Final Report

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"Free-Electron Laser from Wave-Mechanical Beats

of Two Electron Beams."

by

Roland M. Lichtenstein
Professor of Physics, Emeritus
Rensselaer Polytechnic Institute
Troy, NY 12181

Abstract

It is possible, though technically difficult, to produce beams of free electrons that exhibit beats of a quantum-mechanical nature. One may readily think of the following two applications:

1) The generation of electromagnetic radiation, e.g. light, based on the fact that the beats give rise to alternating charge and current densities.

2) A frequency shifter, based on the fact that a beam with beats constitutes a moving grating. When such a grating is exposed to external radiation of suitable frequency and direction, the reflected radiation will be shifted in frequency, since the grating is moving. A twofold increase of the frequency is readily attainable.

In this report we show that

1). It is impossible to generate radiation, because the alternating electromagnetic fields that accompany the beats cannot reform themselves into freely propagating waves.

2) The frequency shifter is useless as a practical device, because its reflectance is extremely low for realizable beams.

Of course, when the work on this grant was started, one could not foresee that, at a later date, somebody (like this writer) would arrive at such disappointing conclusions. It simply takes a lot of time to go through the analysis.

The Main Part (with page numbers M1, M2, etc.) of this report and its Appendix (with page numbers A1, A2, etc.) contain a complete record of how this writer arrived at his conclusions. The report is addressed to someone who has some application for electron beats in mind, and who wishes to find out whether or not his idea has any chance of success.

Are there any useful applications for electrons that are made to exhibit quantum-mechanical beats?

by

Roland M. Lichtenstein
Professor of Physics, Emeritus
Rensselaer Polytechnic Institute
Troy, NY 12181

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Preface and Guide to the Reader.

This report concerns the use that one might make of free electrons with quantum mechanical beats. The Main Part explains what the beats and what the contemplated applications are. Two applications are investigated in detail, the generation of light and a selective moving mirror. The conclusions are:

1. It is impossible to generate light.

2. The mirror device is useless, because its reflectance is essentially zero.

The negative results in these two instances induce the writer to believe that there are no other possible applications and that further work should be suspended, until somebody else comes up with a fruitful idea.

The reader should read the Main Part first. Then he may consult the Appendix, where the physical theories and mathematical methods are explained.

This writer is well aware of the fact that this report is not easy to read. He apoligizes to the reader for making his task so difficult. But it seems to be inherent in the subject that so many strands of argument have to be employed. Perhaps after two or more revisions, a more readable report might be produced. But in view of the negative results, such revisions are not worth the effort.

Main Part of the Report

I. Introduction.

A few years ago, H. Schwarz (in Phys. Rev. Letters 42, 1141 (1979) and 43, 238(E) (1979) suggested that quantum-mechanical beats of electrons could be exploited in a novel form of a free-electron laser. In this introduction we explain the meaning of the word "beats". Throughout this report, we shall describe electrons with the formalism of non-relativistic quantum mechanics, in the style of Schrödinger. A relativistic theory, in the style of Dirac, is not needed, because the speeds of the electrons are much smaller than the speed of light, c, in the device proposed by Schwarz.

A single electron is described by a complex Schrodinger wave function $\psi(\bar{r},ct)$, where $\bar{r}$ is the position vector, and t is the time. We find it more convenient to express the time by means of the product ct, instead of by t itself, because ct and the position $\bar{r}$ come in the same unit, e.g. the meter. This usage facilitates dimension checks. For the same reason, we use the product $c\rho$, whenever we deal with the electric charge density ρ, because $c\rho$ and the electric current density $\bar{J}$ come in the same unit, e.g. the amp m^{-2}. The wave function ψ determines the associated charge and current densities, which are given by

$$c\rho(\bar{r},ct) = (-ec)\psi^*\psi, \tag{1}$$

$$\bar{J}(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\tfrac{1}{2}(-i\psi^*\bar{\nabla}\psi + i\psi\bar{\nabla}\psi^*) . \tag{2}$$

Here, $i = \sqrt{-1}$, (-e) is the electronic charge ($e = +1.6 \times 10^{-19}$ coul), m is the mass of an electron, $\hbar$ is Planck's constant divided by 2π, $\frac{\hbar}{mc} = 3.86 \times 10^{-11}$ cm is the Compton wavelength divided by 2π (which implies that

$\frac{mc}{\hbar}$ is the Compton wave number); the star denotes the complex conjugate, and the symbol $\bar{\nabla}$ denotes the gradient. (Later on, the symbols $\bar{\nabla}\cdot$ and $\bar{\nabla}\times$ denote the divergence and the curl.) The wave function ψ is normalized by the normalization condition

$$\int \Delta\tau_r \psi^* \psi = 1 \ , \tag{3}$$

where the integration is over the entire position space, and where $\Delta\tau_r$ is the volume element in this $\bar{r}$-space.

An electron is called "free" when no electromagnetic forces act on it. In that case, the wave function ψ satisfies the simplest form of the Schrödinger equation

$$i \frac{\partial\psi}{\partial ct} = - \tfrac{1}{2} \frac{\hbar}{mc} \bar{\nabla}\cdot\bar{\nabla}\psi \ . \tag{4}$$

A particular solution of (4) is the plane wave

$$\psi_{plane} = \text{const. } \exp\left(i \bar{\kappa}\cdot\bar{r} - \frac{i\hbar}{mc} \tfrac{1}{2}\kappa^2 ct\right) \ , \tag{5}$$

where $\bar{\kappa}$ is the vectorial wave number, and $\kappa^2 = \bar{\kappa}\cdot\bar{\kappa}$. The general solution of (4) is the wave packet

$$\psi(\bar{r},ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa F(\bar{\kappa}) \exp\left(i\bar{\kappa}\cdot\bar{r} - \frac{i\hbar}{mc} \tfrac{1}{2}\kappa^2 ct\right) \ , \tag{6}$$

where $F(\bar{\kappa})$ is a complex amplitude factor that depends on the wave number $\bar{\kappa}$. The integration is over the wave number space. $\Delta\tau_\kappa \equiv \Delta\kappa_x \Delta\kappa_y \Delta\kappa_z$ is the volume element in this $\bar{\kappa}$-space. The structure and development of a wave packet is completely specified by the function $F(\bar{\kappa})$ in the $\bar{\kappa}$-space.

Let us introduce the spatial Fourier transform $\hat{\psi}(\bar{\kappa},ct)$ (pronounced psi hat) and the temporal Fourier transform $\tilde{\psi}(\bar{r}, \frac{\omega}{c})$ (pronounced psi tilde) of the wave function $\psi(\bar{r},ct)$. (Whenever we deal with a frequency ω, we use the ratio $\frac{\omega}{c}$ because $\frac{\omega}{c}$ and $\bar{\kappa}$ come in the same unit, e.g. m^{-1}). These transforms are defined by

$$\hat{\psi}(\bar{\kappa},ct) = \int \Delta\tau_r e^{-i\bar{\kappa}\cdot\bar{r}} \psi(\bar{r},ct) \ , \tag{7}$$

(The integration is over the position space, $\Delta\tau_r = \Delta x\Delta y\Delta z$ is the volume elemeny in this $\bar{r}$-space.) and

$$\tilde{\psi}(\bar{r}, \frac{\omega}{c}) = \int_{ct=-\infty}^{+\infty} dct \ e^{-i \frac{\omega}{c} ct} \psi(\bar{r},ct) \ . \tag{8}$$

The theory of Fourier transforms yields the inversion formulas

$$\psi(\bar{r},ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}} \hat{\psi}(\bar{\kappa},ct) \ , \tag{9}$$

and

$$\psi(\bar{r},ct) = \frac{1}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{+\infty} d \frac{\omega}{c} e^{i \frac{\omega}{c} ct} \tilde{\psi}(\bar{r}, \frac{\omega}{c}) \ . \tag{10}$$

A consequence of the Fourier transform theorems are the Parseval relations

$$\int \Delta\tau_r \psi^* \psi = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa \hat{\psi}^* \hat{\psi} \ , \tag{11}$$

and

$$\int_{ct=-\infty}^{+\infty} dct \psi^* \psi = \frac{1}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{+\infty} d \frac{\omega}{c} \tilde{\psi}^* \tilde{\psi} \ . \tag{12}$$

When we compare (6) and (9) we see that

$$\hat{\psi}(\bar{\kappa},ct) = F(\bar{\kappa}) \exp(-i \frac{\hbar}{mc} \frac{1}{2} \kappa^2 ct) \ . \tag{13}$$

Then the Parseval relation (11) combined with (3) gives us the following normalization condition for the amplitude factor $F(\bar{\kappa})$.

$$\int \Delta\tau_\kappa F^*(\bar{\kappa}) F(\bar{\kappa}) = (2\pi)^3 \tag{14}$$

(Whereas a wave packet can be normalized, the plane wave (5) cannot be normalized, because the latter extends with constant absolute value throughout the infinite $\bar{r}$-space.)

Now let us write the charge density $\rho(\bar{r},ct)$ in terms of the temporal Fourier transforms $\tilde{\psi}$ and $\tilde{\psi}^*$. For the ψ in (1) we use (10). For the ψ^* in (1) we use a similar formula, but with a renamed integration variable, $\frac{\sigma}{c}$.

Thus

$$\psi^*(\bar{r},ct) = \frac{1}{2\pi} \int_{\frac{\sigma}{c}=-\infty}^{+\infty} d\,\frac{\sigma}{c}\, e^{-i\frac{\sigma}{c}ct}\, \tilde{\psi}^*(\bar{r},\tfrac{\sigma}{c}) \ . \tag{15}$$

The reason for this renaming is that we wish to write the product of two integrals as the double integral over the product of the two integrands. Here confusion would result, had we not renamed. Then (1), (10) and (15) yield

$$c\rho(\bar{r},ct) = \frac{(-ec)}{(2\pi)^2} \int_{-\infty}^{-\infty}\!\!\int d\,\frac{\omega}{c}\, d\,\frac{\sigma}{c}\, e^{i(\frac{\omega}{c}-\frac{\sigma}{c})ct}\, \tilde{\psi}(\bar{r},\tfrac{\omega}{c})\tilde{\psi}^*(\bar{r},\tfrac{\sigma}{c}) \ . \tag{16}$$

We introduce two new integration variables $\frac{\alpha}{c}$ and $\frac{\beta}{c}$ defined by

$$\left.\begin{aligned} \frac{\alpha}{c} &= \frac{\omega}{c} - \frac{\sigma}{c} \\ \frac{\beta}{c} &= \frac{\sigma}{c} \end{aligned}\right\}, \tag{17}$$

and vice versa,

$$\left.\begin{aligned} \frac{\omega}{c} &= \frac{\alpha}{c} + \frac{\beta}{c} \\ \frac{\sigma}{c} &= \frac{\beta}{c} \end{aligned}\right\} . \tag{18}$$

The Jacobian of this transformation is unity. Furthermore, as $\frac{\omega}{c}$ and $\frac{\sigma}{c}$ range over the entire $(\frac{\omega}{c}\ ,\ \frac{\sigma}{c})$-plane, $\frac{\alpha}{c}$ and $\frac{\beta}{c}$ range over the entire $(\frac{\alpha}{c}\ .\ \frac{\beta}{c})$-plane. Thus,

$$c\rho(\bar{r},ct) = \frac{(-ec)}{(2\pi)^2} \int_{-\infty}^{+\infty}\!\!\int d\,\frac{\alpha}{c}\, d\,\frac{\beta}{c}\, e^{i\frac{\alpha}{c}ct}\, \tilde{\psi}(\bar{r},\ \tfrac{\alpha}{c}+\tfrac{\beta}{c})\tilde{\psi}^*(\bar{r},\ \tfrac{\beta}{c}) \ ,$$

or, after a change of notation for the integration or dummy variables, (back to $\frac{\omega}{c}$ and $\frac{\sigma}{c}$)

$$c\rho(\bar{r},ct) = \frac{(-ec)}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{+\infty} d\,\frac{\omega}{c}\, e^{i\frac{\omega}{c}ct}\, \frac{1}{2\pi} \int_{\frac{\sigma}{c}=-\infty}^{+\infty} d\,\frac{\sigma}{c}\, \tilde{\psi}(\bar{r},\ \tfrac{\omega}{c}+\tfrac{\sigma}{c})\tilde{\psi}^*(\bar{r},\ \tfrac{\sigma}{c}) \ . \tag{19}$$

If we compare (19) with (10), the latter equation being applied to $c\rho$ instead of ψ, we see that the temporal Fourier transform $\widetilde{c\rho}(\bar{r},\ \frac{\omega}{c})$ of the charge

density $c\rho(\bar{r},ct)$ is given by

$$\widetilde{c\rho}(\bar{r}, \frac{\omega}{c}) = \frac{(-ec)}{2\pi} \int_{\frac{\sigma}{c}=-\infty}^{\infty} d\,\frac{\sigma}{c}\,\tilde{\psi}(\bar{r}, \frac{\omega}{c} + \frac{\sigma}{c})\tilde{\psi}^{*}(\bar{r}, \frac{\sigma}{c}) \ , \tag{20}$$

where, of course,

$$c\rho(\bar{r},ct) = \frac{1}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{+\infty} d\,\frac{\omega}{c}\, e^{i\,\frac{\omega}{c}\,ct}\, \widetilde{c\rho}(\bar{r}, \frac{\omega}{c}) \ . \tag{21}$$

It is helpful to express the function $\tilde{\psi}(\bar{r}, \frac{\omega}{c})$, which occurs in (20), in terms of the amplitude factor $F(\bar{\kappa})$. We start with (6) and use spherical polar coordinates $\kappa = |\bar{\kappa}|$, θ, ϕ in the $\bar{\kappa}$-space. Then

$$\Delta\tau_{\kappa} = d\kappa\kappa\, d\theta\kappa \sin\theta d\phi = d\kappa\kappa^{2} d\Omega \ ,$$

where

$$d\Omega = d\theta\, \sin\theta\, d\phi$$

is the solid angle element. Then (6) becomes

$$\psi(\bar{r},ct) = \frac{1}{(2\pi)^3} \int_{\kappa=0}^{\infty} d\kappa\ \kappa\ \exp(-i\,\frac{\hbar}{mc}\,\frac{1}{2}\,\kappa^{2}ct) \oiint_{\kappa} d\Omega\kappa F(\bar{\kappa}) e^{i\bar{\kappa}\cdot\bar{r}}, \tag{22}$$

where $\oiint_{\kappa}$ denotes the surface integral over the sphere of radius κ. We express κ in terms of the frequency $\frac{\omega}{c}$, i.e. by way of the equation

$$\frac{\omega}{c} = -\,\frac{\hbar}{mc}\,\tfrac{1}{2}\kappa^{2} \ . \tag{23}$$

Then (22) becomes

$$\psi(\bar{r},ct) = \frac{1}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{0} d\,\frac{\omega}{c}\, e^{i\,\frac{\omega}{c}\,ct}\, \frac{mc}{\hbar}\,\frac{1}{(2\pi)^2} \oiint d\Omega\ \kappa F(\kappa) e^{i\bar{\kappa}\cdot\bar{r}} \ . \tag{24}$$

for $\kappa = \sqrt{-2\,\frac{mc}{\hbar}\,\frac{\omega}{c}}$

We compare (23) with (10) and conclude that

$$\tilde{\psi}(\bar{r}, \frac{\omega}{c}) = \frac{mc}{\hbar}\,\frac{1}{(2\pi)^2} \oiint d\Omega\kappa F(\bar{\kappa}) e^{i\bar{\kappa}\cdot\bar{r}} \text{ for } \frac{\omega}{c} \le 0$$

for $\kappa = \sqrt{-2\,\frac{mc}{\hbar}\,\frac{\omega}{c}}$ (25)

$$= 0 \text{ for } \frac{\omega}{c} \ge 0$$

As an example for an application of equation (25), we consider an approximately mono-energetic wave packet, for which $F(\bar{\kappa}) = 0$ unless $\bar{\kappa}$ lies on a very thin spherical shell (with center at $\bar{\kappa} = \bar{0}$) in the $\bar{\kappa}$-space. Then (25) tells us that $\tilde{\psi}(\bar{r}, \frac{\omega}{c}) = 0$ unless $\frac{\omega}{c}$ lies in a very narrow interval I that straddles the frequency which is related to the radius of the shell by (23). As a consequence, the integral in (20) is zero, unless $\frac{\omega}{c}$ lies in a very narrow interval that straddles the frequency zero. The reason is that one of the factors in the integrand is definitely zero when the other is non-zero, unless $\frac{\omega}{c} = 0$, so that the whole integral is zero. ($\frac{\omega}{c} + \frac{\sigma}{c}$ and $\frac{\sigma}{c}$ cannot both lie in the narrow interval I that we mentioned above, unless $\frac{\omega}{c} = 0$.) Thus, for an approximately mono-energetic wave packet, the temporal Fourier transform $\widetilde{c\rho}(\bar{r}, \frac{\omega}{c})$ of the charge density $\rho(\bar{r},ct)$ vanishes unless $\frac{\omega}{c}$ lies in a very narrow interval that straddles the frequency zero. We express this state of affairs briefly, by saying that $c\rho(\bar{r},ct)$ is apprximately d.c. ("d.c." for "direct current").

On the other hand, for a wave packet that is not mono-energetic, equation (25) permits $\tilde{\psi}(r, \frac{\omega}{c})$ to be non-zero over an extended range of $\frac{\omega}{c}$. And then (20) permits $\widetilde{c\rho}(\bar{r}, \frac{\omega}{c})$ to be non-zero over an extended domain of the frequency $\frac{\omega}{c}$, beyond a very narrow interval around $\frac{\omega}{c} = 0$. We express this state of briefly by saying that $c\rho(\bar{r},ct)$ has alternating components or beats. Specifically, the beat at a given frequency $\frac{\omega}{c}$ is the product of the temporal Fourier transform $\widetilde{c\rho}(r, \frac{\omega}{c})$, regarded as a function of the position $\bar{r}$, and the time factor $e^{i \frac{\omega}{c} ct}$. The first factor is the (complex) amplitude function (it depends on $\bar{r}$) of the beat. The second factor produces the alternating or a.c. behavior ("a.c." for "alternating current"). According to equation (21),

the charge density $c\rho(\bar{r},ct)$ is a superposition of beats.

Everything that we have said about the charge density $c\rho(\bar{r},ct)$ and its beats $\tilde{c\rho}(\bar{r}, \frac{\omega}{c})e^{i\frac{\omega}{c}ct}$ can be extended - mutatis mutandis - to the current density $\bar{J}(\bar{r},ct)$ and its beats $\tilde{\bar{J}}(r, \frac{\omega}{c})e^{i\frac{\omega}{c}ct}$. The analogs of equations (20) and (21) are

$$\tilde{\bar{J}}(\bar{r}, \frac{\omega}{c}) = \frac{(-ec)\hbar}{2\pi mc} \int_{\frac{\sigma}{c}=-\infty}^{+\infty} d\frac{\sigma}{c} \frac{1}{2}(-i\,\tilde{\psi}^*(\bar{r}, \frac{\sigma}{c})\bar{\nabla}\tilde{\psi}(\bar{r}, \frac{\omega}{c} + \frac{\sigma}{c}) +$$

$$+ i\tilde{\psi}(\bar{r}, \frac{\omega}{c} + \frac{\sigma}{c})\bar{\nabla}\tilde{\psi}^*(\bar{r}, \frac{\sigma}{c})) \,, \qquad (26)$$

where, of course,

$$\bar{J}(\bar{r},ct) = \frac{1}{2\pi} \int_{\frac{\omega}{c}=-\infty}^{+\infty} d\frac{\omega}{c}\, e^{i\frac{\omega}{c}ct}\, \tilde{\bar{J}}(\bar{r}, \frac{\omega}{c}) \,. \qquad (27)$$

To summarize; Both the charge density $c\rho(\bar{r},ct)$ and the current density $\bar{J}(\bar{r},ct)$ are linear superpositions of the beats $\tilde{c\rho}(r, \frac{\omega}{c})e^{i\frac{\omega}{c}ct}$ and $\tilde{\bar{J}}(\bar{r}, \frac{\omega}{c})e^{i\frac{\omega}{c}ct}$, as shown by equations (21) and (27). The complex beat amplitudes $\tilde{c\rho}(\bar{r}, \frac{\omega}{c})$ and $\tilde{\bar{J}}(\bar{r}, \frac{\omega}{c})$ are given by (20) and (26). The amplitude $\tilde{\psi}(r, \frac{\omega}{c})$, which occurs in the latter two equations can be calculated according to (25). For an approximately mono-energetic wave packet, there are only beats of very low frequency. In the limit of a strictly mono-energetic wave packet (It cannot be normalized, but is a useful construct.), the charge density and current density do not depend on the time ct; they are strictly d.c. For a wave packet that is not mono-energetic, the charge density and the current density may contain beats of appreciable frequency. The word "beat" refers to the fact that, as shown by (20) and (26) the beat amplitudes $\tilde{c\rho}(\bar{r},\frac{\omega}{c})$ and $\tilde{\bar{J}}(\bar{r}, \frac{\omega}{c})$ are of second order in the temporal Fourier transforms of the wave function, and that the beat frequency $\frac{\omega}{c}$ is the difference $(\frac{\omega}{c} + \frac{\sigma}{c}) - \frac{\sigma}{c}$ of the

two frequencies that occur in the integrands of (20) and (26).

In the device that was proposed by H. Schwarz a swarm of electrons is employed, each exhibiting beats in the optical frequency range. Since the charge and current densities $c\rho(\bar{r},ct)$ and $\bar{J}(\bar{r},ct)$ are the sources of the electromagnetic field, and since both densities contain beats in the optical frequency range, one might expect that light is produced in Schwarz's device.

However, this expectation is illusory. Two authors, A. Peres (Phys. Rev. A, 2627 (1979) and M. Peshkin (ibid. page 2629), attempted to prove that free electrons, even though they were made to exhibit beats, cannot produce electromagnetic radiation. But these proofs are not very convincing to this writer, because they employ only verbal arguments. (One of these arguments, namely the use of the superposition principle, is wrong, because beats involve products of wave functions, whereas the invoked principle applies only to linear expressions.) We, therefore, supplement the work of Peres and Peshkin with a more detailed mathematical treatment, which - though a bit tedious - can demonstrate exactly where the attempt to generate light fails. This analysis, which is based on the principles derived in the Appendix, will be presented in Section 3. But there we shall have to make use of the decomposition of a vector field into its longitudinal and transverse part. This matter will be explained in Section 2.

We conclude the present section with some remarks about the physical meaning of $c\rho(\bar{r},ct)$ and $\bar{J}(\bar{r},ct)$ as given by equations (1) and (2). These quantities are really the quantum-mechanical expectation values of the charge

and current density. But one can show, as it is done in the Appendix, that these expectation values are the sources of the electromagnetic field if this field is treated classically, while the electrons are described quantum-mechanically. The use of quantum mechanics for the electrons and of classical physics for the electromagnetic field is called the semi-classical method. It is described in the Appendix. We use it throughout this report, because we deem it accurate enough for our purposes, and because it is more easily handled than a fully quantized theory, in which also the electromagnetic field would be described quantum-mechanically.

II. The Decomposition of a Vector Field Into Its Longitudinal and Transverse Part.

We start with a vector field, e.g. the current density $\bar{J}(\bar{r},ct)$ and take its spatial Fourier transform $\hat{\bar{J}}(\bar{\kappa},ct)$ (pronounced "Jay hat") defined by

$$\hat{\bar{J}}(\bar{\kappa},ct) = \int \Delta\tau_r e^{-i\bar{\kappa}\cdot\bar{r}} \bar{J}(\bar{r},ct) \ . \tag{1}$$

This definition is the vectorial analog of (1,7). By the Fourier integral theorem, we have the inversion formula

$$\bar{J}(r,ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}} \hat{\bar{J}}(\bar{\ },ct) \ , \tag{2}$$

the analog of (1,9). Now we define the longitudinal part $\bar{J}_L(\bar{r},ct)$ of $\bar{J}(\bar{r},ct)$ by way of its spatial Fourier transform $\hat{\bar{J}}_L(\bar{\kappa},ct)$. The definition of $\hat{\bar{J}}_L(\bar{\kappa},ct)$ is

$$\hat{\bar{J}}_L(\bar{\kappa},ct) = \frac{1}{\kappa^2} \bar{\kappa}\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct), \text{ for } \bar{\kappa} \neq \bar{0}. \tag{3}$$

This equation states that $\hat{\bar{J}}_L(\bar{\kappa},ct)$ is the projection of $\hat{\bar{J}}(\bar{\kappa},ct)$ onto an axis parallel to the wave number vector $\bar{\kappa}$. For $\bar{\kappa} = \bar{0}$, the definition (3) becomes indeterminate, so that we must use a separate definition for this case. We

define $\hat{\bar{J}}_L(\bar{0},ct)$ by

$$\hat{\bar{J}}_L(\bar{0},ct) = \frac{1}{3}\hat{\bar{J}}(\bar{0},ct) \ . \tag{4}$$

Equation (4) results from (3) if we first take the average of (3) as $\bar{\kappa}$ ranges over the surface of a small sphere in $\bar{\kappa}$-space (with its center at the origin $\bar{0}$); and then we let the radius of this sphere go to zero. The factor $\frac{1}{3}$ arises from the fact that the average $\langle\bar{\kappa}\bar{\kappa}\rangle$ of the tensor $\bar{\kappa}\bar{\kappa}$ is equal to $\frac{1}{3}\kappa^2\bar{\bar{I}}$, where $\bar{\bar{I}} = \bar{I}\bar{I} + \bar{J}\bar{J} + \bar{k}\bar{k}$ is the unit tensor or idemfactor. The definition of $\hat{\bar{J}}_L(\bar{\kappa},ct)$ permits us to obtain $\bar{J}_L(\bar{r},ct)$ by taking the inverse Fourier transform, in analogy to the general formula(2). We have

$$\bar{J}_L(\bar{r},ct) = \frac{1}{(2\pi)^3}\int\Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\hat{\bar{J}}_L(\bar{\kappa},ct) = \frac{1}{(2\pi)^3}\int\Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct). \tag{5}$$

We assume that the convergence of the integrals in the $\bar{\kappa}$-space is good enough so that we may take spatial derivatives of $\bar{J}_L(\bar{r},ct)$, such as the divergence $\bar{\nabla}\cdot\bar{J}_L$ and the curl $\bar{\nabla}\times\bar{J}_L$, by taking the derivatives of the integrand. Then ($\bar{\nabla}_r$ denotes the gradient with respect to $\bar{r}$)

$$\bar{\nabla}\cdot\bar{J}_L = \frac{1}{(2\pi)^3}\int\Delta\tau_\kappa(\bar{\nabla}_r e^{i\bar{\kappa}\cdot\bar{r}})\cdot\frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct) \ ,$$

and

$$\bar{\nabla}\times\bar{J}_L = \frac{1}{(2\pi)^3}\int\Delta\tau_\kappa(\bar{\nabla}_r e^{i\bar{\kappa}\cdot\bar{r}})\times\frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct) \ .$$

And since

$$\bar{\nabla}_r e^{i\bar{\kappa}\cdot\bar{r}} = i\bar{\kappa}e^{i\bar{\kappa}\cdot\bar{r}} \ , \tag{6}$$

we obtain

$$\bar{\nabla}\cdot\bar{J}_L = \frac{1}{(2\pi)^3}\int\Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\, i\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct) \tag{7}$$

and

$$\bar{\nabla}\times\bar{J}_L = 0 \tag{8}$$

Equation (8) states that the longitudinal part of a vector field is irrotational.

If we take the divergence of (2) we obtain

$$\bar{\nabla}\cdot\bar{J} = \frac{1}{(2\pi)^3}\int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\, i\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct). \tag{9}$$

On comparing (7) and (9), we see that

$$\bar{\nabla}\cdot\bar{J}_L = \bar{\nabla}\cdot\bar{J}\ . \tag{10}$$

Inspection of equation (7) and (9) shows that the Fourier transforms $\widehat{(\bar{\nabla}\cdot\bar{J}_L)}(\bar{\kappa},ct)$ and $\widehat{(\bar{\nabla}\cdot\bar{J})}(\bar{\kappa},ct)$ are given by

$$\widehat{(\bar{\nabla}\cdot\bar{J}_L)}(\bar{\kappa},ct) = \widehat{(\bar{\nabla}\cdot\bar{J})}(\bar{\kappa},ct) = i\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct)\ . \tag{11}$$

Then equation (5) may be written in the form

$$\bar{J}_L(\bar{r},ct) = -\frac{1}{(2\pi)^3}\int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\, i\bar{\kappa}\,\frac{1}{\kappa^2}\,\widehat{(\bar{\nabla}\cdot\bar{J})}(\bar{\kappa},ct)$$

or

$$\bar{J}_L(r,ct) = -\bar{\nabla}\psi\ , \tag{12a}$$

with

$$\psi(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}}\,\frac{1}{\kappa^2}\,\widehat{(\bar{\nabla}\cdot\bar{J})}(\bar{\kappa},ct)\ . \tag{12b}$$

(There is no connection between the ψ of equations (12a, b) and the Schrödinger wave functions of Section 1.)

Now, the inverse Fourier transform of $\frac{1}{\kappa^2}$ is $\frac{1}{4\pi r}$ as one can easily show by direct calculation. Thus, by (12b), the Fourier transform of $\psi(\bar{r},ct)$ is the product of two Fourier transforms, that of $\frac{1}{4\pi r}$ and that of $\bar{\nabla}\cdot\bar{J}$. Hence, by the convolution theorem of Fourier transforms, $\psi(\bar{r},t)$ is the convolution of $\frac{1}{4\pi r}$ and $\bar{\nabla}\cdot\bar{J}$. Thus, (12) may be written in the form

$$\bar{J}_L(\bar{r},ct) = -\bar{\nabla}\psi\ , \tag{13a}$$

with

$$\psi(\bar{r},ct) = \frac{1}{4\pi}\int \Delta\tau_s\,\frac{1}{|\bar{s}-\bar{r}|}\,(\bar{\nabla}\cdot\bar{J})(\bar{s},ct)\ . \tag{13b}$$

Equations (13) may be found in many textbooks, e.g. Morse and Feshbach, Methods of Theoretical Physics, McGraw-Hill 1953, pages 53, 54 or Panofsky, and

Phillips, Classical Electricity and Magnetism, Addison-Wesley 1962, page 2. However, we find it more convenient to define $\bar{J}_L(\bar{r},ct)$ by way of its Fourier transform (3).

We are finished with the discussion of the longitudinal part $\bar{J}_L(\bar{r},ct)$. The transverse part $\bar{J}_T(\bar{r},ct)$ is defined by the requirement that both parts add up to $\bar{J}(\bar{r},ct)$, i.e. that

$$\bar{J}(\bar{r},ct) = \bar{J}_L(\bar{r},ct) + \bar{J}_T(\bar{r},ct) \ . \tag{14}$$

Then, a similar equation, namely

$$\hat{\bar{J}}(\bar{\kappa},ct) = \hat{\bar{J}}_L(\bar{\kappa},ct) + \hat{\bar{J}}_T(\bar{\kappa},ct) \tag{15}$$

must hold for the Fourier transforms, so that

$$\hat{\bar{J}}_T(\bar{\kappa},ct) = \hat{\bar{J}}(\bar{\kappa},ct) - \frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\hat{\bar{J}}(\bar{\kappa},ct) =$$

$$= -\frac{1}{\kappa^2}\bar{\kappa} \times (\bar{\kappa} \times \hat{\bar{J}}(\bar{\kappa},ct)), \text{ for } \bar{\kappa} \neq 0 \ , \tag{16}$$

and

$$\hat{\bar{J}}_T(\bar{o},ct) = \frac{2}{3}\hat{\bar{J}}(\bar{o},ct) \ . \tag{17}$$

Equation (16) shows that $\hat{\bar{J}}_T(\bar{\kappa},ct)$ is the projection of $\hat{\bar{J}}(\bar{\kappa},ct)$ onto a plane that is normal to $\bar{\kappa}$.

The remainder of the discussion is pretty much a repetition of what was done for $\bar{J}_L$. So we can be brief. The analogs of equations (5), (7), (8) are

$$\bar{J}_T(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\kappa \, e^{i\bar{\kappa}\cdot\bar{r}} \, \hat{\bar{J}}_T(\bar{\kappa},ct) =$$

$$= \frac{1}{(2\pi)^3}\int \Delta\tau_\kappa \, e^{i\bar{\kappa}\cdot\bar{r}} \, \frac{1}{\kappa^2}(-\bar{\kappa} \times (\bar{\kappa} \times \hat{\bar{J}}(\bar{\kappa},ct))) \ , \tag{18}$$

$$\bar{\nabla} \times \bar{J}_T = \frac{1}{(2\pi)^3}\int \Delta\tau_\kappa \, e^{i\bar{\kappa}\cdot\bar{r}} \, i\bar{\kappa} \times \hat{\bar{J}}(\bar{\kappa},ct) \ , \tag{19}$$

$$\bar{\nabla} \cdot \bar{J}_T = 0 \ . \tag{20}$$

Equation (20) states that $\bar{J}_T(\bar{r},ct)$ is solenoidal. The analogs of equation (10) and (11) are

$$\bar{\nabla} \times \bar{J}_T = \bar{\nabla} \times \bar{J} \ , \tag{21}$$

$$\widehat{(\bar{\nabla} \times \bar{J}_T)}(\bar{\kappa},ct) = \widehat{(\bar{\nabla} \times \bar{J})}(\bar{\kappa},ct) = i\bar{\kappa} \times \hat{\bar{J}}(\bar{\kappa},ct) \ . \tag{22}$$

Instead of (12), we have

$$\bar{J}_T(\bar{r},ct) = \bar{\nabla} \times \bar{C} \ , \tag{23a}$$

with

$$\bar{C}(\bar{r},ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa e^{i\bar{\kappa}\cdot\bar{r}} \frac{1}{\kappa^2} (\bar{\nabla} \times \bar{J})(\bar{\kappa},ct) \ . \tag{23b}$$

When we take the divergence of (23b) by differentiating the integrand and when we also use (22), we see that

$$\bar{\nabla}\cdot\bar{C} = 0 \ , \tag{24}$$

which implies that $\bar{C}(\bar{r},ct)$ is purely transverse. (Because of (13), $\bar{\nabla}\cdot\bar{C} = 0$ yields $\bar{C}_L = 0$.)

Finally, the analog of (13) is

$$\bar{J}_T(\bar{r},ct) = \bar{\nabla} \times \bar{C} \ , \tag{25a}$$

with

$$\bar{C}(\bar{r},ct) = \frac{1}{4\pi} \int \Delta\tau_s \frac{1}{|\bar{s}-\bar{r}|} (\bar{\nabla} \times \bar{J})(\bar{s},ct) \tag{25b}$$

This is a well-known relation. [See the references quoted after (13).]

Let us consider two real vector fields $\bar{F}(\bar{r},ct)$ and $\bar{G}(\bar{r},ct)$. We take the longitudinal part of the first and the transverse part of the second field. Then we consider the scalar product $\bar{F}_L \cdot \bar{G}_T$. Now, by (13), $\bar{F}_L$ is the negative gradient of some scalar field ψ, and, by (25), $\bar{G}_T$ is the curl of some vector field $\bar{C}$. Then

$$\bar{F}_L\cdot\bar{G}_T = -(\bar{\nabla}\psi)\cdot(\bar{\nabla} \times \bar{C}) = -\bar{\nabla}\cdot(\psi\bar{\nabla} \times \bar{C}) + \psi\bar{\nabla}\cdot(\bar{\nabla} \times \bar{C}) \ ,$$

or, since the divergence of a curl is zero,

$$\bar{F}_L\cdot\bar{G}_T = -\bar{\nabla}\cdot(\psi\bar{\nabla} \times \bar{C})$$

We integrate this equation over the interior of some large sphere of radius R, and convert the integral of the right-hand side into a surface integral, by virtue of the theorem of Gauss. Thus

$$\int_{\text{sphere}} \Delta\tau_r \bar{F}_L \cdot \bar{G}_T = - \oint\!\!\oint \Delta\bar{f} \cdot \psi \bar{\nabla} \times \bar{C}$$

where $\Delta\bar{f}$ is the vectorial surface element. We assume that $\bar{\nabla} \cdot \bar{F}$ and $\bar{\nabla} \times \bar{G}$ vanish outside a finite region of space, as it usually happens in practice. (Somewhat less stringent requirements will suffice for the argument that follows. For instance, $\bar{\nabla}\cdot\bar{F}$ and $\bar{\nabla} \times \bar{G}$ should tend to zero for $|\bar{r}| \to \infty$ at a sufficiently fast rate.) Then, by (13) and (25), ψ and $\bar{G}$ are of order R^{-1} for $R \to \infty$. Then $\bar{\nabla} \times \bar{C}$ is of order R^{-2}, and the surface integral in (26) is of order R^{-1}. Thus, when we go to the limit $R \to \infty$, equation (26) becomes

$$\int \Delta\tau_r \bar{F}_L \cdot \bar{G}_T = 0 \ , \tag{27}$$

which is an important orthogonality relation.

Another demonstration of (27) is by way of the Parseval relation

$$\int \Delta\tau_r \bar{F}_L(\bar{r},ct) \cdot \bar{G}_T(\bar{r},ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa \hat{\bar{F}}_L(-\bar{\kappa},ct) \cdot \hat{\bar{G}}_T(\bar{\kappa},ct) \ . \tag{28}$$

But the definitions (3) and (16) show that the integrand of the right-hand side of (28) is zero (except at the single point $\bar{\kappa} = \bar{0}$; this exception does not affect the integral.).

A consequence of (27) is: When a vector field $\bar{F}$ is zero everywhere, then its longitudinal and transverse part must be zero individually. For, with $\bar{F} = \bar{F}_L + \bar{F}_T$, we have (if $\bar{F} = 0$)

$$\int \Delta\tau_r \bar{F}_L \cdot \bar{F}_L + \int \Delta\tau_r \bar{F}_T \cdot \bar{F}_T + 2\int \Delta\tau_r \bar{F}_L \cdot \bar{F}_T = 0$$

The third integral is zero, by (27). The remaining two integrals (their integrands are never negative) can add up to zero only if individually $\bar{F}_L = 0$ and $\bar{F}_T = 0$. In the same way one shows that a longitudinal field $\bar{F}_L$

and a transverse field $\bar{G}_T$ can never add up to zero. For we have

$$\int \Delta\tau_r (\bar{F}_L+\bar{G}_T)\cdot(\bar{F}_L+\bar{G}_T) = \int \Delta\tau_r \bar{F}_L\cdot\bar{F}_L + \int \Delta\tau_r \bar{G}_T\cdot\bar{G}_T + 2\int \Delta\tau_r \bar{F}_L\cdot\bar{G}_T \ .$$

By (27), the third integral on the right is zero. The other two are definitely positive, unless $\bar{F}_L = 0$ and $\bar{G}_T = 0$ everywhere. Therefore, if and only if these two equations are satisfied, can $\bar{F}_L + \bar{G}_T$ be zero everywhere.

We also remark that the longitudinal part of the curl of a vector field vanishes. For $\bar{\nabla}\cdot(\bar{\nabla} \times \bar{F}) = 0$, and hence $(\bar{\nabla} \times \bar{F})_L = 0$, as seen from (13). Also from (13) we see that a solenoidal vector field (i.e. a field whose divergence vanishes) is purely transverse because its longitudinal part vanishes. And (25) shows that an irrotational vector field (i.e. a field whose curl vanishes) is purely longitudinal because its transverse part vanishes. Vice versa: A purely longitudinal vector field is irrotational, since - by (13) - it is the negative gradient of a scalar ψ and $\bar{\nabla} \times (\bar{\nabla}\psi) = 0$. And a purely transverse vector field is solenoidal, since - by (25) - it is the curl of a vector $\bar{C}$ and $\bar{\nabla}\cdot(\bar{\nabla} \times \bar{C}) = 0$. Thus, the properties "purely longitudinal" and "irrotational" are equivalent, as are the properties "purely transverse" and "solenoidal". A non-vanishing vector field $\bar{F}$ cannot be both purely longitudinal (meaning $\bar{F}_T = 0$) and purely transverse (meaning $\bar{F}_L = 0$) at the same time, since $\bar{F} = \bar{F}_L + \bar{F}_T$ yields $\bar{F} = 0$ under these conditions. (Of course, the assumption is always that $\bar{F}$ tends to zero for $|\bar{r}| \to \infty$ rapidly enough so that the Fourier transform theory, on which everything was based, is applicable.) Therefore, because of the equivalences of properties spelled out above, we conclude that a field that is both irrotational and purely transverse is zero everywhere. The same conclusion holds for a field that is both solenoidal and purely longitudinal.

We apply the results of this section to the Maxwell equations of the electromagnetic field.

$$\bar{\nabla} \times \bar{E} + \frac{\partial}{\partial ct} c\bar{B} = 0 \ , \tag{29a}$$

$$\bar{\nabla} \times c\bar{B} - \frac{\partial}{\partial ct} \bar{E} = \eta_o \bar{J} \ , \tag{29b}$$

$$\bar{\nabla} \cdot \bar{E} = \eta_o c\rho \ , \tag{29c}$$

$$\bar{\nabla} \cdot c\bar{B} = 0 \ , \tag{29d}$$

Here

$\bar{E}$ = Electric field strength,

$\bar{B}$ = Magnetic induction,

η_o = Impedance of free space = 377 ohm.

The quantity η_o is related to

μ_o = Permeability of free space = $4\pi\ 10^{-7}\ \frac{\text{volt sec}}{\text{amp m}}$,

c = Speed of light = $3 \times 10^8\ \frac{\text{m}}{\text{sec}}$,

ε_o = Permittivity of free space = $\frac{1}{\mu_o c^2}$,

through

$$\eta_o = \sqrt{\frac{\mu_o}{\varepsilon_o}} = \mu_o c = \frac{1}{\varepsilon_o c} \ .$$

Of course, the electric charge density ρ and the electric current density $\bar{J}$ must be coupled by the continuity equation

$$\bar{\nabla} \cdot \bar{J} + \frac{\partial}{\partial ct} c\rho = 0 \ . \tag{30}$$

We apply (29) in the following manner: $c\rho(\bar{r},t)$ and $\bar{J}(\bar{r},ct)$ are given; $\bar{E}(\bar{r},ct)$ and $c\bar{B}(\bar{r},ct)$ are to be found. Equation (29a) tells us that $c\bar{B}$ is solenoidal, hence purely transverse. Thus

$$c\bar{B} = c\bar{B}_T \ . \tag{31}$$

Then, by (24) and (25), there exists a purely transverse vector field $c\bar{A}_T$ such that

$$c\bar{B} = \bar{\nabla} \times c\bar{A}_T \ . \tag{32}$$

The vector $c\bar{A}_T$ is called the "vector potential in the Coulomb gauge". We decompose $\bar{E}$ and also $\bar{J}$ into their longitudinal and transverse parts, so that

$$\bar{E} = \bar{E}_L + \bar{E}_T \ , \tag{33}$$

$$\bar{J} = \bar{J}_L + \bar{J}_T \ . \tag{34}$$

Then the equations (29) become (Note that $\bar{\nabla} \times \bar{E}_L = 0$ and $\bar{\nabla} \cdot \bar{E}_T = 0$)

$$\bar{\nabla} \times (\bar{E}_T + \frac{\partial}{\partial ct} c\bar{A}_T) = 0 \tag{35a}$$

$$\bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_T) - \frac{\partial}{\partial ct} \bar{E}_L - \frac{\partial}{ct} \bar{E}_T = \eta_o \bar{J}_L + \eta_o \bar{J}_T \tag{35b}$$

$$\bar{\nabla} \cdot \bar{E}_L = \eta_o c\rho \tag{35c}$$

$$\bar{\nabla} \cdot (\bar{\nabla} \times c\bar{A}_T) = 0 \tag{35d}$$

Equation (35d) is redundant. Equation (35a) tells us that $\bar{E}_T + \frac{\partial}{\partial ct} c\bar{A}_T$, which is obviously purely transverse, is also solenoidal, hence purely longitudinal. Therefore $\bar{E}_T + \frac{\partial}{\partial ct} c\bar{A}_T$, being both purely transverse and purely longitudinal, must be zero everywhere, so that

$$\bar{E}_T = - \frac{\partial}{\partial ct} c\bar{A}_T \ . \tag{36}$$

We no longer need equations (35a) and (35d). Equation (35b) must hold separately for its transverse and longitudinal part. Thus, with (36), this equation yields

$$\bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_T) + \frac{\partial^2}{(\partial ct)^2} c\bar{A}_T = \eta_o \bar{J}_T \ , \tag{37a}$$

and

$$- \frac{\partial}{\partial ct} \bar{E}_L = \eta_o \bar{J}_L \ . \tag{37b}$$

We also have [see (35c)]

$$\bar{\nabla} \cdot \bar{E}_L = \eta_o c\rho \ . \tag{37c}$$

Now, by (13), there exists a scalar field ϕ, such that

$$\bar{E}_L = - \bar{\nabla}\phi \ . \tag{38}$$

The quantity ϕ is called the "scalar potential in the Coulomb gauge". Then (37b) and (37c) become

$$\bar{\nabla} \frac{\partial \phi}{\partial ct} = \eta_o \bar{J}_L \ , \tag{39a}$$

and

$$- \bar{\nabla}\cdot\bar{\nabla}\phi = \eta_o c\rho \ . \tag{39b}$$

Equation (39b) states that at any instant ct, the scalar potential ϕ is equal to the electrostatic potential associated with the charge density at that instant. But one should keep in mind that ϕ depends on the time, because $c\rho$ depends on the time.

The procedure for obtaining the electromagnetic field from a given charge density $c\rho(\bar{r},ct)$ and current density $\bar{J}(\bar{r},ct)$ is then as follows. First one determines the potentials $\phi(\bar{r},ct)$ and $c\bar{A}_T(\bar{r},ct)$ from [See (37a) and (39b)].

$$\bar{\nabla}\cdot\bar{\nabla}\phi = - \eta_o c\phi \ , \tag{40a}$$

and

$$\bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_T) + \frac{\partial^2}{(\partial ct)^2} c\bar{A}_T = \eta_o \bar{J}_T \ . \tag{40b}$$

Here, $\eta_o \bar{J}_T$ may be obtained either by way of ϕ, namely by [See (39a)].

$$\eta_o \bar{J}_T = \eta_o \bar{J} - \bar{\nabla} \frac{\partial \phi}{\partial ct} \ ; \tag{40c}$$

or one may bypass the determination of ϕ and obtain $\bar{J}_T$ from $\bar{J}$ itself through (16) or (25). After ϕ and $c\bar{A}_T$ have been determined, one obtains the fields $\bar{E}(\bar{r},ct)$ and $c\bar{B}(\bar{r},ct)$ from

$$\bar{E} = \bar{E}_L + \bar{E}_T \ , \tag{41a}$$

$$\bar{E}_L = - \bar{\nabla}\phi \ , \tag{41b}$$

$$\bar{E}_T = -\frac{\partial}{\partial ct} c\bar{A}_T \ , \qquad (41c)$$

$$c\bar{B} = \bar{\nabla} \times c\bar{A}_T \ . \qquad (41d)$$

Equations (40) and (41) are, of course, well-known. We showed how they are derived, not only for the sake of completeness, but also because we wanted to exhibit why the source function for $c\bar{A}_T$, i.e. the right-hand side of (40b) is $\eta_o \bar{J}_T$, not $\eta_o \bar{J}$.

One of the favorite ways of dealing with equations (40) and (41) is by way of their spatial Fourier transforms. What corresponds to the operation $\bar{\nabla}$ in the $\bar{r}$-space is the multiplication by $i\bar{\kappa}$ in the $\bar{\kappa}$-space. Thus the transforms of $\bar{\nabla}\cdot\bar{\nabla}\phi$ and $\bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_T)$ are

$$i\bar{\kappa} \cdot i\bar{\kappa}\hat{\phi} = -\kappa^2\hat{\phi}$$

and

$$i\bar{\kappa} \times (i\bar{\kappa} \times c\hat{\bar{A}}_T) = \kappa^2 c\hat{\bar{A}}_T - \bar{\kappa}\bar{\kappa}\cdot c\hat{\bar{A}}_T$$

But since $\bar{\nabla}\cdot c\bar{A}_T = 0$, we have $i\bar{\kappa}\cdot c\hat{\bar{A}}_T = 0$, so that

$$i\bar{\kappa} \times (i\bar{\kappa} \times c\hat{\bar{A}}_T) = \kappa^2 c\hat{\bar{A}}_T \ .$$

Thus, equations (40) and (41) become

$$\kappa^2\hat{\phi}(\bar{\kappa},ct) = \eta_o c\hat{\rho}(\bar{\kappa},ct) \ , \qquad (42a)$$

$$\kappa^2 c\hat{\bar{A}}_T(\bar{\kappa},ct) + \frac{\partial^2}{(\partial ct)^2} c\hat{\bar{A}}_T(\bar{\kappa},ct) = \eta_o \hat{\bar{J}}_T(\bar{\kappa},ct) \ , \qquad (42b)$$

$$\eta_o \hat{\bar{J}}_T(\bar{\kappa},ct) = \eta_o \bar{J}(\bar{\kappa},ct) - i\bar{\kappa}\frac{\partial}{\partial ct}\hat{\phi}(\bar{\kappa},ct) \ , \qquad (42c)$$

and

$$\hat{\bar{E}}(\bar{\kappa},ct) = \hat{\bar{E}}_L(\bar{\kappa},ct) + \hat{\bar{E}}_T(\bar{\kappa},ct) \ , \qquad (43a)$$

$$\hat{\bar{E}}_L(\bar{\kappa},ct) = -i\bar{\kappa}\hat{\phi}(\bar{\kappa},ct) \ , \qquad (43b)$$

$$\hat{\bar{E}}_T(\bar{\kappa},ct) = -\frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct) \ , \qquad (43c)$$

$$c\hat{\bar{B}}(\bar{\kappa},ct) = i\bar{\kappa} \times c\hat{\bar{A}}_T(\bar{\kappa},ct) \ . \qquad (43d)$$

Equation (42b) states that the Fourier transform $c\hat{\bar{A}}(\bar{\kappa},ct)$ behaves like the excursion of a driven harmonic oscillator, whose resonance frequency $\Omega(\bar{\kappa})$ is given by

$$(\frac{\Omega}{c})^2(\bar{\kappa}) = \kappa^2 \ . \tag{44}$$

The "driving force" for such an oscillator is $\eta_o \hat{\bar{J}}_T(\bar{\kappa},ct)$. We shall return to this remark in the next section.

The energy density ρ_{energy} of the electromagnetic field is given by

$$\rho_{energy} = \frac{1}{2\eta_o c}(\bar{E}\cdot\bar{E} + c\bar{B}\cdot c\bar{B}) \tag{45}$$

or, since $\bar{E} = \bar{E}_L + \bar{E}_T$,

$$\rho_{energy} = \frac{1}{2\eta_o c}(\bar{E}_L\cdot\bar{E}_L + 2\bar{E}_L\cdot\bar{E}_T + \bar{E}_T\cdot\bar{E}_T + c\bar{B}\cdot c\bar{B}) \tag{46}$$

When we integrate this expression over the entire $\bar{r}$-space we obtain the stored electromagnetic energy U. According to the orthogonality relation (27), the integral of $\bar{E}_L\cdot\bar{E}_T$ vanishes. Thus

$$U = U_{stat} + U_{rad} \ , \tag{47a}$$

with

$$U_{stat} = \frac{1}{2\eta_o c}\int \Delta\tau_r \bar{E}_L\cdot\bar{E}_L = \frac{1}{2\eta_o c}\int \Delta\tau_r (\bar{\nabla}\phi)\cdot(\bar{\nabla}\phi) \ , \tag{47b}$$

$$U_{rad} = \frac{1}{2\eta_o c}\int \Delta\tau_r (\bar{E}_T\cdot\bar{E}_T + c\bar{B}\cdot c\bar{B}) = \tag{47c}$$

$$= \frac{1}{2\eta_o c}\int \Delta\tau_r [(\frac{\partial}{\partial ct} c\bar{A}_T)\cdot(\frac{\partial}{\partial ct} c\bar{A}_T) + (\bar{\nabla}\times c\bar{A}_T)\cdot(\bar{\nabla}\times c\bar{A}_T)] .$$

The energy U is therefore the sum of two parts, the electrostatic energy U_{stat} associated with the longitudinal field $\bar{E}_L$ and the energy U_{rad} of what may be called the radiation field, i.e., the field specified by $c\bar{B}$ and the transverse part $\bar{E}_T$ of $\bar{E}$. The decomposition (47a) is a natural one. We shall be interested mainly in U_{rad}, since we can regard U_{stat} as a purely configurational energy. For it depends, by way of ϕ, only on the instantaneous charge distribution.

We can convert the integrals over $\bar{r}$-space in (47) into integrals over $\bar{\kappa}$-space by means of the Parseval relation for Fourier transforms. This relation states that for two complex vector fields $\bar{F}(\bar{r},t)$ and $\bar{G}(\bar{r},t)$ we have

$$\int \Delta\tau_r (\bar{F}(\bar{r},ct))^* \cdot \bar{G}(\bar{r},ct) = \frac{1}{(2\pi)^3} \int \Delta\tau_\kappa (\hat{\bar{F}}(\bar{\kappa},ct))^* \cdot \hat{\bar{G}}(\bar{\kappa},ct) \ . \tag{48}$$

We use

$$\overbrace{(\bar{\nabla} \times c\bar{A}_T)}^{\ }{}^* \cdot \overbrace{(\bar{\nabla} \times c\bar{A}_T)}^{\ } = (-i\bar{\kappa} \times (c\hat{\bar{A}}_T)^*) \cdot (i\bar{\kappa} \times c\hat{\bar{A}}_T) =$$

$$= \kappa^2 (c\hat{\bar{A}}_T)^* \cdot c\hat{\bar{A}}_T - \bar{\kappa} \cdot (c\hat{\bar{A}}_T)^* \bar{\kappa} \cdot c\bar{A}_T = \kappa^2 (c\hat{\bar{A}}_T)^* \cdot c\hat{\bar{A}} - 0 \ .$$

(Note that $\bar{\kappa} \cdot c\hat{\bar{A}}_T = 0$, since $\bar{\nabla} \cdot c\bar{A}_T = 0$). Then (47) becomes

$$U = U_{stat} + U_{rad}, \tag{49a}$$

with

$$U_{stat} = \frac{1}{2\eta_o c} \int \Delta\tau_\kappa \kappa^2 (\hat{\phi}(\bar{\kappa},ct))^* \hat{\phi}(\bar{\kappa},ct) \ , \tag{49b}$$

$$U_{rad} = \frac{1}{2\eta_o c} \int \Delta\tau_\kappa [(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct))]^* \cdot \frac{\partial}{\partial ct} c\bar{A}_T(\bar{\kappa},ct) +$$

$$+ \kappa^2 (c\hat{\bar{A}}_r(\bar{\kappa},ct))^* \cdot c\hat{\bar{A}}_T(\bar{\kappa},ct)] \ . \tag{49c}$$

Equation (49c) states that U_{rad} is the sum (actually an integral) of the energies of the individual field oscillators, whose excursions are given by $c\hat{\bar{A}}_T(\bar{\kappa},ct)$. Seemingly, each oscillator has three degrees of freedom, since $c\hat{\bar{A}}_T(\bar{\kappa},ct)$ is a vector. But since this vector is constrained by the condition that it be normal to the wave number vector $\bar{\kappa}$, each field oscillator has only two degrees of freedom.

We are now ready to show (in the next section) that free electrons, even though they may have beats, cannot radiate.

III. Proof of the Statement that "Quantum-mechanical beats cannot enable free electrons to radiate in free space".

We start with the expression (2, 49c) for the energy U_{rad} of the radiation field. We repeat it here for the sake of convenience.

$$U_{rad}(ct) = \frac{1}{2\eta_o c} \int_\kappa \Delta\tau [(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct))^* \cdot \frac{\partial}{\partial ct} c\bar{A}_T(\bar{\kappa},ct) +$$

$$+ \kappa^2 (c\hat{\bar{A}}_T(\bar{\kappa},ct))^* \cdot (c\hat{\bar{A}}_T(\bar{\kappa},ct))] \ . \tag{1}$$

We assume that in the distant past, $ct \to -\infty$, there was no electromagnetic field present as yet. Then what we wish to show is that in the distant future, $ct \to +\infty$, the radiation energy is zero, i.e., we wish to prove that

$$\lim_{ct \to +\infty} U_{rad}(ct) = 0 \ . \tag{2}$$

In the meantime, there may be a build-up of radiation energy. But this energy will be reabsorbed again (not radiated away) in the end.

We determine $c\hat{\bar{A}}_T(\bar{\kappa},ct)$ by means of equation (2-42b), which we repeat here for the sake of convenience,

$$\frac{\partial^2}{(\partial ct)^2} c\hat{\bar{A}}_T(\bar{\kappa},ct) + \kappa^2 c\hat{\bar{A}}_T(\bar{\kappa},ct) = \eta_o \hat{\bar{J}}_T(\bar{\kappa},ct) \ . \tag{3}$$

As we said before, this is the equation for a driven harmonic oscillator. We determine the driving "force" $\eta_o \hat{\bar{J}}_T(\bar{\kappa},ct)$ by taking the spatial Fourier transform of (see (1-42))

$$\bar{J}(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\ (-i\psi^*\bar{\nabla}\psi + i\psi\bar{\nabla}\psi^*) \ . \tag{4}$$

(Afterwards, we extract the transverse part.)

In order to do this, we start with (1,6), but use a different dummy variable, namely $\bar{\xi}$. Thus

$$\psi(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\xi F(\bar{\xi}) \exp\left(i\bar{\xi}\cdot\bar{r} - i\frac{\hbar}{mc}\frac{\xi^2}{2}ct\right) \ . \tag{5}$$

Similarly, this time with the dummy variable $\bar{\eta}$,

$$\psi^*(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\eta F^*(\bar{\eta}) \exp\left(-i\bar{\eta}\cdot\bar{r} + i\frac{\hbar}{mc}\frac{\eta^2}{2}ct\right) \ . \tag{6}$$

On taking the gradient of (5) and (6), we obtain

$$(\bar{\nabla}\psi)(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\xi\ (i\bar{\xi}) F(\bar{\xi}) \exp\left(i\bar{\xi}\cdot\bar{r} - i\frac{\hbar}{mc}\frac{\xi^2}{2}ct\right) \ , \tag{7}$$

$$(\bar{\nabla}\psi^*)(\bar{r},ct) = \frac{1}{(2\pi)^3}\int \Delta\tau_\eta (-i\bar{\eta}) F^*(\bar{\eta}) \exp\left(-i\bar{\eta}\cdot\bar{r} + i\frac{\hbar}{mc}\frac{\eta^2}{2}ct\right). \tag{8}$$

We insert the expressions (5) - (8) into (4). But we write the product of two integrals as the double integral of the products of the integrands. We obtain

$$\bar{J}(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^6}\iint\Delta\tau_\xi\Delta\tau_\eta\,\frac{(\bar{\xi}+\bar{\eta})}{2}F(\bar{\xi})F^*(\bar{\eta})$$

$$\exp(i(\bar{\xi}-\bar{\eta})\cdot\bar{r} - i\frac{\hbar}{mc}\tfrac{1}{2}(\xi^2-\eta^2)ct)\ . \qquad (9)$$

Instead of $\bar{\xi}$ and $\bar{\eta}$, we use two new dummy variables $\bar{\kappa}$ and $\bar{\lambda}$ defined by

$$\left.\begin{aligned}\bar{\kappa} &= \bar{\xi} - \bar{\eta}\ ,\\ \bar{\lambda} &= \tfrac{1}{2}\bar{\xi} + \tfrac{1}{2}\bar{\eta}\end{aligned}\right\}. \qquad (10)$$

Vice versa:

$$\left.\begin{aligned}\bar{\xi} &= +\tfrac{1}{2}\bar{\kappa} + \bar{\lambda}\ ,\\ \bar{\eta} &= -\tfrac{1}{2}\bar{\kappa} + \bar{\lambda}\ .\end{aligned}\right\}. \qquad (11)$$

The Jacobian of the transformation (11) is equal to unity, as one can see when one examines the three Jacobians for each of the three cartesian components; all three are equal to unity, and $1^3 = 1$. Thus $\Delta\tau_\xi\Delta\tau_\eta = \Delta\tau_\kappa\Delta\tau_\lambda$, and equation (9) becomes

$$\bar{J}(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^6}\iint\Delta\tau_\kappa\Delta\tau_\lambda e^{i\bar{k}\cdot\bar{r}}\bar{\lambda}F(\bar{\lambda}+\tfrac{1}{2}\bar{\kappa})F^*(\bar{\lambda}-\tfrac{1}{2}\bar{\kappa})\ .$$

$$\exp(-i\frac{\hbar}{mc}\bar{\kappa}\cdot\bar{\lambda}ct)\ . \qquad (12)$$

From this equation one can read out the spatial Fourier transform $\hat{\bar{J}}(\bar{\kappa},ct)$. See (2,2).) It is given by

$$\hat{\bar{J}}(\bar{\kappa},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^3}\int\Delta\tau_\lambda\bar{\lambda}F(\bar{\lambda}+\tfrac{1}{2}\bar{\kappa})F^*(\bar{\lambda}-\tfrac{1}{2}\bar{\kappa})\exp(-i\frac{\hbar}{mc}\bar{\kappa}\cdot\bar{\lambda}ct)\ . \qquad (13)$$

However, in the equation of motion (3), we need $\hat{\bar{J}}_T(\bar{\kappa},ct)$, the Fourier transform of the transverse part $\bar{J}_T$ of $\bar{J}$. The definitions (2,16) and (2,17) relate $\hat{\bar{J}}_T$ to $\hat{\bar{J}}$. Thus

$$\hat{\bar{J}}_T(\bar{\kappa},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^3}\int\Delta\tau_\lambda(\bar{\lambda}-\frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\bar{\lambda})F(\bar{\lambda}+\tfrac{1}{2}\bar{\kappa})F^*(\bar{\lambda}-\tfrac{1}{2}\bar{\kappa})$$

$$\exp(-i\frac{\hbar}{mc}\bar{\kappa}\cdot\bar{\lambda}\ ct),\ \text{for}\ \bar{\kappa}\neq\bar{0}\ , \qquad (14)$$

and

$$\hat{\bar{J}}_T(\bar{0},ct) = \frac{2}{3}(-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^3}\int\Delta\tau_\lambda\bar{\lambda}F(\bar{\lambda})F^*(\bar{\lambda})\ . \qquad (15)$$

We now make the assumption that the energy $\frac{(\hbar\kappa)^2}{2m}$ associated with each Fourier component $\hat{\psi}(\bar{\kappa},ct)$ of the wave function $\psi(\bar{r},ct)$ is limited to a value

that is much smaller than the rest energy mc^2. This assumption is fulfilled in the device that Schwarz proposed. Furthermore, we have to adopt this assumption already in view of the decision, made at the outset, to use a non-relativistic treatment. This assumption implies that $F(\vec{\kappa})$ be zero whenever κ exceeds some maximum value κ_m, which is chosen in such a way that the corresponding energy $\frac{(\hbar\kappa_m)^2}{2m}$, reckoned non-relativistically, is much smaller than mc^2. For instance, we might choose κ_m to be equal to $\frac{1}{8}\frac{mc}{\hbar}$, so that $\frac{(\hbar\kappa_m)^2}{2m} = \frac{1}{64} mc^2$, which is in the order of 60 kilo-electronvolt. We summarize these remarks by the statement that

$$F(\vec{\kappa}) = 0, \text{ for } \kappa > \kappa_m . \tag{16}$$

One consequence of (16) is that

$$\hat{J}_n(\vec{\kappa},ct) = 0, \text{ for } \kappa > 2\kappa_m . \tag{17}$$

The reason is that $F(\vec{\lambda} + \frac{1}{2}\vec{\kappa})F^*(\vec{\lambda} - \frac{1}{2}\vec{\kappa})$ in (14) is zero, unless $\vec{\lambda}$ lies simultaneously in the two spheres (drawn in $\vec{\lambda}$-space) $|\vec{\lambda} - \frac{1}{2}\vec{\kappa}| \leq \kappa_m$ and $|\vec{\lambda} - (-\frac{1}{2}\vec{\kappa})| \leq \kappa_m$. (Their centers are at $\frac{1}{2}\vec{\kappa}$ and $-\frac{1}{2}\vec{\kappa}$ respectively; and both have the radius κ_m.) But when $|\frac{1}{2}\vec{\kappa}| > \kappa_m$, the two spheres do not overlap. Thus the integrand in (14) is zero for every $\vec{\lambda}$, and (17) results.

A more important consequence of (16) is that, for each $\vec{\kappa}$, the quantity $\hat{J}_n(\vec{\kappa},ct)$ is band-limited to a low-pass frequency band. In order to see this, we examine the frequencies $\frac{\omega}{c} = -\frac{\hbar}{mc}\vec{\kappa}\cdot\vec{\lambda}$ that occur in the time factor $\exp(-i\frac{\hbar}{mc}\vec{\kappa}\cdot\vec{\lambda}\,ct)$ of (14). Then, what we are looking for, are the extreme values of $\vec{\kappa}\cdot\vec{\lambda}$, when $\vec{\lambda}$ is restricted to lie in the domain that is common to the two spheres $|\vec{\lambda} - \frac{1}{2}\vec{\kappa}| \leq \kappa_m$ and $|\vec{\lambda} - (-\frac{1}{2}\vec{\kappa})| \leq \kappa_m$. A sketch of the two spheres will show that the extreme values of $\vec{\kappa}\cdot\vec{\lambda}$ occurs when $\vec{\lambda}$ lies at the two points $\pm(-\frac{1}{2}\vec{\kappa} + \vec{\kappa}_m\frac{\vec{\kappa}}{\kappa})$. [The surface of each sphere intersects the axis that goes

through $-\frac{1}{2}\bar{\kappa}$ and $\frac{1}{2}\bar{\kappa}$ in two points, whose distances from the origin are $\kappa_m + \frac{1}{2}\kappa$ and $\kappa_m - \frac{1}{2}\kappa$. The two critical vectors $\bar{\lambda}$ that we need lie at the intersection points that are closest to the origin. And that gives us the two points $\pm\,(-\frac{1}{2}\bar{\kappa} + \kappa_m \frac{1}{\kappa}\bar{\kappa})]$. Therefore, for a given wave vector $\bar{\kappa}$, the frequencies $\frac{\omega}{c} = -\frac{\hbar}{mc}\bar{\kappa}\cdot\bar{\lambda}$ that occur in the excitation function $\eta_o\hat{\bar{J}}_T(\bar{\kappa},ct)$ of (3) are limited to the band

$$-\kappa\frac{\hbar}{mc}(\kappa_m - \tfrac{1}{2}\kappa) \leq \frac{\omega}{c} \leq +\kappa\frac{\hbar}{mc}(\kappa_m - \tfrac{1}{2}\kappa)\ . \tag{18}$$

The excitation function $\eta_o\hat{\bar{J}}(\bar{\kappa},ct)$ is thus band-limited to the low-pass band (18).

We could substantiate this conclusion by a detailed calculation of the temporal Fourier transform $\eta_o\tilde{\hat{\bar{J}}}_T(\kappa,\frac{\omega}{c})$ (pronounced jay-tee-hat-tilde) of the excitation function $\hat{\bar{J}}_T(\bar{\kappa},ct)$. This transform is defined by

$$\tilde{\hat{\bar{J}}}_T(\bar{\kappa},\tfrac{\omega}{c}) = \int_{ct=-\infty}^{+\infty} dct\ e^{-i\frac{\omega}{c}ct}\ \hat{\bar{J}}_T(\bar{\kappa},ct)\ . \tag{19}$$

The inversion formula of (19) is

$$\hat{\bar{J}}_T(\bar{\kappa},ct) = \frac{1}{2\pi}\int_{\frac{\omega}{c}=-\infty}^{+\infty} d\,\frac{\omega}{c}\,e^{i\frac{\omega}{c}ct}\,\tilde{\hat{\bar{J}}}_T(\bar{\kappa},\tfrac{\omega}{c}) \tag{20}$$

However we do not need to perform this straight-forward calculation (which is done most convincingly with (20) as the starting point). The reason is that, as we shall see later, we need $\tilde{\hat{\bar{J}}}_T(\bar{\kappa},\frac{\omega}{c})$ only for one particular value of the frequency $\frac{\omega}{c}$. And this value corresponds to the resonance frequency κ of the harmonic oscillator type equation of motion (3). Now, κ lies well outside the low-pass band (18). (For our numerical example $\kappa_m = \frac{1}{2}\frac{mc}{\hbar}$, the resonance frequency κ lies outside the low-pass band (18) by a margin that is better than 2 to 1.) Thus we arrive at the important equations.

$$\left.\begin{aligned}\tilde{\hat{\bar{J}}}_T(\bar{\kappa},\kappa) &= 0\ ,\\ \tilde{\hat{\bar{J}}}_T(\bar{\kappa},-\kappa) &= 0\ ,\end{aligned}\right\}\quad \text{for } |\bar{\kappa}| \neq 0\ . \tag{21a, 21b}$$

Now we take up the reason that we are interested mainly in the temporal Fourier transform $\eta_o \tilde{\tilde{J}}_T(\bar{\kappa},\kappa)$ at the single frequency value $\frac{\omega}{c} = \kappa$, rather than in the complete time function $\hat{\bar{J}}_T(\bar{\kappa},ct)$. We assume that the electromagnetic field was in its quiescent state in the distant past, so that

$$\lim_{ct\to-\infty} c\bar{A}_T(\bar{r},ct) = 0, \quad \lim_{ct\to-\infty} \frac{\partial}{\partial ct} c\bar{A}_T(\bar{r},ct) = 0, \quad \lim_{ct\to-\infty} U_{rad}(ct) = 0 \ .^{\dagger} \tag{22}$$

The first two equations of (22) imply that similar equations hold also for the spatial Fourier transforms, so that

$$\lim_{ct\to\infty} c\hat{\bar{A}}_T(\bar{\kappa},ct) = 0, \quad \lim_{ct\to-\infty} \frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct) = 0 \ . \tag{23}$$

We wish to evaluate how much radiation energy will have been produced in the distant future, i.e., we wish to calculate $\lim_{ct\to+\infty} U_{rad}(ct)$. We start with the expression (1) for $U_{rad}(ct)$. We then need $\lim_{ct\to+\infty} c\hat{\bar{A}}_T(\bar{\kappa},ct)$ and $\lim_{ct\to+\infty} \frac{\partial}{\partial ct} c\bar{A}_T(\bar{\kappa},ct)$. We could determine $c\hat{\bar{A}}_T(\bar{\kappa},ct)$ directly from the equation of motion (3). However, we find it more convenient to determine the two auxiliary functions $\hat{\bar{F}}(\bar{\kappa},ct)$ and $\hat{\bar{G}}(\bar{\kappa},ct)$ which are defined by

$$\begin{aligned} \hat{\bar{F}}(\bar{\kappa},ct) &= \left(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct) - i\kappa c\hat{\bar{A}}_T(\bar{\kappa},ct)\right)e^{i\kappa ct} \ , \\ \hat{\bar{G}}(\bar{\kappa},ct) &= \left(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct) + i\kappa c\hat{\bar{A}}_T(\bar{\kappa},ct)\right)e^{-i\kappa ct} \ , \end{aligned} \tag{24}$$

where, as always, $\kappa = |\bar{\kappa}|$.* Note that both auxiliary functions vanish in the distant past because of (23). For the complex conjugates, we have

$$\begin{aligned} \hat{\bar{F}}^*(\bar{\kappa},ct) &= \left(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T^*(\bar{\kappa},ct) + i\kappa\, c\hat{\bar{A}}_T(\bar{\kappa},ct)\right)e^{-i\kappa ct} \ , \\ \hat{\bar{G}}^*(\bar{\kappa},ct) &= \left(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T^*(\bar{\kappa},ct) - i\kappa c\hat{\bar{A}}_T^*(\bar{\kappa},ct)\right)e^{i\kappa ct} \ . \end{aligned} \tag{25}$$

From (24) and (25) we obtain

$$\begin{aligned} &\tfrac{1}{2}\left(\hat{\bar{F}}^*(\bar{\kappa},ct)\cdot\hat{\bar{F}}(\bar{\kappa},ct) + \hat{\bar{G}}^*(\bar{\kappa},ct)\cdot\hat{\bar{G}}(\bar{\kappa},ct)\right) = \\ &= \left(\frac{\partial}{\partial ct} c\hat{\bar{A}}_T^*(\bar{\kappa},ct)\right)\cdot \frac{\partial}{\partial ct} c\hat{\bar{A}}_T(\bar{\kappa},ct) + \kappa^2 c\hat{\bar{A}}_T^*(\bar{\kappa},ct)\cdot c\hat{\bar{A}}_T(\bar{\kappa},ct) \ . \end{aligned} \tag{26}$$

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*One should not confuse the (vectorial and time-dependent) $\hat{\bar{F}}$ in (24) with the the (scalar and time-independent) F in (5).

†What makes it possible to stipulate these initial conditions is that, in the distant past, the beats have not yet developed and that the wave packet is of infinite size.

The right-hand side of (26) is the integrand of equation (1). Thus, (1) may be written in the form

$$U_{rad}(ct) = \frac{1}{4\eta_o c}\int \Delta_k [\hat{\bar{F}}^*(\bar{\kappa},ct)\cdot\hat{\bar{F}}(\bar{\kappa},ct) + \hat{\bar{G}}^*(\bar{\kappa},ct)\cdot\hat{\bar{G}}(\bar{\kappa},ct)] \ . \qquad (27)$$

Now we calculate the two auxiliary functions $\hat{\bar{F}}(\bar{\kappa},ct)$ and $\hat{\bar{G}}(\bar{\kappa},ct)$. We take the time derivative of (24) and use the equation of motion (3). Then (there are two terms that cancel)

$$\begin{aligned}\frac{\partial}{\partial ct}\hat{\bar{F}} &= \left(\frac{\partial^2}{(\partial ct)}\, c\hat{\bar{A}}_T + \kappa^2 c\hat{\bar{A}}_T\right)e^{i\kappa ct} = \eta_o \hat{\bar{J}}_T e^{i\kappa ct}, \\ \frac{\partial}{\partial ct}\hat{\bar{G}} &= \left(\frac{\partial^2}{(\partial ct)^2}\, c\hat{\bar{A}}_T + .^2 c\hat{\bar{A}}_T\right)e^{-i\kappa ct} = \eta_o \hat{\bar{J}}_T e^{-i\kappa ct} \ .\end{aligned} \qquad (28)$$

The functions $\hat{\bar{F}}$ and $\hat{\bar{G}}$ can then be determined by simple quadratures. Because these functions vanish for $ct \to -\infty$, we have

$$\begin{aligned}\hat{\bar{F}}(\bar{\kappa},ct) &= \int_{cs=-\infty}^{ct} ds\, e^{i\kappa cs}\, \eta_o \hat{\bar{J}}_T(\bar{\kappa},cs) \ , \\ \hat{\bar{G}}(\bar{\kappa},ct) &= \int_{cs=-\infty}^{ct} ds\, e^{-i\kappa cs}\, \eta_o \hat{\bar{J}}_T(\bar{\kappa},cs) \ .\end{aligned} \qquad (29)$$

Now we take the limit $ct \to +\infty$. In view of the definition (19) for the temporal Fourier transform, we have

$$\begin{aligned}\lim_{ct\to+\infty} \hat{\bar{F}}(\bar{\kappa},ct) &= \eta_o \tilde{\hat{\bar{J}}}_T(\bar{\kappa},-\kappa) \ , \\ \lim_{ct\to+\infty} \hat{\bar{G}}(\bar{\kappa},ct) &= \eta_o \tilde{\hat{\bar{J}}}_T(\bar{\kappa},\kappa) \ . \ .\end{aligned} \qquad (30)$$

We use these expressions in equation (27). Then the radiation energy in the distant future becomes

$$\begin{aligned}\lim_{ct\to+\infty} U_{rad}(ct) = \frac{\eta_o}{4c}\int \Delta\tau_\kappa [&(\tilde{\hat{\bar{J}}}_T(\bar{\kappa},-\kappa))^* \cdot \tilde{\hat{\bar{J}}}_T(\bar{\kappa},-\kappa) + \\ &+ (\tilde{\hat{\bar{J}}}_T(\bar{\kappa},\kappa))^* \cdot \tilde{\hat{\bar{J}}}_T(\bar{\kappa},\kappa)] \ .\end{aligned} \qquad (31)$$

But according to (21), all the Fourier transforms in (31) are zero. Thus we have the final result

$$\lim_{ct\to+\infty} U_{rad}(ct) = 0 \ . \qquad (32)$$

In words: A single free electron in free space, even though it may have quantum-mechanical beats, cannot produce any radiation energy in the end. Of course, there may be some temporary production of radiation energy. But, in the end, this energy is reabsorbed by the electron. What made it impossible to generate radiation is that, for a beat of wave number $\bar{\kappa}$, the frequency ω/c is well below the required value $\kappa = |\bar{\kappa}|$. And the reason for that was the band width limitation (18).

So far we have considered just one electron. Now let us consider a swarm of electrons. We enumerate the electrons with some digit $p = 1,2,3, \ldots$ Let ${}_p\bar{J}(\bar{r},ct)$ be the current density that belongs to electron #p. When we wish to adapt our previous calculation to the swarm of electrons, then we merely have to replace $\bar{J}$ by the sum $\sum_p \bar{J}$. In equation (30) and (31) there appear the sums $\sum_p \tilde{\bar{J}}(\bar{\kappa},-\kappa)$ and $\sum_p \tilde{\bar{J}}(\bar{\kappa},\kappa)$. Since each term in the sums is zero, the sums themselves are zero. Thus, equation (32) holds also for a swarm of free electrons in free space. Note that we did not make any assumption about the instants at which the electrons are emitted. The conclusion (32) holds not only when the electrons are emitted at random instants, but also when the electrons are bunched by some gating device.

This finishes the proof for the absence of radiation. We conclude this section with some miscellaneous comments.

Several times we have mentioned the spatial and temporal Fourier transform $\tilde{\bar{J}}_T(\bar{\kappa}, \frac{\omega}{c})$ of the transverse current density $\bar{J}_T(\bar{r},ct)$. We never needed to calculate it, because only the special values $\tilde{\bar{J}}_T(\bar{\kappa},\kappa)$ and $\tilde{\bar{J}}_T(\bar{\kappa},-\kappa)$ were required in our proof. And these values were seen to be zero. Nevertheless, for the sake of completeness, we exhibit an expression for the general value $\tilde{\hat{\bar{J}}}_T(\bar{\kappa}, \frac{\omega}{c})$. We start with equation (14) for the spatial Fourier transform

$\hat{\bar{J}}_T(\bar{\kappa},ct)$. We repeat this equation for the sake of convenience.

$$\hat{\bar{J}}_T(\bar{\kappa},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^3}\int \Delta\tau_\lambda(\bar{\lambda} - \frac{1}{\kappa^2}\bar{\kappa}\bar{\kappa}\cdot\bar{\lambda})F(\bar{\lambda} + \tfrac{1}{2}\bar{\kappa})F^*(\bar{\lambda} - \tfrac{1}{2}\bar{\kappa})$$

$$\exp(-i\frac{\hbar}{mc}\bar{\kappa}\cdot\bar{\lambda}\,ct) \qquad (14, \text{ repeated})$$

In the $\bar{\lambda}$-space, over which the integration in (14) is performed, we introduce cartesian coordinates ξ, η, ζ referred to the three mutually orthogonal unit vectors $\frac{\bar{\kappa}}{\kappa}$, $\bar{a}$, $\bar{b}$. The first of these depends on the given wave number vector $\bar{\kappa}$, which appears on the left-hand side of (14). Then we can always choose the remaining unit vectors $\bar{a}$ and $\bar{b}$ in such a way that $\frac{\bar{\kappa}}{\kappa}$, $\bar{a}$, $\bar{b}$ are mutually orthogonal. Thus we can write

$$\bar{\lambda} = \xi\bar{a} + \eta\bar{b} + \zeta\frac{\bar{\kappa}}{\kappa}$$

and

$$\Delta\tau_\lambda = d\xi d\eta d\zeta.$$

Equation (14) then becomes

$$\hat{\bar{J}}_T(\bar{\kappa},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^3}\iiint_{\xi,\eta,\zeta=-\infty}^{+\infty} d\xi d\eta d\zeta(\xi\bar{a} + \eta\bar{b})F(\xi\bar{a} + \eta\bar{b} + (\zeta + \frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa})$$

$$F^*(\xi\bar{a} + \eta\bar{b} + (\zeta - \frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa})\exp(-i\frac{\hbar}{mc}\zeta\kappa ct)\,. \qquad (33)$$

Here we replace the integration variable ζ by the integration variable $\frac{\omega}{c}$, such that

$$\frac{\omega}{c} = -\frac{\hbar}{mc}\kappa\zeta\,.$$

Then

$$d\zeta = -\frac{mc}{\hbar}\frac{1}{\kappa}d\frac{\omega}{c}\,,$$

and $\frac{\omega}{c}$ runs from $+\infty$ to $-\infty$. We can remove the minus sign that results from the equation for $d\zeta$ by making $\frac{\omega}{c}$ run from $-\infty$ to $+\infty$ again. Then equation (33) becomes

$$\hat{\vec{J}}_T(\bar{\kappa},ct) = (-ec)\frac{1}{\kappa}\frac{1}{(2\pi)^3}\iiint_{\xi,\eta,\omega/c=-\infty}^{+\infty} d\frac{\omega}{c}\,d\xi d\eta(\xi\bar{a}+\eta\bar{b})F(\xi\bar{a}+\eta\bar{b}+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}+\frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa})$$

$$F^*(\xi\bar{a}+\eta\bar{b}+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}-\frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa})\exp(i\frac{\omega}{c}ct)\ . \qquad (34)$$

Next we note that the spatial Fourier transform $\hat{\vec{J}}_T(\bar{\kappa},ct)$ is related to the spatial and temporal Fourier transform $\tilde{\hat{\vec{J}}}_T(\bar{\kappa},\frac{\omega}{c})$ by

$$\hat{\vec{J}}_T(\bar{\kappa},ct) = \frac{1}{2\pi}\int_{\frac{\omega}{c}=-\infty}^{+\infty} d\frac{\omega}{c}\,\tilde{\hat{\vec{J}}}_T(\bar{\kappa},\frac{\omega}{c})\exp(i\frac{\omega}{c}ct). \qquad (35)$$

On comparing (34) and (35) we obtain the final result

$$\tilde{\hat{\vec{J}}}_T(\bar{\kappa},\frac{\omega}{c}) = (-ec)\frac{1}{\kappa}\frac{1}{(2\pi)^2}\iint_{\xi,\eta=-\infty}^{+\infty} d\xi d\eta(\xi\bar{a}+\eta\bar{b})F(\xi\bar{a}+\eta\bar{b}+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}+\frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa})$$

$$F^*(\xi\bar{a}+\eta\bar{b}+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}-\frac{\kappa}{2})\frac{\bar{\kappa}}{\kappa}). \qquad (36)$$

Here, as always in our calculations, the quantity κ stands for $|\kappa|$. On the other hand, $\frac{\omega}{c}$ takes on both positive and negative values.

According to our assumption about the energies encountered in the wave packet, the functions F and F^* in (36) vanish unless their vectorial arguments are smaller in magnitude than some maximum value κ_m, for which we suggested, by way of an example, the quantity $\frac{1}{2}\frac{mc}{\hbar}$. Thus the effective domain of the (ξ,η) - integration is constrained by the two inequalities

$$\xi^2+\eta^2+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}+\frac{\kappa}{2})^2 < \kappa_m^2\ ,$$

$$\xi^2+\eta^2+(\frac{mc}{\hbar}\frac{1}{\kappa}\frac{\omega}{c}-\frac{\kappa}{2})^2 < \kappa_m^2 \qquad (37)$$

Therefore, the effective domain of the integral in (36) is finite, in spite of the $\pm\infty$ marked on the integration signs. Hence, there are no convergences problems.

Again, let us take the example $\kappa_m = \frac{1}{2}\frac{mc}{\hbar}$. Let us now calculate $\tilde{\hat{\vec{J}}}_T(\bar{\kappa},\frac{\omega}{c})$ for $\frac{\omega}{c} = \pm\kappa$. Then, it cannot ever happen that both inequalities (37) are satisfied.

(For $\frac{\omega}{c} = +\kappa$, the first is definitely violated, and for $\frac{\omega}{c} = -\kappa$, the second is definitely violated). Thus the effective domain for the integration in (36) has shrunk to zero, so that

$$\left.\begin{aligned}\tilde{\bar{J}}_T(\bar{\kappa},\kappa) &= 0,\\ \tilde{\bar{J}}_T(\bar{\kappa},-\kappa) &= 0,\end{aligned}\right\} \quad \text{for } |\bar{\kappa}| \neq 0 . \tag{38}$$

This result agrees with the equations (21a,b), which were established without a detailed calculation of the spatial and temporal Fourier transform.

We may establish the validity of equations (38), on which the impossibility of radiation was based, also directly from equation (9). We modify this equation so that it yields the transverse part $\bar{J}_T$. The modified equation is

$$\bar{J}_T(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^6}\iint \Delta\tau_\xi \Delta\tau_\eta \left[\frac{\bar{\xi}+\bar{\eta}}{2} - \frac{(\bar{\xi}-\bar{\eta})(\bar{\xi}-\bar{\eta})}{(\bar{\xi}-\bar{\eta})\cdot(\bar{\xi}-\bar{\eta})}\cdot\frac{\bar{\xi}+\bar{\eta}}{2}\right]$$

$$F(\bar{\xi})F^*(\bar{\eta})$$

$$\exp\left[i(\bar{\xi}-\bar{\eta})\cdot\bar{r} - i\frac{\hbar}{mc}(\xi^2-\eta^2)ct\right] . \tag{39}$$

We generalize this equation to a form which is valid also in the relativistic region of velocities. But we still adhere to the description in terms of scalar Schrödinger waves, i.e., we refrain from using the Dirac spinors. The relativistic formulation allows us to dispense with the introduction of some maximum wave number κ_m, as we did in connection with equations (16) and (17). In order to obtain the relativistic generalization we have to replace the quantities $\frac{\hbar}{mc}\frac{1}{2}\xi^2$ and $\frac{\hbar}{mc}\frac{1}{2}\eta^2$ in the exponent of (14) by $\sqrt{(\frac{mc}{\hbar})^2 + \xi^2}$ and $\sqrt{(\frac{mc}{\hbar})^2 + \eta^2}$. These replacements follow from the relativistic relation

$$E^2 = (mc^2)^2 + (cp)^2 \tag{40}$$

between the energy E and the momentum p, as well as from the de Broglie relations

$$E = \hbar c\frac{\omega}{c} , \quad \bar{p}_\xi = \hbar\bar{\xi}, \quad \bar{p}_\eta = \hbar\bar{\eta} . \tag{41}$$

The relativistic generalization of (39) is then

$$\bar{J}_T(\bar{r},ct) = (-ec)\frac{\hbar}{mc}\frac{1}{(2\pi)^6}\iint\Delta\tau_\xi\Delta\tau_\eta\left[\frac{\bar{\xi}+\bar{\eta}}{2} - \frac{(\bar{\xi}-\bar{\eta})(\bar{\xi}-\bar{\eta})}{(\bar{\xi}-\bar{\eta})\cdot(\bar{\xi}-\bar{\eta})}\cdot\frac{\bar{\xi}+\bar{\eta}}{2}\right]$$

$$F(\xi)F^*(\eta)$$

$$\exp\left[i(\bar{\xi}-\bar{\eta})\cdot\bar{r} - i\left(\sqrt{(\tfrac{mc}{\hbar})^2+\xi^2}-\sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}\right)ct\right] . \qquad (42)$$

This equation shows that each doublet $(\bar{\xi},\bar{\eta})$ of wave number vectors contributes a sinusoidal wave to $\bar{J}_T$. The wave number vector $\bar{\kappa}$ and the frequency $\frac{\omega}{c}$ of such an elementary wave are given by

$$\left.\begin{aligned}\bar{\kappa} &= \bar{\xi} - \bar{\eta} ,\\ \frac{\omega}{c} &= \sqrt{(\tfrac{mc}{\hbar})^2+\xi^2} - \sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}\end{aligned}\right\} . \qquad (43)$$

(Different doublets $(\bar{\xi},\bar{\eta})$ can produce a common $\bar{\kappa}$ and $\frac{\omega}{c}$. But this lack of a one-to-one correspondence need not concern us.) Now let us examine the ratio $\frac{|\omega/c|}{|\bar{\kappa}|}$ of an elementary wave. We have

$$\frac{|\omega/c|}{|\bar{\kappa}|} = \frac{\left|\sqrt{(\tfrac{mc}{\hbar})^2+\xi^2} - \sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}\right|}{|\bar{\xi}-\bar{\eta}|}$$

But since

$$|\bar{\xi}-\bar{\eta}| \geq \left||\bar{\xi}| - |\bar{\eta}|\right| = \left|\sqrt{\xi^2} - \sqrt{\eta^2}\right| ,$$

we obtain

$$\frac{|\omega/c|}{|\bar{\kappa}|} \leq \left|\frac{\sqrt{(\tfrac{mc}{\hbar})^2+\xi^2} - \sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}}{\sqrt{\xi^2} - \sqrt{\eta^2}}\right|$$

Now

$$\left|\frac{\sqrt{(\tfrac{mc}{\hbar})^2+\xi^2} - \sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}}{\sqrt{\xi^2} - \sqrt{\eta^2}}\right| \left|\frac{\sqrt{(\tfrac{mc}{\hbar})^2+\eta^2} + \sqrt{(\tfrac{mc}{\hbar})^2+\eta^2}}{\sqrt{\xi^2} + \sqrt{\eta^2}}\right| = \left|\frac{\xi^2-\eta^2}{\xi^2-\eta^2}\right| = 1$$

so that

$$\frac{|\omega/c|}{|\bar{\kappa}|} \leq \frac{\sqrt{\xi^2} + \sqrt{\eta^2}}{\sqrt{(\frac{mc}{\hbar})^2+\xi^2} + \sqrt{(\frac{mc}{\hbar})^2+\eta^2}}$$

The expression on the right-hand side is clearly less than unity. Thus we arrive at the result

$$\frac{|\omega/c|}{|\bar{\kappa}|} < 1 \, . \tag{44}$$

The inequality (44) tells us that every elementary wave in (42) has a frequency-to-wave number ratio that is less than unity. But $\hat{\tilde{J}}_T(\bar{\kappa},\kappa)$ and $\hat{\tilde{J}}_T(\bar{\kappa},\dot{\kappa})$ are the amplitude factors of elementary waves whose frequency-to-wave number ratio is equal to unity. Since we have seen that elementary waves with a ratio equal to unity do not occur in (42), we conclude that

$$\left.\begin{aligned} \hat{\tilde{J}}_T(\bar{\kappa},\kappa) &= 0 \, , \\ \hat{\tilde{J}}_T(\bar{\kappa},-\kappa) &= 0 \, , \end{aligned}\right\} \text{ for } |\bar{\kappa}| \neq 0 \, . \tag{45}$$

And these equations are identical with (38).

We conclude this section with a remark about the spirit of the calculations we have performed. We started with a given free wave packet of Schrödinger waves. The word "free" indicates that the wave packet is not influenced by electromagnetic forces. Then we calculated the electromagnetic field that is generated by the electric current density associated with the wave packet. Now in principle, this field would influence the behavior of the Schrödinger waves. However, we neglected to take into account this back-reaction that proceeds from the electro-magnetic field to the Schrödinger waves. We only considered the forward action that proceeds from the Schrödinger waves to the electromagnetic field. What we have done then is in accordance with the perturbation calculus, whose principles are explained in Section 10 of the Appendix. We had to resort to the perturbation calculua

because an exact calculation is impracticable. It is believed that the accuracy of the perturbation calculus is good enough for our purposes. One could, in principle, adduce some evidence for this belief by carrying out the perturbation calculus to the next higher order of approximation. But this would entail a lot of effort, more than we can afford to devote to this task. As far as this writer knows, there are no general principles that could obviate the necessity of those cumbersome calculations. Even if the next order of approximation were to predict some radiation, it would be too weak to be of practical use.

We have seen that no radiation can be expected from free electrons, even if they exhibit beats. Naturally, there comes up the following question: Can one use the beats in some other way? For instance, one may ask whether electrons with beats interact with externally produced radiation in some peculiar, and perhaps useful, way. We explore this question in the next section.

IV. A Selective Moving Mirror .

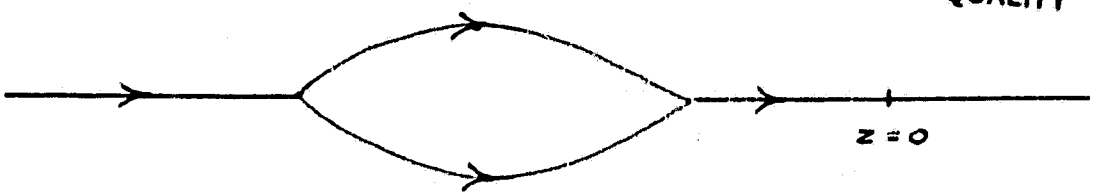
H. Schwarz suggested a device that produces an electron beam which is a superposition of two plane waves of different wavelength. In mathematical language: The Schrödinger wave that describes the electron beam is of the form

$$\psi(z,ct) = C\{\exp(i\kappa_1 z - i \frac{\hbar}{mc} \frac{\kappa_1^2}{2} ct) + \exp(i\kappa_2 z - i \frac{\hbar}{mc} \frac{\kappa_2^2}{2} ct)\} . \qquad (1)$$

Here C is an amplitude factor. The beam travels in the z-direction of some cartesian coordinate system. Each of the two partial waves is a plane wave. The first partial wave has the wave number κ_1 and the kinetic energy $\frac{\hbar^2}{2m} \kappa_1^2$. The frequency ω_1 is therefore given by $\frac{\omega_1}{c} = \frac{\hbar}{mc} \frac{\kappa_1^2}{2}$. Similarly, κ_2 and $\frac{\hbar^2}{2m} \kappa_2^2$

are the wave number and kinetic energy of the second partial wave. Both kinetic energies are of the order of 30×10^3 electrovolt. And their difference is in the optical range, i.e. we have $\frac{\hbar}{2m}(\kappa_2^2 - \kappa_1^2) \approx 3$ electron-volt. The constants $\hbar$, m, c have their usual meaning, namely $\frac{1}{2\pi}$ · Planck's constant, electronic mass, and speed of light in vacuo.

We give a brief description of Schwarz's design. An electron beam is sent through a beam splitter that splits it into two divergent beams #1 and #2. Several inches down their paths, they are made to converge again into the working region of the apparatus (near z = 0), where they form a single beam again. This writer is not competent in the field of electron optics. Therefore, we will refrain from describing how this may be accomplished. Perhaps one may imagine that the beam splitter and, further down the line, the beam joiner consist of diffraction gratings, presumably in the form of single crystals. What is important to keep in mind is that the beam splitter does not sort out different individual electrons. Instead, it splits the Schrödinger wave of each electron into two divergent portions. Similar remarks may be made about the beam joiner. So far then, the lay-out of the beams is as follows. First there is a straight and narrow beam along the z-axis. The beam enters the beam splitter and becomes two beams, diverging off to the north and the south respectively. After a few inches down the line, these two beams are bent back to the z-axis. Where they meet, they are joined by the beam joiner and form again a straight beam along the z-axis. (The beam joiner will waste some of the beam by sending off additional beams to the sides.) Eventually this beam enters the working region of the apparatus near z = 0.



In the region between the two curving beams, a device is installed that contains a magnetic field in the vertical direction. This field is made to change with time. According to Faraday's induction law, an electric vortex field arises that speeds up the northern partial beam and slows down the southern partial beam. The beam that emergies beyond the beam joiner is then a superposition of two beams with different energies, the energy difference being chosen to be in the optical range. Because the beam splitter and the beam joiner act on the Schrödinger wave of each electron, the superposition is linear as described by equation (1).

If, in a more realistic manner, we consider that the Schrödinger wave of an individual electron would be a localized wave packet instead of a c.w. wave (c.w. = continuous wave) of infinite extent, then we conclude that an additional device is needed. After all, since the northern beam was sped up whereas the southern beam was slowed down, the southern wave packet would lag behind the northern wave packet beyond the beam joiner, so that the superposition described by equation (1) could not take place. Therefore, we have to install a delay section in the northern partial beam to remove the lag.

From now on, we shall assume that a perfect design of the electron beam in the working region has been achieved. By this we mean that the Schrödinger wave $\psi(z,ct)$ is the linear superpostion of two partial waves $\psi_1(z,ct)$ and $\psi_2(z,ct)$,

$$\psi(z,t) = \psi_1(z,t) + \psi_2(z,t) \ , \qquad (2)$$

and that at the center of the working region (i.e. at z = 0) the quantities $\psi_2(o,ct)$ and $\psi_1(o,ct)$ are related by

$$\psi_2(o,ct) = \psi_1(o,ct)e^{-iFct} , \tag{3}$$

where F is a constant. In terms of κ_2 and κ_1 we have

$$F = \frac{\hbar}{mc} \tfrac{1}{2}(\kappa_2^2 - \kappa_1^2) . \tag{4}$$

Of course, $\hbar cF$ is the energy difference for the two partial beams. We assume that (3) holds, no matter how $\psi_1(o,ct)$ depends on the time t. As we implied by the notation $\psi(z,ct)$, we ignore any dependence on x and y. That is, we assume that the Schrödinger waves are plane waves. Certainly the c.w. wave (1) conforms to the specification (2) - (4). The specification (3) permits the investigation not only of c.w. waves but also of wave packets.

To begin with, we examine c.w. waves. We will discuss wave packets later on. We start with the example of equation (1). The density of electrons is given by $\psi^*\psi$. In our case, we obtain

$$\psi^*\psi = 2C^*C\{1 + \cos[(\kappa_2-\kappa_1)(z - \tfrac{\kappa_2+\kappa_1}{2} \tfrac{\hbar}{mc} ct)]\} \tag{5}$$

The first term in the curled bracket describes a constant background, whereas the second term exhibits the beats. The beats persist with constant strength for all values of z. The beats have the wave number $\kappa_2 - \kappa_1$, and their velocity v is given by

$$\frac{v}{c} = \frac{\hbar}{mc} \frac{\kappa_1+\kappa_2}{2} \tag{6}$$

Now we come to the matter of wave packets. Let us first consider the partial wave #1. Instead of the c.w. wave

$$\psi_1(z,ct) = C \exp[i\kappa_1 z - i \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} ct] , \tag{7}$$

we consider a superposition of plane waves, each with a different wave number κ. However the κ-values should be closely clustered around the nominal

value κ_1. Accordingly we write

$$\psi_1(z,ct) = N_1 \int_{\kappa=-\infty}^{+\infty} d\kappa\ f(\kappa)\ \exp[i\kappa z - i\,\tfrac{1}{2}\kappa^2\,\frac{\hbar}{mc}\,ct]\ , \qquad (8)$$

where $|f(\kappa)|^2$ is sharply peaked near $\kappa = \kappa_1$. The quantity N_1 is a (complex) normalization factor, which we determine later. The conclusions that we wish to draw do not depend on the choice of the weighting function $f(\kappa)$, as long as it is sharply peaked. We choose $f(\kappa)$ to be equal to unity when κ lies in a narrow range centered at κ_1, and we set $f(\kappa)$ equal to zero when κ lies outside this narrow range. We therefore write

$$\psi_1(z,t) = N_1 \int_{\kappa=\kappa_1-\alpha_1}^{\kappa_1+\alpha_1} d\kappa\ \exp[i\kappa z - i\,\tfrac{1}{2}\kappa^2\,\frac{\hbar}{mc}\,ct]\ . \qquad (9)$$

We demand that

$$\alpha_1 \ll \kappa_2 - \kappa_1\ , \qquad (10)$$

where κ_1 and κ_2 ($\kappa_2 > \kappa_1$) are the nominal wave numbers of the first and secnd partial beam respectively. We replace the integration variable κ by $\xi = \kappa - \kappa_1$. Then (9) becomes

$$\psi_1(z,ct) = N_1 \int_{\xi=-\alpha_1}^{+\alpha_1} d\xi\ \exp[i(\kappa_1+\xi)z - i\tfrac{1}{2}(\kappa_1{}^2+2\kappa_1\xi+\xi^2)\,\frac{\hbar}{mc}\,ct]\ . \qquad (10a)$$

So that we may evaluate the integral in a convenient closed form, we decide to keep track of the wave packet only for those times that satisfy the condition

$$\alpha_1{}^2\,\frac{\hbar}{mc}\,|ct| \ll 1. \qquad (11)$$

Then we may delete the term ξ^2 in (10a) and obtain

$$\psi_1(z,ct) = N_1\ \exp[\,i\kappa_1 z - i\tfrac{1}{2}\,\kappa_1{}^2\,\frac{\hbar}{mc}\,ct] \int_{\xi=-\alpha_1}^{\alpha_1} d\xi\ \exp[\,i(z-\kappa_1\,\frac{\hbar}{mc}\,ct)\xi]$$

or

$$\psi_1(z,ct) = N_1 \exp[i\kappa_1 z - i\,\tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} ct] \frac{2\sin[\alpha_1(z-\kappa_1 \frac{\hbar}{mc} ct)]}{z-\kappa_1 \frac{\hbar}{mc} ct} . \qquad (12)$$

We might express the approximation we made when we deleted the ξ^2-term in a different way: We replace the exact parabolic relation

$$\frac{\omega}{c} = \tfrac{1}{2}\kappa^2 \frac{\hbar}{mc} \qquad (13)$$

between frequency $\frac{\omega}{c}$ and wave number κ by its tangent line at κ_1, i.e. by

$$\frac{\omega}{c} = \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} + \kappa_1 \frac{\hbar}{mc} (\kappa-\kappa_1) . \qquad (14)$$

After having made this replacement we can afford to abandon the inequality (11). Thus the substitution of the new "dispersion relation" (14) for the old relation (13) makes the wave packet formula (12) an exact one.

The exponential in (12) describes the ripples of the wave packet. The last factor in (12) describes the envelope. The envelope consists of a central peak with its center at $z_c = \kappa_1 \frac{\hbar}{mc} ct$. The height of the peak is $2\alpha_1$ and its width is $\frac{2\pi}{\alpha_1}$. On both sides of the central peak, the envelope factor decays, with ups and downs, to zero. The envelope pattern moves rigidly with the velocity v_1 given by

$$\frac{v_1}{c} = \kappa_1 \frac{\hbar}{mc} \qquad (15)$$

The rigidity of the envelope pattern is a consequence of our approximation [(14) instead of (13)]. An exact calculation would show that the peak becomes wider and lower for times that do not satisify the inequality (11). But this is of no concern to us.

The expression (12) describes a wave packet whose center passes the origin $z = 0$ at the time zero. If the center passes $z = 0$ at some other time s, then we merely need to replace ct by $ct - cs$. We are allowed to multiply by the constant phase factor $\exp[-i\,\tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} cs]$, or - expressed

differently - to absorb $\exp[+ i \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} cs]$ into the normalization factor N_1. Thus, for a wave packet whose center passes $z = 0$ at time s, we have

$$\psi_1(z,ct) = N_1 \exp[i\kappa_1 z - i \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} ct] \frac{2\sin[\alpha_1(z-\kappa_1 \frac{\hbar}{mc}(ct-cs))]}{z-\kappa_1 \frac{\hbar}{mc}(ct-cs)} \qquad (16)$$

The concomitant wave packet in the partial beam #2 is described by an analogous expression, namely

$$\psi_2(z,ct) = N_2 \exp[i\kappa_2 z - i \tfrac{1}{2}\kappa_2^2 \frac{\hbar}{mc} ct] \frac{2\sin[\alpha_2(z-\kappa_2 \frac{\hbar}{mc}(ct-cs))]}{z-\kappa_2 \frac{\hbar}{mc}(ct-cs)} . \qquad (17)$$

We relate the constants α_2, N_2 in (17) to the constants α_1, N_1 in (16) with the aid of the design conditions (3), (4). To this end, we examine the ratio

$$\frac{\psi_2(o,ct)}{\psi_1(o,ct)} = \exp[-i\tfrac{1}{2}(\kappa_2^2-\kappa_1^2) \frac{\hbar}{mc} ct] \frac{N_2}{N_1} \frac{\kappa_1}{\kappa_2} \frac{\sin[\alpha_2\kappa_2 \frac{\hbar}{mc}(ct-cs)]}{\sin[\alpha_1\kappa_1 \frac{\hbar}{mc}(ct-cs)]} . \qquad (18)$$

The factor that follows the exponential should come out to be unity because of the design condition (3). This requirement yields

$$\alpha_2\kappa_2 = \alpha_1\kappa_1 \qquad (19)$$

$$\frac{N_2}{N_1} = \frac{\kappa_2}{\kappa_1} , \text{ or with (19), } N_2\alpha_2 = N_1\alpha_1 . \qquad (20)$$

The heights of the central peaks of the two wave packets are respectively $|N_1\alpha_1|$ and $|N_2\alpha_2|$. They are equal to each other, by virtue of (20).

Next, we determine the normalization factors N_1 and N_2. As we are dealing with a single electron, we have the condition

$$\int_{z=-\infty}^{\infty} dz\psi^*\psi = 1 \qquad (21)$$

And, since $\psi = \psi_1+\psi_2$, we obtain

$$\int_{z=-\infty}^{+\infty} dz\psi_1^*\psi_1 + \int_{z=-\infty}^{+\infty} dz\psi_2^*\psi_2 + \int_{z=-\infty}^{+\infty} dz\psi_1^*\psi_2 + \int_{z=-\infty}^{+\infty} dz\psi_2^*\psi_1 = 1 \qquad (22)$$

These four integrals are evaluated most easily by way of the Fourier transforms $\hat{\psi}_1(\kappa,ct)$ and $\hat{\psi}_2(\kappa,ct)$. For, according to the Parseval relation, we have

$$\int_{z=-\infty}^{+\infty} dz\psi_1^* \psi_2 = \frac{1}{2\pi} \int_{\kappa=-\infty}^{+\infty} d\kappa \hat{\psi}_1^* \hat{\psi}_2 \tag{23}$$

and similarly for the other three integrals. We can read out the Fourier transform $\hat{\psi}(\kappa,ct)$ from the definition (9). But we must remember that we linearized the dispersion relation, i.e., we replaced $\frac{\kappa^2}{2}$ by $\frac{\kappa_1^2}{2} + \kappa_1(\kappa-\kappa_1)$. Also we replaced ct by ct - cs, and we multiplied by the constant phase factor $\exp[-i\kappa\tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} cs]$. Thus, instead of (9), we now have

$$\psi_1(z,ct) = N_1 \int_{\kappa=\kappa_1-\alpha_1}^{\kappa_1+\alpha_1} d\kappa \exp[i\kappa z - i \frac{\hbar}{mc}(\tfrac{1}{2}\kappa_1^2 + \kappa_1(\kappa-\kappa_1)(ct-cs) - i \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} cs] . \tag{24}$$

We compare (24) with the inverse Fourier transform formula

$$\psi_1(z,ct) = \frac{1}{2\pi} \int_{\kappa=-\infty}^{\infty} d\kappa\ e^{ikz}\hat{\psi}_1(\kappa,ct) \tag{25}$$

and read out

$$\hat{\psi}_1(\kappa,ct) = 2\pi N_1 \exp[-i \frac{\hbar}{mc}(\tfrac{1}{2}\kappa_1^2 + \kappa_1(\kappa-\kappa_1))(ct-cs) - i \tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} cs]$$

$$\text{for } |\kappa-\kappa_1| \leq \alpha_1$$

$$\hat{\psi}_1(\kappa,ct) = 0 \text{ for } |\kappa-\kappa_1| > \alpha_1$$

A similar formula holds for $\hat{\psi}_2(\kappa,ct)$. We merely have to replace the subscript 1 by 2. Because of the inequality (10) and the related inequality $\alpha_2 << \kappa_2-\kappa_1$, the intervals in which $\hat{\psi}_1(\kappa,ct)$ and $\hat{\psi}_2(\kappa,ct)$ are non-zero do not overlap. Consequently, the integrand on the right-hand side of (23) is always zero. Thus we obtain

$$\int_{z=-\infty}^{+\infty} dz\psi_1^* \psi_2 = 0, \text{ and similarly } \int_{z=-\infty}^{+\infty} dz\psi_2^* \psi_1 = 0 \tag{27}$$

Therefore, the functions $\psi_1(z,ct)$ and $\psi_2(z,ct)$ are orthogonal to each other. Since

$$\hat{\psi}_1^*(\kappa,ct)\hat{\psi}_1(\kappa,ct) = (2\pi)^2 N_1^* N_1 \text{ for } |\kappa-\kappa_1| \leq \alpha_1$$
$$= 0 \text{ for } |\kappa-\kappa_1| < \alpha_1 \tag{28}$$

we obtain [from an equation similar to (23)]

$$\int_{z=-\infty}^{+\infty} dz\, \psi_1^* \psi_1 = 2\pi N_1^* N_1 2\alpha_1. \tag{29}$$

Similarly,

$$\int_{z=-\infty}^{+\infty} dz\, \psi_2^* \psi_2 = 2\pi N_2^* N_2 2\alpha_2 \ . \tag{30}$$

The normalization condition (22) then gives us

$$4\pi(\alpha_1 N_1^* N_1 + \alpha_2 N_2^* N_2) = 1 \ . \tag{31}$$

When we combine this result with (20), we obtain

$$\left.\begin{aligned} N_1^* N_1 &= \frac{1}{4\pi(\alpha_1+\alpha_2)} \frac{\alpha_2}{\alpha_1}, \\ N_2^* N_2 &= \frac{1}{4\pi(\alpha_1+\alpha_2)} \frac{\alpha_1}{\alpha_2}. \end{aligned}\right\} \tag{32}$$

Let us divide (30) by (29). With the aid of (32) and (19) we obtain

$$\frac{\int_{-\infty}^{+\infty} dz \psi_2^* \psi_2}{\int_{-\infty}^{+\infty} dz \psi_1^* \psi_1} = \frac{\alpha_1}{\alpha_2} = \frac{\kappa_2}{\kappa_1} = \frac{v_2}{v_1} \tag{33}$$

(See (15) and the related equation for v_2). This equation shows that the electron has a slightly higher probability ($\kappa_2 > \kappa_1$, $\frac{\kappa_2-\kappa_1}{\kappa_1} \ll 1$) to be in beam #2 than in beam #1, if the design conditions (3), (4) are fulfilled.

Now we shall investigate the probability density $\psi^*\psi$. We calculate $\psi = \psi_1 + \psi_2$ from (16) and (17). In order to simplify the notation, we introduce the abbreviation

$$\zeta = \alpha_1\kappa_1 \frac{\hbar}{mc}(cs-ct) = \alpha_2\kappa_2 \frac{\hbar}{mc}(cs-ct) \ , \tag{34}$$

where we have used $\alpha_1\kappa_1 = \alpha_2\kappa_2$ [see (19)]. We also use $\alpha_1 N_1 = \alpha_2 N_2$ [see (20)]. Then

$$\psi = 2\alpha_1 N_1 \{ \frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z} \exp[i\kappa_1 z - i\,\tfrac{1}{2}\kappa_1^2 \frac{\hbar}{mc} ct] + \frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_2 z} \exp[i\kappa_2 z - i\,\tfrac{1}{2}\kappa_2^2 \frac{\hbar}{mc} ct]\} , \tag{35}$$

so that

$$\psi^*\psi = 4(\alpha_1)^2 N_1^* N_1 \left\{ \left(\frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z}\right)^2 + \left(\frac{\sin(\zeta+\alpha_2 z)}{\zeta+\alpha_2 z}\right)^2 + 2\,\frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z}\,\frac{\sin(\zeta+\alpha_2 z)}{\zeta+\alpha_2 z} \cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc} ct] \right\} . \tag{36}$$

The factors containing ζ are envelope factors. The cosine term describes the pattern of beats. We see that - apart from the envelope factors - the beat factor is universal. This means that the peaks and valleys of the beat pattern of any particular electron coincides with those of its sister electrons. The Schrödinger wave packets of different electrons are incoherent, because the normalization factors N_1 for each electron contain uncontrollable phase factors. Nevertheless, as we have seen, the beat patterns are coherent, because they depend only on the product $N_1^* N_1$ in which the uncontrollable phase factors cancel. This coherence of the beat patterns is important in the application that we wish to examine later on.

So far we have considered a single electron. Now we are going to evaluate the electron density for an electron beam, which consists of a great many electrons. We will ignore fluctuations (the shot effect). Thus we consider the electrons as evenly spaced, which means that the time interval ds between the instants when two consecutive electrons pass the origin $z = 0$ is given by $ds = \frac{1}{R}$, where R is the rate at which electrons pass the origin. Let us

express this statement in a different way. We are going to assign integer order numbers n to the electrons, in the order of their zero-passage time s. Thus, as the order number advances from n to n + dn, the zero-passage time advances from s to s + ds, and we have

$$dn = Rds \ . \tag{37}$$

When we combine this with (34), we obtain (keeping z and ct fixed)

$$dn = \frac{R}{c} \frac{1}{\alpha_1 \kappa_1 \frac{\hbar}{mc}} d\zeta \ . \tag{38}$$

The (linear) electron density $\rho(z,ct)$ (number of electrons per unit length along the beam) is given by

$$\rho(z,ct) = \int_{n=-\infty}^{+\infty} \psi^* \psi dn \ , \tag{39}$$

or with (38),

$$\rho(z,ct) = \frac{R}{c} \frac{1}{\alpha_1 \kappa_1 \frac{\hbar}{mc}} \int_{\zeta=-\infty}^{+\infty} d\zeta \psi^* \psi \tag{40}$$

The integrand $\psi^* \psi$ is given by (36).

We then have to evaluate integrals of the type

$$I_{1,2} = \int_{\zeta=-\infty}^{+\infty} d\zeta \frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z} \frac{\sin(\zeta+\alpha_2 z)}{\zeta+\alpha_2 z} \ . \tag{41}$$

We use the Parseval theorem. It states that for two function $f(\zeta)$ and $g(\zeta)$ we have

$$\int_{\zeta=-\infty}^{+\infty} d\zeta [f(\zeta)]^* g(\zeta) = \frac{1}{2\pi} \int_{=-\infty}^{+\infty} dk [\hat{f}(k)]^* \hat{g}(k) \ , \tag{42}$$

where $\hat{f}(k)$ and $\hat{g}(k)$ are the Fourier transforms of $f(\zeta)$ and $g(\zeta)$. In our case we have

$$f(\zeta) = \frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z} \ , \ g(\zeta) = \frac{\sin(\zeta+\alpha_2 z)}{\zeta+\alpha_2 z} \ . \tag{43}$$

Since

$$\frac{\sin(\zeta+\alpha_1 z)}{\zeta+\alpha_1 z} = \frac{1}{2\pi} \int_{k=-1}^{+1} dk \, e^{ik\zeta} \, e^{ik\alpha_1 \zeta} \ , \tag{44}$$

we see that

$$\hat{f}(k) = \pi e^{ik\alpha_1 z} \text{ for } |k| \leq 1 ,$$
$$= 0 \text{ for } |k| > 1 . \qquad (45)$$

Similarly for $\hat{g}(k)$. Thus

$$\frac{1}{2\pi}\int_{k=-\infty}^{+\infty} dk[\hat{f}(k)]^* \hat{g}(k) = \frac{\pi}{2}\int_{k=-1}^{+1} dk\, e^{ik(\alpha_2-\alpha_1)z} = \pi \frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z} ,$$

so that

$$I_{1,2} = \pi \frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z} . \qquad (46)$$

The other two integrals we need are $I_{1,1}$ and $I_{2,2}$. Their values follow from (46) when we make $\alpha_2 \to \alpha_1$ and $\alpha_1 \to \alpha_2$. Thus

$$I_{1,1} = \pi, \; I_{2,2} = \pi . \qquad (47)$$

We insert (46) and (47) into (40), where the integrand was given by (36). We obtain

$$\rho(z,ct) = \frac{R}{c}\frac{1}{\alpha_1\kappa_1 \frac{\hbar}{mc}} 4(\alpha_1)^2 N_1^* N_1 2\pi \cdot$$
$$\cdot \{1 + \frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z}\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct]\}.$$

Finally we use the expression (32) for $N_1^* N_1$ and also the relation (19). The end result is

$$\rho(z,ct) = \frac{R}{c}\left(\frac{\hbar}{mc}\frac{\kappa_1+\kappa_2}{2}\right)^{-1}\{1+\frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z}\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct]\}. \qquad (48)$$

We see that there is a constant background, attributable to the 1 in the curled bracket, and a beat pattern, attributable to the cosine term. This beat pattern fades with increasing distance from the origin, as described by the $\frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z}$ - term.

We shall now discuss this fading term. According to equation (9), the quantity α_1 is of the order of the quantum-mechanical wave number uncertainty

of the ψ_1-packet. Thus $\hbar\alpha_1$ is of the order of the momentum uncertainty. Similarly, $\hbar\alpha_2 = \hbar \frac{\kappa_1}{\kappa_2} \alpha_1 \approx \hbar\alpha_1$ is of the order of the quantum-mechanical momentum uncertainty of the ψ_2-packet. Nothing is known about these uncertainties. In the absence of any hard information about this matter, we use the simplest assumption, namely that we can make α_1 and α_2 in (48) go to zero. Then the fading factor $\frac{\sin(\alpha_2-\alpha_1)z}{(\alpha_2-\alpha_1)z}$ tends to unity, and (48) simplifies to

$$\rho(z;ct) = \frac{R}{c} \left(\frac{\hbar}{mc} \cdot \frac{\kappa_1+\kappa_2}{2}\right)^{-1} \{1+\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2) \frac{\hbar}{mc} ct]\} . \qquad (49)$$

According to (49), the beats persist for all values of z. There is no fading.

We feel fairly confident that we are permitted to replace (48) by (49), because it is very likely that any fading of the quantum-mechanical nature is overridden by a fading of thermal origin, which we shall describe now. The electrons are emitted by a themionic cathode. So they come off with an energy uncertainty δE, which is of the order of kT, where k is the Boltzmann constant and T is the cathode temperature. Since the cathode is hot, δE is of the order of $\frac{1}{5}$ electronvolt. The same energy uncertainty δE obtains after acceleration and hence in the working region (near z=0) of the apparatus. Now let us examine the ψ_1-packet in the partial beam #1. Since

$$E_1 = \frac{\hbar^2}{2m} \kappa_1^2,$$

we have

$$\frac{\delta E_1}{E_1} = 2 \frac{\delta \kappa_1}{\kappa_1} ,$$

so that the thermal wave number uncertainty $\delta_{\kappa 1}$ is given by

$$\delta\kappa_1 = \kappa_1 \frac{\delta E_1}{E_1} . \qquad (50)$$

Now there is no uncertainty in the difference $\kappa_2^2 - \kappa_1^2$ because of the design condition (4), namely

$$F = \frac{\hbar}{mc}\,\tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\ , \qquad \text{(4, repeated)}$$

where F is a precise constant. If we take the variation of (4) and use $\delta F = 0$, we obtain

$$\kappa_2\delta\kappa_2 - \kappa_1\delta\kappa_1 = 0\ ,$$

so that

$$\delta\kappa_2 = \frac{\kappa_1}{\kappa_2}\,\delta\kappa_1\ . \qquad (51)$$

Then we get [from (50) and (51)]

$$\delta(\kappa_2-\kappa_1) = -\frac{\kappa_2-\kappa_1}{\kappa_2}\,\delta\kappa_1 = -\frac{\kappa_1}{\kappa_2}\,(\kappa_2-\kappa_1)\,\frac{\delta E_1}{E_1} \approx -\tfrac{1}{2}(\kappa_2-\kappa_1)\,\frac{\delta E_1}{E_1}\ . \qquad (52)$$

Therefore the quantity $(\kappa_2-\kappa_1)$ in the cosine-term of (49) has an uncertainty which is given by (52), whereas the quantity $\kappa_2^2-\kappa_1^2$ is still exact. We take care of this uncertainty by taking a suitable average of the formula (49). The easiest average to take is the Gaussian average, as then the resulting integrals can be evaluated in closed form. We can afford to treat the quantity $\frac{\kappa_1+\kappa_2}{2}$ in the prefactor of (49) as exact, the resulting error is not important. Thus, if we denote averages by carets $\langle\ \rangle$, we have

$$\langle\rho(z,ct)\rangle = \frac{R}{c}\left(\frac{\hbar}{mc}\,\frac{\kappa_1+\kappa_2}{2}\right)^{-1}\{1 + \langle\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\,\frac{\hbar}{mc}\,ct]\rangle\}. \qquad (53)$$

Now

$$\langle\cos[\ldots]\rangle = \tfrac{1}{2}\langle\exp i[\ldots]\rangle + \text{c.c.}\ , \qquad (54)$$

where c.c. stands for "complex conjugate". And, since we decided to take a Gaussian average,

$$\begin{aligned}\langle\exp i[\ldots]\rangle &= \langle\exp[i(\kappa_2-\kappa_1)z - \tfrac{i}{2}(\kappa_2^2-\kappa_1^2)\,\tfrac{\hbar}{mc}\,ct]\rangle = \\ &= \exp[-\tfrac{i}{2}(\kappa_2^2-\kappa_1^2)\,\tfrac{\hbar}{mc}\,ct]\ \langle\exp(i(\kappa_2-\kappa_1)z)\rangle = \\ &= \exp[-\tfrac{i}{2}(\kappa_2^2-\kappa_1^2)\,\tfrac{\hbar}{mc}\,ct]\ \frac{\int_{\eta=-\infty}^{+\infty} d\eta\,\exp(i(\kappa_2-\kappa_1+\eta)z - (a^2/2)\eta^2)}{\int_{\eta=-\infty}^{+\infty} d\eta\,\exp(-(a^2/2)\eta^2)}\ , \qquad (55)\end{aligned}$$

where the quantity a is of the order of the reciprocal of $\delta(k_2-k_1)$, as given by (52). Thus we may write

$$a = \frac{2}{\kappa_2-\kappa_1}\frac{E_1}{\delta E_1} . \tag{56}$$

The integrals N and D in the numerator and denominator of (55) have the values

$$N = \frac{\sqrt{2\pi}}{a}\exp(i(\kappa_2-\kappa_1)z)\exp(-\frac{z^2}{2a^2}) ,$$

and

$$D = \frac{\sqrt{2\pi}}{a} .$$

Thus, (55) yields

$$\langle\exp[i(\kappa_2-\kappa_1)z - i\,\tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct]\rangle =$$
$$= \exp(-\frac{z^2}{2a^2})\exp[i(\kappa_2-\kappa_1)z - i\,\tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct] . \tag{57}$$

Then (54) becomes

$$\langle\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct]\rangle =$$
$$= \exp(-\frac{z^2}{2a^2})\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}ct] . \tag{58}$$

When we insert this into (53), we obtain the final answer

$$\langle\rho(z,ct)\rangle = \frac{R}{c}(\frac{\hbar}{mc}\frac{\kappa_1+\kappa_2}{2})^{-1}\{1+\exp(-\frac{z^2}{2a^2})\cos[(\kappa_2-\kappa_1)z - \tfrac{1}{2}(\kappa_2^2-\kappa_1^2)\frac{\hbar}{mc}t]\}, \tag{59}$$

or, when written in a slightly different form,

$$\langle\rho(z,ct)\rangle = \frac{R}{c}(\frac{\hbar}{mc}\frac{\kappa_1+\kappa_2}{2})^{-1}\{1+\exp(-\frac{z^2}{2a^2})\cos[(\kappa_2-\kappa_1)(z - \frac{\kappa_1+\kappa_2}{2}\frac{\hbar}{mc}ct)]\}. \tag{60}$$

So now we again have a fading factor, namely $\exp(-\frac{z^2}{2a^2})$. Let us calculate the fading length a. From (56) we have

$$a = 4\,\frac{\kappa_1+\kappa_2}{2}\frac{1}{\kappa_2^2-\kappa_1^2}\frac{E_1}{\delta E_1} \tag{61}$$

Since the energy difference $\Delta E = E_2 - E_1$ of the two partial beams is given by

$$\Delta E = \frac{\hbar^2}{2m}(\kappa_2^2-\kappa_1^2) ,$$

we may write (61) as

$$a = 4\,\frac{\kappa_1+\kappa}{2}\,\frac{\hbar^2}{2m}\,\frac{1}{\Delta E}\,\frac{E_1}{\delta E_1}\ ,$$

or, with $E_1 = \frac{\hbar^2}{2m}\,\kappa_1^2$,

$$a = 4\,\frac{1}{\kappa_1^2}\,\frac{\kappa_1+\kappa_2}{2}\,\frac{E_1}{\Delta E}\,\frac{E_1}{\delta E}\ . \tag{62}$$

Since $\kappa_2-\kappa_1 \ll \kappa_1$ and $E_2-E_1 \ll E_1$, we need no longer distinguish between κ_1 and κ_2 or between E_1 and E_2. Thus we can drop the subscripts 1 and 2 in (62) and write this formula simply as

$$a = \frac{4}{\kappa}\,\frac{E}{\Delta E}\,\frac{E}{\delta E}\ .$$

Finally we use $E = \frac{\hbar^2}{2m}\,\kappa^2$ or $\frac{1}{\kappa} = \frac{\hbar}{mc}\sqrt{\frac{mc^2}{2E}}$, and obtain

$$a = 4\,\frac{\hbar}{mc}\sqrt{\frac{mc^2}{2E}}\,\frac{E}{\Delta E}\,\frac{E}{\delta E}\ . \tag{63}$$

To repeat: ΔE is the energy difference between the two partial beams, it is typically of the order of 3 electronvolt. And δE is the thermal energy uncertainty, which is of the order of $\frac{1}{5}$ electronvolt. With E about 30 kiloelectronvolt, we have $\frac{E}{\Delta E} \sim 10^4$ and $\frac{E}{\delta E} \sim (1.5) \times 10^5$. Also $mc^2 \approx 500$ kiloelectronvolt, so that $\sqrt{\frac{mc^2}{2E}} = \sqrt{\frac{500}{60}} \sim 3$. Thus $a \sim 4 \times 3 \times 1.5 \times 10^9\,\frac{\hbar}{mc} \sim 2 \times 10^{10}\,\frac{\hbar}{mc}$. Now $\frac{\hbar}{mc}$ is $\frac{1}{2\pi}$ timesthe Compton wavelength, or $\frac{\hbar}{mc} = (3.86) \times 10^{-11}$ cm. Thus finally,

$$a \sim 1 \text{ cm}\ . \tag{64}$$

So the best we can hope for is that the beats persist over a length of about 1 cm. (Actually 2 cm, as there is 1 cm on either side of the origin. But we are only making rough estimates.) Of course we could stretch this length by installing a narrow-band energy filter in front of the beam splitter, thus reducing δE. But then we would reduce the beam intensity. How the electron beam with beats will perform in its comtemplated use, which we shall discuss presently, will depend not only on the fading length but also on the beam

intensity. So, most probably, we would be no better off in the end, had we installed the energy filter.

We shall now describe the contemplated use of an electron beam with beats. The (linear) electron density in this beam is given by equation (60). Apart from a constant background (attributable to the 1 in the curled brakcet) there exists a sinusoidal density pattern, the beats, (attributable to the remaining term in the curled bracket). This beat pattern moves in the positive z-direction with a speed v given by

$$\frac{v}{c} = \frac{\kappa_1+\kappa_2}{2}\frac{\hbar}{mc} \quad . \tag{65}$$

The wave number of this beat pattern is $\kappa_2 - \kappa_1$. Let us send a plane electromagnetic wave in the direction of the negative z-axis, i.e. against the electron beam. We assume that this wave is polarized with the electric field parallel to the x-axis, i.e. normal to the z-axis. This electric field acts on the electrons in the beam and makes them oscillate in the x-direction. This oscillatory motion is, of course, superimposed on the steady motion, which is in the z-direction. The oscillating electrons give rise to a new wave, the reflected wave which propagates in the positive z-direction, i.e. against the incident electromagnetic wave. (The oscillating electrons produce also a wave in the negative z-direction, i.e. in the direction of the incident wave. But this wave is of no interest to us.) Since the electrons in the beam exhibit a beat pattern, the process of reflection is similar to the reflection from a grating, as in x-ray crystallography. The reflected wave will be strongest when the Bragg condition is fulfilled, i.e. when the wave number κ_{in} of the incident wave is related to the wave number $\kappa_2-\kappa_1$ of the beats by

$$\kappa_{in} = \tfrac{1}{2}(\kappa_2-\kappa_1)(1-v/c) \quad . \tag{66}$$

The factor (1-v/c) comes in because the beat pattern is moving. We shall derive (66) after the discussion of the Doppler-shift formula (67). Since the beats move with a speed given by (65), we are dealing with a moving grating. Because of this, the wave number κ_r of the reflected beam will be Doppler-shifted upward, according to

$$\kappa_r = \kappa_{in} \frac{1+v/c}{1-v/c} = \tfrac{1}{2}(\kappa_2-\kappa_1)(1+v/c) \qquad (67)$$

Now we are ready to derive equation (66). The Bragg condition is

$$\kappa_r - (-\kappa_{in}) = \kappa_{beat} = \kappa_2-\kappa_1 \ . \qquad (67a)$$

(Later on, when we develop the detailed theory of the reflection, we shall meet an independent proof of the Bragg condition for a moving grating.) And indeed, with (66) and (67), the Bragg condition (67a) is satisfied. We thus have the possibility of constructing a highly selective frequency shifter. The selectivity comes from the fact that, for good reflection, the Bragg condition (66) must be satisfied. Expressed differently: One may construct a selective moving mirror. The speed of the mirror is a good fraction of the speed of light. For electrons with an energy of 30 kilo electronvolt, equation (65) gives a v/c-ratio of the order of 1/3. The frequency shift is appreciable. For v/c = 1/3, equation (67) shows that the wave number, and hence also the frequency, of the reflected wave is twice that of the incident wave.

All of this sounds rather attractive. Nevertheless, the device is useless, because the reflection coefficient, i.e. the ratio of the reflected power density to the incident power density is exceedingly small. The reason is that there just are not enough electrons available for a strong reflection to occur. Let us make a rough estimate to show that this is the case. A realistic

estimate for the electric current density J in the electron beam is J = 1 milliamp per millimeter squared = 10^{-3} amp ÷ 10^{-2} cm^2 = 10^{-1} amp/cm^2, about what may be found in a television tube. The electron current density is then $\frac{1}{e} J$, where e is the electronic charge = 1.6 x 10^{-19} coul. Thus $\frac{1}{e} J$ is of the order of 10^{18} electrons/sec cm^2. The spatial electron density is then $\frac{1}{e} J \frac{1}{v}$, where v is the speed of the electrons. With v = 10^{10} cm/sec (for v/c = 1/3), we get $\frac{1}{e} J \frac{1}{v} \approx 10^{8}$ electrons/cm^3. But only a length of the order of the fading length a ≈ 1 cm contributes to the reflection by the beam. The areal density σ (number of electrons per unit cross sectional area of the incident electromagnetic wave) is than $\sigma = \frac{1}{e} J \frac{a}{v} \approx 10^{8}$ electrons/cm^2. This is much less (by a factor of 10^{-8} to 10^{-7}) than the areal density of optically active electrons in a monomolecular layer of a solid. Now we certainly do not get much reflection from a monomolecular layer, let alone a layer that is sparser by a factor of 10^{-8} to 10^{-7}.

The reader whom the preceding estimate convinces that the moving-mirror device is useless can stop reading right here. We continue a formal demonstration to satisfy the more skeptical reader. Another reason is that the derivations that follow are instructive. They may be helpful for the feasibility analysis of other devices that one may wish to consider.

We start with the equations (256) - (262) of the Appendix. These equations are the result of the perturbation calculus. We repeat these equations for the sake of easier reference.

$$(i\hbar\bar{\nabla}\psi_0 + m\bar{\chi}_0)_p = 0 \ , \tag{68}$$

$$(i\hbar \frac{\partial \psi_0}{\partial t} + \frac{i\hbar}{2} \bar{\nabla}\cdot\bar{\chi}_0)_p = 0 \ , \tag{69}$$

$$(i\hbar\bar{\nabla}\psi_1 + m\bar{\chi}_1)_p = -(\psi_0)_p \frac{1}{c}(-e)c\bar{A}_o , \tag{70}$$

$$(i\hbar\frac{\partial\psi_1}{\partial t} + \frac{i\hbar}{2}\bar{\nabla}\cdot\bar{\chi}_1)_p = -\tfrac{1}{2}(\bar{\chi}_0)_p \cdot \frac{1}{c}(-e)c\bar{A}_o , \tag{71}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_o + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_o) = 0 , \tag{72}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) = \frac{1}{\varepsilon_o c} \mathcal{P}_{T,low} \sum_{\substack{\text{electrons} \\ \#p}} (-e)\tfrac{1}{2}(\bar{\chi}_0^* \psi_0 + \bar{\chi}_0 \psi_0^*)_p , \tag{73}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2)$$

$$= \frac{1}{\varepsilon_o c} \mathcal{P}_{T,low} \sum_{\substack{\text{electrons} \\ \#p}} (-e)\tfrac{1}{2}(\bar{\chi}_0^* \psi_1 + \bar{\chi}_1^* \psi_0 + \bar{\chi}_0 \psi_1^* + \bar{\chi}_1 \psi_0^*)_p . \tag{74}$$

Here m and (-e) are the electronic mass and charge. The index p refers to electron #p. The quantities with the subscript 0 are the zero-order approximations. Those with subscripts 1 and 2 are the first-order and second-order corrections.

We are not interested in equation (73), which tells us how to calculate the first-order correction of the electromagnetic field. To be sure, this correction does not vanish in general. However, as we showed in Section 3, there is no radiation that is attributable to these fields. It is for this reason that we are not interested in $c\bar{A}_1$. Furthermore, in our example in which the zero-order Schrödinger waves of the electrons are plane waves in z-direction, the sum in (73) is purely longitudinal in character. Thus, when the projection operator $\mathcal{P}_{T,low}$ acts on this sum, the result is zero, since $\mathcal{P}_{T,low}$ retains only the transverse part, which is zero. Therefore, the right-hand side of (73) is zero in our example, so that (73) is satisfied by $c\bar{A}_1 = 0$. As a consequence, the first-order correction $c\bar{B}_1 = \bar{\nabla} \times c\bar{A}_1$ to the magnetic

field vanishes, and the first-order correction $\bar{E}_1 = -\frac{\partial cA_1}{\partial ct} - \bar{\nabla}\phi$, is simply $\bar{E}_1 = -\bar{\nabla}\phi$, where ϕ, in the electrostatic potential associated with the zero-order approximation to the charge density. A straightforward calculation of electrostatics, which we will not reproduce here, shows that the alternating part of $\bar{E}_1$, which is attributable to the beats, is only of the order of 10^{-4} volt/cm, much too small to be of any interest. (This magnitude of an electric field occurs in a laser beam with a power density of less than 10^{-10} watt/cm^2.)

Having disposed of the first-order correction $c\bar{A}_1$ as something that is of no interest, we concentrate our attention on the second-order correction $c\bar{A}_2$, which we can calculate from equation (74). Even though $c\bar{A}_2$ will turn out to be a genuine radiation field, it will be too weak to be of any use. Let us substantiate this prediction by means of an explicit calculation. First we have to evaluate the quantities $(\psi_1)_p$ and $(\bar{\chi}_1)_p$ on the right-hand side of (74). The remaining quantities $(\psi_0)_p$ and $(\bar{\chi}_0)_p$ are given by the properties of the electron beam. First we note that equations (70) and (71) are satisfied by

$$(\psi_1)_p = 0 \quad , \tag{75}$$

$$m(\bar{\chi}_1)_p = -(\psi_0)_p \frac{1}{c}(-e)c\bar{A}_0 \, . \tag{76}$$

The reason is first that $\bar{\chi}_0 = -\frac{i\hbar}{m}\bar{\nabla}\psi_0$ (from (68)) has only a non-vanishing z-component, since ψ_0 does not depend on x and y. Furthermore, by assumption, $c\bar{A}_0$ has only a non-vanishing x-component, so that the dot product on the right-hand side of (71) vanishes. In the second place, on taking the divergence of (70), we obtain

$$i\hbar(\bar{\nabla}\cdot\bar{\nabla}\psi_1)_p + m(\bar{\nabla}\cdot\bar{\chi}_1)_p = -\frac{1}{c}(-e)\{(\bar{\nabla}\psi_0)_p \cdot c\bar{A}_0 + (\psi_0)_p \, \bar{\nabla}\cdot c\bar{A}_0\} \, .$$

But the right-hand side of this equation vanishes, since $\bar{\nabla}\cdot c\bar{A}_0 = 0$ (because of the Coulomb gauge) and the dot product vanishes ($\bar{\nabla}\psi_0$ has only a non-vanishing

z-component and $c\bar{A}_0$ has only a non-vanishing x-component). This equation then becomes

$$i\hbar(\bar{\nabla}\cdot\bar{\nabla}\psi_1)_p + m(\bar{\nabla}\cdot\bar{\chi}_1)_p = 0 \ . \tag{77}$$

When we combine (77) with (71) and use the fact that the right-hand side of (71) vanishes, we obtain

$$(i\hbar\frac{\partial\psi_1}{\partial t} + \frac{\hbar^2}{2m}\bar{\nabla}\cdot\bar{\nabla}\psi_1)_p = 0 \ . \tag{78}$$

This equation is satisfied by $(\psi_1)_p = 0$, so that (75) holds. Equation (76) then follows from (70) and (75).

Equation (74) then simplifies to*

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_2) = -\frac{(-e)^2}{\varepsilon_0 mc^2}\left[\sum_{\substack{\text{electrons}\\ \#p}} (\psi_0^*\psi_0)_p\right] c\bar{A}_0 . \tag{79}$$

But the expression in the square bracket is the spatial electron density. It is related to the linear electron density $\langle\rho(z,ct)\rangle$ of equation (60). We merely have to divide by the cross section Q of the electron beam. Thus, with the abbreviation (65),

$$\sum_{\substack{\text{electrons}\\ \#p}} (\psi_0^*\psi_0)_p = \frac{1}{c}\frac{R}{Q}\left(\frac{v}{c}\right)^{-1}\{1+\exp(-\frac{z^2}{2a^2})\cos[(k_2-k_1)(z-\frac{v}{c}ct)]\} \ . \tag{80}$$

We note that $\frac{R}{Q}$ is the electron current density of the beam. The electrical current density is then $(-e)\frac{R}{Q}$.

Now we combine equation (79) and (80). In order to simplify the writing, we introduce the classical electron radius

$$r_o = \frac{e^2}{4\pi\varepsilon_0 mc^2} = (2.82)\cdot 10^{-13}\ \text{cm} \ , \tag{81}$$

and the symbol

$$J_e = \frac{R}{Q} \tag{82}$$

for the electron current density of the beam. Thus

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*We can delete the projection operator $P_{T,low}$, because the right-hand side of (79) is purely transverse and has only low-modes components.

$$\frac{\partial^2}{(\partial ct)^2}\, c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) =$$

$$= -\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e \{1+\exp(-\frac{z^2}{2a^2})\cos[(\kappa_2-\kappa_1)(z-\frac{v}{c}\,ct)]\}c\bar{A}_0 . \qquad (83)$$

Finally, we use the fact that, by assumption, the incident electromagnetic field is polarized in the x-direction. Then the desired field $c\bar{A}_2$ will also be polarized in the x-direction. Then, with the Cartesian unit vectors $\bar{I}$, $\bar{J}$, $\bar{K}$, we can write

$$\left.\begin{aligned} c\bar{A}_0(z,ct) &= \bar{I}cA_0(z,t) , \\ c\bar{A}_2(z,ct) &= \bar{I}cA_2(z,ct) . \end{aligned}\right\} \qquad (84)$$

where we are stipulating that both fields do not depend on x and y. We also have

$$\bar{\nabla} \times c\bar{A}_2 = \bar{K} \times \bar{I}\, \frac{\partial}{\partial z}\, cA_2 = \bar{J}\, \frac{\partial}{\partial z}\, cA_2 ,$$

and

$$\bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) = \bar{K} \times \bar{J}\, \frac{\partial^2}{\partial z^2}\, cA_2 = -\bar{I}\, \frac{\partial^2}{\partial z^2}\, cA_2 .$$

Then, when we delete the unit vector $\bar{I}$, which is common to all terms, equation (83) becomes

$$\frac{\partial^2}{(\partial ct)^2}\, cA_2 - \frac{\partial^2}{\partial z^2}\, cA_2 =$$

$$= -\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e \{1+\exp(-\frac{z^2}{2a^2})\cos[(\kappa_2-\kappa_1)(z-\frac{v}{c}\,ct)]\}cA_0 . \qquad (85)$$

We then have to find the solution $\psi(z,ct)$ of a partial differential equation of the type

$$\frac{\partial^2\psi}{(\partial ct)^2} - \frac{\partial^2\psi}{\partial z^2} = f(z,ct) . \qquad (86)$$

Here both z and ct run from $-\infty$ to $+\infty$, and $f(z,ct)$ vanishes in the distant past, i.e. for $ct \to -\infty$. The explicit solution of this differential equation is

$$\psi(z,ct) = \tfrac{1}{2} \int_{c\tau=-\infty}^{ct} dc\tau \int_{\zeta=z-(ct-c\tau)}^{z+(ct-c\kappa)} d\zeta\, f(\zeta,c\tau) \qquad (87)$$

There is no connection between the dummy variable ζ of this equation and the ζ of equation (34).

This writer could find the explicit formula (87) in only one book, namely "Mathematical Physics" by Eugene Butkov, Addison-Wesley, 1968, pg. 607. As this book is not readily available, we establish the validity of (87) here. We will not go through the process of creating this equation. This process is based on physical intuition, which comes from the examination of vibrating strings; officially it goes by the name of Green function techniques. Instead, we will check that the differential equation (86) is satisfied by the solution (87). We calculate the required partial derivatives. We start with $\frac{\partial}{\partial ct}\psi$. In (87), the ct occurs in 3 places. On taking the derivative with respect to each place in turn we obtain

$$\frac{\partial}{\partial ct}\psi = \tfrac{1}{2}\left[\int_{\zeta=z-(ct-c\tau)}^{z+(ct-c\tau)} d\zeta\, f(\zeta,c\tau)\right]_{\text{at } c\tau=ct}^{+}$$

$$+ \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} dc\tau\, f(z+(ct-c\tau),c\tau) +$$

$$+ \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} dc\tau f(z-(ct-c\tau),c\tau) .$$

The first term vanishes, because the domain of integration has shrunk to zero. In each of the other terms, the ct occurs in two places. If we denote the first partial derivative of f(z,ct) with respect to the first argument by g(z,ct), we obtain

$$\frac{\partial^2}{(\partial ct)^2}\psi = \tfrac{1}{2}\{f(z,ct) + \int_{c\tau=-\infty}^{ct} dc\tau\, g(z+(ct-c\tau),c\tau) +$$

$$+ f(z,ct) - \int_{c\tau=-\infty}^{ct} dc\tau\, g(z-(ct-c\tau),c\tau)\} ,$$

or

$$\frac{\partial^2}{(\partial ct)^2}\psi = f(z,ct) + \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} d\tau\,[g(z+(ct-c\tau),c\tau)-g(z-(ct-c\tau),c\tau)] \ . \qquad (88)$$

Now we come to the z-derivatives. In (87), the z occurs in 2 places. Proceeding, as we did before, we obtain

$$\frac{\partial\psi}{\partial z} = \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} d\tau\,[f(z+(ct-c\tau)-f(z-(ct-c\tau),c\tau)] \ ,$$

and

$$\frac{\partial^2\psi}{\partial z^2} = \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} d\tau\,[g(z+(ct-c\tau) - g(z-(ct-c\tau),c\tau)] \ . \qquad (89)$$

When we subtract (80) from (88), we see that (86) is satisfied indeed.

We should require not only that the differential equation (86) is satisfied by the solution (87), but also that the solution contains only outgoing waves. Let us check that the second requirement is fulfilled as well. We assume that the excitation f(z,ct) is confined to a finite domain of the z-axis, say to the domain $|z| < b$, where b is some constant length. We therefore assume that

$$f(z,ct) = 0 \text{ for } |z| > b \ .$$

Now let us examine the time derivative $\frac{\partial\psi}{\partial ct}$, rather than ψ itself. We already calculated this derivative and found

$$\frac{\partial\psi}{\partial ct} = \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} d\tau\, f(z+(ct-c\tau),c\tau) +$$
$$+ \tfrac{1}{2}\int_{c\tau=-\infty}^{ct} d\tau\, f(z-(ct-c\tau),c\tau) \ .$$

Let us pick a point z to the right of the excitation domain; thus $z > b$. Since $ct-c\tau > 0$, we have $z + (ct-c\tau) > b$, so that the integrand in the first term vanishes. Therefore only the second term survives. But in this term, z and ct occur only in the combination z-ct, which signifies waves that travel in the positive z-direction, i.e. outgoing waves. Similar statements apply to a

point z which is to the left of the excitation domain. Thus, (87) contains only outgoing waves.

Let us now apply the solution (87) to the problem of equation (85). We obtain

$$cA_2(z,ct) = -\tfrac{1}{2}\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e \cdot$$

$$\cdot \int_{c\tau=-\infty}^{ct} dc\tau \int_{\zeta=z-(ct-c\tau)}^{z+(ct-c\tau)} d\zeta\{1+\exp(-\frac{\zeta^2}{2a^2})\cos[(\kappa_2-\kappa_1)(\zeta-\frac{v}{c}c\tau)]\}cA_o(\zeta,c\tau) \ . \qquad (90)$$

We observe that this result is a linear functional of the incident electromagnetic vector potential cA_0. Let us assume that cA_0 is a monochromatic wave, whose wave number is matched to the wave number $\kappa_2-\kappa_1$ of the beats, so that we can obtain the strongest possible response. Accordingly, we write (with (66))

$$cA_0(\zeta,c\tau) = cA_0'\cos[(1-\frac{v}{c})\frac{\kappa_2-\kappa_1}{2}(\zeta+c\tau)] \ , \qquad (91)$$

where cA_0 is a constant amplitude factor. The plus sign in the $(\zeta+c\tau)$-term indicates that the incident wave travels in the negative z-direction.

A precise interpretation of the formula (87) would require that we make the right-hand side of (85) tend to zero in the distant past. We can achieve this by first decomposing (91) into two exponential terms, i.e. by writing

$$cA_0(\zeta,c\ ) = \tfrac{1}{2}cA_0'\exp[(1-\frac{v}{c})(i\frac{\kappa_2-\kappa_1}{2})(\zeta+c\tau)]$$
$$+ \tfrac{1}{2}cA_0'\exp[(1-\frac{v}{c})(-i\frac{\kappa_2-\kappa_1}{2})(\zeta+c\tau)] \ . \qquad (92)$$

And then we should replace the wave numbers $i\frac{\kappa_2-\kappa_1}{2}$ and $-i\frac{\kappa_2-\kappa_1}{2}$ by $i\frac{\kappa_2-\kappa_1}{2}+\beta$ and $i\frac{\kappa_2-\kappa_1}{2}+\beta$ respectively, where β is a positive real quantity. We then would replace (92) by

$$cA_0(\zeta,c\tau) = \tfrac{1}{2}cA_0'\exp[(1-\frac{v}{c})(i\frac{\kappa_2-\kappa_1}{2})+\beta)(\zeta+c\tau)]$$
$$+ \tfrac{1}{2}cA_0'\exp[(1-\frac{v}{c})(-i\frac{\kappa_2-\kappa_1}{2}+\beta)(\zeta+c_\tau)] \ . \qquad (93)$$

The presence of the quantity β in (93) would ensure that $cA_0(\zeta,c\sigma)$ tends to zero for $c\tau \to -\infty$ with sufficient rapidity. We would then calculate the respence cA_2 separately for each exponential term in (93) and add the results, which we are permitted to do because of the linearity of the functional (90). In the end we would make β approach zero. But this concession to logical precision is not worth the effort. Therefore, we shall evaluate (90) on the basis of expression (91).

Furthermore, we shall ignore the constant background of the electron beam, when we calculate the response cA_2, as being of no great interest. Accordingly we delete the term "1" in the curled bracket of (90). Thus, with (91), we obtain

$$cA_2(z,ct) \underset{\text{beats}}{=} -\tfrac{1}{2}\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e \, cA_0' \cdot$$

$$\cdot \int_{c\tau=-\infty}^{ct} d\sigma \int_{\zeta=z-(ct-c\tau)}^{z+(ct-c\tau)} d\zeta \, \exp\left(-\frac{\zeta^2}{2a^2}\right)\cos\left[(\kappa_2-\kappa_1)\left(\zeta-\frac{v}{c}c\tau\right)\right] \cdot$$

$$\cdot \cos\left[\left(1-\frac{v}{c}\right)\frac{\kappa_2-\kappa_1}{2}(\zeta+c\tau)\right] .$$

For the sake of greater convenience, we calculate, not cA_2 itself, but its time derivative $\frac{\partial}{\partial ct}cA_2$ We repeat the differentiation process that we used when we checked the validity of (87) and obtain

$$\frac{\partial cA_2}{\partial ct}(z,ct) \underset{\text{beats}}{=} -\tfrac{1}{2}\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e cA_0' \cdot$$

$$\int_{c\tau=-\infty}^{ct} d c\tau \Big\{ \exp\left(-\frac{(z+(ct-c\tau))^2}{2a^2}\right)\cos\left[(\kappa_2-\kappa_1)\left(z+ct-\left(1+\frac{v}{c}\right)c\tau\right)\right] \cdot$$

$$\cdot \cos\left[\left(1-\frac{v}{c}\right)\frac{\kappa_2-\kappa_1}{2}(z+ct)\right] +$$

$$+ \exp\left(-\frac{(z-(ct-c\tau))^2}{2a^2}\right)\cos\left[(\kappa_2-\kappa_1)\left(z-ct+\left(1-\frac{v}{c}\right)c\tau\right)\right]$$

$$\cdot \cos\left[\left(1-\frac{v}{c}\right)\frac{\kappa_2-\kappa_1}{2}(z-ct+c\tau)\right]\Big\} . \qquad (95)$$

We assume that the field point z is far beyond the region of beats in the direction of the positive z-axis. Then $z > 0$, and $z \gg a$. Since also $ct-c\tau$ is positive, we see that the exponential fading factor in the first term of (95) is essentially zero. We can therefore delete the first term. In the second term we rewrite the product of cosines according to the formula

$$\cos\xi\cos\eta = \tfrac{1}{2}\cos(\xi+\eta)+\tfrac{1}{2}\cos(\xi-\eta) .$$

Then

$$\frac{\partial cA_2}{\partial ct}(z,ct) = -\tfrac{1}{4}\frac{4\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e cA_0' \cdot$$

$$\text{beats}$$

$$\cdot \int_{c\tau=-\infty}^{ct} d c\tau \exp\left(-\frac{(z-(ct-c\tau))^2}{2a^2}\right) \cdot$$

$$\cdot \left\{\cos\left[\frac{\kappa_2-\kappa_1}{2}\left(2+\left(1-\frac{v}{c}\right)(z-ct) + 2(\kappa_2-\kappa_1)\left(1-\frac{v}{c}\right)c\tau\right] + \right.\right.$$

$$\left.\left. + \cos\left[\frac{\kappa_2-\kappa_1}{2}\left(1+\frac{v}{c}\right)(z-ct)\right]\right\} . \qquad (96)$$

Now we perform the integration over $c\tau$. Let us look at the first cosine term in (96). This is a rapidly varying function of $c\tau$ with average value 0. The rapid variation is attributable to the term $2(\kappa_2-\kappa_1)(1-\frac{v}{c})c\tau$ in the argument of the cosine. On the other hand the exponential fading factor is a comparatively smooth function of $c\tau$. It is comparatively smooth, because $(\kappa_2-\kappa_1)(1-\frac{v}{c})$ is much larger than the inverse fading length $\frac{1}{a}$. As a result, the contribution of the first cosine term to the integral is essentially zero. There remains the second cosine term, which does not depend on the dummy variable $c\tau$ and can therefore be factored out. The only thing that needs to be done is the intergral over the exponential fading factor. With the substitution $\xi = c\tau + cz - ct$, we obtain

$$\int_{c\tau=-\infty}^{ct} d c\tau \exp\left(-\frac{(z-(ct-c\tau))^2}{2a^2}\right) = \int_{\xi=-\infty}^{z} d\xi \exp\left(-\frac{\xi^2}{2a^2}\right) .$$

Since $z >> a$, we may replace the upper limit by $+\infty$, without making an appreciable error. Thus

$$\int_{c\tau=-\infty}^{ct} dc\tau \exp\left(-\frac{(z-(ct-c\tau))^2}{2a^2}\right) \approx a\sqrt{2\pi} \quad . \tag{97}$$

On combining (96) and (97) we obtain

$$\left(\frac{\partial cA_2}{\partial ct}\right)_{\text{beats}}(z,ct) = -a\sqrt{2\pi}\,\frac{\pi}{c}\left(\frac{v}{c}\right)^{-1} r_o J_e cA_0' \cos[\kappa_r(z-ct)] \ , \tag{98}$$

where we have used the expression (67) for the wave number κ_r of the reflected wave. This wave propagates in the positive z-direction, as indicated by the minus sign in the cosine term, i.e. in the direction opposite to that of the incident wave.

The transverse electric field $E_2\bar{I}$ of the reflected wave is given by

$$E_2 = -\frac{\partial}{\partial ct} cA_2. \tag{99}$$

(There is no contribution $-\bar{\nabla}\phi_{2_{\text{beats}}}$ from the scalar potential $\phi_{2_{\text{beats}}}$. In the first place, the domain of non-zero values of $\phi_{2_{\text{beats}}}$ is confined to the region of the beats, since $\phi_{2_{\text{beats}}}$ is a solution of the electrostatic Poisson equation

$$\bar{\nabla} \cdot \bar{\nabla}\phi_{2_{\text{beats}}} = -\frac{1}{\varepsilon_0 c} c\rho_{\text{beats}} \ ,$$

which does not yield any propagating waves. On the other hand, the region for which we calculated the reflected wave is beyond the region of the beats. In the second place, where the scalar potential does not vanish, its gradient is in the z-direction, thus purely longitudinal). We compare the x-components of the reflected and the incident waves. For the incident wave, we have, from (91) and (66),

$$E_0(z,ct) = -\frac{\partial}{\partial ct} cA_0 = \kappa_{in}\, cA_0' \sin[\kappa_{in}(z+ct)] \ , \tag{100}$$

whereas, for the reflected wave, we have, from (98) and (99),

$$E_{2_{beats}}(z,ct) = a\sqrt{2\pi}\,\frac{\pi}{c}\,(\frac{v}{c})^{-1}\,r_o J_e c A_0' \cos[\kappa_r(z-ct)] \qquad (101)$$

The ratio R of the reflected to incident power density is the square of the ratio of the amplitude factors in (101) and (100), so that

$$R = (\frac{a}{\kappa_{in}}\sqrt{2\pi}\,\frac{\pi}{c}\,(\frac{v}{c})^{-1}\,r_o J_e)^2 \,. \qquad (102)$$

If we introduce the wavelength $\lambda_{in} = \frac{2\pi}{\kappa_{in}}$ of the incident radiation, equation (102) becomes

$$R = (a\,\lambda_{in}\sqrt{\frac{\pi}{2}}\frac{1}{c}\,(\frac{v}{c})^{-1}\,r_o J_e)^2 \,. \qquad (103)$$

Let us insert numbers. For the fading length a we take the optimistic value of 1 cm. Suppose we adjust the device to an optical wavelength $\lambda_{in} = 5 \times 10^{-5}$ cm. We also have $\frac{v}{c} \sim \frac{1}{3}$. Then for $J_e \sim 10^{18}$ cm^{-2} sec, corresponding to an electrical current density of the order of 10^{-1} amp/cm^2, we obtain, with (81),

$$R \sim 10^{-18} \,. \qquad (104)$$

This exceedingly small value of the reflection coefficient R shows that the device is useless. This verdict stands, even if we boost the electron beam current by many orders of magnitude. Our detailed calculation substantiates our previous estimate, which was based on the sparseness of scattering electrons.

Appendix: The Semiclassical Method.

The problem that we wish to address in this appendix is that of the interaction between an atom (or molecule) and electromagnetic radiation. We confine ourselves to the semiclassical method in which the atom is treated quantum-mechanically, i.e. by way of the Schrödinger equation, whereas the radiation is treated classically, i.e. by way of the Maxwell equations. Of course, quantum mechanics could be used also for the electromagnetic field. But for the kind of applications we have in mind this is not necessary.

Most textbooks of quantum mechanics discuss how a given electromagnetic field influences an atom. But what is hardly ever explained is how, in return, the atom reacts back on the field. This aspect is, of course, important in laser physics. Only a rule is sometimes used, but hardly ever explicitly stated nor derived. According to this rule, the atomic sources of the electron-magnetic field are the quantum-mechanical averages of the electric charge densities and the electric current densities. Here we wish to derive this rule.

The derivation is based on the following consideration. We are dealing with a two-way process: Forward from field to atom and, in reverse, from atom to field. We know the equations of motion for the forward process, and we wish to infer the equations of motion for the reverse process. In order to make this inference one employs the action principle of analytical dynamics. One finds, as we shall see, that with the application of this principle the equations of motion for the forward process will determine those of the reverse process. In order to instill confidence in this procedure we shall employ it first in the case where both the atom and the radiation are treated classically. In this case the outcome is, of course, known: The Maxwell equations will be the result. This

case, then, provides a good confirmation of the procedure. Later on we shall apply the procedure to the case where the atom is treated quantum-mechanically.

In order to state and use the action principle one has to define a number of terms. We will give these definitions, not in abstract generality, but for the concrete example at hand, an atom interacting with electromagnetic radiation. The terms that we wish to define are, in this order, the instantaneous configuration, the history, the instantaneous dynamical state, and the driver fields.

1. The Instantaneous Configuration.

As far as the atom is concerned, its configuration is specified by the locations of each of the atomic particles, if we neglect the spins of the particles. These locations may be specified by a set of n cartesian coordinates, three for each particle. Thus n, the number of degrees of freedom of the atom, is three times the number of particles. In order to avoid cumbersome language and notation, we will say that the configuration is specified by a point q in the n-dimensional "configuration space" of the atom. If we so desire, we may specify the point q by the set $\{q^1, q^2, \ldots q^n\}$, abbreviated by $\{q^i\}$, of n "configurational coordinates" chosen in any convenient way. ({...} means "set of". Latin indices run from 1 to n.)

Each point of the configuration space determines an electric charge pattern in the three-dimensional space in which all of us live, our "home-space". Because of the point-like nature of the atomic particles, this pattern is, technically speaking, a distribution. The electric charge is concentrated in a number of discrete points (one for each particle); everywhere else the charge density is zero. So as to avoid the technicalities of the distribution theory we will envision the atomic particles as being of finite, though small, extent.

We also imagine that the charge density of each particle gradually decreases from a high value at the center to zero at the surface of the particle. We can then regard the charge density ρ of the atom as a whole as being a smooth function of the home-space position vector $\bar{r}$ and of the n configurational coordinates q^i. When we wish to indicate what variables the charge density ρ depends on we denote it by $\rho(q^i,\bar{r})$ or sometimes by $\rho(q,\bar{r})$. - As the text of this paragraph shows, two spaces are involved in the theory, the home-sapce and the atomic configuration space. Vectors in the home-space will be denoted by an upper bar, as we have already done it for the position vector $\bar{r}$.

We have completed the discussion of the atomic configuration. We can now go ahead and define what is meant by the instantaneous configuration of the electromagnetic field. Here we shall use the familiar notation and terminology of engineering electromagnetics, although there exists a more felicitous notation, namely that of the exterior calculus, which conforms more closely to the geometric imagination. As most readers may not be familiar with the latter notation, we use the former, thus trading ease of visualization for familiarity. All quantities and formulas will be expressed in the SI system of units (Système International).

One's first inclination might be to describe the instantaneous configuration of the electromagnetic field by means of the following two fields: the electric field strength $\bar{E}$ and the magnetic induction $\bar{B}$. But then one does not account for the fact that $\bar{E}$ and $\bar{B}$ are subject to the constraint expressed by the first pair of the Maxwell equations, namely

$$\bar{\nabla} \times \bar{E} + \frac{\partial}{\partial ct} c\bar{B} = 0 \text{ and } \bar{\nabla} \cdot c\bar{B} = 0 \,. \qquad (1)$$

(We have inserted the factor c (c = speed of light in vacuo) in various places. The advantage is that $\bar{E}$ and $c\bar{B}$ are expressed in the same unit, namely volt m^{-1} and that the differential operators $\bar{\nabla}$ and $\frac{\partial}{\partial ct}$ bring in the same unit, namely m^{-1}). In order to enforce this constraint, one adopts the usual procedure of expressing $\bar{E}$ and $c\bar{B}$ in terms of the vector potential $\bar{A}$ and the scalar potential ϕ, as shown by

$$\bar{E} = -\left(\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi\right) \text{ and } c\bar{B} = \bar{\nabla} \times c\bar{A} \qquad (2)$$

(Both $c\bar{A}$ and ϕ come in the same unit, namely volt.) The fields of $c\bar{A}$ and ϕ are free of constraints. We use them to specify the instantaneous configuration of the electromagnetic field.

At this point we must say something about the boundary conditions for the electromagnetic field. We imagine that the atom is located inside a large room (singly connected and bounded by a single surface, like a room in a house) with perfectly reflecting walls. The boundary conditions for $\bar{E}$ and $c\bar{B}$ are then that $\bar{E}$ is normal to the wall and that $c\bar{B}$ is tangential to the wall, i.e. that

$$\Delta\bar{f} \times \bar{E} = 0, \text{ and } \Delta\bar{f} \cdot c\bar{B} = 0 , \qquad (3)$$

where $\Delta\bar{f}$ is the vectorial surface element, directed outward. We can enforce (3) by stipulating the following boundary conditions for $c\bar{A}$ and ϕ.

$$\Delta\bar{f} \times c\bar{A} = 0, \text{ and } \phi = 0 \text{ at the wall.} \qquad (4)$$

The instantaneous configuration of the entire system comprising the atom and the electromagnetic field is given by the point q (or the n configurational coordinates q^i) of the atomic configuration space and the two field functions $\phi(\bar{r})$ and $c\bar{A}(\bar{r})$ in the three-dimensional home-space.

2. The History.

The history of a system is determined, when we specify the instantaneous configuration as a function of the time t of its occurrence. In our case then

we specify the history by the functions $q^i(t)$, $\phi(\bar{r},t)$, and $c\bar{A}(\bar{r},t)$. In general the history may be made to conform to any prearranged plan. But then the system will have to be drivenby means of suitably chosen driving agencies, which will be discussed in section 4.

3. The Instantaneous Dynamical State.

The instantaneous dynamical state of a system is determined, when we specify the time t of its occurrence, the configuration $\{q^i,\phi(\bar{r}),\ c\bar{A}(\bar{r})\}$ at that time, and also the time derivatives of the configurational parameters at that time, i.e. the set $\{v^i,\ \frac{\partial}{\partial t}\phi,\ \frac{\partial}{\partial t}c\bar{A}\}$, where we have used the customary abbreviation v^i for $\frac{d}{dt}q^i$. The partial derivatives $\frac{\partial}{\partial t}$ indicate that the time derivatives are to be taken while the position $\bar{r}$ in the home-space is held fixed. Altogether then, the instantaneous dynamical state is given by the set $\left\{t,\ q^i,\ v^i,\ \phi,\ c\bar{A},\ \frac{\partial}{\partial t}\phi,\ \frac{\partial}{\partial t}c\bar{A}\right\}$. As far as the fields ϕ, $c\bar{A}$, etc. in this set are concerned, they have to be specified throughout the room in which the fields exist. The utility of the concept "instantaneous dynamical state" arises from the fact that the specification of this state at one single time, e.g. at t = 0, is enough to determine the entire history, provided that the system is "free-running", i.e. not driven.

We have seen that the instantaneous configuration of the atom, i.e. the set $\{q^i\}$, determines a charge density field $\rho(q^i,\bar{r})$. Similarly the instantaneous dynamical state of the atom, i.e. the set $\{t,\ q^i,\ v^i\}$, determines not only a charge density field $\rho(q^i,\bar{r})$ at the time t, but also a current density field $\bar{J}(q^i,v^i,\bar{r})$ at that time. The current density field will be linear in the v^i so that we can write

$$\bar{J}(q^i,v^i,\bar{r}) = v^j\bar{J}_j(q^i,\bar{r}) \ , \qquad (5)$$

where we have used the summation convention: We will always sum over any repeated index, here j, which appears both as a superscript and a subscript. Latin indices, range from 1 to n, where n is the number of degrees of freedom of the atom.

One should keep in mind that the functions $\rho(q^i,\bar{r})$ and $\bar{J}_j(q^i,\bar{r})$ do not explicitly depend on the time t. The time-dependence of the charge density field and of the current density field is implicit; it arises from the fact that, when the history is examined, the q^i and v^i are seen to be functions of the time.

The continuity equation

$$\frac{\partial}{\partial t}\rho + \bar{\nabla}\cdot\bar{J} = 0 \tag{6}$$

entails a relation between the functions $\rho(q^i,\bar{r})$ and $\bar{J}_j(q^i,\bar{r})$. Since ρ depends cn t by way of the q^i, we have

$$\frac{\partial}{\partial t}\rho = (\frac{d}{dt}q^j)\frac{\partial}{\partial q^j}\rho = v^j\frac{\partial}{\partial q^j}\rho.$$

Also, from (5),

$$\bar{\nabla}\cdot\bar{J} = v^j\,\bar{\nabla}\cdot\bar{J}_j,$$

since the v^j do not depend on $\bar{r}$. Thus the continuity equation yields

$$v^j[\frac{\partial}{\partial q^j}\rho + \bar{\nabla}\cdot\bar{J}_j] = 0\ .$$

This equation must hold for any arbitrary choice of the velocity components v^j. Thus we get

$$\frac{\partial}{\partial q^j}\rho + \bar{\nabla}\cdot\bar{J}_j = 0\ . \tag{7}$$

One should note that the derivative $\frac{\partial}{\partial q^j}$ attacks one of the q^i in the functional form $\rho(q^i,\bar{r})$ whereas the divergence $\bar{\nabla}\cdot$ attacks the $\bar{r}$ in $\bar{J}_j(q^i,\bar{r})$.

Equation (7) is not the only relation connecting the functions $(q^i,\bar{r})$ and $\bar{J}_j(q^i,\bar{r})$. There is another important relation, which we derive in Note #1. It is

$$\frac{\partial}{\partial q^i}\bar{J}_j - \frac{\partial}{\partial q^j}\bar{J}_i = \bar{\nabla} \times \left(\frac{1}{\rho}\bar{J}_i \times \bar{J}_j\right) . \qquad (8)$$

The origin of equation (8) is more subtle than that of the continuity equation (6), on which equation (7) was based. Equation (8) is derived from the principle of "gene-identity". This word, meaning identifiability, was coined in Germany, perhaps around the turn of the century, probably because it is easier to pronounce than its synonym. We say that the atomic system obeys the principle of gene-identity, if each element of charge can be regarded as an identifiable object, i.e. if it can be tagged. This is certainly the case if each atomic particle is a point-like object. We shall make the assumption that the n + 1 functions $\rho(q^i,\bar{r})$, $\bar{J}_j(q^i,\bar{r})$ are structured in such a way that gene-identity is fulfilled even for smeared-out, i.e. continuous, charge and current densities. Equation (8) is the necessary and sufficient condition for gene-identity.

Equation (8) is an important link between the history of a system and the driver fields. These fields will be discussed in the next section.

4. The Driver Fields .

In Section 2 we introduced the notion of driving agencies. These agencies are fields in the home-space, namely a force field with force density $\bar{F}^d(\bar{r},t)$, an electric charge field with charge density $\rho^d(\bar{r},t)$ and an electric current field with current density $\bar{J}^d(\bar{r},t)$. These three driver fields have to be impressed from the outside, i.e. from sources that are external to the system. Figuratively speaking, the driver fields are impressed "by hand".

We have affixed the superscript d ("d" for driver), mainly in order to distinguish the driver fields ρ^d and $\bar{J}^d$ from the atomic fields ρ and $\bar{J}$ (without a superscript), which were discussed in the previous sections. The driver fields ρ^d and $\bar{J}^d$ have to be superimposed on the atomic fields ρ and $\bar{J}$, so that the total

fields ρ^t and $\bar{J}^t$ ("t" for total) are given by $\rho^t = \rho + \rho^d$ and $\bar{J}^t = \bar{J} + \bar{J}^d$. In actual practice the driver fields ρ^d and $\bar{J}^d$ are spatially well separated from the atomic fields ρ and $\bar{J}$, so that the superposition, when viewed as a technical task, is easily accomplished.

We have to make a comment about the forces whose density we denoted by F^d. Here only those forces are included which are impressed directly on the atomic constitutents by the "man" who steers the system to make its history conform to a prearranged plan. Of course, this "man"would also have to impress forces on the electrical drivers, whose densities we denoted by ρ^d and $\bar{J}^d$, in order to overcome inertia effects and to counteract the electromagnetic forces on the drivers. (The density of these electromagnetic forces is given by the usual expression $\rho^d\bar{E} + \bar{J}^d \times \bar{B}$). Perhaps the word "interface" used by computer engineers may help to explain why the density F^d should pertain only to those forces that are impressed directly on the atomic constituents. The interface between the system under study (namely the atom and the radiation field) and the external world (namely the "man" who steers the system and his actions) consists of nothing but the three driver fields F^d, ρ^d, and $\bar{J}^d$. Thus the forces that the "man" impresses on the two electrical drivers (whose densities are ρ^d and $\bar{J}^d$) are entirely within the external world; they do not penetrate the interface.

When the history of the system is made to conform to some prearranged plan, then the system has to be "steered" by means of the three driver fields F^d, ρ^d, and $\bar{J}^d$. The required driver fields can be calculated by way of the action principle, which is the subject of the next section. The case that is usually treated in the literature is that of a "free-running" system, i.e. a system whose history unfolds according to spontaneous evolution. A free-running system

then need not be driven, so that the condition that a system be free-running is that all three driver fields be zero. This condition yields the well-known Lagrangian equations of motion.

5. The Action Principle.

With each history $\{q^i(t),\ \phi(\bar{r},t),\ c\bar{A}(\bar{r},t)\}$ and a set of two times $t = a$, $t = b > a$ there is associated a quantity $A_{a,b}$, the action accumulated between these two times. The units in which $A_{a,b}$ is expressed are those of an action, for instance joule sec or joule hertz^{-1}. It is given by

$$A_{a,b} = \int_{t=a}^{b} dt\ L, \tag{9}$$

where L, the Lagrangian, is a function of the instantaneous dynamical state. The units in which L is expressed are those of an energy, for instance joule. The nature of the function L is obtained essentially through revelation, of course not divine revelation, but revelation stemming from the long tradition of science. But one ought to check the revealed result against other things we know. And that we shall do to some extent later on. For the system consisting of an atom and an electromagnetic field, the Lagrangian L is the sum of three terms, the atomic Lagrangian L_{atom}, the electromagnetic Lagrangian $L_{e.m.}$, and the interaction Lagrangian L_{int}.

$$L = L_{atom} + L_{e.m.} + L_{int}\ . \tag{10}$$

We now proceed to write down these three terms. In the non-relativistic approximation, to which we shall adhere, the atomic Lagrangian is given by

$$L_{atom} = \frac{1}{2}\, v^i M'_{ij} v^j + U'_i v^i - V';\ v^i \equiv \frac{dq^i}{dt}\ , \tag{11}$$

where the quantities M'_{ij}, U'_i, V' depend on the atomic configuration $\{q^k\}$, but not explicitly on the time t. (In general these quantities could be permitted

to depend explicitly on t, but such a t-dependence is not needed for our system.) We have affixed primes to M_{ij}, U_i, V, because we wish to reserve the unprimed symbols for related quantities that are of more immediate practical importance. They will appear later on in our development. The first term in (11) is the kinetic energy, the last term is the potential energy. And the U_i' are the components of a vector potential in the configuration space. For particles without spin all the U_i' are zero. We shall restrict our treatment to spin-less particles.

The electromagnetic Lagrangian $L_{e.m.}$ is the volume integral of the Lagrange density $\mathcal{L}_{e.m.}$ of the electromagnetic field.

$$L_{e.m.} = \iiint \Delta\tau \mathcal{L}_{e.m.} , \tag{12}$$

where $\Delta\tau$ is the volume element. The integral is taken over the whole room in which the atom is situated. The Lagrange density $\mathcal{L}_{e.m.}$ is given by

$$\mathcal{L}_{e.m.} = \frac{\varepsilon_o}{2} \bar{E}\cdot\bar{E} - \frac{\varepsilon_o}{2} c\bar{B}\cdot c\bar{B} , \tag{13}$$

where ε_o is the permittivity of vacuum. The two terms in (13) are, respectively, the electric energy density, and the magnetic energy density. Equations (2) enable us to express $\mathcal{L}_{e.m.}$ more directly in terms of the configurational parameters $c\bar{A}$ and ϕ of the electromagnetic field:

$$\mathcal{L}_{e.m.} = \frac{\varepsilon_o}{2} \left(\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi\right)\cdot\left(\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi\right) - \frac{\varepsilon_o}{2} (\bar{\nabla} \times c\bar{A})\cdot(\bar{\nabla} \times c\bar{A}) . \tag{14}$$

The interaction Lagrangian L_{int} is a similar volume integral, this time of the interaction Lagrange density $\mathcal{L}_{int}$.

$$L_{int} = \iiint \Delta r \mathcal{L}_{int} . \tag{15}$$

The integrand $\mathcal{L}_{int}$ is given by

$$\mathcal{L}_{int} = \frac{1}{c} (c\bar{A}\cdot\bar{J} - \phi c\rho) . \tag{16}$$

Note that $\bar{J}$ and $c\rho$ are expressed in the same units, for instance amp m^{-2}. According to (5), equation (16) may be written in the more directly useful form

$$L_{int} = \frac{1}{c}\,(c\bar{A} \cdot \bar{J}_i v^i - \phi c\rho)\ . \qquad (17)$$

Perhaps it is advisable to repeat (17), this time with all the independent variables indicated:

$$L_{int}(q^i, v^i, \bar{r}, t) = \frac{1}{c}[c\bar{A}(\bar{r},t) \cdot \bar{J}_i(q^j,\bar{r})v^i - \phi(\bar{r},t)c\rho(q^j,\bar{r})]\ . \qquad (18)$$

The action principle is concerned with the variation $\delta A_{a,b}$ of the action, when the actual history $\{q^i(t),\ \phi(\bar{r},t),\ c\bar{A}(\bar{r},t)\}$ is replaced by a slightly varied history $\{q^i(t) + \delta q^i(t),\ \phi(\bar{r},t) + \delta\phi(\bar{r},t),\ c\bar{A}(\bar{r},t) + \delta c\bar{A}(\bar{r},t)\}$. Here the variations δq^i, $\delta\phi$, $\delta c\bar{A}$ of the configurational parameters are very small in some sense (i.e. almost infinitesimals), but otherwise arbitrary. One then evaluates the variation of the action $\delta A_{a,b} \equiv A_{a,b}$ (varied history) $- A_{a,b}$ (actual history) to first order in the δq^i, $\delta\phi$, $\delta c\bar{A}$ with the aid of the rules of the calculus of variations. Although this is a very common calculation, we will repeat it here, because it uses and generates some interesting ideas.*

But before we start with this calculation, we should adopt a policy of prudence and eliminate the somewhat vague concepts of "very small in some sense" and "almost infinitesimal". The procedure that we shall follow is also common. Instead of examining just two histories, namely the actual one and the varied one, we examine a whole family of histories, ordered and labeled by some "variational parameter" η. The case of $\eta = 0$ corresponds to the actual history; and the more η deviates from zero, the more does the history labeled by η deviate from the history labeled by 0. Accordingly, the configurational parameters q^i, ϕ, and $c\bar{A}$ will also depend on the label η. Thus the history labeled by η is given by the set $\{q^i(\eta,t),\ \phi(\eta,\bar{r},t),\ c\bar{A}(\eta,\bar{r},t)\}$. Since q^i depends not only on the

*When we vary the action $A_{a,b}$, we keep the end points a and b of the surveillance-time interval fixed. However, in some investigations, one finds it useful to vary also the end points by the amounts δa and δb. But we can get along without the introduction of these more general variations.

time t, but on the variational parameter η as well, the configurational velocity component v^i is given by the partial derivative $\frac{\partial q^i}{\partial t}$. Then we simply <u>define</u> δq^i, $\delta\phi$, $\delta c\bar{A}$, and $\delta A_{a,b}$ by

$$\delta q^i \equiv \frac{\partial q^i}{\partial \eta}\,\delta\eta,\quad \delta\phi \equiv \frac{\partial \phi}{\partial \eta}\,\delta\eta,\quad \delta c\bar{A} \equiv \frac{\delta c\bar{A}}{\partial \eta}\,\delta\eta,\quad \delta A_{a,b} \equiv \frac{\partial A_{a,b}}{\partial \eta}\,\delta\eta\ ,$$

$$\delta v^i \equiv \frac{\partial v^i}{\partial \eta}\,\delta\eta = \frac{\partial^2 q^i}{\partial \eta \partial t}\,\delta\eta\ . \tag{19}$$

And the $\delta\eta$ that appears in these equations could be of any magnitude; it need not be "small" of "infinitesimal". In fact, all we need to calculate is the partial derivative $\frac{\partial}{\partial \eta} A_{a,b}$. In a way, the $\delta\eta$ is mere decoration. In the end, if we wish to do so, we may multiply the resulting equations by $\delta\eta$ and use (19) to recover the δq^i, $\delta\phi$, $\delta c\bar{A}$, $\delta A_{a,b}$. During the calculation we will make free use of the fact that second partial derivatives do not depend on the order in which they are taken. Thus we may replace $\frac{\partial}{\partial \eta}\frac{\partial q^i}{\partial t}$ by $\frac{\partial}{\partial t}\frac{\partial q^i}{\partial \eta}$, $\frac{\partial}{\partial \eta}\bar{\nabla}\phi$ by $\bar{\nabla}\frac{\partial \phi}{\partial \eta}$, etc. In order to make it easier to read what is being done, we perform the calculation for each of the three portions of the action separately. These three portions are

$$A_{\substack{a,b\\ atom}} = \int_{t=a}^{b} dt\, L_{atom},\quad A_{\substack{a,b\\ e.m.}} = \int_{t=a}^{b} dt\, L_{e.m.}\ , \tag{20}$$

$$A_{\substack{a,b\\ int}} = \int_{t=a}^{b} dt\, L_{int}\ .$$

a. The Portion $\delta A_{\substack{a,b\\ atom}}$.

We have

$$\frac{\partial}{\partial \eta} A_{\substack{a,b\\ atom}} = \int_{t=a}^{b} dt\, \frac{\partial}{\partial \eta} L_{atom}\ .$$

In order to write the integrand in a useful form, we use the fact that $L_{atom}(t, q^i, v^i)$ depends on η by way of the q^i and v^i. Thus

$$\frac{\partial}{\partial \eta} L_{atom} = \left(\frac{\partial}{\partial v^i} L_{atom}\right)\frac{\partial v^i}{\partial \eta} + \left(\frac{\partial}{\partial q^i} L_{atom}\right)\frac{\partial q^i}{\partial \eta}\ .$$

We use the customary abbreviation

$$\frac{\partial}{\partial v^i} L_{atom} = p_i' \ .$$

The p_i' are the configurational momentum components. In our case, we have

$$p_i' = M'_{ij} v^j + U_i' \ ,$$

where we have used the symmetry condition $M'_{ij} = M'_{ji}$, which does not entail any loss of generality. This expression for p_i', involving the primed quantities M'_{ij} and U_i', shows why we have affixed a prime to p_i. We use

$$\frac{\partial v^i}{\partial \eta} \equiv \frac{\partial}{\partial \eta} \frac{\partial q^i}{\partial t} = \frac{\partial}{\partial t} \frac{\partial q^i}{\partial \eta} \ .$$

Thus

$$\frac{\partial}{\partial \eta} L_{atom} = p_i' \frac{\partial}{\partial t} \frac{\partial q^i}{\partial \eta} + \left(\frac{\partial}{\partial q^i} L_{atom}\right) \frac{\partial q^i}{\partial \eta} =$$

$$= \frac{\partial}{\partial t} \left(p_i' \frac{\partial q^i}{\partial \eta}\right) - \frac{\partial p_i'}{\partial t} \frac{\partial q^i}{\partial \eta} + \left(\frac{\partial}{\partial q^i} L_{atom}\right) \frac{\partial q^i}{\partial \eta} \ .$$

Next we integrate over the time t. Afterwards we multiply by $\delta\eta$ (Note that $\delta\eta$ does not depend on t.), thus obtaining the final result

$$\delta A_{\substack{a,b \\ atom}} = (p_i' \delta q^i)\Big|_{t=a}^{b} - \int_{t=a}^{b} dt \left(\frac{\partial p_i'}{\partial t} - \frac{\partial}{\partial q^i} L_{atom}\right) \delta q^i \ , \qquad (21)$$

b. The Portion $\delta A_{\substack{a,b \\ e.m.}}$.

We have

$$\frac{\partial}{\partial \eta} A_{\substack{a,b \\ e.m.}} = \int_{t=a}^{b} dt \ \frac{\partial}{\partial \eta} L_{e.m.} \ ,$$

and

$$\frac{\partial}{\partial \eta} L_{e.m.} = \iiint \Delta\tau \ \frac{\partial}{\partial \eta} \ L_{e.m.}$$

Equations (14) yields

$$\frac{\partial}{\partial \eta} L_{e.m.} = - \left(\frac{\partial}{\partial ct} \frac{\partial c\bar{A}}{\partial \eta}\right) \cdot \varepsilon_o \bar{E} - (\bar{\nabla} \frac{\partial \phi}{\partial \eta}) \cdot \varepsilon_o \bar{E} - (\bar{\nabla} \times \frac{\partial c\bar{A}}{\partial \eta}) \cdot \varepsilon_o c\bar{B} ,$$

where we have used equations (2) to shorten the notation. We rewrite each of the three terms in a way that is preliminary to an integration by parts.

$$\frac{\partial}{\partial \eta} L_{e.m.} = - \frac{\partial}{\partial ct} \{\frac{\partial c\bar{A}}{\partial \eta} \cdot \varepsilon_o \bar{E}\} + \frac{\partial c\bar{A}}{\partial \eta} \cdot \frac{\partial}{\partial ct} \varepsilon_o \bar{E} -$$

$$- \bar{\nabla} \cdot \{\frac{\partial \phi}{\partial \eta} \varepsilon_o \bar{E}\} + \frac{\partial \phi}{\partial \eta} \bar{\nabla} \cdot \varepsilon_o \bar{E} -$$

$$- \bar{\nabla} \cdot \{\frac{\partial c\bar{A}}{\partial \eta} \times \varepsilon_o c\bar{B}\} - \frac{\partial c\bar{A}}{\partial \eta} \cdot (\bar{\nabla} \times \varepsilon_o c\bar{B}) .$$

We integrate this equation over the volume of the room that contains the atoms and the radiation field. As for the first term on the right-hand side, we may interchange the space-integration and the time-differentiation, obtaining

$$- \frac{\partial}{\partial ct} \{\iiint \Delta\tau \frac{\partial c\bar{A}}{\partial \eta} \cdot \varepsilon_o \bar{E}\} .$$

By virtue of the theorem of Gauss, the contributions made by the third and the fifth term gets transformed into the surface integrals.

$$- \oiint \Delta\bar{f} \cdot \varepsilon_o \bar{E} \frac{\partial \phi}{\partial \eta} ,$$

and

$$- \oiint \Delta\bar{f} \cdot \{\frac{\partial c\bar{A}}{\partial \eta} \times \varepsilon_o c\bar{B}\} = - \oiint (\Delta\bar{f} \times \frac{\partial c\bar{A}}{\partial \eta}) \cdot \varepsilon_o c\bar{B} .$$

Now, the derivatives $\frac{\partial c\bar{A}}{\partial \eta}$ and $\frac{\partial \phi}{\partial \eta}$ fulfill the same kind of boundary conditions that were given by equations (4), namely

$$\Delta\bar{f} \times \frac{\partial c\bar{A}}{\partial \eta} = 0, \text{ and } \frac{\partial \phi}{\partial \eta} = 0 \text{ at the wall.} \qquad (22)$$

(Simply differentiate (4) with respect to η.) As a consequence, the two surface integrals vanish. Thus we get

$$\frac{\partial}{\partial \eta} L_{e.m.} = - \frac{\partial}{\partial ct} \{\iiint \Delta\tau \frac{\partial c\bar{A}}{\partial \eta} \cdot \varepsilon_o \bar{E}\} + \iiint \Delta\tau \frac{\partial \phi}{\partial \eta} \bar{\nabla} \cdot \varepsilon_o \bar{E} -$$

$$- \iiint \Delta\tau \frac{\partial c\bar{A}}{\partial \eta} \cdot [\bar{\nabla} \times \varepsilon_o c\bar{B} - \frac{\partial}{\partial ct} \varepsilon_o \bar{E}] .$$

Next we integrate over the time t. Afterwards we multiply by $\delta\eta$ (Note that $\delta\eta$ does not depend on $\bar{r}$ and t), and obtain the final result

$$\delta A_{\substack{a,b \\ e.m.}} = -\left\{\frac{1}{c}\iiint \Delta\tau(\delta c\bar{A})\cdot\varepsilon_o\bar{E}\right\}\Big|_{t=a}^{b} +$$

$$+\int_{t=a}^{b} dt\left\{\iiint \Delta\tau(\delta\phi)\bar{\nabla}\cdot\varepsilon_o\bar{E}\right\} -$$

$$-\int_{t=a}^{b} dt\left\{\iiint \Delta\tau(\delta c\bar{A})\cdot[\bar{\nabla}\times\varepsilon_o c\bar{B} - \frac{\partial}{\partial ct}\varepsilon_o\bar{E}]\right\} . \qquad (23)$$

c. The Portion $\delta A_{\substack{a,b \\ int}}$.

Here our development will become a bit more perspicuous, if we vary the atomic configurational parameters q^i and the electromagnetic configurational parameters ϕ and $c\bar{A}$ separately. We are not forced to do it that way, but it eases the task of writing and reading the equations. Accordingly we examine a family of histories that depend on two variational parameters η and ζ. The history labeled by the pair $\{\eta,\zeta\}$ is given by the set $\{q^i(\eta,t), \phi(\zeta,\bar{r},t), c\bar{A}(\zeta,\bar{r},t)\}$. Then we define $\delta A_{\substack{a,b \\ int}}$ by

$$\delta A_{\substack{a,b \\ int}} = (\frac{\partial}{\partial\eta} A_{\substack{a,b \\ int}})\delta\eta + (\frac{\partial}{\partial\zeta} A_{\substack{a,b \\ int}})\delta\zeta .$$

First we calculate $\frac{\partial}{\partial\eta} A_{\substack{a,b \\ int}}$. We have

$$\frac{\partial}{\partial\eta} A_{\substack{a,b \\ int}} = \int_{t=a}^{b} dt\, \frac{\partial}{\partial\eta} L_{int} ,$$

and

$$\frac{\partial}{\partial\eta} L_{int} = \iiint \Delta\tau\, \frac{\partial}{\partial\eta} L_{int} .$$

We obtain $\frac{\partial}{\partial\eta} L_{int}$ from equation (16). But there only $\bar{J}$ and ρ depend on the variational parameter η. So we have

$$\frac{\partial}{\partial\eta} L_{int} = \frac{1}{c}\left(c\bar{A}\cdot\frac{\partial\bar{J}}{\partial\eta} - \phi c\,\frac{\partial\rho}{\partial\eta}\right) . \qquad (24)$$

The next task is to express $\frac{\partial \bar{J}}{\partial \eta}$ and $\frac{\partial \rho}{\partial \eta}$ in terms of the $\frac{\partial q^i}{\partial \eta}$. Equation (5) yields

$$\frac{\partial \bar{J}}{\partial \eta} = \bar{J}_i \frac{\partial v^i}{\partial \eta} + \frac{\partial \bar{J}_i}{\partial \eta} v_i = \bar{J}_i \frac{\partial}{\partial t} \frac{\partial q^i}{\partial \eta} + \frac{\partial \bar{J}_i}{\partial \eta} v^i .$$

We rewrite the first term in a way that is preliminary to an integration by parts. And in the second term we replace the dummy index i by j. Thus

$$\frac{\partial \bar{J}}{\partial \eta} = \frac{\partial}{\partial t} (\bar{J}_i \frac{\partial q^i}{\partial \eta}) - \frac{\partial q^i}{\partial \eta} \frac{\partial \bar{J}_i}{\partial t} + v^j \frac{\partial \bar{J}_j}{\partial \eta} .$$

Since the $\bar{J}_i$ and $\bar{J}_j$ depend on t and η by way of the q^k, we get (Note: $\frac{\partial q^j}{\partial t} = v^j$)

$$\frac{\partial \bar{J}}{\partial \eta} = \frac{\partial}{\partial t} (\bar{J}_i \frac{\partial q^i}{\partial \eta}) + \frac{\partial q^i}{\partial \eta} v^j (\frac{\partial \bar{J}_j}{\partial q^i} - \frac{\partial \bar{J}_i}{\partial q^j}) .$$

Now we use equation (8), which followed from the principle of gene-identity. At the same time we can bring the $\frac{\partial q^i}{\partial \eta}$ and v^j behind the curl $\bar{\nabla}\times$, since neither of these quantities depends on $\bar{r}$. Thus we obtain

$$\frac{\partial \bar{J}}{\partial \eta} = \frac{\partial}{\partial t} (\bar{J}_i \frac{\partial q^i}{\partial \eta}) + \bar{\nabla} \times [(\frac{1}{\rho} \bar{J}_i \frac{\partial q^i}{\partial \eta}) \times \bar{J}_j v^j] .$$

We use (5) to replace $\bar{J}_j v^j$ by $\bar{J}$. Also, since the combination $\frac{1}{\rho} \bar{J}_i \frac{\partial q^i}{\partial \eta}$ will occur frequently later on, we rewrite the first term in such a way that this combination will appear. Thus

$$\frac{\partial \bar{J}}{\partial \eta} = \frac{\partial}{\partial t} [\rho(\frac{1}{\rho} \bar{J}_i \frac{\partial q^i}{\partial \eta})] + \bar{\nabla} \times [(\frac{1}{\rho} \bar{J}_i \frac{\partial q^i}{\partial \eta}) \times \bar{J}] . \qquad (25)$$

Next we calculate $\frac{\partial \rho}{\partial \eta}$ in a similar manner. We have

$$\frac{\partial \rho}{\partial \eta} = \frac{\partial \rho}{\partial q^i} \frac{\partial q^i}{\partial \eta} ,$$

or, with (7),

$$\frac{\partial \rho}{\partial \eta} = - \frac{\partial q^i}{\partial \eta} \bar{\nabla} \cdot \bar{J}_i .$$

The $\frac{\partial q^i}{\partial \eta}$ may be brought behind the divergence $\bar{\nabla}\cdot$, since this quantity does not depend on $\bar{r}$. Thus

$$\frac{\partial \rho}{\partial \eta} = - \bar{\nabla} \cdot [\rho(\frac{1}{\rho} \bar{J}_i \frac{\partial q^i}{\partial \eta})] . \qquad (26)$$

Equations (25) and (26) may be written in a shorter way. We multiply these equations by $\delta\eta$. The left-hand sides then become

$$\delta\bar{J} \equiv \frac{\partial \bar{J}}{\partial \eta}\,\delta\eta \text{ and } \delta\rho \equiv \frac{\partial \rho}{\partial \eta}\,\delta\eta \ . \tag{27}$$

On the right-hand sides we may bring the $\delta\eta$ behind the differentiation operators $\frac{\partial}{\partial t}$, $\bar{\nabla}\times$, $\bar{\nabla}\cdot$, since $\delta\eta$ does not depend on $\bar{r}$ and t. Then there will appear the combination

$$\frac{1}{\rho}\,\bar{J}_i\,\frac{\partial q^i}{\partial \eta}\,\delta\eta \equiv \frac{1}{\rho}\,\bar{J}_i\,\delta q^i \ ,$$

for which the customary abbreviation is $\delta\bar{r}$. The physical significance of $\delta\bar{r}$ will be explained presently. Then, with

$$\delta\bar{r} \equiv \frac{1}{\rho}\,\bar{J}_i\,\delta q^i \ , \tag{28}$$

equations (25) and (26) become

$$\delta\bar{J} = \frac{\partial}{\partial t}\,(\rho\,\delta\bar{r}) + \bar{\nabla}\times(\delta\bar{r}\times\bar{J}) \ , \tag{29}$$

$$\delta\rho = -\,\bar{\nabla}\cdot(\rho\,d\bar{r}) \ . \tag{30}$$

Another derivation of equations (29) and (30), which are used in our subsequent discussions, may be found in Note #2. There the derivation is based on the vector calculus.

We interrupt the process of calculating $\delta A_{a,b}^{int}$ in order to discuss the meaning of $\delta\bar{r}$, called the field of virtual displacements. According to the principle of gene-identity, each element of charge may be tagged, i.e. it may be considered as an identifiable object. Let us consider one such element, and let $\bar{a}$ be its position in the home-space. Now $\bar{a}$ depends explicitly only on the atomic configurational parameters q^i. When the q^i depend on the time t, the velocity $\frac{d\bar{a}}{dt}$ of this charge element is given by

$$\frac{d\bar{a}}{dt} = \frac{\partial \bar{a}}{\partial q^i}\,\frac{dq^i}{dt} = \frac{\partial \bar{a}}{\partial q^i}\,v^i \ .$$

But the velocity ought to be related to the local charge density ρ and the local current density $\bar{J}$ by $\rho \frac{d\bar{a}}{dt} = \bar{J}$. With the aid of (5), this equation yields

$$\frac{d\bar{a}}{dt} = \frac{1}{\rho} \bar{J}_i \, v^i \ .$$

We compare the two expressions for $\frac{d\bar{a}}{dt}$ and use the fact that the set $\{v^i\}$ of the configurational velocity components may be chosen arbitrarily. Then we find

$$\frac{\partial \bar{a}}{\partial q^i} = \frac{1}{\rho} \bar{J}_i \ . \tag{31}$$

Now let the q^i also depend on the variational parameters η, as before. Then we have

$$\delta\bar{a} \equiv \frac{\partial \bar{a}}{\partial \eta} \delta\eta = \frac{\partial \bar{a}}{\partial q^i} \frac{\partial q^i}{\partial \eta} \delta\eta \equiv \frac{\partial \bar{a}}{\partial q^i} \delta q^i \ .$$

With the aid of (31), this equation becomes

$$\delta\bar{a} = \frac{1}{\rho} \bar{J}_i \delta q^i \ . \tag{32}$$

An equation of this type holds not only for this particular charge element, but for every charge element. Of course, the ρ and the $\bar{J}_i$ in (32) have to be evaluated at the position at which the charge element is situated. We may therefore regard (32) as a generic relation. The customary symbol for a generic $\delta\bar{a}$ is $\delta\bar{r}$, although $\delta\bar{a}$ would be preferable on strictly logical grounds. With this change of notation, (32) becomes

$$\delta\bar{r} = \frac{1}{\rho} \bar{J}_i \delta q^i \qquad \text{(28), repeated.}$$

According to (28), each set of $\{\delta q^i \equiv \frac{\partial q^i}{\partial \eta} \delta\eta\}$ engenders a field of virtual displacements $\delta\bar{r}$. Additional material, especially as it concerns equation (31), may be found in Note #1.

We may resume the calculation of $\frac{\partial}{\partial \eta} A_{a,b}$. At this point we have become so accustomed to the use of quantities which are prefixed by a δ that we can skip a few steps and calculate $(\frac{\partial}{\partial \eta} A_{a,b})\delta\eta$ directly. To repeat: No infinitesimals
int int

are involved. A quantity, say Q, that is prefixed by a δ simply stands for the η-derivative $\frac{\partial Q}{\partial \eta}$ multiplied by $\delta\eta$. And $\delta\eta$ is of finite magnitude. Furthermore, $\delta\eta$ does not depend on $\bar{r}$ and t; it is a constant. We have

$$(\frac{\partial}{\delta\eta}\,\delta A_{\substack{a,b\\ int}})\delta\eta = \int_{t=a}^{b} \delta L_{int} \ ,$$

and

$$\delta L_{int} = \iiint \Delta r \ \delta \mathcal{L}_{int}$$

Equation (24) yields

$$\delta \mathcal{L}_{int} = \frac{1}{c}(c\bar{A} \cdot \delta\bar{J} - \phi c\delta\rho) \ .$$

With the aid of (29) and (30), this equation becomes

$$\delta \mathcal{L}_{int} = \frac{1}{c}\{c\bar{A} \cdot \frac{\partial}{\partial t}(\rho\delta\bar{r}) + c\bar{A} \cdot [\bar{\nabla} \times (\delta\bar{r} \times \bar{J})] + \phi c\bar{\nabla} \cdot (\rho\delta\bar{r})\}$$

We rewrite each term in a way that is preliminary to an integration by parts, and obtain

$$\begin{aligned}\delta \mathcal{L}_{int} = {} & \frac{\partial}{\partial ct}(c\bar{A} \cdot \rho\delta\bar{r}) - \frac{\partial c\bar{A}}{\partial ct} \cdot \rho\delta\bar{r} \ + \\ & + \frac{1}{c}\bar{\nabla} \cdot [(\delta\bar{r} \times \bar{J}) \times c\bar{A}] + \frac{1}{c}(\bar{\nabla} \times c\bar{A}) \cdot (\delta\bar{r} \times \bar{J}) \ + \\ & + \frac{1}{c}\bar{\nabla} \cdot [\phi c\rho\delta\bar{r}] - \frac{1}{c}(\bar{\nabla}\phi) \cdot c\rho\delta\bar{r} \ ,\end{aligned}$$

or, with the aid of equation (2),

$$\begin{aligned}\delta \mathcal{L}_{int} = {} & \frac{\partial}{\partial ct}(c\bar{A} \cdot \rho\delta\bar{r}) + \frac{1}{c}\bar{\nabla} \cdot [(\delta\bar{r} \times \bar{J}) \times c\bar{A} + \phi c\rho\delta\bar{r}] \\ & + \frac{1}{c}(c\rho\bar{E} + \bar{J} \times c\bar{B}) \cdot \delta\bar{r} \ .\end{aligned}$$

We integrate this equation over the volume of the room that contains the atom and the radiation field. As for the first term, we may interchange space-integration and time-differentiation. The second term gets transformed into a surface integral by virtue of the theorem of Gauss. But this surface integral vanishes because of the boundary conditions (4); it is treated in a way that

is very similar to what was done in the preceding section. We then obtain

$$\delta L_{int} = \frac{\partial}{\partial t}\{\iiint \Delta\tau \bar{A} \cdot \rho\delta\bar{r}\} + \frac{1}{c}\iiint \Delta\tau(c\rho\bar{E} + \bar{J} \times c\bar{B}) \cdot \delta\bar{r}$$

Finally we integrate over the time t and obtain

$$(\frac{\partial}{\partial\eta} A_{a,b}{}_{int})\delta\eta = \{\iiint \Delta\tau \bar{A} \cdot \rho\delta\bar{r}\}\Big|_{t=a}^{b} + \int_{t=a}^{b} dt\,\{\iiint \Delta\tau(\bar{E} + \bar{J} \times \bar{B}) \cdot \delta\bar{r}\} . \qquad (33)$$

Next we calculate $(\frac{\partial}{\partial\zeta} A_{a,b}{}_{int})\delta\zeta$. Again we work with quantities that have a δ as a prefix. Here, of course, the δ indicates the ζ-derivative multiplied by $\delta\zeta$. Equation (16) yields

$$\delta L_{int} = \frac{1}{c}(\bar{J} \cdot \delta c\bar{A} - c\rho\delta\phi) .$$

The only thing we have to do here is to integrate this equation over space and time. We obtain

$$(\frac{\partial}{\partial\zeta} A_{a,b}{}_{int})\delta\zeta = \int_{t=a}^{b} dt\{\iiint \Delta\tau \frac{1}{c}(\bar{J} \cdot \delta c\bar{A} - c\rho\delta\phi)\} . \qquad (34)$$

Finally we add equations (33) and (34). Then, according to the first equation of this subsection, we obtain the desired quantity $\delta A_{a,b}{}_{int}$. We arrive at

$$\delta A_{a,b}{}_{int} = \{\iiint \Delta\tau \bar{A} \cdot \rho\delta\bar{r}\}\Big|_{t=a}^{b} +$$

$$+ \int_{t=a}^{b} dt\{\iiint \Delta\tau[(\rho\bar{E} + \bar{J} \times \bar{B}) \cdot \delta\bar{r} + \frac{1}{c}(\bar{J} \cdot \delta c\bar{A} - c\rho\delta\phi)]\} , \qquad (35)$$

which is the last equation of this subsection.

Now that we have finished expressing each of the three portions of $\delta A_{a,b}$ in a form that is useful for our purposes, we obtain $\delta A_{a,b}$ itself by adding equations (21), (23), and (35). We change the order of the various terms so that related terms appear together. Since in the final expression the variational parameters η and ζ no longer occur, we can replace the partial

derivative $\frac{\partial p_i'}{\partial t}$ in (21) by the total time-derivative $\frac{dp_i'}{dt}$. (The partial derivative $\frac{\partial p_i'}{\partial t}$ appeared at an earlier stage of our discussion, because then the p_i' were considered to depend not only on the time t but also on the variational parameter η. From now on we can ignore the η-dependence, since in essence it was only a procedural artifact in our derivations.) We obtain

$$\delta A_{a,b} = \{p_i' \delta q^i + \iiint \Delta\tau \rho \bar{A} \cdot \delta \bar{r} - \iiint \Delta\tau \varepsilon_o \bar{E} \cdot \delta \bar{A}\}\Big|_{t=a}^{b} -$$

$$- \int_{t=a}^{b} dt\{(\frac{dp_i'}{dt} - \frac{\partial}{\partial q^i} L_{atom})\delta q^i - \iiint \Delta\tau(\rho \bar{E} + \bar{J} \times \bar{B}) \cdot \delta \bar{r} +$$

$$+ \iiint \Delta\tau[(\bar{\nabla} \times \frac{1}{\mu_o} \bar{B} - \frac{\partial}{\partial t} \varepsilon_o \bar{E} - \bar{J}) \cdot \delta \bar{A} - (\bar{\nabla} \cdot \varepsilon_o \bar{E} - \rho)\delta\phi]\} , \qquad (36)$$

where we have introduced the permeability μ_o of the vacuum, given by $\mu_o = \frac{1}{\varepsilon_o c^2}$.

Later on, when we will state the action principle, it will be helpful if we replace those terms in (36) that contain the δq^i by terms in $\delta \bar{r}$. To this end we introduce n vector fields $\bar{s}^i$ in the home-space. (Note that n was the number of atomic degrees of freedom) which are "reciprocal" to the n vector fields $\bar{J}_i$, i.e. which fulfil the relation

$$\iiint \Delta\tau \bar{s}^i \cdot \bar{J}_j = \delta^i_j . \qquad (37)$$

Here δ^i_j is the Kronecker-delta: $\delta^i_j = 1$ for $i = j$, $\delta^i_j = 0$ for $i \neq j$. The $\bar{s}^i$ are not uniquely determined by (37). But our further considerations do not depend on the feature of uniqueness. At any rate, later on the $\bar{s}^i$ will occur only in the products $\rho \bar{s}^i$; and these are determined uniquely, because the atomic configurations are not subject to the kind of constraints that we find in engineering mechanics, in the form of mechanical linkages.

We can express the δq^i in terms of the $\delta \bar{r}$-field if we multiply equation (28) by $\rho \bar{s}^j$ and then integrate over the volume. Then, by virtue of (37), we obtain

$$\delta q^j = \iiint \Delta\tau \rho \bar{s}^j \cdot \delta\bar{r} \ . \qquad (38)$$

We use this result to rewrite equation (36). Here the p_i' and the expression $(\frac{dp_i'}{dt} - \frac{\partial}{\partial q^i} L_{atom})$ may be moved behind the integration signs $\iiint$, since these quantities do not depend on $\bar{r}$. We obtain

$$\delta A_{a,b} = \{\iiint \Delta\tau \rho (\bar{s}^i p_i' + \bar{A}) \cdot \delta\bar{r} - \iiint \Delta\tau \varepsilon_o \bar{E} \cdot \delta\bar{A}\}\Big|_{t=a}^{b}$$
$$- \int_{t=a}^{b} dt \{\iiint \Delta\tau [(\frac{dp_i'}{dt} - \frac{\partial}{\partial q^i} L_{atom}) \rho \bar{s}^i - (\rho\bar{E} + \bar{J} \times \bar{B})] \cdot \delta\bar{r}$$
$$+ \iiint \Delta\tau [(\bar{\nabla} \times \frac{1}{\mu_o} \bar{B} - \frac{\partial}{\partial t} \varepsilon_o \bar{E} - \bar{J}) \cdot \delta\bar{A} - (\bar{\nabla} \cdot \varepsilon_o \bar{E} - \rho)\delta\phi]\} \ . \qquad (39)$$

At this point we are ready to state the action principle. But before we do so, we briefly review what we have done so far. We started with an expression for the action $A_{a,b}$ as a functional of the history. This step was a part of Physics. Then there followed a rather lengthy derivation resulting in the expression (39) for the variation of the action. This derivation was mostly of a purely formal nature, except for the use of the principle of gene-identity [as in equation (8)], which is a part of Physics.

The action principle, a part of Physics, states that the driver fields $\bar{F}^d$, ρ^d, and $\bar{J}^d$ are related to the variation of the action by the equation

$$\delta A_{a,b} = \{\iiint \Delta\tau \bar{\rho}_{mom} \cdot \delta\bar{r} - \iiint \Delta\tau \bar{D} \cdot \delta\bar{A}\}\Big|_{t=a}^{b} -$$
$$- \int_{t=a}^{b} \{dt \{\iiint \Delta\tau \bar{F}^d \cdot \delta\bar{r} + \iiint \Delta\tau [\bar{J}^d \cdot \delta\bar{A} - \rho^d \delta\phi]\} \ , \qquad (40)$$

where $\bar{\rho}_{mom}$ is the momentum density of the atomic constituents, and where $\bar{D}$ is the electric displacement.

When we subtract equation (39) from equation (40) we obtain

$$\{\iiint \Delta\tau [\bar{\rho}_{mom} - \rho(\bar{s}^i p_i' + \bar{A})] \cdot \delta\bar{r} - \iiint \Delta\tau [\bar{D} - \varepsilon_o \bar{E}] \cdot \delta\bar{A}\}\Big|_{t=a}^{b} =$$
$$= \int_{t=a}^{b} dt \{\iiint \Delta\tau [\bar{F}^d - (\frac{dp_i'}{dt} - \frac{\partial}{\partial q^i} L_{atom}) \rho \bar{s}^i + (\bar{E} + \bar{J} \times \bar{B})] \cdot \delta\bar{r} -$$
$$- \iiint \Delta\tau [(\bar{\nabla} \times \frac{1}{\mu_o} \bar{B} - \frac{\partial}{\partial t} \varepsilon_o \bar{E} - \bar{J} - \bar{J}^d) \cdot \delta\bar{A} - (\bar{\nabla} \cdot \varepsilon_o \bar{E} - \rho - \rho^d)\delta\phi]\} \ . \qquad (41)$$

In order to extract useful information from equation (41), we remember that the atom possesses enough degrees of freedom so that there are no restrictions on the displacement variations $\delta\bar{r}$. (Where there are no atomic constituents the $\delta\bar{r}$ is completely arbitrary by default.) Furthermore there are no restrictions on $\delta\bar{A}$ and $\delta\phi$, except that, at the walls of the room, these variations are subject to the boundary conditions

$$\Delta\bar{f} \times \delta\bar{A} = 0, \text{ and } \delta\phi = 0 \text{ at the wall.}$$

These conditions are merely a different version of (22). In addition, the end points t = a and t = b of the time interval of surveillance are arbitrary. We observe that the left-hand side of (41) is contributed only by the end points of this time interval, whereas the right-hand side is contributed only by the interior points. Each side is therefore a linear functional of a different set of quantities. Thus they can be equal to each other only if they are zero. Because of the arbitrariness of $\delta\bar{r}$, $\delta\bar{A}$, and $\delta\phi$ each side can vanish only if the factors of these quantities are zero. Thus we obtain

$$\bar{\rho}_{mom} = \rho(\bar{s}^i p_i' + \bar{A}) \ , \tag{42}$$

$$\bar{D} = \varepsilon_o \bar{E} \ , \tag{43}$$

$$\bar{F}^d = \left(\frac{dp_i'}{dt} - \frac{\partial}{\partial q^i} L_{atom}\right)\rho\bar{s}^i - (\rho\bar{E} + \bar{J} \times \bar{B}) \ , \tag{44}$$

$$\bar{J}^d = \bar{\nabla} \times \frac{1}{\mu_o}\bar{B} - \frac{\partial}{\partial t}\varepsilon_o\bar{E} - \bar{J} \ , \tag{45}$$

$$\rho^d = \bar{\nabla} \cdot \varepsilon_o\bar{E} - \rho \ . \tag{46}$$

Equation (44) - (46) serve to determine the required driver fields $\bar{F}^d$, $\bar{J}^d$, and ρ^d. Additional information is furnished by equations (42) and (43).

But we will not use them. Equation (44) is of great interest. It states that in the absence of electromagnetic fields the required driving force density is given by the first term, whereas in the presence of electromagnetic fields the required force density is reduced by the amount $\rho\bar{E} + \bar{J} \times \bar{B}$. This means that the electromagnetic fields exert forces on the atomic constituents with a force density equal to $\rho\bar{E} + \bar{J} \times \bar{B}$. Since this agrees with the predictions of electromagnetic theory, our choice of L_{int}, as given by equation (16), has been confirmed. [It was the interaction part of the total action that produced the term $\rho\bar{E} + \bar{J} \times \bar{B}$, as shown by equation (35).] It is hard to imagine - and probably also impossible - that any other choice for L_{int} would have produced the same result. But then equations (45) and (46) follow automatically. In terms of the total charge density $\rho^t = \rho + \rho^d$ and the total current density $\bar{J}^t = \bar{J} + \bar{J}^d$, these equations yield the second pair of the Maxwell equations

$$\bar{\nabla} \times \frac{1}{\mu_o} \bar{B} - \frac{\partial}{\partial t} \varepsilon_o \bar{E} = \bar{J}^t \text{ and } \bar{\nabla} \cdot \varepsilon_o \bar{E} = \rho^t, \tag{47}$$

which supplement the first pair (1).

The most familiar application of the action principle concerns the behavior of a free-running system. In this case the three driver fields $\bar{F}^d$, $\bar{J}^d$, and ρ^d are zero. Before we set $\bar{F}^d$ equal to zero in (44), we multiply this equation by $\frac{1}{\rho} \bar{J}_j$ and then integrate over the volume. With the aid of (37), we obtain

$$\frac{dp'_i}{dt} - \frac{\partial}{\partial q^i} L_{atom} = \iiint \Delta\tau \frac{1}{\rho} \bar{J}_j \cdot (\rho\bar{E} + \bar{J} \times \bar{B}). \tag{48}$$

This equation tells us how the electromagnetic field influences the atom. Equations (45) and (46) yield directly

$$\bar{\nabla} \times \frac{1}{\mu_o} \bar{B} - \frac{\partial}{\partial t} \varepsilon_o \bar{E} = \bar{J}\ , \tag{49}$$

and

$$\bar{\nabla} \cdot \varepsilon_o \bar{E} = \rho. \qquad (50)$$

These two equations tell us how the atom influences the electromagnetic field. Of course, in all three of these equations we have to express $\bar{E}$ and $\bar{B}$ by the potentials $c\bar{A}$ and ϕ, as shown by (2). At this point we can appreciate the great utility of the action principle. If the action functional is formulated in such a way that it yields the expected equation of motion (48) for the forward process "radiation → atom", then it will automatically produce the equations of motion (49), (50) for the reverse process "atom → radiation".

We have written down the equations of motion (48) - (50) for the free-running system in order to show that something we are familiar with results from the action principle. But it is more useful to work directly with the action principle, even in the case of a free-running system, and to leave the equations of motion as something that is implied by the principle. In this case the action principle may be stated in a rather concise form. Equation (40) shows that, when the three driver fields $\bar{F}^d$, $\bar{J}^d$, and ρ^d are zero, the terms contributed by the interior of the time interval t = a to t = b vanish and that only the terms contributed by the end points t = a and t = b survive. Thus the action principle states simply that

$$\delta A_{a,b} = \text{E.T.O.} \ , \qquad (51)$$

where E.T.O. stands for "End Terms Only". In order to apply the principle (51), one first writes down the action functional $A_{a,b}$. For the system consisting of an atom and a radiation field both treated according to classical physics, this functional is given by

$$A_{a,b} = \int_{t=a}^{b} dt\{\frac{1}{2} \frac{dq^i}{dt} M'_{ij} \frac{dq^j}{dt} + U'_i \frac{dq^i}{dt} - V +$$
$$+ \iiint \Delta\tau[\frac{\varepsilon_o}{2} (\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) \cdot (\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) - \frac{\varepsilon_o}{2} (\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A}) +$$
$$+ \frac{1}{c} (c\bar{A} \cdot \bar{J}_i \frac{dq^i}{dt} - \phi c\rho)]\} \ , \qquad (52)$$

as we have seen. Then one works out the variation $\delta A_{a,b}$ by purely mathematical manipulations and obtains (39). The next step is to set the "interior term" $\int_{t=a}^{b}\{dt \ldots\}$ equal to zero. Here one uses the fact that the variations $\delta\bar{r}$, $\delta\bar{A}$, and $\delta\phi$ are arbitrary. The result is the equations of motion (48) - (50). The end terms themselves are of no interest in the applications we have in mind.

We shall follow the same procedure later on when we treat the atom according to the quantum mechanics. The only modification occurs in the very first step, namely in the formulation of the action functional. This step will be made easier, if we rewrite the various terms of (52) in a different order, namely

$$A_{a,b} = \int_{t=a}^{b} dt\{\frac{1}{2}\frac{dq^i}{dt} M'_{ij} \frac{dq^i}{dt} + [U'_i + \iiint \Delta\tau \bar{J}_i \cdot \bar{A}]\frac{dq^i}{dt} - [V' + \iiint \Delta\tau\rho\phi] +$$

$$+ \iiint \Delta\tau[\frac{\varepsilon_o}{2}(\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) \cdot (\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) - \frac{\varepsilon_o}{2}(\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A})]\} \ . \quad (53)$$

We see that the vector potential component U'_i in the atomic configuration space is augmented by $\iiint \Delta\tau \bar{J}_i \cdot \bar{A}$, and that the potential energy V' is augmented by $\iiint \Delta\tau\rho\phi$. We may regard $\iiint \Delta\tau \bar{J}_i \cdot \bar{A}$ as the "pull-back" of the home-space vector potential and $\iiint \Delta\tau\rho\phi$ as the pull back of the scalar potential ϕ. In the pull-back operation one starts with a quantity defined in the home-space and constructs a related quantity in the configuration space. A third example of a pull-back is furnished by equation (48). In treatises an analytical dynamics this equation is usually written as

$$\frac{dp'_j}{dt} - \frac{\partial}{\partial q'^j} L_{atom} = F_j^{e.m.} \ ,$$

where $F_j^{e.m.}$ is the component of the generalized force (here of electromagnetic origin as indicated by the superscript e.m.). We see then that $F_J^{e.m.}$ is given by

$$F_j^{e.m.} = \iiint \Delta r \, \frac{1}{\rho} \bar{J}_j \cdot (\bar{E} + \bar{J} \times \bar{B}) \qquad (54)$$

Thus $F_j^{e.m.}$ may be regarded as the pull-back of the electromagnetic force density $\rho\bar{E} + \bar{J} \times \bar{B}$. A fourth example is furnished by equation (38), which describes the pull-back of a displacement field $\delta\bar{r}$. A related equation would be the pull-back of a velocity field $\bar{w}$ from the home-space into configurational velocity components v^j, namely

$$v^j = \iiint \Delta\tau\rho\bar{s}^j \cdot \bar{w} \, . \qquad (55)$$

The inverse of the pull-back is the "push-out". In this operation we start with a quantity defined in the atomic configuration space and construct a related quantity in the home-space. We can always recover one of these two operations from its inverse by means of equation (37). For instance the push-out that is related to the pull-back (55) is

$$\bar{w} = \frac{1}{\rho} \, \bar{J}_i v^i \, . \qquad (56)$$

As we go from pull-back to push-out we use (37) to check the result, whereas we use (37) directly when we go from push-out to pull-back. Equations (28) and (38) constitute another pair of these two inverse operations.

The action principle (51) in conjunction with (52) or (53) seems to be all that is required for the analysis of the free-running system. But when one comes to the equations of motion (48) - (50), one meets a difficult situation. For the sake of simplicity and physical reality one would like to treat the atomic particles as point-like objects. But $\bar{E}$ and $\bar{B}$ tend to infinity as we approach the object. As a consequence, the meaning of the right-hand side of (48) becomes obscure, as the following consideration will show. The factor $\frac{1}{\rho} \bar{J}_i$ in the integrand presents no difficulties. As equation (56) shows, this factor

must be finite, so that $\bar{w}$, which here is the velocity of the particle in question, comes out to be finite for any arbitrary choice of the set $\{v^i\}$. Integrals of the type $\iiint \Delta\tau (\frac{1}{\rho}\bar{J}_j)\rho$ and $\iiint \Delta\tau (\frac{1}{\rho}\bar{J}_j)\bar{J}$ present no difficulties, even though ρ and $\bar{J}$ become infinite at the location of the particle. The values of these integrals are $(\frac{1}{\rho}\bar{J}_j)Q$ and $(\frac{1}{\rho}\bar{J}_j)\, Q\,\bar{w}$, where Q is the charge of the particle. But unfortunately the integrand in (48) contains also $\bar{E}$ and $\bar{B}$, which tend to infinity as the particle is approached. And it is this feature that makes the meaning of the integral obscure. As far as equations (49) and (50) are concerned, the situation is manageable, as the theory of the Liénard-Wiechert potentials would show. But we will not pursue this matter, since the difficulty about equation (48) still remains.

The discipline of quantum electrodynamics was created for the purpose of coping with this difficulty. But we shall not use this discipline here, because it is too complex. Furthermore it treats the particles relativistically, and the electromagnetic field quantum-mechanically, whereas we decided at the outset to treat the particles non-relativistically and to use the classical theory for the fields. Instead of quantum electrodynamics, we are going to employ a more elementary method. This method is based on two approximations, which will be explained in Section 7.

But before we deal with these approximations we will describe some simplifications that result from the choice of a particular "gauge" for the electromagnetic potentials $c\bar{A}$ and ϕ. Choosing a gauge means to subject the divergence of $c\bar{A}$ to any requirement that will assist further developments of the analysis. Our ability to stipulate what $\bar{\nabla} \cdot c\bar{A}$ should be is based on the following argument. According to equations (2) the electromagnetic fields $\bar{E}$ and $c\bar{B}$ remain unchanged

if we subject $c\bar{A}$ and ϕ to a gauge transformation, i.e., if we replace $c\bar{A}$ and ϕ by $c\bar{A} + \bar{\nabla}\chi$ and $\phi - \frac{\partial}{\partial ct}\chi$ respectively, where χ is an arbitrary function of the position $\bar{r}$ and the time t. There is then some redundancy in $c\bar{A}$ and ϕ, which we can exploit to impose conditions on $\bar{\nabla} \cdot c\bar{A}$. The most common conditions are

$$\bar{\nabla} \cdot c\bar{A} + \frac{\partial}{\partial ct}\phi = 0 \ , \tag{57}$$

which embodies the choice of the Lorentz gauge, and

$$\bar{\nabla} \cdot c\bar{A} = 0 \ , \tag{58}$$

which embodies the choice of the Coulomb or radiation gauge. We choose the latter. The consequences of this choice will be described in the next section. Besides the constraint (58) we will also impose a similar constraint on the variation $\delta c\bar{A}$, namely

$$\bar{\nabla} \cdot (\delta c\bar{A}) = 0 \tag{59}$$

The statement that we are going to use the Coulomb gauge is not quite precise enough. What we are really going to do is to expand the vector field $c\ddot{A}$ in terms of longitudinal and transverse cavity modes. And then we impose the constraint that $c\bar{A}$ be a linear combination of only the transverse modes. In other words: Those expansion coefficients that belong to the longitudinal modes are set equal to zero. The equations (58) and (59) still hold. But $c\bar{A}$ and $\delta c\bar{A}$ when constrained in this manner will have additional properties. For instance, the boundary conditions

$$\Delta\bar{f} \times c\bar{A} = 0 \text{ and } \Delta\bar{f} \times \delta c\bar{A} = 0 \tag{60}$$

will be fulfilled. [See (4) and (22)]. All of this will be explained in the next section. Instead of saying that we will subject the vector potential $c\bar{A}$ to the Coulomb gauge (58), we will say that we constrain $c\bar{A}$ to be "transverse".

6. The Transverse Gauge.

We shall base our discussions on the formalism that may be found in the book "Microwave Electronics" by John C. Slater, (Van Nostrand 1950). As this book may be out of print we shall repeat the arguments that are presented there but sometimes in modified form. We shall use the word "cavity", customary in this context, for the room that contains the atom and the radiation field. This cavity is assumed to have perfectly conducting walls, which implies that the electric field $\vec{E}$ and the magnetic induction $c\vec{B}$ satisfy the boundary conditions

$$\Delta\vec{f} \times \vec{E} = 0, \text{ and } \Delta\vec{f} \cdot c\vec{B} = 0 \qquad (2) \text{ repeated}$$

Slater's formalism pertains to the expansion of fields in terms of cavity modes.

Before we get started we review three theorems of geometry. The first theorem states that the surface integral of the curl of an arbitrary smooth vector field $\vec{V}$ is zero, when this integral is taken over a closed surface. That is, we have

$$\oiint \Delta\vec{f} \cdot \vec{\nabla} \times \vec{V} = 0 \,. \qquad (61)$$

In order to prove (61) we transform the surface integral into a volume integral over the enclosed space, by virtue of the theorem of Gauss. Thus

$$\oiint \Delta\vec{f} \cdot \vec{\nabla} \times \vec{V} = \iiint \Delta\tau \; \vec{\nabla} \cdot \vec{\nabla} \times \vec{V} \,.$$

Since the divergence of a curl is zero, equation (61) follows.

The second theorem states that, for a scalar function ψ which has the constant value 0 on some smooth surface F, we have

$$\Delta\vec{l} \times \vec{\nabla}\psi = 0, \text{ if } \psi = 0 \text{ on } F, \qquad (62)$$

i.e. the gradient is normal to the surface. This should be clear, when the geometrical situation is visualised. A more formal proof goes as follows. We

can always extend the surface, so that it forms a part of a closed surface.* Equation (62) is equivalent to the statement that

$$\oiint(\Delta\bar{f} \times \bar{\nabla}\psi) \cdot \bar{w} = 0$$

for any arbitrary smooth vector field $\bar{w}$. And this statement results from the following calculation.

$$\oiint(\Delta\bar{f} \times \bar{\nabla}\psi) \cdot \bar{w} = \oint\int\Delta\bar{f} \cdot (\bar{\nabla}\psi \times \bar{w}) = \oint\int\Delta\bar{f} \cdot [\bar{\nabla} \times (\psi\bar{w}) - \psi\bar{\nabla} \times \bar{w}] .$$

The integral of the first term is zero by virtue of (61). The integral of the second term vanishes, because $\psi = 0$ on the surface. Since $\bar{\nabla}\psi$ is not affected, when we add a constant to ψ, the statement (62) may be generalized to read

$$\Delta\bar{f} \times \bar{\nabla}\psi = 0, \text{ if } \psi = \text{const on } F. \tag{63}$$

The third theorem states that, for a vector field $\bar{E}$, which is normal to a smooth surface , i.e. for which $\Delta\bar{f} \times \bar{E} = 0$, the curl is tangential to the surface, so that

$$\Delta\bar{f} \cdot \bar{\nabla} \times \bar{E} = 0, \text{ if } \Delta\bar{f} \times \bar{E} = 0 \text{ on } F. \tag{64}$$

In order to prove (64), we again extend the surface, so that it forms a part of a closed surface.† Equation (64) is equivalent to the statement that

$$\oint\int \Delta\bar{f} \cdot (\bar{\nabla} \times \bar{E})w = 0$$

for any arbitrary smooth scalar field w. And this statement results from the following calculation.

$$\oint\int\Delta\bar{f} \cdot (\bar{\nabla} \times \bar{E})w = \oint\int\Delta\bar{f} \cdot [\bar{\nabla} \times (\bar{E}w) - (\bar{\nabla}w) \times \bar{E}]$$

$$= \oiint\Delta\bar{f} \cdot \bar{\nabla} \times (\bar{E}w) + \oiint\Delta\bar{f} \times \bar{E}w .$$

The first term vanishes by virtue of (61). The second term vanishes because of the assumption $\Delta\bar{f} \times \bar{E} = 0$.

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*We assume that $\psi = 0$ on the extended surface.

†We assume that $\Delta\bar{f} \times \bar{E} = 0$ on the extended surface.

We now consider the following two eigenvalue-eigenfunction problems:

$$\bar{\nabla}(\bar{\nabla} \cdot \bar{F}_a) + \ell_a^2 \bar{F}_a = 0, \text{ with the boundary condition } \bar{\nabla} \cdot \bar{F}_a = 0, \tag{65}$$

and

$$\bar{\nabla}(\bar{\nabla} \cdot \bar{G}_a) + m_a^2 \bar{G}_a = 0, \text{ with the boundary condition } \Delta\bar{f} \cdot \bar{G}_a = 0. \tag{66}$$

Here the ℓ_a^2 and m_a^2 are the (positive) eigenvalues, and the $\bar{F}_a$ and $\bar{G}_a$ are the vectorial eigenfunctions. These eigenfunctions are irrotational (i.e. the curls vanish), as one can see when one takes the curl of (65) and (66). (Note that the curl of a gradient is zero.) The index "a" labels the eigenvalues and eigenfunctions;there is an infinite number of them. We assign the indices "a" in such a way that the eigenvalues are ordered according to their magnitude, so that

$$\ell_1^2 \leq \ell_2^2 \leq \ell_3^2 \leq \ldots ,$$

$$m_1^2 \leq m_2^2 \leq m_3^2 \leq \ldots .$$

In order to make sure that the problems (65) and (66) conform to the classical paradigm of such problems, we have to prove that the operator $\bar{\nabla}\bar{\nabla}\cdot$ is self-adjoint. The self-adjointness conditions are:

$\iiint_{\Delta\tau} [\bar{F} \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}') - \bar{F}' \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F})] = 0$ for two functions $\bar{F}$ and $\bar{F}'$ that satisfy the boundation conditions $\bar{\nabla} \cdot \bar{F} = 0$ and $\bar{\nabla} \cdot \bar{F}' = 0$, (67)

and

$\iiint_{\Delta\tau} [\bar{G} \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{G}') - \bar{G}' \ \bar{\nabla}(\bar{\nabla} \cdot \bar{G})] = 0$ for two functions $\bar{G}$ and $\bar{G}'$ that satisfy the boundary conditions $\Delta\bar{f} \cdot \bar{G} = 0$ and $\Delta\bar{f} \cdot \bar{G}' = 0$. (68)

To prove these relations we note that

$$\bar{F} \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}') = \bar{\nabla} \cdot [\bar{F}\bar{\nabla} \cdot \bar{F}'] - (\bar{\nabla} \cdot \bar{F})(\bar{\nabla} \cdot \bar{F}') .$$

Similarly

$$\bar{F}' \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}) = \bar{\nabla} \cdot [\bar{F}'\bar{\nabla} \cdot \bar{F}] - (\bar{\nabla} \cdot \bar{F}')(\bar{\nabla} \cdot \bar{F}) .$$

On subtracting, we obtain

$$\bar{F} \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}') - \bar{F}' \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}) = \bar{\nabla} \cdot [\bar{F}\bar{\nabla} \cdot \bar{F}' - \bar{F}'\bar{\nabla} \cdot \bar{F}] .$$

We integrate this equation over the cavity and transform the right-hand side into a surface integral with the aid of the theorem of Gauss. Thus

$$\iiint \Delta\tau[\bar{F} \cdot \bar{\nabla}(\bar{\nabla} \cdot F') - F' \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F})] = \iint \Delta\bar{f} \cdot [\bar{F}\bar{\nabla} \cdot \bar{F}' - \bar{F}'\bar{\nabla} \cdot \bar{F}] .$$

But the surface integral vanishes because of the boundary conditions that are stated in (67). Hence (67) is established. We prove (68) in the same way. The only change is that here the surface integral vanishes because of $\Delta\bar{f} \cdot \bar{G} = 0$ and $\Delta\bar{f} \cdot \bar{G}' = 0$.

Next we prove the orthogonality relations

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{F}_b = 0, \text{ for } \ell_a^2 \neq \ell_b^2 , \tag{69}$$

and

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{G}_b = 0, \text{ for } m_a^2 \neq m_b^2 . \tag{70}$$

We take the scalar product of (65) with $\bar{F}_b$ and obtain

$$\ell_a^2 \bar{F}_a \cdot \bar{F}_b = - \bar{F}_b \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}_a) .$$

Similarly,

$$\ell_b^2 \bar{F}_b \cdot \bar{F}_a = - \bar{F}_a \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}_b) .$$

We subtract and integrate over the cavity. Then, with the aid of the self-adjointness relation (67), we obtain

$$(\ell_a^2 - \ell_b^2) \iiint \Delta\tau \bar{F}_a \cdot \bar{F}_b = 0 .$$

And, since we assumed $\ell_a^2 - \ell_b^2 \neq 0$, equation (69) follows. Equation (70) is proved in the same way.

So far we have proved (69) under the assumption that $\ell_a^2 \neq \ell_b^2$. But when an eigenvalue is degenerate, i.e. when it admits several different eigenfunctions, we may always redefine these functions (by taking suitable linear combinations)

in such a way that (69) still holds, even when $\ell_a^2 = \ell_b^2$. Similar comments apply to equation (70). Finally we normalize the eigenfunctions so that

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{F}_a = 1 \ , \tag{71}$$

and

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{G}_b = 1 \ . \tag{72}$$

On combining (69) and (71), we obtain the orthonormality relation

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{F}_b = \delta_{ab} \ . \tag{73}$$

Similarly

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{G}_b = \delta_{ab} \ . \tag{74}$$

Here, δ_{ab} is the Kronecker delta: $\delta_{ab} = 0$ for $a \neq b$, $\delta_{ab} = 1$ for $a = b$. There is no orthonormality relation between an $\bar{F}_a$ and a $\bar{G}_b$.

We can get a better insight into the behavior of the vectorial eigenfunctions $\bar{F}_a$ and $\bar{G}_a$, if we relate them to scalar functions ψ_a and χ_a defined by

$$\ell_a \psi_a = - \bar{\nabla} \cdot \bar{F}_a \ , \tag{75}$$

and

$$m_a \chi_a = - \bar{\nabla} \cdot \bar{G}_a \tag{76}$$

Here ℓ_a and m_a are the positive square roots of the eigenvalues ℓ_a^2 and m_a^2. By direct substitution of these relations into the first terms of (65) and (66), we obtain the inverses of (75) and (76), namely

$$\ell_a \bar{F}_a = \bar{\nabla}\psi_a \ , \tag{77}$$

and

$$m_a \bar{G}_a = \bar{\nabla}\chi_a \ . \tag{78}$$

Inspection of (75) and (78) in conjunction with the boundary conditions for the $\bar{F}_a$ and $\bar{G}_a$ stated in (65) and (66) yields the following boundary conditions for ψ_a and χ_a.

$$\psi_a = 0 \text{ at the wall,} \tag{79}$$

and

$$\Delta\bar{f} \cdot \bar{\nabla}\chi_a = 0 \text{ at the wall} \tag{80}$$

On combining (62), (77) and (79) we see that the $\bar{F}_a$ automatically satisfy also the boundary condition

$$\Delta\bar{f} \times \bar{F}_a = 0 , \tag{81}$$

i.e. the $\bar{F}_a$ are normal to the wall.

When we take the divergence of (65) and (66), divide by $-\ell_a$ and $-m_a$ respectively, use (75) and (76), and adjoin the boundary conditions (79) and (80), we see that the ψ_a and χ_a could have been determined also directly from the following two eigenvalue-eigenfunction problems:

$$\bar{\nabla} \cdot \bar{\nabla}\psi_a + \ell_a^2\psi_a = 0, \text{ with the boundary condition } \psi_a = 0, \tag{82}$$

and

$$\bar{\nabla} \cdot \bar{\nabla}\chi_a + m_a^2\chi_a = 0, \text{ with the boundary condition } \Delta\bar{f} \cdot \bar{\nabla}\chi_a = 0 . \tag{83}$$

Here the self-adjointness relations for the operator $\bar{\nabla} \cdot \bar{\nabla}$ are:

$$\iiint \Delta\tau[\psi\bar{\nabla} \cdot \bar{\nabla}\psi' - \psi'\bar{\nabla} \cdot \bar{\nabla}\psi] = 0 \text{ for two functions } \psi \text{ and } \psi'$$

that satisfy the boundary conditions $\psi = 0$ and $\psi' = 0$, (84)

and

$$\iiint \Delta\tau[\chi\bar{\nabla} \cdot \bar{\nabla}\chi' - \chi'\bar{\nabla} \cdot \bar{\nabla}\chi] = 0 \text{ for two functions } \chi \text{ and } \chi'$$

that satisfy the boundary conditions $\Delta\bar{f} \cdot \bar{\nabla}\chi = 0$ and $\Delta\bar{f} \cdot \bar{\nabla}\chi' = 0$ (85)

These relations are established by the same technique that was used in the proof of (67) and (68). One starts with the formula

$$\psi\bar{\nabla} \cdot \bar{\nabla}\psi' - \psi'\bar{\nabla} \cdot \bar{\nabla}\psi = \bar{\nabla} \cdot [\psi\bar{\nabla}\psi' - \psi'\bar{\nabla}\psi] .$$

Consequences of the orthonormality by relations (73) and (74) are the following orthonormality relations for the ψ_a and χ_a:

$$\iiint_\Delta \tau \psi_a \psi_b = \delta_{ab} , \tag{86}$$

and

$$\iiint_\Delta \tau \chi_a \chi_b = \delta_{ab} . \tag{87}$$

In order to prove (86), we use (75) and arrive at

$$\ell_a \psi_a \ell_b \psi_b = (\bar{\nabla} \cdot \bar{F}_a)(\bar{\nabla} \cdot \bar{F}_b) = \bar{\nabla} \cdot [\bar{F}_a (\bar{\nabla} \cdot \bar{F}_b)] - \bar{F}_a \cdot \bar{\nabla}(\bar{\nabla} \cdot \bar{F}_b) ,$$

or, with the aid of (65),

$$\ell_a \ell_b \psi_a \psi_b = \bar{\nabla} \cdot [\bar{F}_a (\bar{\nabla} \cdot \bar{F}_b)] + \ell_b^2 \bar{F}_a \cdot \bar{F}_b .$$

We integrate this equation over the cavity. By virtue of the theorem of Gauss, the first term gets transformed into a surface integral, which vanishes because of the boundary condition $\bar{\nabla} \cdot \bar{F}_b = 0$. Then (86) follows. Equation (87) is proved in the same way.

According to established eigenvalue-eigenfunction theory the set $\{\psi_a\}$ is complete, i.e. any function ψ that occurs in practice may be expanded in terms of the ψ_a, so that we may write

$$\psi = \sum_{a=1}^{\infty} C_a \psi_a . \tag{88}$$

We can determine the expansion coefficients C_a in the following manner. We multiply (88) by ψ_b and integrate over the cavity. It is permissible to use term-by-term integration on the right-hand side.* Then the orthonormality relation (86) yields

$$C_b = \iiint_\Delta \tau \psi \psi_b . \tag{89}$$

Similarly the set $\{\chi_a\}$ is complete, if we adjoin the (constant) function $\chi_o = \frac{1}{\sqrt{\text{Vol}}}$, where Vol is the volume of the cavity. Here we have to supplement (87) by the orthonormality relation

$$\iiint_\Delta \tau \chi_o \chi_b = \delta_{ob} , \tag{90}$$

*Term-by-term integration is permissible when the expansion (88) converges in the mean. See equations (107) - (111), which pertain to the analogous case of vector fields.

which is easily proved. For $b = 0$, (90) is obvious. For $b \neq 0$, we have, with (83),

$$\chi_o \chi_b = -\frac{1}{m_b^2} \chi_o \bar{\nabla} \cdot \bar{\nabla} \chi_b \ .$$

Then (χ_o = const), with the theorem of Gauss,

$$\iiint \Delta\tau \chi_o \chi_b = -\frac{1}{m_b^2} \chi_o \iint \Delta\bar{f} \cdot \bar{\nabla} \chi_b \ .$$

But the surface integral vanishes because of the boundary condition $\Delta\bar{f} \cdot \bar{\nabla}\chi_b = 0$. The eigenvalue m_o^2 is, of course, zero.

The convergence of the expansion series is most rapid, when the function ψ that is to be expanded satisfies the same boundary conditions that the eigenfunctions satisfy. Thus we would prefer to expand a function ψ with the boundary condition $\psi = 0$ (alternatively $\Delta\bar{f} \cdot \bar{\nabla}\psi = 0$) in terms of the ψ_a (alternatively χ_a).

Any irrotational vector field may be expanded in terms of the eigenfunctions $\bar{F}_a$, or in terms of the eigenfunctions $\bar{G}_a$. But we are not going to pursue this matter yet, because we are interested in the expansion of general vector fields, not just of irrotational ones. For general fields, the sets $\{\bar{F}_a\}$ or $\{\bar{G}_a\}$ are not complete. Therefore we must construct additional sets of vectorial eigenfunctions. There will be two sets $\{\bar{E}_a\}$ and $\{\bar{H}_a\}$ of solenoidal eigenfunctions. ('Solenoidal' means: the divergence is zero.) They arise from the eigenvalue-eigenfunction problem

$$\bar{\nabla} \times (\bar{\nabla} \times \bar{E}_a) - k_a^2 \bar{E}_a = 0, \text{ with the boundary condition } \Delta\bar{f} \times \bar{E}_a = 0, \qquad (91)$$

and

$$\bar{\nabla} \times (\bar{\nabla} \times \bar{H}_a) - k_a^2 \bar{H}_a = 0, \text{ with the boundary condition } \Delta\bar{f} \times (\bar{\nabla} \times \bar{H}_a) = 0. \qquad (92)$$

The (positive) eigenvalues k_a^2 are the same in both problems, as we shall see shortly. Again we assign the indices "a" in such a way that the eigenvalues are ordered by magnitude, so that

$$k_1^2 \leq k_2^2 \leq k_3^2 \leq \dots .$$

That the $\bar{E}_a$ and $\bar{H}_a$ are solenoidal is seen easily when we take the divergence of (91) and (92) and observe that the divergence of a curl is zero. Here the self-adjointness relations are

$\iiint_{\Delta\tau}[\bar{E} \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E}') - \bar{E}' \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E})] = 0$ for two functions $\bar{E}$ and $\bar{E}'$ that satisfy the boundary conditions $\Delta\bar{f} \times \bar{E} = 0$ and $\Delta\bar{f} \times \bar{E}' = 0$, (93)

and

$\iiint_{\Delta\tau}[\bar{H} \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{H}') - \bar{H}' \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{H})] = 0$ for two functions $\bar{H}$ and $\bar{H}'$ that satisfy the boundary conditions $\Delta\bar{f} \times (\bar{\nabla} \times \bar{H}) = 0$ and $\Delta\bar{f} \times (\bar{\nabla} \times \bar{H}') = 0$. (94)

In order to prove (93), we note that

$$\bar{E} \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E}') = \bar{\nabla} \cdot [(\bar{\nabla} \times \bar{E}') \times \bar{E}] + (\bar{\nabla} \times \bar{E}') \cdot (\bar{\nabla} \times \bar{E}) .$$

Similarly

$$\bar{E}' \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E}) = \bar{\nabla} \cdot [(\bar{\nabla} \times \bar{E}) \times \bar{E}'] + (\bar{\nabla} \times \bar{E}) \cdot (\bar{\nabla} \times \bar{E}') .$$

Subtraction, integration, and the theorem of Gauss yield

$$\iiint_{\Delta\tau}[\bar{E} \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E}') - \bar{E}' \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E})]$$
$$= \oiint_{\Delta f} \cdot [(\bar{\nabla} \times \bar{E}') \times \bar{E} - (\bar{\nabla} \times \bar{E}) \times \bar{E}'] .$$

But the surface integral vanishes because of the boundary conditions. The relation (94) is proved in the same way.

Now we show that the eigenvalues k_a^2 are the same in the two eigenvalue-eigenfunction problems (91) and (92). Instead of determining the $\bar{H}_a$ by way of (92), we can obtain them also through the definition

$$k_a \bar{H}_a \equiv \bar{\nabla} \times \bar{E}_a \qquad (95)$$

from the $\bar{E}_a$. Here k_a denotes the positive square root of k_a^2. If we substitute (95) in the first term of (91) we obtain the inverse of (95), namely

$$k_a \bar{E}_a = \bar{\nabla} \times \bar{H}_a \ . \tag{96}$$

Then, when we take the curl of (91) (and also divide by k_a), and use (95) and (96), we see that (92) is a direct consequence of (91).

Equation (95), in conjunction with the theorem (64), tells us that the $\bar{H}_a$ automatically satisfy the boundary condition

$$\Delta\bar{f} \cdot \bar{H}_a = 0 \ . \tag{97}$$

Just as we established the orthonormality by relations (73) for the $\bar{F}_a$, we obtain the orthonormality relations

$$\iiint \Delta\tau \bar{E}_a \cdot \bar{E}_b = \delta_{ab} \ . \tag{98}$$

All we need to do, is to substitute $\bar{E}_a$ for $\bar{E}$ and $\bar{E}_b$ for $\bar{E}'$ in the self-adjointness relation (93) and to use equation (91). The use of the formula

$$k_a \bar{H}_a \cdot k_b \bar{H}_b = (\bar{\nabla} \times \bar{E}_a) \cdot (\bar{\nabla} \times \bar{E}_b) = \bar{\nabla} \cdot [\bar{E}_a \times (\bar{\nabla} \times \bar{E}_b)] +$$
$$+ \bar{E}_a \cdot \bar{\nabla} \times (\bar{\nabla} \times \bar{E}_b) = \bar{\nabla} \cdot [\bar{E}_a \times (\bar{\nabla} \times \bar{E}_b)] + k_b^2 \bar{E}_a \cdot \bar{E}_b \ ,$$

integration, the theorem of Gauss, and the boundary condition $\Delta\bar{f} \times \bar{E}_a = 0$, give us the orthonormality relations

$$\iiint \Delta\tau \bar{H}_a \cdot \bar{H}_b = \delta_{ab} \tag{99}$$

as a direct consequence of (98). There is no orthonormality relation between an $\bar{E}_a$ and an $\bar{H}_b$.

Finally we prove the orthogonality relations

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{E}_b = 0 \ , \tag{100}$$

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{H}_b = 0 \ . \tag{101}$$

and

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{H}_b = 0 \ . \tag{102}$$

For we have

$$\bar{F}_a \cdot k_b \bar{E}_b = \bar{F}_a \cdot \bar{\nabla} \times \bar{H}_b = \bar{\nabla} \cdot (\bar{H}_b \times \bar{F}_a) + \bar{H}_b \cdot \bar{\nabla} \times \bar{F}_a ,$$

$$\bar{G}_a \cdot k_b \bar{H}_b = \bar{G}_a \cdot \bar{\nabla} \times \bar{E}_b = \bar{\nabla} \cdot (\bar{E}_b \times \bar{G}_a) + \bar{E}_b \cdot \bar{\nabla} \times \bar{G}_a ,$$

and

$$\bar{F}_a \cdot k_b \bar{H}_b = \bar{F}_a \cdot \bar{\nabla} \times \bar{E}_b = \bar{\nabla} \cdot (\bar{E}_b \times \bar{F}_a) + \bar{E}_b \cdot \bar{\nabla} \times \bar{F}_a .$$

But $\bar{\nabla} \times \bar{F}_a = 0$ and $\bar{\nabla} \times \bar{G}_a = 0$. Then, integration and the theorem of Gauss give us

$$k_b \iiint \Delta\tau \bar{F}_a \cdot \bar{E}_b = \oint\oint \Delta\bar{f} \cdot \bar{H}_b \times \bar{F}_a ,$$

$$k_b \iiint \Delta\tau \bar{G}_a \cdot \bar{H}_b = \oint\oint \Delta\bar{f} \cdot \bar{E}_b \times \bar{G}_a .$$

and

$$k_b \iiint \Delta\tau \bar{F}_a \cdot \bar{H}_b = \oint\oint \Delta\bar{f} \cdot (\bar{E}_b \times \bar{F}_a)$$

But the surface integrals vanish, because $\bar{F}_a$ and $\bar{E}_b$ are parallel to $\Delta\bar{f}$.

Before we continue with our discussions, we summarize the most important properties of the eigenfunctions in boxes, in order to facilitate the task of referring to an equation.

Box #1. Eigenvalue-eigenfunction problems. (BC stands for boundary condition.)

$\bar{\nabla}(\bar{\nabla} \cdot \bar{F}_a) + \ell_a^2 \bar{F}_a = 0$, BC: $\bar{\nabla} \cdot \bar{F}_a = 0$,	(65)
$\bar{\nabla} \cdot \bar{\nabla}\psi_a + \ell_a^2 \psi_a = 0$, BC: $\psi_a = 0$.	(82)
$\bar{\nabla}(\bar{\nabla} \cdot \bar{G}_a) + m_a^2 \bar{G}_a = 0$, BC: $\Delta\bar{f} \cdot \bar{G}_a = 0$.	(66)
$\bar{\nabla} \cdot \bar{\nabla}\chi_a + m_a^2 \chi_a = 0$, BC: $\Delta\bar{f} \cdot \bar{\nabla}\chi_a = 0$.	(83)
$\bar{\nabla} \times (\bar{\nabla} \times \bar{E}_a) - k_a^2 \bar{E}_a = 0$, BC: $\Delta\bar{f} \times \bar{E}_a = 0$.	(91)
$\bar{\nabla} \times (\bar{\nabla} \times \bar{H}_a) - k_a^2 \bar{H}_a = 0$, BC: $\Delta\bar{f} \times (\bar{\nabla} \times \bar{H}_a) = 0$.	(92)

We note that there is a duality in the BC's for each pair. One BC involves the function itself, whereas the other BC involves a derivative.

Box #2. Relations between eigenfunctions.

$$\bar{\nabla}\psi_a = \ell_a \bar{F}_a \,. \qquad (77)$$

$$\bar{\nabla} \cdot \bar{F}_a = -\ell_a \psi_a \,. \qquad (75)$$

$$\bar{\nabla}\chi_a = m_a \bar{G}_a \qquad (78)$$

$$\bar{\nabla} \cdot \bar{G}_a = -m_a \chi_a \qquad (76)$$

$$\bar{\nabla} \times \bar{E}_a = k_a \bar{H}_a \qquad (95)$$

$$\bar{\nabla} \times \bar{H}_a = k_a \bar{E}_a \qquad (96)$$

Box #3. Additional boundary conditions.

$$\Delta\bar{f} \times \bar{F}_a = 0 \,. \qquad (81)$$

$$\Delta\bar{f} \times \bar{\nabla}\psi_a = 0 \,. \qquad (77 + 81)$$

$$\Delta\bar{f} \cdot \bar{H}_a = 0 \qquad (97)$$

$$\Delta\bar{f} \cdot (\bar{\nabla} \times \bar{E}_a) = 0 \qquad (95 + 97)$$

Box #4. Properties of derivatives, as obtained from Box #2.

$$\bar{\nabla} \times \bar{F}_a = 0,\ \bar{\nabla} \times \bar{G}_a = 0,\ \bar{\nabla} \cdot \bar{H}_a = 0,\ \bar{\nabla} \cdot \bar{E}_a = 0 \,.$$

Box #5. Orthonormality relations.

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{r}_b = \delta_{ab} \,. \tag{73}$$

$$\iiint \Delta\tau \psi_a \psi_b = \delta_{ab} \,. \tag{86}$$

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{G}_b = \delta_{ab} \tag{74}$$

$$\iiint \Delta\tau \chi_a \chi_b = \delta_{ab} \tag{87}$$

$$\iiint \Delta\tau \bar{E}_a \cdot \bar{E}_b = \delta_{ab} \tag{98}$$

$$\iiint \Delta\tau \bar{H}_a \cdot \bar{H}_b = \delta_{ab} \tag{99}$$

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{E}_b = 0 \tag{100}$$

$$\iiint \Delta\tau \bar{G}_a \cdot \bar{H}_b = 0 \tag{101}$$

$$\iiint \Delta\tau \bar{F}_a \cdot \bar{H}_b = 0 \tag{102}$$

So far our treatment of the eigenfunctions was strictly formal. But they allow a direct physical interpretation. For instance, a possible free-running (no charges, no currents, except in the walls) electromagnetic field in the cavity is given by

$$\begin{aligned} \bar{E}(\bar{r},t) &= C_a \bar{E}_a(\bar{r}) \sin k_a ct \,, \\ cB(\bar{r},t) &= C_a \bar{H}_a(\bar{r}) \cos k_a ct \,, \end{aligned} \tag{103}$$

where C_a is a constant. One easily checks that the Maxwell equations (1), (47), (for $\rho^t = 0$, $J^t = 0$) and the boundary conditions (3) are fulfilled. In this case the fields oscillate in the single (normal) mode #a. Therefore the functions $\bar{E}_a(\bar{r})$ and $\bar{H}_a(\bar{r})$ are called the electric and magnetic part of the mode pattern #a. The other eigenfunctions, namely the pair $\psi_a(\bar{r})$, $\bar{F}_a(\bar{r})$ and

the pair $\chi_a(\bar{r})$, $\bar{G}_a(\bar{r})$, do not permit such an interpretation in terms of electromagnetic oscillations. But they are associated in a similar way with acoustic vibrations in an air-filled cavity. Thus, the pressure excursion p and the velocity $\bar{v}$ in a cavity with "hard" walls, which impose the boundary condition $\Delta\bar{r} \cdot \bar{v} = 0$, are given by

$$\begin{aligned} p &= C_a \chi_a \sin m_a ct \ , \\ \bar{v} &= C_a \frac{1}{sc} \bar{G}_a \cos m_a ct \ , \end{aligned} \tag{104}$$

for mode #a. Here, of course, c is the speed of sound, and s is the ambient mass density of the air. One easily checks that (104) is consistent with the first-order (for vibrations of small amplitude) equations of motion and continuity, namely

$$\begin{aligned} s \frac{\partial}{\partial t} \bar{v} &= - \bar{\nabla} p \ , \\ \frac{\partial}{\partial t} p &= - sc^2 \bar{\nabla} \cdot \bar{v} \ , \end{aligned} \tag{105}$$

where we have used the relation $B = sc^2$ for the bulk modulus $B \equiv s \frac{dp}{ds}$. We may also contemplate a cavity with "soft" walls, which impose the boundary conditions $p = 0$, even though it is hard to envision how such walls might be constructed. (A liquid drop may be one way in which such a soft-walled "cavity" can be realized.) In this case, the motion for a single mode #a is given by

$$\begin{aligned} p &= C_a \psi_a \sin m_a ct \\ \bar{v} &= C_a \frac{1}{sc} \bar{F}_a \cos m_a ct \end{aligned} \tag{106}$$

We have related the modes with the patterns $(\bar{E}_a, \bar{H}_a)$ to electromagnetic oscillations and the two classes of modes with the patterns $(\chi_a, \bar{G}_a)$ and $(\psi_a, \bar{F}_a)$ to acoustic oscillations. Since plane electromagnetic waves are transverse, and since plane acoustic waves are longitudinal, one uses the term "transverse modes" for the $(\bar{E}_a, \bar{H}_a)$ - modes and the term "longitudinal modes"

for the $(\chi_a, \bar{G}_a)$ - modes and for the $(\psi_a, \bar{F}_a)$ - modes. This terminology is somewhat inaccurate, because the words "transverse" and "longitudinal" make sense only for plane waves, which are characterized by a definite direction. No such direction can be assigned to the complex patterns of the cavity modes. Nevertheless, these two words are commonly used, because they simplify the language.

We accept, without giving a proof here, that the two sets $\{\bar{E}_a\}$ and $\{\bar{F}_a\}$ taken together are complete. This means that any vector field $\bar{V}$ in the cavity that occurs in practice may be expanded in terms of the $\bar{E}_a$ and $\bar{F}_a$, so that we can write

$$\bar{V} = \sum_{a=1}^{\infty} C'_a \bar{F}_a + \sum_{a=1}^{\infty} C_a \bar{E}_a \, . \tag{107}$$

Here, the C'_a and C_a are the expansion coefficients. The first series in (107) is called the longitudinal part of $\bar{V}$ and is denoted by $\bar{V}_L$, the second series is called the transverse part of $\bar{V}$ and is denoted by $\bar{V}_T$. The series in (107) are "convergent in the mean". Thus, if we approximate $\bar{V}$ by the first N terms, i.e. if we replace it by

$$\bar{V}_{appr,N} = \sum_{a=1}^{N} C'_a \bar{F}_a + \sum_{a=1}^{N} C_a \bar{E}_a \, , \tag{108}$$

the error $\bar{V} - \bar{V}_{appr,N}$ has the property that the integral of the square of its magnitude tends to zero, as N tends to infinity, so that

$$\lim_{N \to \infty} \iiint \Delta\tau (\bar{V} - \bar{V}_{appr,N}) \cdot (\bar{V} - \bar{V}_{appr,N}) = 0 \tag{109}$$

The expansion coefficients C_a' and C_a may be determined from $\bar{V}$ in terms of integrals, as shown by the following argument. We start with the inequality of Schwarz

$$[\iiint \Delta\tau \bar{U} \cdot \bar{W}]^2 \leq [\iiint \Delta\tau \bar{U} \cdot \bar{U}][\iiint \Delta\tau \bar{W} \cdot \bar{W}] \, , \tag{110}$$

which holds for any pair $\bar{U},\bar{W}$ of vectorial functions. Let us make the choice $\bar{U} = \bar{V} - \bar{V}_{appr,N}$ and $\bar{W} = \bar{F}_b$. Then, with the normalization condition

$$\iiint \Delta\tau \bar{F}_b \cdot \bar{F}_b = 1$$

we obtain

$$[\iiint \Delta\tau(\bar{V} - \bar{V}_{appr,N}) \cdot \bar{F}_b]^2 \leq \iiint \Delta\tau(\bar{V} - \bar{V}_{appr,N}) \cdot (\bar{V} - \bar{V}_{appr,N})$$

Now let us take the limit for $N \to \infty$. According to (109), the right-hand side tends to zero. Thus we get

$$\lim_{N\to\infty} \iiint \Delta \cdot \bar{V}_{appr,N} \cdot \bar{F}_b = \iiint \Delta\ \bar{V} \cdot \bar{F}_b$$

But as soon as the index N exceeds the index b, the integral on the left assumes the value C_b', by the orthonormality relations. Thus the limit is also equal to C_b', and we obtain

$$C_b' = \iiint \Delta\tau \bar{V} \cdot \bar{F}_b$$

Similarly,

$$C_b = \iiint \Delta\tau \bar{V} \cdot \bar{E}_b \ . \qquad (111)$$

The result (111) agrees with the following procedure: Take the scalar product of (107) with $\bar{F}_b$ (or $\bar{E}_b$), integrate term-by-term, and use the orthonormality relations. Now that we have established the legitimacy of term-by-term integration, we can use it freely in our future work.

Let us assume that the vector field $\bar{V}$ is of sufficient smoothness so that the derivatives $\bar{\nabla} \cdot \bar{V}$ and $\bar{\nabla} \times \bar{V}$ exist and that these derivatives can be expanded in terms of eigenfunctions. We choose the types of eigenfunctions in the expansion for $\bar{\nabla} \cdot \bar{V}$ and $\bar{\nabla} \times \bar{V}$ in such a way that the new expansion coefficients can be easily expressed in terms of the coefficients C_a' and C_a, which occurred in the expansion (107) for $\bar{V}$. Accordingly we write

$$\bar{\nabla} \cdot \bar{V} = \sum_a K_a' \psi_a \ , \tag{112}$$

and

$$\bar{\nabla} \times \bar{V} = \sum_a D_a' \bar{G}_a + \sum_a D_a \bar{H}_a \tag{113}$$

Indeed, we have

$$K_a' = \iiint \Delta\tau \psi_a \bar{\nabla} \cdot \bar{V} = \iiint \nabla\tau [\bar{\nabla} \cdot (\psi_a \bar{V}) - \bar{V} \cdot \bar{\nabla}\psi_a]$$

$$= \oiint \Delta\bar{f} \cdot \psi_a \bar{V} - \ell_a \iiint \Delta\tau \bar{V} \cdot \bar{F}_a \ .$$

The surface integral vanishes because of the boundary condition $\psi_a = 0$. Then, with (111), we obtain

$$K_a' = - \ell_a C_a' \ , \tag{114}$$

so that

$$\bar{\nabla} \cdot \bar{V} = - \sum_a C_a' \ell_a \psi_a \ . \tag{115}$$

We would have obtained the same result (115), if we had taken the divergence of (107) term-by-term, since

$$\bar{\nabla} \cdot \bar{F}_a = - \ell_a \psi_a \text{ and } \bar{\nabla} \cdot \bar{E}_a = 0 \ .$$

Next we calculate the expansion coefficients D_a' and D_a in (113). We have

$$D_a' = \iiint \Delta\tau \bar{G}_a \cdot \bar{\nabla} \times \bar{V} = \iiint \Delta\tau [\bar{\nabla} \cdot (\bar{V} \times \bar{G}_a) + \bar{V} \cdot \bar{\nabla} \times \bar{G}_a] =$$

$$= \oiint \Delta\bar{f} \cdot \bar{V} \times \bar{G}_a + \iiint \Delta\tau \ \bar{V} \cdot \bar{\nabla} \times \bar{G}_a =$$

$$= \oiint \Delta\bar{f} \cdot \bar{V} \times \bar{G}_a + 0 \ ,$$

since $\bar{\nabla} \times \bar{G}_a = 0$. Similarly

$$D_a = \iiint \Delta\tau \bar{H}_a \cdot \bar{\nabla} \times \bar{V} = \oiint \Delta\bar{f} \cdot \bar{V} \times \bar{H}_a + \iiint \Delta\tau \bar{V} \cdot \bar{\nabla} \times \bar{H}_a$$

$$= \oiint \Delta\bar{f} \cdot \bar{V} \times \bar{H}_a + k_a C_a \ ,$$

where we have used the relation $\bar{\nabla} \times \bar{H}_a = k_a \bar{E}_a$ and the second formula (111). On inserting these results for D_a and D_a' into (113) we obtain

$$\bar{\nabla} \times \bar{V} = \sum [\oiint \Delta\bar{f} \cdot \bar{V} \times \bar{G}_a] \bar{G}_a + \sum [\oiint \Delta\bar{f} \cdot \bar{V} \times \bar{H}_a + k_a C_a] \bar{H}_a \ . \tag{116}$$

Had we taken the curl of (113) term-by-term, we would have obtained a different result. For we would have lost the surface integrals that appear in the expansion coefficients of (116). However, if $\bar{V}$ happens to satisfy the boundary condition

$$\Delta\bar{f} \times \bar{V} = 0 \ , \tag{117}$$

then these surface integrals vanish. In this case then, we are permitted to evaluate the curl term-by-term.

If the series (107), (112), (113) for the fields $\bar{V}$, $\bar{\nabla} \cdot \bar{V}$, and $\bar{\nabla} \times \bar{V}$ were uniformly convergent, then we could deduce (by the usual continuity arguments) that these fields satisfy the same boundary conditions that the eigenfunctions satisfy. Thus, for uniform convergence, we would have

$$\Delta\bar{f} \times \bar{V} = 0, \ \bar{\nabla} \cdot \bar{V} = 0, \ \Delta\bar{f} \cdot (\bar{\nabla} \times \bar{V}) = 0, \text{ at the wall.} \tag{118}$$

Unfortunately, the proofs for uniform convergence, at any rate those that are most easily carried out, start with conditions that are not satisfied in the application we wish to make. (What foils these proofs is the point-like nature of the atomic particles.) However, later on we are going to make an approximation in the Lagrangian. As a result of this approximation, the infinite series will be replaced by finite series, so that all the convergence problems will disappear. And then the boundary conditions (118) are certainly satisfied.

So far we have considered a general vector field $\bar{V}$ and its derivatives $\bar{\nabla} \cdot \bar{V}$ and $\bar{\nabla} \times \bar{V}$. Now we apply what we have seen to a specific case, the vector potential $c\bar{A}$. In analogy to (107) we write

$$c\bar{A} = \sum_a Q'_a \bar{F}_a + \sum_a Q_a \bar{E}_a \ , \tag{119}$$

where the Q_a' and Q_a are the expansion coefficients. And in analogy to (118), we have the boundary conditions

$$\Delta\bar{f} \times c\bar{A} = 0,\ \bar{\nabla} \cdot c\bar{A} = 0,\ \Delta\bar{f} \cdot (\bar{\nabla} \times c\bar{A}) = 0, \text{ at the wall.} \tag{120}$$

The third of these conditions is a consequence of the first, as we have seen in the proof for (64). Again we remind ourselves of the circumstance that, in the end, the series (119) will have only a finite number of terms, so that we will not be bothered by convergence problems. [See the remarks following (118)].

Now we are ready to formulate the gauge condition for the vector potential $c\bar{A}$. We require that all the primed expansion coefficients Q_a' be zero. Then the longitudinal part of $c\bar{A}$, i.e. the first series in (119) vanishes, and only the transverse part, i.e., the second series, remains. Our gauge condition is then that the vector potential $c\bar{A}$ is purely transverse. As a consequence [see (115)] the divergence of $c\bar{A}$ vanishes everywhere. Thus we have

$$\bar{\nabla} \cdot c\bar{A} = 0 . \tag{121}$$

But, in addition, the boundary conditions (120) are satisfied. The second of these is already implied by (121). Thus

$$\Delta\bar{f} \times c\bar{A} = 0,\ \Delta\bar{f} \cdot \bar{\nabla} \times c\bar{A} = 0, \text{ at the wall.} \tag{122}$$

Similar remarks apply to the variation $\delta c\bar{A}$: Merely insert the symbol δ as a prefix to $c\bar{A}$, Q_a', and Q_a.

We summarize the discussion of this long section by the statement that we choose the "transverse gauge" for the vector potential. This term is more restrictive than the term "Coulomb gauge". The latter implies only (121). But the former implies that $c\bar{A}$ can be expanded as a series in the eigenfunctions $\bar{E}_a$ alone, the $\bar{F}_a$ are not needed. A particular consequence is that the boundary

(122) are satisfied.

In the next section we will introduce the approximationswe have already alluded to. They will make it possible to replace infinite series by finite ones.

7. Two Approximations .

We start with the expression (53) for the action functional, which we write down again for the sake of easier reference.

$$A_{a,b} = \int_{t=a}^{b} dt\{\frac{1}{2}\frac{dq^i}{dt} M'_{ij} \frac{dq^j}{dt} + [U_i' + \iiint \Delta\tau \bar{J}_i \cdot \bar{A}]\frac{dq^i}{dt} - [V' + \iiint \Delta\tau\rho\phi]$$
$$+ \iiint \Delta\tau[\frac{\varepsilon_o}{2}(\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) \cdot (\frac{\partial}{\partial ct} c\bar{A} + \bar{\nabla}\phi) - \frac{\varepsilon_o}{2}(\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A})]\} .$$

(53 repeated)

The functions that are to be obtained from the action principle are $q^i(t)$, $\phi(\bar{r},t)$, and $c\bar{A}(\bar{r},t)$. Since we agreed to use the transverse gauge for the vector potential $c\bar{A}$, we can simplify (53). For, when we multiply out the scalar product that contains $\bar{\nabla}\phi$, the following sum of three integrals appears in (53).

$$\iiint \Delta\tau \frac{\varepsilon_o}{2} \bar{\nabla}\phi \cdot \bar{\nabla}\phi + \iiint \Delta\tau \frac{\varepsilon_o}{2}(\frac{\partial}{\partial ct} c\bar{A}) \cdot (\frac{\partial}{\partial ct} c\bar{A}) + \iiint \Delta\tau\, \varepsilon_o \bar{\nabla}\phi \cdot \frac{\partial}{\partial ct} c\bar{A} .$$

The last of these vanishes because of our choice of the transverse gauge for $c\bar{A}$. For we have

$$\iiint \Delta\tau \varepsilon_o \bar{\nabla}\phi \cdot \frac{\partial}{\partial ct} c\bar{A} = \varepsilon_o \iiint \Delta\tau [\bar{\nabla} \cdot (\phi \frac{\partial}{\partial ct} c\bar{A}) - \phi \frac{\partial}{\partial ct} \bar{\nabla} \cdot c\bar{A}] ,$$

where we have interchanged $\frac{\partial}{\partial ct}$ and $\bar{\nabla}$ in the last term. But since $\bar{\nabla} \cdot c\bar{A} = 0$, we obtain

$$\iiint \Delta\tau \varepsilon_o \bar{\nabla}\phi \cdot \frac{\partial}{\partial ct} c\bar{A} = \varepsilon_o \oiint \Delta\bar{f} \cdot \phi \frac{\partial}{\partial ct} c\bar{A} ,$$

when we convert the remaining volume integral into a surface integral with the aid of the theorem of Gauss. But this surface integral vanishes because

of the boundary condition $\phi = 0$. As a result, the expression (53) is simplified to

$$A_{a,b} = \int_{t=a}^{b} dt\{\frac{1}{2}\frac{dq^i}{dt} M'_{ij} \frac{dq^j}{dt} + [U'_i + \iiint \Delta\tau \bar{J}_i \cdot \bar{A}] \frac{dq^i}{dt} - [V' + \iiint \Delta\tau \rho\phi]$$

$$+ \iiint \Delta\tau[\frac{\varepsilon_o}{2} \bar{\nabla}\phi \cdot \bar{\nabla}\phi + \frac{\varepsilon_o}{2} (\frac{\partial}{\partial ct} c\bar{A}) \cdot (\frac{\partial}{\partial ct} c\bar{A}) - \frac{\varepsilon_o}{2} (\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A})]\} . \quad (123)$$

We see that the scalar potential ϕ and the vector potential $c\bar{A}$ have become "decoupled", since terms that are mixed in ϕ and $c\bar{A}$ no longer occur in (123).

One of the consequences of the action principle is equation (46), namely

$$\rho^d = \bar{\nabla} \cdot \varepsilon_o \bar{E} - \rho . \qquad \text{(46) repeated}$$

(It results, when we examine $\delta A_{a,b}$ under the assumption that only ϕ is varied.) For a free-running system, to which we confine our attention here, the driver field ρ^d is zero. Thus (46) yields

$$\bar{\nabla} \cdot \varepsilon_o \bar{E} = \rho \quad .$$

And with

$$\bar{E} = - \bar{\nabla}\phi - \frac{\partial}{\partial ct} c\bar{A}, \; \bar{\nabla} \cdot c\bar{A} = 0 \; ,$$

we obtain

$$\varepsilon_o \bar{\nabla} \cdot \bar{\nabla}\phi = - \rho. \qquad (124)$$

This equation shows that ϕ is equal to the electrostatic potential associated with the atomic charge density ρ. Since ρ depends explicitly only on the configuration $\{q^i\}$ and the position $\bar{r}$, the scalar potential ϕ will depend explicitly only on these variables. Then the two integrals

$$\iiint \Delta\tau \rho\phi \text{ and } \frac{\varepsilon_o}{2} \iiint \Delta\tau \bar{\nabla}\phi \cdot \bar{\nabla}\phi \; ,$$

which appear in (123), will depend only on $\{q^i\}$, since the $\bar{r}$-dependence of ϕ and ρ was wiped out by the integration process. These two integrals are closely related. Indeed with (124), we have

$$\iiint_{\Delta\tau}\rho\phi = -\varepsilon_o\iiint_{\Delta\tau}\phi\bar{\nabla}\cdot\bar{\nabla}\phi = -\varepsilon_o\iiint_{\Delta\tau}[\bar{\nabla}\cdot(\phi\bar{\nabla}\phi) - \bar{\nabla}\phi\cdot\bar{\nabla}\phi] .$$

The integral over the first term is converted into the surface integral $\iint_{\Delta\bar{f}}\cdot\phi\bar{\nabla}\phi$, which vanishes because of the boundary condition $\phi = 0$. Thus

$$\iiint_{\Delta\tau}\rho\phi = \varepsilon_o\iiint_{\Delta\tau}\bar{\nabla}\phi\cdot\bar{\nabla}\phi . \tag{125}$$

We use this result to simplify (123). With the abbreviation

$$V(q^i) = V'(q^i) + \frac{\varepsilon_o}{2}\iiint_{\Delta\tau}\bar{\nabla}\phi\cdot\bar{\nabla}\phi , \tag{126}$$

equation (123) becomes

$$A_{a,b} = \int_{t=a}^{b} dt\{\frac{1}{2}\frac{dq^i}{dt}M'_{ij}\frac{dq^j}{dt} + [U_i' + \iiint_{\Delta\tau}\bar{J}_i\cdot\bar{A}]\frac{dq^i}{dt} - V +$$
$$+ \iiint_{\Delta\tau}[\frac{\varepsilon_o}{2}(\frac{\partial}{\partial ct}c\bar{A})\cdot(\frac{\partial}{\partial ct}c\bar{A}) - \frac{\varepsilon_o}{2}(\bar{\nabla}\times c\bar{A})\cdot(\bar{\nabla}\times c\bar{A})]\} . \tag{127}$$

We note that the quantity V depends explicitly only on the atomic configuration $\{q^i\}$, and that the scalar potential ϕ has disappeared from the action functional.

The procedure that enabled us to eliminate the scalar potential ϕ from the action functional may be applied also to the vector potential $c\bar{A}$. In order to get ready for it, we use the eigenfunction expansion (119). Since we are using the transverse gauge, in which all the coefficients Q_a' are zero, the expansion simplifies to

$$c\bar{A} = \sum_a Q_a\bar{E}_a . \tag{128}$$

Similarly,

$$\frac{\partial}{\partial ct}c\bar{A} = \frac{1}{c}\sum_a\frac{dQ_a}{dt}\bar{E}_a , \tag{129}$$

and, because term-by-term differentiation is permissible ,

$$\bar{\nabla}\times c\bar{A} = \sum_a k_a Q_a\bar{H}_a \tag{130}$$

Next we express the three volume integrals in (127) that contain the vector potential in terms of the expansion coefficients Q_a. We have

$$\iiint_{\Delta\tau} \frac{\varepsilon_o}{2} \left(\frac{\partial}{\partial ct} c\bar{A}\right) \cdot \left(\frac{\partial}{\partial ct} c\bar{A}\right) = \frac{\varepsilon_o}{2c^2} \iiint_{\Delta\tau} \left(\sum_a \frac{dQ_a}{dt} \bar{E}_a\right) \cdot \left(\sum_b \frac{dQ_b}{dt} \bar{E}_b\right) =$$

$$= \frac{\varepsilon_o}{2c^2} \sum_a \sum_b \frac{dQ_a}{dt} \frac{dQ_b}{dt} \iiint_{\Delta\tau} \bar{E}_a \cdot \bar{E}_b = \frac{\varepsilon_o}{2c^2} \sum_a \left(\frac{dQ_a}{dt}\right)^2, \qquad (131)$$

where we have used the orthonormality relations (98). (See Box #5.) Similarly

$$\iiint_{\Delta\tau} \frac{\varepsilon_o}{2} (\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A}) = \frac{\varepsilon_o}{2} \sum_a (k_a Q_a)^2 .$$

In the remaining integral we expand the functions $\bar{J}_i$ in terms of the $\bar{F}_a$ and $\bar{E}_a$, i.e. we write

$$\bar{J}_i = \sum_a J'_{i,a} \bar{F}_a + \sum_a J_{i,a} \bar{E}_a . \qquad (132)$$

The expansion coefficients $J'_{i,a}$ and $J_{i,a}$ depend on the atomic configuration $\{q^j\}$. The first series in (132) is the longitudinal part $\bar{J}_{i,L}$ of $\bar{J}_i$, the second series is the transverse part $\bar{J}_{i,T}$. Then, with the aid of the orthonormality relations (98), (100) (See Box #5) we obtain

$$\iiint_{\Delta\tau} \bar{J}_i \cdot \bar{A} = \frac{1}{c} \sum_a J_{i,a} Q_a . \qquad (133)$$

When we insert (131) - (133) into (127), we obtain

$$A_{a,b} = \int_{t=a}^{b} dt \{\frac{1}{2} \frac{dq^i}{dt} M'_{ij} \frac{dq^j}{dt} + [U_i' + \frac{1}{c} \sum_a J_{i,a} Q_a] \frac{dq^i}{dt} - V +$$

$$+ \frac{\varepsilon_o}{2c^2} \sum_a \left(\frac{dQ_a}{dt}\right)^2 - \frac{\varepsilon_o}{2} \sum_a (k_a Q_a)^2\} \qquad (134)$$

(We have used the same symbol "a" for two different purposes. It indicates not only the lower limit in the time-integration, but also the mode-numbers. This double usage should not cause any confusion, since the place where the "a" is written makes its meaning unambiguous.) The functions that are to be determined from the action principle are the n functions $q^i(t)$ and the infinite set $\{Q_a(t)\}$.

In order to derive the equation of motion for one of the $Q_a(t)$, we examine the variation of the action under the assumption that only this particular Q_a is varied. With the aid of the calculation

$$\delta[\frac{1}{2}(\frac{dQ_a}{dt})^2] = \frac{dQ_a}{dt}\,\delta(\frac{dQ_a}{dt}) = \frac{dQ_a}{dt}\,\frac{d}{dt}(\delta Q_a) = \frac{d}{dt}[\frac{dQ_a}{dt}\,\delta Q_a] - \frac{d^2Q_a}{dt^2}\,\delta Q_a ,$$

we obtain

$$\delta A_{a,b} = \frac{\varepsilon_o}{c^2}[\frac{dQ_a}{dt}\,\delta Q_a]\Big|_{t=a}^{b} + \int_{t=a}^{b} dt[\frac{1}{c}\,J_{i,a}\,\frac{dq^i}{dt} - \frac{\varepsilon_o}{c^2}\,\frac{d^2Q_a}{dt^2} - \varepsilon_o(k_a)^2 Q_a]\delta Q_a . \qquad (135)$$

The action principle

$$\delta A_{a,b} = \text{E.T.O.} \qquad (51)\ \text{repeated}$$

for a free-running system causes the square bracket in the integral of (135) to vanish. Thus

$$\frac{d^2Q_a}{dt^2} + (ck_a)^2 Q_a = \frac{c}{\varepsilon_o}\,J_{i,a}\,\frac{dq^i}{dt} . \qquad (136)$$

This equation shows that the expansion coefficient $Q_a(t)$ behaves like the excursion of a harmonic oscillator that is driven by the "force" $\frac{c}{\varepsilon_o}\,J_{i,a}\,\frac{dq^i}{dt}$. The resonance frequency Ω_a of this oscillator is given by

$$\Omega_a = ck_a \qquad (137)$$

Equation (136) suggests the kind of approximation we are going to make. We will first go through the procedure of this approximation. Only later will we discuss the motivation for it. At this point we merely mention that it serves to eliminate infinities that arise when the atomic particles are treated as point-like entities. We divide the modes into two groups: the "low" modes whose resonance frequencies lie below some critical frequency Ω_{crit}, which will be selected later, and the "high" modes whose resonance frequencies lie above Ω_{crit}. For the low modes, we retain equation (136). But in the high modes, the "intertia term" $\frac{d^2Q_a}{dt^2}$ is small when it is compared to the "stiffness term" $(ck_a)^2 Q_a$. We may therefore neglect the inertia term. Accordingly, we replace (136) by

$$\frac{d^2Q_a}{dt^2} + (ck_a)^2 Q_a = \frac{c}{\varepsilon_o}\,J_{i,a}\,\frac{dq^i}{dt} , \text{ for the low modes,} \qquad (138a)$$

and

$$(ck_a)^2 Q_a = \frac{c}{\varepsilon_o} J_{i,a} \frac{dq^i}{dt} \text{ , for the high modes,} \qquad (138b)$$

We decompose the sums over the modes in (134) into two sums, one over the low modes, the other over the high modes, so that

$$\sum_a = \sum_{a,\text{low}} + \sum_{a,\text{high}} . \qquad (139)$$

The deletion of the inertia term in (138b) is accounted for by a change in the action functional (134), where we would have to omit the term $\sum_{a,\text{high}} (\frac{dQ_a}{dt})^2$. Accordingly, we approximate $A_{a,b}$ by

$$A_{\substack{a,b \\ \text{appr}}} = \int_{t=a}^{b} dt \{ \frac{1}{2} \frac{dq^i}{dt} M'_{ij} \frac{dq^j}{dt} + U_i' \frac{dq^i}{dt} + \frac{1}{c} \sum_{a,\text{high}} J_{i,a} Q_a \frac{dq^i}{dt} +$$
$$+ \frac{1}{c} \sum_{a,\text{low}} J_{i,a} Q_a \frac{dq^i}{dt} - V + \frac{\varepsilon_o}{2c^2} \sum_{a,\text{low}} (\frac{dQ_a}{dt})^2 -$$
$$- \frac{\varepsilon_o}{2} \sum_{a,\text{high}} (k_a Q_a)^2 - \frac{\varepsilon_o}{2} \sum_{a,\text{low}} (k_a Q_a)^2 \} . \qquad (140)$$

We express the expansion coefficients Q_a for the high modes by means of (138b). We therefore write

$$Q_a = \frac{1}{(ck_a)^2} \frac{c}{\varepsilon_o} J_{i,a} \frac{dq^i}{dt} = \frac{1}{(ck_a)^2} \frac{c}{\varepsilon_o} J_{j,a} \frac{dq^j}{dt} .$$

Here we must be prepared to use two different summation indices i and j, in order to avoid confusion later on. The two terms in (140) that contain the Q_a of the high modes are then

$$\frac{1}{c} \sum_{a,\text{high}} J_{i,a} Q_a \frac{dq^i}{dt} = \frac{1}{\varepsilon_o} \frac{dq^i}{dt} \Big(\sum_{a,\text{high}} \frac{1}{(ck_a)^2} J_{i,a} J_{j,a} \Big) \frac{dq^j}{dt} .$$

and

$$\frac{\varepsilon_o}{2} \sum_{a,\text{high}} (k_a Q_a)^2 = \frac{1}{2\varepsilon_o} \frac{dq^i}{dt} \Big(\sum_{a,\text{high}} \frac{1}{(ck_a)^2} J_{i,a} J_{j,a} \Big) \frac{dq^j}{dt} .$$

We see that they resemble each other. We combine these two terms and use the abbreviation

$$M_{ij} = M'_{ij} + \frac{1}{\varepsilon_o} \sum_{a,\text{high}} \frac{1}{(ck_a)^2} J_{i,a} J_{j,a} \ . \tag{141}$$

Then (140) becomes

$$A_{\substack{a,b \\ \text{appr}}} = \int_{t=a}^{b} dt\{[\frac{1}{2} \frac{dq^i}{dt} M_{ij} \frac{dq^j}{dt} + U'_i \frac{dq^i}{dt} - V] + \frac{1}{c} \sum_{a,\text{low}} J_{i,a} Q_a \frac{dq^i}{dt} +$$

$$+ \frac{\varepsilon_o}{2c^2} \sum_{a,\text{low}} (\frac{dQ_a}{dt})^2 - \frac{\varepsilon_o}{2} \sum_{a,\text{low}} (k_a Q_a)^2\} \ . \tag{142}$$

The functions that are to be determined from the action principle (51) are the n functions $q^i(t)$ and the, now finite, set $\{Q_a(t)\}$ for the low modes.

When we reverse some of the procedures that led from (127) to (134), we can write (142) also in the form

$$A_{\substack{a,b \\ \text{appr}}} = \int_{t=a}^{b} \{[\frac{1}{2} \frac{dq^i}{dt} M_{ij} \frac{dq^j}{dt} + U'_i \frac{dq^i}{dt} - V] + \iiint \Delta\tau \bar{J} \cdot \bar{A}_{\text{low}} +$$

$$+ \iiint \Delta\tau [\frac{\varepsilon_o}{2} (\frac{\partial}{\partial ct} c\bar{A})_{\text{low}} \cdot (\frac{\partial}{\partial ct} c\bar{A}_{\text{low}}) - \frac{\varepsilon_o}{2} (\bar{\nabla} \times c\bar{A}_{\text{low}}) \cdot (\bar{\nabla} \times c\bar{A}_{\text{low}})]\} \ , \tag{143}$$

where

$$c\bar{A}_{\text{low}} = \sum_{a,\text{low}} Q_a \bar{E}_a \ . \tag{144}$$

Because of the orthonormality relations, we may also replace the complete current density $\bar{J}$ in (143) by $\bar{J}_{T,\text{low}}$, the low-mode part of the transverse portion of $\bar{J}$, which is given by

$$\bar{J}_{T,\text{low}} = \sum_{a,\text{low}} \frac{dq^i}{dt} J_{i,a} \bar{E}_a \ . \tag{145}$$

However, the best policy is to work with equation (142).

We are now in the position to discuss the motivation for the approximation we have made. The expression (123) contains the integral

$$\iiint \Delta\tau \frac{\varepsilon_o}{2} \bar{\nabla}\phi \cdot \bar{\nabla}\phi \ ,$$

which is equal to the electrostatic energy associated with the atomic particles. (Remember that ϕ was the electrostatic potential, as shown by (124). But for point-like particles, this energy is infinitely large, because $|\bar{\nabla}\phi|$ increases to infinity with decreasing distance from the particle so rapidly that the energy integral diverges. The other terms represented by triple integrals in (123) offer similar difficulties. For instance, the term

$$\frac{\varepsilon_o}{2} \iiint \Delta\tau (\bar{\nabla} \times c\bar{A}) \cdot (\bar{\nabla} \times c\bar{A}) \ ,$$

which is the magnetic energy, is infinitely large for moving point-like particles, because the immediate vicinity of a particle contributes a diverging amount to the integral. Thus for point-like atomic particles, equation (127) is really without meaning.

On the other hand, the approximation described by (142) appears to be meaningful, as neither diverging triple integrals nor infinite series occur in this equation. Of course, this appearance is deceptive, because the second terms in the equations

$$V = V' + \frac{\varepsilon_o}{2} \iiint \Delta\tau \bar{\nabla}\phi \cdot \bar{\nabla}\phi \ , \qquad \text{(125) repeated}$$

and

$$M_{ij} = M'_{ij} + \frac{1}{\varepsilon_o} \sum_{a,\text{high}} \frac{1}{(ck_a)^2} J_{i,a} J_{j,a} \qquad \text{(141) repeated}$$

are infinitely large for point-like particles. But it is conceivable that the infinities of the second terms in (125) and (141) are compensated by infinities of the opposite sign in the first terms, so that the left-hand sides V and M_{ij} turn out to be finite. It is generally believed, although there are no rational foundations for this belief, that this actually happens. It is

believed furthermore that the square bracket in (142), which looks like an atomic Lagrangian, is in fact equal to the conventional atomic Lagrangian, if the critical frequency Ω_{crit}, which formed the dividing point between low and high modes, is chosen low enough. This means that, for $\Omega_{crit} \to 0$, the expression $\frac{1}{2} \frac{dq^i}{dt} M_{ij} \frac{dq^i}{dt}$ is equal to the conventional kinetic energy (in the sense of elementary particles) of the atomic particles, that V is their conventional potential energy (again in the sense of elementary particles) and that the quantities U_i' are zero.

We have introduced two approximations.

(1) The approximation that was made when we deleted the inertial term for the high modes, as in (138b).

(2) The approximation that was made when we replaced the square bracket in (142) by the conventional Lagrangian of the atom.

The quality of the first approximation is improved, when we raise the critical frequency Ω_{crit}. And the quality of the second approximation is improved when we lower the critical frequency Ω_{crit}. Therefore, we have to make a compromise when we choose Ω_{crit}. We believe that the quality of the overall approximation is good enough for our purposes, when we choose Ω_{crit} to be of the order of ten times the dominant frequencies, e.g. ten times the frequency of visible light for the example of the laser. Unfortunately we have no evidence for this belief at the moment. But to adhere to this belief is the best we can do.

At any rate, the approximations we have made and the beliefs we have adopted furnish us with the definite action functional (142). Since our future work is based on it, we write it down again in a box. We use the statement that all

the U_i' are zero, and we indicate the variables on which the various quantities depend.

$$A_{\substack{a,b \\ appr}} = \int_{t=a}^{b} dt\{[[\tfrac{1}{2}[\tfrac{d}{dt} q^i(t)]M_{ij}(q^k)[\tfrac{d}{dt} q^j(t)] - V(q^k)]] +$$
$$+ \frac{1}{c} \sum_{a,low} J_{i,a}(q^k)Q_a(t)[\tfrac{d}{dt} q^i(t)] +$$
$$+ \frac{\epsilon_o}{2c^2} \sum_{a,low} [\tfrac{d}{dt} Q_a(t)]^2 - \frac{\epsilon_o}{2} \sum_{a,low} [k_a Q_a(t)]^2\} . \qquad (146)$$

The expression in the double square bracket is the conventional Lagrangian of the atom, when the atom is isolated from the radiation field.

This action functional is of the standard type that one always meets in classical dynamics. It pertains to a system with (n + N) degrees of freedom. Here n is the number of the degrees of freedom of the atom, and N is the number of transverse modes whose resonance frequencies are less than the critical frequency Ω_{crit}. The configurational coordinates are the n quantities q^i, and the N expansion coefficients Q_a. The action functional depends on the functions $Q_a(t)$ in a particularly simple way, characteristic of harmonic oscillators. There is no direct coupling among these oscillators, as shown by the absence of mixed terms of the type $Q_a Q_b$ etc. However, the "radiation field" oscillators are coupled to the atom by the term on the second line of (146). Hence they are coupled to each other in an indirect way.

The other form, analogous to (143), of the action functional is

$$
\begin{aligned}
A_{\substack{a,b\\ appr}} = \int_{t=a}^{b} dt\{&[[\tfrac{1}{2}[\tfrac{d}{dt}\, q^i(t)]M_{ij}(q^k)[\tfrac{d}{dt}\, q^j(t)] - V[q^k)]] + \\
&+ \iiint_{\Delta\tau} \bar{J}_{T,low}(\bar{r},q^k) \cdot \bar{A}_{low}(\bar{r},t) + \\
&+ \frac{\varepsilon_o}{2} \iiint_{\Delta\tau}[\tfrac{\partial}{\partial ct}\, c\bar{A}_{low}(\bar{r},t)] \cdot [\tfrac{\partial}{\partial ct}\, c\bar{A}_{low}(\bar{r},t)] - \\
&- \frac{\varepsilon_o}{2} \iiint_{\Delta r}[\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)] \cdot [\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)]\} \,. \qquad (147)
\end{aligned}
$$

We note that $\bar{J}_{T,low}(\bar{r},q^k)$ depends on the time t in an indirect way through the functions $q^k(t)$.

There is another way of looking at (146). We retain the first and second lines as they are. But in the third line we delete the subscript "low". Then equation (138a) holds for all transverse modes, not just the low ones. But the excitation term, i.e. the right-hand side of (138a) vanishes for the high modes. Thus if we use the initial conditions

$$Q_a = 0,\ \frac{d}{dt}\, Q_a = 0 \text{ at } t = 0 \text{ for the high modes,} \qquad (148)$$

we find that the high modes are never excited, so that the $Q_{a,high}$ are automatically zero at all times. The preceding remarks may be interpreted in the following way. Since, in the spirit of our approximation, the interaction term (i.e. the second line of (146)) is a sum that extends only over the low modes, the real atom has been converted by our approximation into an object that is completely inert to radiation whose frequencies exceed the critical frequency Ω_{crit}. In this way then our approximate treatment differs from reality. But this deviation is not harmful in the applications we have in mind. In these applications we are interested in radiation whose frequencies lie in or near

those of visible light.

We close this section with a qualitative argument which is designed to show that the approximation in (138b), where we deleted the term $\frac{d^2}{dt^2} Q_a$, is good only in the non-relativistic domain, i.e. when the speeds of the atomic particles satisfy the condition $(\text{speed})^2 << c^2$. Let us consider just one atomic particle of charge e. We assume that it travels with constant velocity w along the x-axis of some cartesian coordinate system. Its position $\bar{r}$ is then given by $\bar{r} = wt\bar{i}$, where $\bar{i}$ is the unit vector in the x-direction. Here we need only one configurational coordinate q^1, which we choose to be equal to x. From the expansion (132) we determine $J_{1,a}$ by integration. We have

$$J_{1,a} = \iiint \Delta\tau \bar{J}_1 \cdot \bar{E}_a$$

Since $\bar{J}_1$ is a distribution that is concentrated in just one point, the integration is easy to carry out. The result is

$$J_{1,a} = e\bar{i} \cdot \bar{E}_a(wt\bar{i})$$

As the time t progresses, the value of $\bar{J}_{1,a}$ will change appreciably when the particle has travelled a distance, which is of the order of $\frac{1}{k_a}$. The elapsed time is then $\frac{1}{wk_a}$. The inverse $\omega_a = wk_a$ is the dominant frequency of $J_{1,a}$. Now we calculate Q_a from (138b). It is proportional to $J_{1,a}$. Thus the dominant frequency of Q_a is also wk_a. Now we ask: Were we permitted to delete the term $\frac{d^2}{dt^2} Q_a$ in (138b)? Since $\frac{d^2}{dt^2} Q_a$ is of the order of $(\text{frequency})^2 Q_a$, our question becomes: Is $(wk_a)^2|Q_a|$ much smaller than $(ck_a)^2|Q_a|$? The answer is yes, if and only if $(\frac{w}{c})^2 << 1$. And this is the condition for the non-relativistic velocity range.

We have seen that the approximation in (138b) is of poor quality, if the particle velocities lie in the relativistic range. The converse of this

statement is not necessarily true. Non-relativistic velocities do not necessarily guarantee that the approximation is of good quality. After all, in the foregoing estimate, we have considered only a particle that moves with constant velocity. Nevertheless, we stick to our approximate treatment, because it is presumably the best that can be done without the use of advanced quantum electrodynamics. Furthermore, it yields a definite action functional, which permits further analysis.

In the next section, we are going to make the transition to quantum mechanics. We shall apply quantum mechanics only to the atom, not to the radiation field. However, the procedure that we are going to use can be easily adapted also to the case in which quantum mechanics is used for the radiation field as well.

8. The Transition to Quantum Mechanics.

The usual method for making the transition to quantum mechanics (or "quantizing") is to define the generalized momenta and the Hamiltonian function, and then to proceed to the Schrödinger equation. But this means that additional concepts must be used. Another drawback of this method is that it can tell us only how the atom responds to the radiation. It will not tell us how, in reverse, the atom influences the radiation field. However, both of these questions are answered, when the action principle is used. Therefore, we stay with the action principle. All we have to do, in order to make the transition to quantum mechanics, is to modify the action functional (146) in the appropriate manner.

In order to simplify the presentation of this approach, we shorten the notation in (146). We use the abbreviations

$$\frac{d}{dt} q^i(t) = v^i(t) \ , \tag{149}$$

(This one we have used before), and

$$\frac{1}{c}\sum_{a,low} J_{i,a}(q^k)Q_a(t) = U_i(q^k,t). \qquad (150)$$

(This U_i is without a prime. The primed quantities U_i' were all zero, as we had mentioned in the paragraph that followed equations (125), (141) (repeated) of the previous section.) We also delete the variables on which the quantities of (146) depend, i.e. we delete the variables in the round parentheses. Then, if we put the term $U_i v^i$ inside the double square bracket, the shortened version of (146) appears as

$$A_{\substack{a,b\\appr}} = \int_{t=a}^{b} dt\{[[\tfrac{1}{2} v^j M_{jk} v^k + U_j v^j - V]] + \frac{\varepsilon_o}{2c^2}\sum_{a,low}[\frac{dQ_a}{dt}]^2 - \frac{\varepsilon_o}{2}\sum_{a,low}[k_a Q_a]^2\} \ . \qquad (151)$$

In order to quantize the atomic subsystem, we introduce a time-dependent complex scalar field $\psi(q^m,t)$ defined throughout the configuration space of the atom. And we also introduce a time-dependent complex vector field in this space, with components $\chi^j(q^m,t)$. These components are referred to axes that, locally, conform to the coordinate lines of the configurational coordinates q^j. Then we replace the double square bracket in (151) by an integral over the entire configuration space of the atom, i.e. we make the replacement

$$[[\tfrac{1}{2} v^j M_{jk} v^k + U_j v^i - V]] \rightarrow$$

$$\rightarrow \int_{ecs} \Delta\sigma[[\frac{i\hbar}{2}((\psi^* \frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t} + \chi^{*j}\frac{\partial}{\partial q^j}\psi - \chi^j\frac{\partial}{\partial q^j}\psi^*)) +$$

$$+ ((\tfrac{1}{2}\chi^{*j}M_{jk}\chi^k + \tfrac{1}{2}(\chi^{*j}\psi + \chi^j\psi^*)U_j - \psi^*\psi V))]] \ . \qquad (152)$$

where the stars indicate the complex conjugate quantities. The symbol $\hbar$ denotes Planck's constant divided by 2π. The "i" in front of $\hbar$ stands for $\sqrt{-1}$. The symbol $\Delta\sigma$ denotes the volume element in the configuration space. In order to

explain the meaning of $\Delta\sigma$, we consider a volume element that is shaped like a small parallelepiped whose edges conform to the coordinate lines of the configurational coordinates q^j. The extents of the edges are Δq^1, Δq^2, ... Δq^n. The volume element $\Delta\sigma$ is proportional to the product of these extents, so that we can write

$$\Delta\sigma = M\Delta q^1 \ \Delta q^2 \ \ldots \Delta q^n \ . \tag{153}$$

The proportionality factor M is equal to the positive square root of the determinate of an n-by-n matrix whose matrix elements are the quantities M_{jk} in (152). Thus, in simplified notation,

$$M = (\mathrm{Det}M_{jk})^{\frac{1}{2}} \ . \tag{154}$$

The letters ecs under the integration sign stand for "entire configuration space." They will be omitted henceforth.

Some insight into the physical meaning of the field quantities ψ and χ^j is gained, when they are related to probabilistic statements. In quantum mechanics, the instantaneous configuration of the atom is no longer given by a definite point $\{q^j\}$ in the configuration space. Instead, we deal with a probability distribution, whose density s is given by

$$s = \psi^*\psi \ . \tag{155}$$

This means that the probability $\Delta(\mathrm{prob})$ of finding the configuration to be in some volume element $\Delta\sigma$ is given by

$$\Delta(\mathrm{prob}) = s\Delta\sigma = \psi^*\psi\Delta\sigma = \psi^*\psi M\Delta q^1\Delta q^2 \ \ldots \ \Delta q^n. \tag{156}$$

(The last member of this string pertains to the case in which the volume element is shaped like a parallelepiped of the type we described earlier.) Since the probability of finding the configuration to lie somewhere in the configuration space is unity, the field quantity ψ should satisfy the

normalization condition

$$\int \Delta\sigma \psi^* \psi = 1 \ . \tag{157}$$

Associated with the probability density s is the probability current density (in the configuration space) whose components K^j are given by

$$K^j = \tfrac{1}{2}(\chi^{*j}\psi + \chi^j \psi^*) \ . \tag{158}$$

The probability density and the probability current density are linked by the continuity equation

$$\frac{\partial}{\partial t} s + \frac{1}{M} \frac{\partial}{\partial q^j} (M K^j) = 0 \tag{159}$$

as we shall see later.

When we make the replacement (152) in (151) we obtain the quantum mechanical action functional.

$$\begin{aligned} M_{\substack{a,b \\ appr,quant}} = \int_{t=a}^{b} dt \{ \int \Delta q^1 \Delta q^2 \ldots \Delta q^n \, M [[\tfrac{i\hbar}{2} ((\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} + \chi^{*j} \frac{\partial \psi}{\partial q^j} - \chi^j \frac{\partial \psi^*}{\partial q^j})) \\ + ((\tfrac{1}{2} \chi^{*j} M_{jk} \chi^k + \tfrac{1}{2}(\chi^{*j}\psi + \chi^j \psi^*) U_j - \psi^* \psi V))]] \\ + \frac{\varepsilon_o}{2c^2} \sum_{a,low} [\frac{dQ_a}{dt}]^2 - \frac{\varepsilon_o}{2} \sum_{a,low} [k_a Q_a]^2 \} \ . \end{aligned} \tag{160}$$

*

The functions that are to be determined from the action principle are $\psi(q^i,t)$, the n functions $\chi^j(q^i,t)$, and the N function $Q_a(t)$. We repeat the definitions of n and N. The number n is equal to the number of the atomic degrees of freedom, and N is the number of transverse modes whose resonance frequencies lie below the critical frequency Ω_{crit}. We might also say that N is the number of electromagnetic degrees of freedom that we retained after the approximations of the preceding section. When we apply the action principle (for a free-running system), we may regard the variations $\delta\psi$, $\delta\psi^*$, $\delta\chi^j$, $\delta\chi^{*j}$ as independent variations,

---

*The U_j in (160) are given by (150).

even though ψ^* is tied to ψ and χ^{*j} is tied to χ^j by the condition that the starred quantities are the complex conjugates of the unstarred ones. What enables us to do this is that we will have to deal with quantities of the type $F\delta\psi + F^*\delta\psi^*$, which have to be equated to zero. Choosing $\delta\psi$ to be purely real yields $F + F^* = 0$. And choosing $\delta\psi$ to be purely imaginary yields $F - F^* = 0$. These two equations imply that $F = 0$ and $F^* = 0$. These are just the results that we would have obtained, had we regarded $\delta\psi$ and $\delta\psi^*$ as independent variations.

Had we desired to quantize also the electromagnetic field, then we could have extended the procedure that led from (151) to (160). In this case we would have used, instead of an integral over the n-dimensional configuration space of the atom, an integral over the (n + N)-dimensional configuration space of the total system. We need not elaborate any further upon this theme, since we decided at the outset to quantize only the atom and to treat the radiation field classically.

Now let us apply the action principle

$$\delta A_{a,b} = \text{E.T.O.} \qquad \text{(51) repeated}$$

for a free-running system. We use the action functional (160). If we vary only the χ^{j*}, we obtain

$$\delta A_{a,b} = \int_{t=a}^{b} dt\{\int \Delta q^1 \Delta q^2 \ldots \Delta q^n \, M \, \delta\chi^{*j}\left(\frac{i\hbar}{2}\frac{\partial\psi}{\partial q^j} + \tfrac{1}{2}M_{jk}\chi^k + \tfrac{1}{2}U_j\psi\right)\}$$

Equation (51) tells us that the factor of $\delta\chi^{*j}$ must vanish. Thus

$$M_{jk}\chi^k = -\,i\hbar\frac{\partial\psi}{\partial q^j} - U_j\psi\,. \qquad (161)$$

We introduce the matrix with elements M^{ij}, which is the inverse to the matrix with the elements M_{ij}. (Both are symmetric.) The condition that these two

matrices are the inverses of each other is reflected by the following equations for the matrix elements

$$M_{ij}M^{jk} = \delta_i^k \; ; \; M^{ij}M_{jk} = \delta_k^i \; . \tag{162}$$

(The summation convention remains in effect), where the δ_i^k are the Kronecker deltas. Then, if we premultiply (161) by $M^{\ell j}$, we obtain

$$\chi^{\ell} = M^{\ell j}\left(- i\hbar \frac{\partial \psi}{\partial q^j} - U_j \psi\right) \tag{163}$$

Similarly,

$$\chi^{*\ell} = M^{\ell j}\left(+ i\hbar \frac{\partial \psi^*}{\partial q^j} - U_j \psi^*\right) \tag{164}$$

Now let us vary only ψ^*. In $\delta A_{a,b}$, there appear the terms $- \psi \frac{\partial}{\partial t} \delta\psi^*$ and $\chi^j \frac{\partial}{\partial q^j} \delta\psi^*$, which require some manipulation. We have

$$- M\psi \frac{\partial}{\partial t} \delta\psi^* = - \frac{\partial}{\partial t}\left(M\psi\delta\psi^*\right) + M \frac{\partial \psi}{\partial t} \delta\psi^* + \frac{\partial M}{\partial t} \psi \delta\psi^* \; .$$

The first term, being a full time-derivative contributes only to the end terms E.T.O. The last term vanishes, since we assumed that the matrix elements M_{jk} do not depend on the time t. Thus $M = (\text{Det } M_{jk})^{1/2}$ does not depend on t, so that $\frac{\partial M}{\partial t} = 0$. Similarly

$$- M\chi^j \frac{\partial}{\partial q^j} \delta\psi^* = - \frac{\partial}{\partial q^j}\left(M\chi^j \delta\phi^*\right) + \delta\psi^* \frac{\partial}{\partial q^j}\left(M\chi^j\right) \; .$$

The first term is a full configurational derivative. When we integrate it over the entire configuration space, the result is zero, because $M\chi^j\delta\psi^*$ vanishes in the far reaches of the configuration space. (We could even require that $\delta\psi^*$ vanishes except in a finite domain.)

Combined with the results of these manipulations, equation (160) yields

$$\delta A_{a,b} = -\frac{i\hbar}{2}\{\int \Delta q^1 \Delta q^2 \ldots \Delta q^n M \psi \delta\psi^*\}\Big|_{t=a}^{b} +$$

$$+ \int_{t=a}^{b} dt\{\int \Delta q^1 \Delta q^2 \ldots \Delta q^n M(\delta\psi^*)[[i\hbar \frac{\partial\psi}{\partial t} + \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi^j) +$$

$$+ \frac{1}{2} U_j \chi^j - V\psi]]\} .$$

The action principle (51) tells us that the expression in the double square bracket must vanish. Thus

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi^j) - \frac{1}{2} U_j \chi^j + V\psi. \qquad (165)$$

Similarly

$$-i\hbar \frac{\partial\psi^*}{\partial t} = +\frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi^{*j}) - \frac{1}{2} U_j \chi^{*j} + V\psi^* . \qquad (166)$$

On combining (163) with (165), we obtain

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(MM^{jk}\frac{\partial\psi}{\partial q^k}) + \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(MM^{jk}U_k\psi)$$

$$+ \frac{i\hbar}{2} U_j M^{jk}\frac{\partial\psi}{\partial q^k} + \frac{1}{2} U_j M^{jk} U_k \psi + V\psi, \qquad (167)$$

or, in somewhat abbreviated notation,

$$i\hbar \frac{\partial\psi}{\partial t} = \frac{1}{2M}\left(-i\hbar\frac{\partial}{\partial q^j} - U_j\right)MM^{jk}\left(-i\hbar\frac{\partial}{\partial q^k} - U_k\right)\psi + V\psi. \qquad (168)$$

Equation (168) is the well-known Schrödinger equation for time-independent "kinetic coefficients" M_{jk}, M^{jk}, M. We will refer to the pair of equations (161) and (165), from which (168) could be derived, as the "pair of Schrödinger equations". The influence of the radiation field is contained in the quantities U_j, which - according to equation (150) - depend on the electromagnetic variables $Q_a(t)$. Similarly, when we consider the variations $\delta\psi$ of ψ, we obtain

$$-i\hbar \frac{\partial\psi^*}{\partial t} = \frac{1}{2M}\left(+i\hbar\frac{\partial}{\partial q^j} - U_j\right)MM^{jk}\left(+i\hbar\frac{\partial}{\partial q^k} - U_k\right)\psi^* + V\psi^*. \qquad (169)$$

This equation is, of course, the complex conjugate of (168).

At this point we are ready to check the continuity equation (159). We have

$$\frac{\partial}{\partial t} s + \frac{1}{M} \frac{\partial}{\partial q^j} (MK^j) = \frac{\partial}{\partial t} (\psi^* \psi) + \frac{1}{M} \frac{\partial}{\partial q^j} [M \tfrac{1}{2}(\psi^* \chi^j + \psi \chi^{*j})] =$$

$$= \psi^* \frac{\partial \psi}{\partial t} + \frac{1}{2} \chi^j \frac{\partial \psi^*}{\partial q^j} + \psi^* \frac{1}{2M} \frac{\partial}{\partial q^j} (M \chi^j) + \text{c.c.} ,$$

where c.c. stands for conjugate complex. With (165) we obtain

$$\psi^* \frac{\partial \psi}{\partial t} + \frac{1}{2} \chi^j \frac{\partial \psi^*}{\partial q^j} + \psi^* \frac{1}{2M} \frac{\partial}{\partial q^j} (M \chi^j) =$$

$$= \frac{1}{i\hbar} \psi^* (- \frac{1}{2} U_j \chi^j + V \psi) + \frac{1}{2} \chi^j \frac{\partial \psi^*}{\partial q^j} =$$

$$= \frac{1}{2i\hbar} \chi^j (- U_j \psi^* + i\hbar \frac{\partial \psi^*}{\partial q^j}) + \frac{1}{i\hbar} \psi^* \psi V =$$

$$= \frac{1}{2i\hbar} \chi^j M_{jk} \chi^{*k} + \frac{1}{i\hbar} \psi^* \psi V ,$$

where, in the last step, we have used the complex conjugate of (161). But this expression is purely imaginary, since the factors of $\frac{1}{i\hbar}$ are purely real. Thus, when we add the complex conjugate "c.c.", we get zero. And this completes the check.

So far we have exploited the action principle only in part, in that we examined what happens when the quantum-mechanical quantities ψ, ψ^*, χ^j, χ^{*j} are varied. Now we subject the electromagnetic quantities Q_a to variations δQ_a. Here we must not forget that, according to equation (150), the Q_a are contained in the U_i. We therefore write down the action functional (160) again, but this time with the Q_a exhibited wherever they occur. All the other terms are indicated by a sequence of dots. Then, with the use of (150), we obtain

$$A_{a,b} = \int_{t=a}^{b} dt \{ \sum_{a,\text{low}} Q_a [\int \Delta q^1 \Delta q^2 \ldots \Delta q^n M \tfrac{1}{2}(\chi^{*j} \psi + \chi^j \psi^*) \tfrac{1}{c} J_{j,a}(q^k)] +$$

$$+ \ldots + \frac{\varepsilon_o}{2c^2} \sum_{a,\text{low}} [\frac{dQ_a}{dt}]^2 - \frac{\varepsilon_o}{2} \sum_{a,\text{low}} [k_a Q_a]^2 \} . \qquad (170)$$

In the variation $\delta A_{a,b}$ there appear the terms $\delta[\frac{dQ_a}{dt}]^2$, which require some manipulation. We have

$$\delta[\frac{dQ_a}{dt}]^2 = 2\frac{dQ_a}{dt}\delta(\frac{dQ_a}{dt}) = 2\frac{dQ_a}{dt}\frac{d}{dt}(\delta Q_a) =$$

$$= 2\frac{d}{dt}[\frac{dQ_a}{dt}\delta Q_a] - 2\frac{d^2Q_a}{dt^2}\delta Q_a.$$

The first term, being a full time-derivative, contributes only to the end terms E.T.O. We then obtain

$$\delta A_{a,b} = \ldots + \frac{\varepsilon_o}{c^2}\sum_{a,low}[\frac{dQ_a}{dt}\delta Q_a]\Big|_{t=a}^{b} +$$

$$+ \int_{t=a}^{b} dt \sum_{a,low}\delta Q_a\{-\frac{\varepsilon_o}{c}\frac{d^2Q_a}{dt^2} - \varepsilon_o(k_a)^2Q_a +$$

$$+ \int\Delta q^1\Delta q^2 \ldots \Delta q^n M\frac{1}{2}(\chi^{*j}\psi + \chi^j\psi^*)\frac{1}{c}J_{j,a}(q^k)\}.$$

The action principle tells us that the expression in the curled brackets must vanish. Thus

$$\frac{\varepsilon_o}{c^2}\frac{d^2Q_a}{dt^2} + \varepsilon_o(k_a)^2Q_a = \frac{1}{c}\int\Delta q^1\Delta q^2 \ldots \Delta q^n M\frac{1}{2}(\chi^{*j}\psi + \chi^j\psi^*)J_{j,a} \qquad (171)$$

These N equations (one for each of the low transverse modes #a) describe how the atom influences the electromagnetic field. Each of these equations is constructed like the equation of motion for a driven harmonic oscillator. With the aid of (153) and (158), we can write (171) in more compact form, namely as

$$\boxed{\frac{d^2Q_a}{(dct)^2} + (k_a)^2Q_a = \frac{1}{\varepsilon_o c}\int\Delta\sigma\, K^j J_{j,a}\,,} \qquad (172)$$

after we have divided it by ε_o. This equation is the main result of this section. It is the quantum-mechanical analog of the classical equation (138a).

In order to explain the meaning of (172), we write it down again in conjunction with (138a), also divided by ε_o. Only this time we indicate the variables on which the various quantities depend. In (138a) we replace $\frac{dq^i}{dt}$ by its

abbrevations v^i.

Classically:

$$\frac{d^2}{(dct)^2} Q_a(t) + (k_a)^2 Q_a(t) = \frac{1}{\varepsilon_o c} v^j(t) J_{j,a}(q^k(t)) \ , \qquad (173)$$

Quantum-mechanically:

$$\frac{d^2}{(dct)^2} Q_a(t) + (k_a)^2 Q_a(t) = \frac{1}{\varepsilon_o c} \int \Delta\sigma K^j(q^k,t) J_{j,a}(q^k) \ . \qquad (174)$$

Of course, the words "Classically" and "Quantum-mechanically" refer only to the treatment of the atomic subsystem. The electromagnetic subsystem is always treated classically in our presentation.

In order to make the transition from (173) to (174) more evident, we rewrite the right-hand side (R.H.S.) of (173) in a cumbersome, but instructive, way. We could regard the precisely defined configuration $\{q^k(t)\}$ as the reflection of a highly concentrated probability distribution in the atomic configuration space. Let $s(q^\ell,t)$ be the density of this distribution. It is sharply peaked near the point $\{q^k(t)\}$ and zero elsewhere. When we integrate s over the entire configuration space, the result must be unity. Of course only the immediate vicinity of the point $q^k(t)$ contributes to the integral. We can therefore write the R.H.S. of (173) in the form

$$\text{R.H.S.} = \frac{1}{\varepsilon_o c} \{\int \Delta\sigma\, s\} v^j(t) J_{j,a}(q^k(t)) \ .$$

Here s in the integral is evaluated at the generic or "running" configuration of the integration process, whereas $J_{j,a}$ is evaluated at the precisely defined configuration $\{q^k(t)\}$. But, because s is so sharply peaked near $\{q^k(t)\}$ we may pull $J_{j,a}$ into the integrand and evaluate it at the running configuration, without changing the value of the R.H.S. We may pull in the $v^j(t)$ as well, because this quantity figures as a constant in the integration process. Thus

$$\text{R.H.S.} = \frac{1}{\varepsilon_o c} \int_{\Delta\sigma} sv^j(t) J_{j,a} \ .$$

But sv^j is the component #j of the probability current density K^j in the atomic configuration space. Like s, the K^j as well are sharply peaked near the point $\{q^i(t)\}$. We then obtain

$$\text{R.H.S.} = \frac{1}{\varepsilon_o c} \int_{\Delta\sigma} K^j J_{j,a} \ . \tag{175}$$

And now the R.H.S. of (173) looks like the R.H.S. of (174). This shows the intimate connection between the classical and quantum-mechanical equations (173) and (174).

We may recapitulate the considerations of the preceding paragraph in the following way. The R.H.S. of the classical equation (173) is deterministic in form and in substance, since it refers to a precisely defined configuration $\{q^k(t)\}$ and velocity with components $\{v^j(t)\}$. But we may contrive to write it in a probabilistic form, as in (175). In substance, it is still deterministic, because the probability current density components K^j are such highly concentrated distributions. When we go over to the quantum-mechanical equation (174), the same probabilistic form is retained. Only now the R.H.S. is probabilistic not only in form but also in substance, because the quantum-mechanical K^j are no longer highly concentrated distributions. We may therefore regard (174) as the direct probabilistic analog of (173).

Now that we have elucidated the meaning of the quantum-mechanical equation (174), we are permitted to make the transition from (173) to (174) in a rather mechanical manner, i.e. by a purely typographical procedure. All we have to do is to replace the symbol v^j in (173) by the symbol $\int_{\Delta\sigma} K^j$ and to pull in the symbol $J_{j,a}$ under the integral. We do this, while the independent variables are deleted. Afterwards we restore the appropriate independent variables. Thus:

$$v^j(t)J_{j,a}(q^k(t)) \rightarrow v^j J_{j,a} \rightarrow \int \Delta\sigma K^j J_{j,a} \rightarrow \int \Delta\sigma K^j(q^k,t) J_{j,a}(q^k) \ . \qquad (176)$$

We ought to make sure that the ultimate independent variable is the same on both sides of (173) and also of (174). The left-hand sides depend only on the time t. And in fact, the right-hand sides have only t as the ultimate independent variable. In (173) this is assured, because the q^k depend on t. And in (174) this is assured, because the q^k get "integrated out".

The equations (173) and (174) tell us how the atom influences the electromagnetic field. In the form we have written them, they describe how the atom affects the individual mode excursions $Q_a(t)$. We may also write down equivalent equation for the vector potential field $c\bar{A}(\bar{r},t)$. To this end, we multiply each of the N equations (173) and (174) (one for each mode #a) by the corresponding transverse mode pattern $\bar{E}_a(\bar{r})$. Then we sum over the low modes #a. We use equation (91) (See Box #1 of Section 6), namely

$$(k_a)^2 \bar{E}_a = \bar{\nabla} \times (\bar{\nabla} \times \bar{E}_a) \ , \qquad \text{(91) repeated}$$

and equation (144), namely

$$c\bar{A}_{low}(\bar{r},t) = \sum_{a,low} Q_a(t) \bar{E}_a(\bar{r}) \ . \qquad \text{(144) repeated}$$

Then we obtain

Classically:

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_{low}(\bar{r},t) + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)) = \frac{1}{\varepsilon_o c} v^j(t) \sum_{a,low} J_{j,a}(q^k(t)) \bar{E}_a(\bar{r}), \qquad (177)$$

Quantum mechanically:

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_{low}(\bar{r},t) + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)) = \frac{1}{\varepsilon_o c} \int \Delta\sigma K^j(q^k,t) J_{j,a}(q^k) \bar{E}_a(\bar{r}). \qquad (178)$$

Next we introduce the abbreviation

$$\sum_{a,low} J_{j,a}(q^k) \bar{E}_a(\bar{r}) = \bar{J}_{j,T,low}(q^k,\bar{r}) \ , \qquad (179)$$

which is suggested by equation (145). Then equations (177) and (178) can be written in more compact form:

Classically:

$$\frac{\partial^2}{(\partial ct)^2}\, c\bar{A}_{low}(\bar{r},t) + \bar{\nabla} \times [\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)] = \frac{1}{\epsilon_o c}\, v^j(t)\bar{J}_{j,T,low}(q^k(t),\bar{r}) \ , \qquad (180)$$

Quantum mechanically:

$$\frac{\partial^2}{(\partial ct)^2}\, c\bar{A}_{low}(\bar{r},t) + \bar{\nabla} \times [(\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)] = \frac{1}{\epsilon_o c} \int \Delta\sigma K^j(q^k,t)\bar{J}_{j,T,low}(q^k,\bar{r}) \ . \qquad (181)$$

We may also reverse the procedure that led from (173) or (174) to (180) or (181). All we have to do is multiply (180) or (181) by the transverse mode pattern $\bar{E}_a(\bar{r})$, and then to integrate over the cavity. As far as the details of the calculation are converned, one uses the series expansions (144) and (179), and also the orthonormality relations (98). (See Box #5 of Section 6.) One also uses term-by-term integration and differentiation of the expansion series. This is certainly permissible, since all the series are finite.

We just went through a procedure that carried us from equations (173) and (174), the equations of motion for the mode excursions, to equations (180) and (181), the equations of motion for the vector potential field $c\bar{A}(\bar{r},t)$ as a whole. We could have gone through this procedure also in the action functional. In the case of classical dynamics for the atom, we have done it already, as we went from (146) to (147). When the atom is treated quantum-mechanically, the field-analog of (160) would have been

$$A_{\substack{a,b \\ \text{appr,quant.}}} = \int_{t=a}^{b} dt\{\int \Delta q^1 \Delta q^2 \ldots \Delta q^n M[[\frac{i\hbar}{2}(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} + \chi^{*j} \frac{\partial \psi}{\partial q^j} - \chi^j \frac{\partial \psi^*}{\partial q^j}) +$$

$$+ ((\frac{1}{2}\chi^{*j} M_{jk} \chi^k + \frac{1}{2}(\chi^j \psi^* + \chi^{*j}\psi)U_j - \psi^* \psi V))]] +$$

$$+ \frac{\varepsilon_o}{2} \iiint \Delta\tau [\frac{\partial}{\partial ct} c\bar{A}_{low}(\bar{r},t)] \cdot [\frac{\partial}{\partial ct} c\bar{A}_{low}(\bar{r},t)] -$$

$$- \frac{\varepsilon_o}{2} \iiint \Delta\tau [\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)] \cdot [\bar{\nabla} \times c\bar{A}_{low}(\bar{r},t)]\} \qquad (182)$$

For $U_j(q^k,t)$ in this expression, we would prefer, instead of (150), the equivalent formula

$$U_j(q^k,t) = \frac{1}{c} \iiint \Delta\tau \bar{J}_{j,T,low}(q^k,\bar{r}) \cdot c\bar{A}_{low}(\bar{r},t) \; . \qquad (183)$$

All the equations of motion for a free-running system follow from the action principle

$$\delta A_{a,b} = \text{E.T.O.} \qquad (51) \text{ repeated}$$

The transition from (173) and (174) to (180) and (181) in the equations of motion for the electromagnetic field does not produce any new results. It is merely a change in the mathematical idiom. However, it affords us some insight into the physical significance of the excitation terms, namely the right hand sides. In the classical equation (180) the excitation term (except for the factor $\frac{1}{\varepsilon_o c}$) is the low-modes portion of the transverse current density

$$\bar{J}_{T,low}(\bar{r},t) = v^j(t)\bar{J}_{j,T,low}(q^k(t),\bar{r}) \qquad (184)$$

In the quantum-mechanical equation (181), this quantity $\bar{J}_{T,low}(\bar{r},t)$ is replaced by its quantum-mechanical expectation value.

So far we have considered only one atom in the cavity. The next question that arises naturally is: How does one proceed when several or many atoms are present? We take up this question in the next section. We omit the classical

treatment of the atoms and proceed right away to the more interesting case in which the atoms are treated quantum-mechanically.

9. The Quantum-Mechanical Problem of Many Atoms.

In order to explain the principle of the method that we shall employ, we first discuss the case of just two atoms. We assume that the two atoms are far enough apart so that they do not influence each other directly. But they are permitted to interact with each other in an indirect way, namely through the low-modes portion of the vector potential field $c\bar{A}(\bar{r},t)$.

The first atom has n' degrees of freedom. Its configuration is described by the n' coordinates $q^{k'}$, (k' = 1,2, ... n'). The second atom has n" degrees of freedom. Its configuration is described by the n" coordinates $q^{k"}$, (k" = 1, 2, ... n"). The correct procedure would be to treat the two atoms as one super-atom with n = n' + n" degrees of freedom. One would then start with the action functional, e.g. of the form (182). But this procedure is much too unwieldy, especially so, when many more than two atoms are involved. Therefore, we shall look for some assumptions that will simplify the treatment. In order to spell out these assumptions, we have to devise a consistent scheme of notation. Single-primed symbols and symbols with single-primed indices refer to the first atom, while double-primed symbols and symbols with double-primed indices refer to the second atom. Unprimed symbols and symbols with unprimed indices refer to the super-atom. Single-primed, double-primed, and unprimed indices run respectively from 1 to n', from 1 to n", and from 1 to n = n' + n". We relabel the index set 1,2, ... n', n' + 1, n' + 2, ... n' + n" as

$$1', 2', \ldots n', 1", 2" \ldots n" .$$

One consequence of this relabeling is that the product of differentials $\Delta q^1 \Delta q^2 \ldots \Delta q^n$ that occurs in (182) can be rewritten as $(\Delta q^{1'} \Delta q^{2'} \ldots \Delta q^{n'})(\Delta q^{1''} \Delta q^{2''} \ldots \Delta q^{n''})$. Next we examine the matrix of the kinetic coefficients with elements M_{jk}. Because of the relabeling, this matrix becomes partitioned into four boxes, namely

$$\text{Matrix}(M_{jk}) = \left.\begin{array}{c|c} M_{j'k'} & M_{j'k''} \\ \hline M_{j''k'} & M_{j''k''} \end{array}\right. .$$

Since the two atoms do not interact with each other in a direct way, we conclude that the matrix elements $M_{j'k''}$, $M_{j''k'}$ in the off-diagonal boxes are zero. Thus

$$\text{Matrix}(M_{jk}) = \left.\begin{array}{c|c} M_{j'k'} & 0 \\ \hline 0 & M_{j''k''} \end{array}\right. . \tag{185}$$

A consequence of (185) is that the appropriate determinants satisfy the relation

$$\text{Det } M_{jk} = (\text{Det } M_{j'k'})(\text{Det } M_{j''k''}) \tag{186}$$

Then the quantity $M = (\text{Det } M_{jk})^{\frac{1}{2}}$ which occurs in (182) can be written as

$$M = M' M'' \tag{187}$$

in rather obvious notation. We note also that M' and the matrix elements $M_{j'k'}$ depend only on the $q^{\ell'}$, while M'' and the matrix elements $M_{j''k''}$ depend only on the $q^{\ell''}$. The nature of these dependences is the same that we find in the single atoms. Again, because of the appearance of the zeros in (185), we have

$$\chi^{*j} M_{jk} \chi^k = \chi^{*j'} M_{j'k'} \chi^{k'} + \chi^{*j''} M_{j''k''} \chi^{k''} . \tag{188}$$

But the $\chi^{k'}$ depend on both sets of coordinates $q^{\ell'}$, $q^{\ell''}$ and the time t. And so do the $\chi^{k''}$.

To continue with our examination of the terms that occur in (182), we note that

$$(\chi^{*j}\psi + \chi^j \psi^*)U_j = (\chi^{*j'}\psi + \chi^{j'}\psi^*)U_{j'} + (\chi^{*j''}\psi + \chi^{j''}\psi^*)U_{j''} \tag{189}$$

The quantity ψ in (189) depends on both sets of coordinates $q^{\ell'}$, $q^{\ell''}$ and the time t. However, the $U_{j'}$ depend only on the set $q^{\ell'}$, and the $U_{j''}$ depend only

on the set of $q^{k''}$. We see this when we examine equation (183), which defines the U_j. In this equation, there occur the quantities $\bar{J}_{j,T,low}(q^k,\bar{r})$, which are of purely kinematical origin, in that the low-modes portion of the current density in our home-space is given by

$$\bar{J}_{T,low}(\bar{r},t) = v^{j'}(t)\bar{J}_{j,T,low}(q^k(t),\bar{r})$$

After the relabeling that we introduced earlier this equation becomes

$$\bar{J}_{T,low}(\bar{r},t) = v^{j'}(t)\bar{J}_{j',T,low}(q^{k'}(t),q^{k''}(t),\bar{r}) + v^{j''}(t)\bar{J}_{j'',T,low}(q^{k'}(t),q^{k''}(t),\bar{r}) \qquad (190a)$$

Since the contribution to $\bar{J}_{T,low}$ made by the first atom (the first term in (190a) cannot depend on the configuration of the second atom, we conclude that $\bar{J}_{j',T,low}$ can depend only on the set $q^{k'}$. Similarly $\bar{J}_{j'',T,low}$ can depend only on the set $q^{k''}$. Equation (190a) thus becomes

$$\bar{J}_{T,low}(\bar{r},t) = v^{j'}(t)\bar{J}_{j',T,low}(q^{k'}(t),\bar{r}) + v^{j''}(t)\bar{J}_{j'',T,low}(q^{k''}(t),\bar{r}) \; . \qquad (190b)$$

The equations that define the $U_{j'}$ and $U_{j''}$ (see (183)) then become

$$U_{j'}(q^{k'},t) = \frac{1}{c}\iiint \Delta\tau \bar{J}'_{j',T,low}(q^{k'},\bar{r}) \cdot c\bar{A}_{low}(\bar{r},t) \; , \qquad (191a)$$

and

$$U_{j''}(q^{k''},t) = \frac{1}{c}\iiint \Delta r \bar{J}''_{j'',T,low}(q^{k''},\bar{r}) \cdot c\bar{A}_{low}(\bar{r},t) \; . \qquad (191b)$$

They show that the $U_{j'}$ can depend only on the set $q^{k'}$ and that the $U_{j''}$ can depend only on the set $q^{k''}$, as we already indicated by the way we wrote the left-hand sides.

Furthermore, since the two atoms do not interact directly, the potential $V(q^k)$ that occurs in (182) will be of the form

$$V(q^k) = V'(q^{k'}) + V''(q^{k''}) \; , \qquad (192)$$

where the two functions V' and V" are the potentials for the single atoms.

Now we are ready to incorporate our previous considerations into the action functional. We shorten the notation somewhat by the use of the volume element in configuration space. On combining (153) and (187), we have

$$\Delta\sigma = \Delta q^1 \Delta q^2 \ldots \Delta q^n M = (\Delta q^{1'} \Delta q^{2'} \ldots \Delta q^{n'} M')(\Delta q^{1''} \Delta q^{2''} \ldots \Delta q^{n''} M'') = \Delta\sigma' \Delta\sigma''$$

Also we use two integration signs in front of $\Delta\sigma'\Delta\sigma''$ in order to remind ourselves that we have to integrate over both configuration spaces. With these changes of notation equation (182) becomes

$$\begin{aligned} A_{\substack{a,b \\ appr,quant}} = \int_{t=a}^{b} dt \{ \iint \Delta\sigma' \Delta\sigma'' [[\tfrac{i\hbar}{2} (\psi^* \tfrac{\partial \psi}{\partial t} - \psi \tfrac{\partial \psi^*}{\partial t} + \chi^{*j'} \tfrac{\partial \psi}{\partial q^{j'}} + \chi^{*j''} \tfrac{\partial \psi}{\partial q^{j''}} - \\ - \chi^{j'} \tfrac{\partial \psi^*}{\partial q^{j'}} - \chi^{j''} \tfrac{\partial \psi^*}{\partial q^{j''}}) + ((\tfrac{1}{2} \chi^{*j'} M_{j'k'} \chi^{k'} + \tfrac{1}{2} \chi^{*j''} M_{j''k''} \chi^{k''} + \\ + \tfrac{1}{2} (\chi^{*j'} \psi + \chi^{j'} \psi^*) U_{j'} + \tfrac{1}{2} (\chi^{*j''} \psi + \chi^{j''} \psi^*) U_{j''} \\ - \psi^* \psi V' - \psi^* \psi V''))]] + \\ + \frac{\varepsilon_o}{2} \iiint \Delta\tau [\tfrac{\partial}{\partial ct} c\bar{A}_{low}] \cdot [\tfrac{\partial}{\partial ct} c\bar{A}_{low}] - \\ - \frac{\varepsilon_o}{2} \iiint \Delta\tau [\bar{\nabla} \times c\bar{A}_{low}] \cdot [\bar{\nabla} \times c\bar{A}_{low}] \} , \end{aligned} \tag{193}$$

where we have omitted the indication of the independent variables in order to keep the notation as short as possible.

And now we come to the statement of the assumptions we are going to make. We shall assume that the $(n' + n'' + 1)$ functions $\chi^{j'}(q^k,t)$, $\chi^{j''}(q^k,t)$, $\psi(q^k,t)$ are of a rather restricted form, namely that

$$\psi(q^k,t) = \psi'(q^{k'},t)\psi''(q^{k''},t) , \tag{194a}$$

$$\chi^{j'}(q^k,t) = \chi^{j'}(q^{k'},t)\psi''(q^{k''},t) , \tag{194b}$$

$$\chi^{j''}(q^k,t) = \chi^{j''}(q^{k''},t)\psi'(q^{k'},t) , \tag{194c}$$

(Similarly for the complex conjugates, the starred quantities.) Furthermore, the functions ψ' and ψ'' shall fulfill the normalization conditions

$$\int \Delta\sigma' \psi'^{*} \psi' = 1, \quad \int \Delta\sigma'' \psi''^{*} \psi'' = 1 \tag{195}$$

(Actually we need to postulate these normalization conditions only for one particular time, say $t = 0$. Then they will be satisfied at all times, since the Schrödinger equations for ψ', $\chi^{j'}$ and those for ψ'', $\chi^{j''}$ turn out to be satisfied. And this, in turn, guarantees the validity of the continuity equations of the type (159), once for the single-primed quantities and then again for the double-primed quantities. And when we integrate the continuity equations over the appropriate configuration spaces, we see that the normalization integrals of (195) do not depend on the time t.)

As we shall see, the assumptions (194a) - (195) will yield a workable action functional, from which - by way of the action principle - equations of motion can be derived that are well defined. Of course, because of the restricted nature of the quantum-mechanical functions as embodied by (194a) - (195), only a restricted class of system histories can be obtained from these equations of motion. The histories that are rejected by our assumptions are, though possible ones, not of technical importance at the moment.

When we use the equations (194a) - (194c), but not yet the equations (195), in the action functional (193), we obtain, after a reordering of the terms, the following expression:

$$A_{\substack{a,b\\ appr,quant}} = \int_{t=a}^{b} dt\{\iint \Delta\sigma' \Delta\sigma'' \psi^{*}{}'' \psi'' [[\frac{i\hbar}{2}(\psi^{*}{}' \frac{\partial \psi'}{\partial t} - \psi' \frac{\partial \psi^{*}{}'}{\partial t} + {}'\chi^{*j'} \frac{\partial \psi'}{\partial q^{j'}} - {}'\chi^{j'} \frac{\partial \psi^{*}{}'}{\partial q^{j'}}) +$$

$$+ ((\tfrac{1}{2}\, {}'\chi^{*j'} M_{j'k'} {}'\chi^{k'} + \tfrac{1}{2}({}'\chi^{*j'}\psi' + {}'\chi^{j'}\psi^{*}{}')U_{j'} - \psi^{*}{}'\psi' V'))]] +$$

$$+ \iint \Delta\sigma' \Delta\sigma'' \psi^{*}{}'' \psi' [[\frac{i\hbar}{2}(\psi^{*}{}'' \frac{\partial \psi''}{\partial t} - \psi'' \frac{\partial \psi^{*}{}''}{\partial t} + {}''\chi^{*j''} \frac{\partial \psi''}{\partial q^{j''}} - {}''\chi^{j''} \frac{\partial \psi^{*}{}''}{\partial q^{j''}}) +$$

$$+ ((\tfrac{1}{2}\, {}''\chi^{*j''} M_{j''k''} {}''\chi^{k''} + \tfrac{1}{2}({}''\chi^{*j''}\psi'' + {}''\chi^{j''}\psi^{*}{}'')U_{j''} - \psi^{*}{}''\psi'' V''))]] +$$

$$+ \frac{\varepsilon_o}{2} \iiint \Delta\tau [\frac{\partial}{\partial ct} c\bar{A}_{low}] \cdot [\frac{\partial}{\partial ct} c\bar{A}_{low}] -$$

$$- \frac{\varepsilon_o}{2} \iiint \Delta\tau [\bar{\nabla} \times c\bar{A}_{low}] \cdot [\bar{\nabla} \times c\bar{A}_{low}]\} . \qquad (196)$$

In the first configuration-space integral of (196) we first integrate over the double-primed space. Because of one of the normalization conditions (195), this portion of the integration yields unity. Thus there is only the integral over the single-primed space left. We proceed in a similar way in the second integral, where we first integrate over the single-primed space. Thus the expression (196) simplifies into

$$A_{\substack{a,b\\ appr,quant}} = \int_{t=a}^{b} dt\{\int \Delta\sigma' [[\frac{i\hbar}{2}(\psi^{*}{}' \frac{\partial \psi'}{\partial t} - \psi' \frac{\partial \psi^{*}{}'}{\partial t} + {}'\chi^{*j'} \frac{\partial \psi'}{\partial q^{j'}} - {}'\chi^{j'} \frac{\partial \psi^{*}{}'}{\partial q^{j'}}) +$$

$$+ ((\tfrac{1}{2}\, {}'\chi^{*j'} M_{j'k'} {}'\chi^{k'} + \tfrac{1}{2}({}'\chi^{*j'}\psi' + {}'\chi^{j'}\psi^{*}{}')U_{j'} - \psi^{*}{}'\psi' V'))]] +$$

$$+ \int \Delta\sigma'' [[\frac{i\hbar}{2}(\psi^{*}{}'' \frac{\partial \psi''}{\partial t} - \psi'' \frac{\partial \psi^{*}{}''}{\partial t} + {}''\chi^{*j''} \frac{\partial \psi''}{\partial q^{j''}} - {}''\chi^{j''} \frac{\partial \psi^{*}{}''}{\partial q^{j''}}) +$$

$$+ ((\tfrac{1}{2}\, {}''\chi^{*j''} M_{j''k''} {}''\chi^{k''} + \tfrac{1}{2}({}''\chi^{*j''}\psi'' + {}''\chi^{j''}\psi^{*}{}'')U_{j''} - \psi^{*}{}''\psi'' V''))]] +$$

$$+ \frac{\varepsilon_o}{2} \iiint \Delta\tau [\frac{\partial}{\partial ct} c\bar{A}_{low}] \cdot [\frac{\partial}{\partial ct} c\bar{A}_{low}] -$$

$$- \frac{\varepsilon_o}{2} \iiint \Delta\tau [\bar{\nabla} \times c\bar{A}_{low}] \cdot [\bar{\nabla} \times c\bar{A}_{low}]\} . \qquad (197)$$

We see that the quantum-mechanical portion of the action functional has been decomposed into two completely separated portions, one for each of the two atoms. A consequence of this observation is that the quantum-mechanical functions ψ', ${}'\chi^{j'}$ of the first atom satisfy their own pair of Schrödinger

equations, namely

$$i\hbar \frac{\partial \psi'}{\partial q^{j'}} + M_{j'k'} \, {}'\chi^{k'} + U_{j'} \psi' = 0 \ , \tag{198}$$

and

$$i\hbar \frac{\partial \psi'}{\partial t} + \frac{i\hbar}{2} \frac{1}{M'} \frac{\partial}{\partial q^{j'}} (M' {}'\chi^{j'}) + \frac{1}{2} U_{j'} {}'\chi^{j'} - V' \psi' = 0 \ , \tag{199}$$

in analogy to (161) and (165). Equations (198) and (199) ensue from the action principle in the usual manner, when we vary ${}'\chi^{*j'}$ and ${}'\psi^{*}$. Similar statements pertain to the second atom. The foregoing remarks do not imply however that the two atoms are completely independent from each other. For they interact through the low-modes portion of the vector potential field $c\bar{A}_{low}$, which is contained in the $U_{j'}$ and $U_{j''}$ according to (191a) and (191b). The equation that governs $c\bar{A}_{low}$ is obtained from the action principle, when we vary $c\bar{A}_{low}$. Of course, when we perform this variation, we must not forget that $c\bar{A}_{low}$ is contained in the $U_{j'}$ and $U_{j''}$. Then, with the abbreviations

$${}'K^{j'} = \frac{1}{2}({}'\chi^{*j'} \psi' + {}'\chi^{j'} \psi^{*}{}') \ , \tag{200}$$

and

$${}''K^{j''} = \frac{1}{2}({}''\chi^{*j''} \psi'' + {}''\chi^{j''} \psi^{*}{}'') \ , \tag{201}$$

in analogy to (158), we obtain

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_{low} + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_{low}) = \frac{1}{\varepsilon_o c} \int \Delta\sigma' \, {}'K^{j'} \, \bar{J}'_{j',T,low} +$$

$$+ \frac{1}{\varepsilon_o c} \int \Delta\sigma'' \, {}''K^{j''} \bar{J}''_{j'',T,low} \tag{202}$$

This equation resembles (181). However, each atom contributes separately and independently to the exciting term, the right-hand side.

We could have skipped the entire preceding discussion of this section. Instead we could have postulated (197) as a workable action functional. But

then we would not know what kind of assumptions lie behind this postulational approach. But now that we have recognized the assumptions, namely the restricted product form for the quantum-mechanical functions, we can use the postulational approach for the case of more than two atoms. Let us tag the atoms with the index p. Then, when we write down the analog of(197) we can afford to omit the index p for most of the symbols. Instead, we write it below the integration sign of the configuration-space integral. In this way, we imply that the p should be appended to each symbol behind the integration sign. This shortened notation should not cause any confusion. Then the generalization of (197) is:

$$
\begin{aligned}
A_{\substack{a,b \\ \text{appr,quant}}} = \int_{t=a}^{b} dt\{ \sum_{\text{atoms}\#p} \int_{p} \Delta\sigma[[\frac{i\hbar}{2}(\psi^* \frac{\partial\psi}{\partial t} - \psi \frac{\partial\psi^*}{\partial t} + \chi^{*j} \frac{\partial\psi}{\partial q^j} - \chi^j \frac{\partial\psi^*}{\partial q^j}) \\
+ ((\tfrac{1}{2}\chi^{*j} M_{jk} \chi^k + \tfrac{1}{2}(\chi^{*j}\psi + \chi^j\psi^*)U_j - \psi^*\psi V)))]] \\
+ \frac{\varepsilon_o}{2} \iiint \Delta\tau [\frac{\partial}{\partial ct} c\bar{A}_{low}] \cdot [\frac{\partial}{\partial ct} c\bar{A}_{low}] \\
- \frac{\varepsilon_o}{2} \iiint \Delta\tau [\bar{\nabla} \times c\bar{A}_{low}] \cdot [\bar{\nabla} \times c\bar{A}_{low}]\} \quad . \qquad (203)
\end{aligned}
$$

where

$$
{}_pU_j = \frac{1}{c} \iiint \Delta\tau \; {}_p\bar{J}_{j,T,low} \cdot c\bar{A}_{low} \quad . \qquad (204)
$$

With each atom #p there is associated its own pair of Schrödinger equations, which are built like (198) and (199). And the generalization of (202) is

$$
\frac{\partial^2}{(\partial ct)^2} c\bar{A}_{low} + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_{low}) = \frac{1}{\varepsilon_o c} \sum_{\text{atoms}\#p} \int_{p} \Delta\sigma \; K^j \bar{J}_{j,T,low} \qquad (205)
$$

This equation shows that each atom contributes separately to the exciting term. Each of these contributions is the quantum-mechanical expectation value of the current density for the atom in question, except for the factor $\frac{1}{\varepsilon_o c}$.

The equations of motion for the whole system consist of the pairs of Schrödinger equations, one for each atom (An example of such a pair is given by (198), (199)), and equation (205) for the vector potential. These equations are intertwined, because the Schrödinger equations contain the vector potential (by way of the U_j), and because equation (205) contains the quantum-mechanical functions (by way of the K^j). It is impossible in practice to solve such an intertwined system exactly. Therefore, one has to use approximate methods for the solution. The favorite method is the perturbation calculus, which we shall discuss in the next section.

10. The Perturbation Calculus .

We start with the action functional (203), in which we regard the term with the U_j as a perturbation. It is this term which causes the equations of motion to become intertwined. As is the custom, we multiply this term by an "expansion parameter" λ, which in the end we set equal to unity. We also expand the quantum-mechanical functions ψ, χ^j for each atom #p and the vector potential $c\bar{A}_{low}$ as power series in λ. Accordingly we write

$$(\psi)_p = (\psi_o + \lambda\psi_1 + \lambda^2\psi_2 + \ldots)_p \ , \tag{206}$$

$$(\chi^j)_p = (\chi^j_0 + \lambda\chi^j_1 + \lambda^2\chi^j_2 + \ldots)_p \ , \tag{207}$$

and similarly for the starred quantities. In the expansion for $c\bar{A}_{low}$, we delete the subscript "low" on the right-hand side, in order to keep the notation as concise as possible. Thus

$$c\bar{A}_{low} = c\bar{A}_0 + \lambda c\bar{A}_1 + \lambda^2 c\bar{A}_2 + \ldots \tag{208}$$

The terms with the index 0 constitute the zero-order approximation, those with index 1 constitute the first-order correction, and so on.

We insert the expansions (206) - (208) into the action functional (203) and multiply the terms with the U_j (which we write out according to (204)) by λ. In doing so, we multiply the inserted series term-by-term, but break off after the terms in λ^N (for the N^{th}-order perturbation calculus). We indicate this breaking-off by the prefix $[B(\lambda^N)]$. In our applications, we will be satisfied with the second-order perturbation calculus. Thus we break off after the terms in λ^2. The action functional (203) is then replaced by an approximation, which we denote by $A_{\substack{a,b \\ pert}}$ ("pert" for perturbation). We refrain from writing out the inserted series and the results of the multiplications in detail, and simply write

$$A_{\substack{a,b \\ pert}} = [B(\lambda^2)] \int_{t=a}^{b} dt\{ \sum_{\text{atoms}\ \#p} \int_{p} \Delta\sigma[[\frac{i\hbar}{2}(\psi^* \frac{\partial\psi}{\partial t} - \psi \frac{\partial\psi^*}{\partial t} + \chi^{*j} \frac{\partial\psi}{\partial q^j} - \chi^j \frac{\partial\psi^*}{\partial q^j})$$

$$+ ((\frac{1}{2}\chi^{*j}M_{jk}\chi^k - V\psi^*\psi + \frac{\lambda}{2}(\chi^{*j}\psi + \chi^j\psi^*)\frac{1}{c}\iiint\Delta\sigma \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_{low}))]]$$

$$+ \frac{\varepsilon_o}{2}\iiint\Delta\tau[\frac{\partial}{\partial ct} c\bar{A}_{low}] \cdot [\frac{\partial}{\partial ct} c\bar{A}_{low}]$$

$$- \frac{\varepsilon_o}{2}\iiint\Delta\tau[\bar{\nabla} \times c\bar{A}_{low}] \cdot [\bar{\nabla} \times c\bar{A}_{low}]\} \qquad (209)$$

This is a workable action functional.

When we apply the action principle, we can vary all the functions ψ_0, ψ_1, ψ_2 ... . $c\bar{A}$ independently. We start by varying the χ^{*j} for atom #p. Then, in the usual manner, we conclude that we must have

$$[B(\lambda^2)]\{(\delta\chi_0^{*j} + \lambda\delta\chi_1^{*j} + \lambda^2\delta\chi_2^{*j})[i\hbar(\frac{\partial\psi_o}{\partial q^j} + \lambda\frac{\partial\psi_1}{\partial q^j} + \lambda^2\frac{\partial\psi_2}{\partial q^j})$$

$$+ M_{jk}(\chi_0^k + \lambda\chi_1^k + \lambda^2\chi_2^k) + \lambda(\psi_0 + \lambda\psi_1)\frac{1}{c}\iiint\Delta\sigma \underset{j,T,low}{\bar{J}} \cdot (c\bar{A}_0 + \lambda c\bar{A}_1)]\}_p = 0$$

(210)

Here we have written out the series in detail. In the last term we could shorten the series, because of the factor λ in front of it. Now we remember that $\delta\chi_0^{*j}$, $\delta\chi_1^{*j}$, $\delta\chi_2^{*j}$ can be chosen independently. We also remember that we break off after the terms in λ^2. Then, on equating to zero the factor of $\delta\chi_2^{*j}$, we obtain

$$\lambda^2[i\hbar \frac{\partial\psi_0}{\partial q^j} + M_{jk}\chi_0^k]_p = 0 . \tag{211}$$

The factor λ^2 may be cancelled, of course. Next, we equate the factor of $\delta\chi_1^{*j}$ in (210) to zero. We obtain

$$\lambda[i\hbar \frac{\partial\psi_0}{\partial q^j} + M_{jk}\chi_0^k]_p + \lambda^2[i\hbar \frac{\partial\psi_1}{\partial q^j} + M_{jk}\chi_1^k + \psi_0 \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0 .$$

Now, the first term vanishes, because of (211). Then, after we cancel the factor λ^2, we obtain

$$[i\hbar \frac{\partial\psi_1}{\partial q^j} + M_{jk}\chi_1^k + \psi_0 \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0 . \tag{212}$$

Finally we equate the factor of $\delta\chi_0^{*j}$ in (210) to zero. We obtain

$$[i\hbar \frac{\partial\psi}{\partial q^j} + M_{jk}\chi_0^k]_p + \lambda[i\hbar \frac{\partial\psi_1}{\partial q^j} + M_{jk}\chi_1^k + \psi_o \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A} \,]_p +$$
$$+ \lambda^2[i\hbar \frac{\partial\psi_2}{\partial q^j} + M_{jk}\chi_2^k + \psi_o \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A} +$$
$$+ \psi_1 \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0 .$$

Now, the first and second terms vanish, because of (211) and (212). Then, after we cancel the factor λ^2, we obtain

$$[i\hbar \frac{\partial\psi_2}{\partial q^j} + M_{jk}\chi_2^k + \psi_0 \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_1 + \psi_1 \frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0$$

In the next step, we vary the ψ^* for atoms #p in (209). In the normal manner, which involves some integrations by parts, we conclude that we must have

$$[B(\lambda^2)]\{(\delta\psi_0^* + \lambda\delta\psi_1^* + \lambda^2\delta\psi_2^*)[i\hbar(\frac{\partial\psi_0}{\partial t} + \lambda\frac{\partial\psi_1}{\partial t} + \lambda^2\frac{\partial\psi_2}{\partial t})$$

$$+ \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M(\chi_0^j + \lambda\chi_1^j + \lambda^2\chi_2^j)) - V(\psi_o + \lambda\psi_1 + \lambda^2\psi_2)$$

$$+ \frac{\lambda}{2}(\chi_0^j + \lambda\chi_1^j)\frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} (c\bar{A}_0 + \lambda c\bar{A}_1)]\}_p = 0 \ . \qquad (214)$$

We apply the same step-by-step procedure that we used before. That is, we equate to zero first the factor of $\delta\psi_2^*$, then the factor of $\delta\psi_1^*$, finally the factor of $\delta\psi_0^*$. And at each step we use the results of the previous steps. Then we obtain

$$[i\hbar\frac{\partial\psi_0}{\partial t} + \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi_0^j) - V\psi_0]_p = 0 \ , \qquad (215)$$

$$[i\hbar\frac{\partial\psi_1}{\partial t} + \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi_1^j) - V\psi_1 + \frac{1}{2}\chi_0^j\frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0 \ , \qquad (216)$$

$$[i\hbar\frac{\partial\psi_2}{\partial t} + \frac{i\hbar}{2}\frac{1}{M}\frac{\partial}{\partial q^j}(M\chi_2^j) - V\psi_2 + \frac{1}{2}\chi_0^j\frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_1 +$$

$$+ \frac{1}{2}\chi_1^j\frac{1}{c}\iiint\Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0]_p = 0 \ . \qquad (217)$$

In the last step we vary $c\bar{A}_{low}$ in (209). In the usual manner, which involves some integrations by part we conclude that we must have

$$[B(\lambda^2)](\delta c\bar{A}_0 + \lambda\delta c\bar{A}_1 + \lambda^2\delta c\bar{A}_2)\cdot\{\sum_{\substack{\text{atoms}\\ \#p}}\int\Delta\sigma\frac{\lambda}{2}[(\chi_0^{*j} + \lambda\chi_1^{*j})(\psi_o + \lambda\psi_1) +$$

$$+ (\chi_0^j + \lambda\chi_1^j)(\psi_0^* + \lambda\chi_1^*)]\ \frac{1}{c}\underset{j,T,low}{\bar{J}} -$$

$$- \varepsilon_o\frac{\partial^2}{(\partial ct)^2}(c\bar{A}_0 + \lambda c\bar{A}_1 + \lambda^2 c\bar{A}_2) - \varepsilon_o\bar{\nabla}\times(\bar{\nabla}\times(c\bar{A}_0 + \lambda c\bar{A}_1 + \lambda^2 c\bar{A}_2))\} = 0 \ . \qquad (218)$$

Now we apply the same step-by-step procedure that we used twice before. It yields

$$- \varepsilon_o\frac{\partial^2}{(\partial ct)^2}c\bar{A}_0 - \varepsilon_o\bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_0) = 0 \ , \qquad (219)$$

$$- \varepsilon_o \frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 - \varepsilon_o \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) +$$

$$+ \sum_{\substack{\text{atoms} \\ \#p}} \int_p \Delta\sigma \, \frac{1}{2}(\chi_0^{*j}\psi_o + \chi_o^j \psi_o^*) \frac{1}{c} \bar{J}_{j,T,low} = 0 , \tag{220}$$

$$- \varepsilon_o \frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 - \varepsilon_o \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) +$$

$$+ \sum_{\substack{\text{atoms} \\ \#p}} \int_p \Delta\sigma \, \frac{1}{2}(\chi_0^{*j}\psi_1 + \chi_1^{*j}\psi_0 + \chi_0^j \psi_1^* + \chi_1^j \psi_0^*) \frac{1}{c} \bar{J}_{j,T,low} = 0 . \tag{221}$$

We may rewrite these equations in a way that appeals to our physical intuition. According to equations (200) and (201), the probability current density components $(K^j)_p$ for atom #p is given by

$$(K^j)_p = \frac{1}{2}(\chi^{*j}\psi + \chi^j \psi^*)_p . \tag{222}$$

On the right-hand side we use the expansions (206), (207). We use a similar expansion for the left-hand side, namely

$$(K^j)_p = (K_0^j + \lambda K_1^j + \lambda^2 K_2^j + \ldots)_p . \tag{223}$$

It will suffice for our purposes, if we break off the ensuing expressions after the term in λ^1. Then equation (222) becomes

$$(K^j{}_0 + \lambda K_1^j)_p = [B(\lambda)]\frac{1}{2}[(\chi_0^{*j} + \lambda\chi_1^{*j})(\psi_0 + \lambda\psi_1) + (\chi_0^j + \lambda\chi_1^j)(\psi_0^* + \lambda\psi_1^*)]_p .$$

Comparing the terms in λ^0 and λ^1, we read out

$$(K_0^j)_p = \frac{1}{2}(\chi_0^{*j}\psi_0 + \chi_0^j \psi_0^*) , \tag{224}$$

$$(K_1^j)_p = \frac{1}{2}(\chi_0^{*j}\psi_1 + \chi_1^{*j}\psi_0 + \chi_0^j \psi_1^* + \chi_1^j \psi_0^*) . \tag{225}$$

Then, instead of (219) - (221), we can write after an obvious rearrangement

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_0 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_0) = 0 , \tag{226}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) = \frac{1}{\varepsilon_o c} \sum_{\text{atoms } \#p} \int_p \Delta\sigma K_0^j \; \bar{J}_{j,T,\text{low}} \,, \tag{227}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) = \frac{1}{\varepsilon_o c} \sum_{\text{atoms } \#p} \int_p \Delta\sigma K_1^j \; \bar{J}_{j,T,\text{low}} \,. \tag{228}$$

We see that the exciting terms for the first and second order correction to the vector potential are the zero-order atomic current density and the first-order correction to it respectively (except for the factor $\frac{1}{\varepsilon_o c}$).

We summarize the results of this section by writing down the equations of motion we have derived, only this time in the order in which they are applied. We can delete equations (213) and (217), since they determine only the second order corrections to the atomic structures, in which we are not interested. The center of our interest is the electromagnetic field, because of its technical importance. And here it is mainly the second order correction that we need to know. For it constitutes the response to the excitation provided by the zero-order approximation to the electromagnetic field. To begin with, we have the equations of motion for the zero-order approximation, namely

$$\left(i\hbar \frac{\partial}{\partial q^j} \psi_o + M_{jk} \chi_0^k\right)_p = 0 \,, \tag{229}$$

$$\left(i\hbar \frac{\partial \psi_0}{\partial t} + \frac{i\hbar}{2} \frac{1}{M} \frac{\partial}{\partial q^j} (M\chi_0^j) - V\psi_0\right)_p = 0 \,, \tag{230}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_0 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_0) = 0 \tag{231}$$

Usually we do not have to solve these equations, because the solutions are given to us as the starting point of a technical problem. Then we determine the first order corrections from the following set of equations.

$$(i\hbar \frac{\partial \psi_1}{\partial q^j} + M_{jk}\chi_1^k)_p = -(\psi_o \frac{1}{c} \iiint \Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0)_p , \tag{232}$$

$$(i\hbar \frac{\partial \psi_1}{\partial t} + \frac{i\hbar}{2} \frac{1}{M} \frac{\partial}{\partial q^j} (M\chi^j) - V\psi_1)_p = -\frac{1}{2}(\chi_0^j \frac{1}{c} \iiint \Delta\tau \underset{j,T,low}{\bar{J}} \cdot c\bar{A}_0)_p , \tag{233}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) = \frac{1}{\varepsilon_o c} \sum_{\text{atoms } \#p} \int_p \Delta\sigma \frac{1}{2}(\chi_0^{*j}\psi_0 + \chi_0^j\psi_0^*) \underset{j,T,low}{\bar{J}} \tag{234}$$

The pair of Schrödinger equations (229), (230) and the pair (232), (233) have similar structures. The only difference is that inhomogeneous exciting terms have been added in the latter pair. Equation (234) is not of great importance in our technical applications, because $c\bar{A}_1$ does not depend on the "incident" field $c\bar{A}_o$, Finally we have the important equation for the second order correction $c\bar{A}_2$, namely

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) =$$

$$= \frac{1}{\varepsilon_o c} \sum_{\text{atoms } \#p} \int_p \Delta\sigma \frac{1}{2}(\chi_0^{*j}\psi_1 + \chi_1^{*j}\psi_0 + \chi_0^j\psi_1^* + \chi_1^j\psi_0^*) \underset{j,T,low}{\bar{J}} . \tag{235}$$

In order to use it we have to first determine the solutions of (232), (233) and their complex conjugates.

Sometimes it may be helpful to rewrite the equations (232) - (235) in such a way that only the symbol $\bar{J}_j$ appears in them, instead of the symbol $\bar{J}_{j,T,low}$. The reason for this is that analytical expressions for $\bar{J}_j$ are more easily formulated than those for $\bar{J}_{j,T,low}$. In order to explain the modification that we are going to make, we review the definition of $\bar{J}_{j,T,low}$. We had (see equation (132))

$$\bar{J}_j = \sum_a J'_{j,a}\bar{F}_a + \sum_a J_{j,a}\bar{E}_a . \tag{236}$$

By definition, $\bar{J}_{j,T,low}$ is the low-modes portion of the transverse part of $\bar{J}_j$, so that

$$\bar{J}_{j,T,low} = \sum_{a,low} J_{j,a}\bar{E}_a \tag{237}$$

By assumption, $c\bar{A}_0$ is purely transverse and its high-modes portion vanishes. This statement implies that $c\bar{A}_0$ may be expressed in the series

$$c\bar{A}_0 = \sum_{a,low} Q_{a,o}\bar{E}_a \ . \tag{238}$$

According to the orthonormality theorems (98), (100) of Box #5, all those terms in the series (236) that are not contained in the series (237) contribute zero to the integrals in (232) and (233). Thus we may delete the subscripts T, low in these integrals.

However, this mere deletion is not permissible in equations (234), (235). Here we must proceed in a different way if we wish to rewrite these equations in terms of $\bar{J}_j$ instead of $\bar{J}_{j,T,low}$. We start with equation (237). This time we write in the independent variables. Thus

$$\bar{J}_{j,T,low}(q^k,\bar{r}) = \sum_{a,low} J_{j,a}(q^k)\bar{E}_a(\bar{r}) \ . \tag{239}$$

We express the expansion coefficients in terms of integrals taken over the home-space. We obtain

$$J_{j,a}(q^k) = \iiint \Delta\tau' (\bar{E}_a(\bar{r}') \cdot \bar{J}_{j,T,low}(q^k,\bar{r}')$$

Here we have affixed primes to $\Delta\tau$ and $\bar{r}$ in order to avoid confusion in the equations that follow. For the reasons that were explained in the paragraph following equation (238), we may delete the subscripts T and low. Thus our last equation becomes

$$J_{j,a}(q^k) = \iiint \Delta\tau' \bar{E}_a(\bar{r}') \cdot \bar{J}_j(q^k,\bar{r}') \ . \tag{240}$$

On combining (237) and (240), we obtain

$$\bar{J}_{j,T,low}(q^k,\bar{r}') = \sum_{a,low} \bar{E}_a(\bar{r}) \iiint \Delta\tau' \bar{E}_a(\bar{r}') \cdot \bar{J}_j(q^k,\bar{r}') ,$$

or

$$\bar{J}_{j,T,low}(q^k,\bar{r}) = \iiint \Delta\tau' [\sum_{a,low} \bar{E}_a(\bar{r}) \bar{E}_a(\bar{r}') \cdot \bar{J}_j(q^k,\bar{r}') . \qquad (241)$$

This equation shows that $\bar{J}_{j,T,low}$ is obtained from $\bar{J}_j$ by means of a linear operation, called a projection (into the sub-space spanned by the low-modes patterns $\bar{E}_a$). We denote this projection by the symbol $P_{T,low}$. Then the shorthand notation for (241) will be

$$\bar{J}_{j,T,low} = P_{T,low} \bar{J}_j \qquad (242)$$

Now we come to the integrals in (234) and (235). Here we use (242). The integral in (234) becomes

$$\int_p \Delta\sigma \, \frac{1}{2} (\chi_0^{*j} \psi_0 + \chi_0^j \psi_0^*) P_{T,low} \bar{J}_j$$

But the projection $P_{T,low}$, being an integration over the home-space (according to (241)) may be interchanged with the integration over the configuration space, so that the integral becomes

$$P_{T,low} \int_p \Delta\sigma \, \frac{1}{2} (\chi_0^{*j} \psi_0 + \chi_0^j \psi_0^*) \bar{J}_j .$$

We may even interchange the projection and the summation over the atoms #p. Similar statements apply to the integral in (235). Therefore, equations (232) - (235) may be replaced by

$$(i\hbar \frac{\partial \psi_1}{\partial q^j} + M_{jk}\chi_1^k)_p = -(\psi_0 \frac{1}{c}\iiint \Delta r \bar{J}_j \cdot c\bar{A}_0)_p , \tag{243}$$

$$(i\hbar \frac{\partial \psi_1}{\partial t} + \frac{i\hbar}{2M}\frac{\partial}{\partial q^j}(M\chi_1^j) - V\psi_1)_p = -\frac{1}{2}(\chi_0^j \frac{1}{c}\iiint \Delta\tau \bar{J}_j \cdot c\bar{A}_0)_p , \tag{244}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) = \frac{1}{\varepsilon_o c} P_{T,low} \sum_{\text{atoms } \#p} \int_p \Delta\sigma \frac{1}{2}(\chi_0^{*j}\psi_0 + \chi_0^j \psi_0^*)\bar{J}_j , \tag{245}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) =$$

$$= \frac{1}{\varepsilon_o c} P_{T,low} \sum_{\text{atoms } \#p} \int_p \Delta\sigma \frac{1}{2}(\chi_0^{*j}\psi_1 + \chi_1^{*j}\psi_0 + \chi_0^j \psi_1^* + \chi_1^j \psi_0^*)\bar{J}_j . \tag{246}$$

The main part of our report is based on these equations. Of course, they are to be supplemented by the equations (229) - (231) for the zero-order approximations.

It may be helpful to rewrite equations (243) - (246) in a more abbreviated form, in which they may appeal to the physical intuition. To this end, we introduce the abbreviation

$$(U_{j,o})_p = (\frac{1}{c}\iiint \Delta\tau \bar{J}_j \cdot c\bar{A}_o)_p . \tag{247}$$

The quantity $(U_{j,o})_p$ is the vector potential component #j in the configuration space of atom #p. The index 0 indicates that $(U_{j,o})$ is based on the zero-order approximation $c\bar{A}_o$ to the electromagnetic field. Furthermore, we abbreviate the two integrals in (245) and (246) by $\langle \bar{J}_o \rangle_p$ and $\langle \bar{J}_1 \rangle_p$. These two quantities are the zero-order approximation and first-order correction to the quantum-mechanical expectation values (as indicated by the carets < >) of the atomic electric current density (in our home-space) of atom #p. With these abbreviations, equations (243) - (246) assume the form

$$\left(i\hbar \frac{\partial \psi_1}{\partial q^j} + M_{jk} x_1^k\right)_p = -\left(\psi_0 U_{j,o}\right)_p , \tag{248}$$

$$\left(i\hbar \frac{\partial \psi_1}{\partial t} + \frac{i\hbar}{2M} \frac{\partial}{\partial q^j} (M x^j) - V\psi_1\right)_p = -\frac{1}{2}\left(x_0^j U_{j,o}\right)_p , \tag{249}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_1) = \frac{1}{\epsilon_o c} P_{T,low} \sum_{\substack{\text{atoms} \\ \#p}} \langle \bar{J}_o \rangle_p , \tag{250}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla} \times (\bar{\nabla} \times c\bar{A}_2) = \frac{1}{\epsilon_o c} P_{T,low} \sum_{\substack{\text{atoms} \\ \#p}} \langle \bar{J}_1 \rangle_p . \tag{251}$$

In fact, someone who is not too concerned about mathematical proofs would be inclined to write down these equations at the outset of an investigation. He could well say to himself: Things just have to be that way, they cannot be otherwise. Perhaps he may have forgotten to include the projection operator $P_{T,low}$. But, after some reflection, he would have spotted the need for it, otherwise $c\bar{A}_1$ and $c\bar{A}_2$ would not turn out to be purely transverse and devoid of the bothersome contributions of the high modes.

11. The Special Case of Free Electrons.

The atoms (or molecules) that we have considered so far are, in general, composite entities consisting of several particles (electrons and nuclei). Now we are going to examine an especially simple example, in which each of these entities consists of a single free electron; no nuclei are present. The electron will be treated non-relativistically and quantum-mechanically. In this simple example, the configuration space of each electron may be considered as being identical with our three-dimensional home-space. We may therefore identify the three configurational coordinates q^1, q^2, q^3 of a given electron with the three cartesian coordinates x, y, z of its position. And we may combine q^1, q^2, q^3 into the position vector $\bar{q} = q^1\bar{e}_1 + q^2\bar{e}_2 + q^3\bar{e}_3$, where the $\bar{e}_j$ are the cartesian unit vectors. The configuration of the electron is then characterized by its position vector $\bar{q}$. We may therefore choose a more appropriate notation for the function $\rho(q^i,\bar{r})$ of Section 1) and the functions $\bar{J}_j(q^i,\bar{r})$ of equation (5). The new notation will be $\rho(\bar{q},\bar{r})$ and $\bar{J}_j(\bar{q},\bar{r})$. Because the charge (-e) of an electron ($e = 1.6 \times 10^{-19}$ coul) is concentrated in a single point, the functions $\rho(\bar{q},\bar{r})$ and $\bar{J}_j(\bar{q},\bar{r})$ have a particularly simple form, namely

$$\rho(\bar{q},\bar{r}) = (-e)\delta(\bar{q}-\bar{r}) \ , \tag{252}$$

and

$$\bar{J}_j(\bar{q},\bar{r}) = (-e)\delta(\bar{q}-\bar{r})\ \bar{e}_j, \ j = 1, 2, 3 \ , \tag{253}$$

where $\delta(\bar{q}-\bar{r})$ is the three-dimensional Dirac delta-function (really a distribution, whose meaning is given in terms of integrals). It has the following properties:

$$\left.\begin{aligned} &\delta(\bar{q}-\bar{r}) = 0 \text{ for } \bar{q} \neq \bar{r} \ , \\ &\iiint \Delta\tau_q \, \delta(\bar{q}-\bar{r}) f(\bar{q}) = f(\bar{r}) \ , \\ &\iiint \Delta\tau_r \, \delta(\bar{q}-\bar{r}) f(\bar{r}) = f(\bar{q}) \ , \end{aligned}\right\} \tag{254}$$

for any arbitrary smooth function f.

We can now proceed to adapt equations (243)-(246) to the case of free electrons. First of all, since each electron #p is free, the function V is zero. Of course, we neglect the direct interaction of the electrons with each other, just as we did for the atoms. This is permissible if the electron density is not too great. In the second place, the coefficients M_{jk} in (243) have rather simple values. Here we go back to the dicussion that followed equations (125, repeated) and (141, repeated), which may be found after equation (145). There we see that the expression $\frac{1}{2}\frac{dq^j}{dt} M_{jk} \frac{dq^k}{dt}$ is equal to the conventional kinetic energy of an electron. And since we are using cartesian coordinates as the q^j, we conclude that $M_{jk} = 0$ for $j \neq k$, and $M_{jk} = m$ for $j = k$, where m is the conventional electronic mass. Then with the aid of (253) and (254), equation (243) becomes

$$(ih\frac{\partial \psi_1}{\partial q^j} + m\chi_1^j)_p = -(-e)\frac{1}{c}(\psi_o \bar{e}_j \cdot c\bar{A}_o)_p .$$

We may regard $\frac{\partial \psi_1}{\partial q^j}$ and χ^j as the cartesian components #j of the vectors $\bar{\nabla}\psi_1$ and $\bar{\chi}_1$. The last equation we wrote stands for three equations, one for each of the three values 1, 2, 3 of the index j. We can combine these three equations into one vectorial equation, namely

$$(ih\bar{\nabla}\psi_1 + m\bar{\chi}_1)_p = -(-e)\frac{1}{c}(\psi_o c\bar{A}_o)_p, \qquad (255)$$

So far the independent variables on which the functions in (255) depend are $(\bar{q})_p$,t. (The $\bar{r}$ that occurred in (253) disappeared by virtue of the integration over the home-space.) But since the configuration space of each electron #p is identical with our home-space, we may just as well use $\bar{r}$,t as the independent variables.

We use the delta-function expression (253) for the $\bar{J}_j$ in the remaining equations (244) - (246). And we also use vectorial notation. For convenience we add the equations for the zero-order approximations $(\psi_o)_p$, $(\bar{\chi}_o)_p$, and $c\bar{A}_o$. We then arrive at the following system of equations, where, as before, the subscript p indicates that the quantum-mechanical functions refer to electron #p.

$$(i\hbar\bar{\nabla}\psi_o + m\bar{\chi}_o)_p = 0 \ , \tag{256}$$

$$(i\hbar \frac{\partial \psi_o}{\partial t} + \frac{i\hbar}{2}\bar{\nabla}\cdot\bar{\chi}_o)_p = 0 \ , \tag{257}$$

$$(i\hbar\bar{\nabla}\psi_1 + m\bar{\chi}_1)_p = -(\psi_o)_p \frac{1}{c}(-e)c\bar{A}_o \ , \tag{258}$$

$$(i\hbar \frac{\partial \psi_1}{\partial t} + \frac{i\hbar}{2}\bar{\nabla}\cdot\bar{\chi}_1)_p = -\frac{1}{2}(\bar{\chi}_o)_p \cdot \frac{1}{c}(-e)c\bar{A}_o \ , \tag{259}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_o + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_o) = 0 \ , \tag{260}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_1 + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_1) = \frac{1}{\varepsilon_o c} P_{T,low} \sum_{\substack{\text{electrons} \\ \#p}} (-e)\frac{1}{2}(\bar{\chi}_o^*\psi_o + \bar{\chi}_o\psi_o^*)_p \ , \tag{261}$$

$$\frac{\partial^2}{(\partial ct)^2} c\bar{A}_2 + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_2) = \frac{1}{\varepsilon_o c} P_{T,low} \sum_{\substack{\text{electron} \\ \#p}} (-e)\frac{1}{2}(\bar{\chi}_o^*\psi_1 + \bar{\chi}_1^*\psi_o + \bar{\chi}_o\psi_1^* + \bar{\chi}_1\psi_0^*) \tag{262}$$

Note that the projection operator $P_{T,low}$, which selects the low-modes part of the transverse portion, appears in (261) and (262). Again we observe that the excitation terms for the vector potentials $c\bar{A}_1$ and $c\bar{A}_2$ are (apart from the operation $P_{T,low}$ and the factor $\frac{1}{\varepsilon_o c}$) the quantum-mechanical expectation values of the current densities. Equation (256) - (262) are the basis of the main part of this report.

It may be helpful to adapt also the expression (203) for the action functional to the case of free electrons, so that equations (256) - (262) may be

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*As we did it before, we have omitted the subscript "low" of the symbols $c\bar{A}_0$, $c\bar{A}_1$, $c\bar{A}_2$.

derived also directly without the detour through the problem of composite atoms. In this derivation one uses the same rules of the calculus of variations and of the calculus of perturbations that we have employed before. For the sake of convenience, we replace the triple integrals $\iiint$ by a single integral $\int$. On the other hand, for the sake of clearness, we will have to indicate the independent variables. In (203) there occur the quantities $U_j(\bar{q},t)$, which are given by (204). We repeat the latter equation, but omit the index p.

$$U_j(\bar{q},k) = \frac{1}{c}\int \Delta\tau \; c\bar{A}_{low}(\bar{r},t) \cdot \bar{J}_{j,T,low}(\bar{q},\bar{r}) \; . \qquad \text{(204), repeated}$$

Then, with (241), we obtain

$$U_j(\bar{q},t) = \frac{1}{c}\iint \Delta\tau\,\Delta\tau' c\bar{A}_{low}(\bar{r},t) \cdot \sum_{a,low} \bar{E}_a(\bar{r})\bar{E}_a(\bar{r}') \cdot \bar{J}_j(\bar{q},\bar{r}') \; .$$

Now we use the delta-function expression (253) for $\bar{J}_j(\bar{q},\bar{r}')$. It permits us to perform the integration over $\bar{r}'$ in a simple way. The result is

$$U_j(\bar{q},t) = \frac{1}{c}(-e)\int \Delta\tau \; c\bar{A}_{low}(\bar{r},t) \cdot \sum_{a,low} \bar{E}_a(\bar{r})\bar{E}_a(\bar{q}) \cdot \bar{e}_j \; .$$

Now, $U_j(\bar{q},t)$ is the cartesian component #j of the vector $\bar{U}(\bar{q},t)$. This vector is therefore given by

$$\bar{U}(\bar{q},t) = \frac{1}{c}(-e)\int \Delta\tau\, c\bar{A}_{low}(\bar{r},t) \cdot \sum_{a,low} \bar{E}_a(\bar{r})\bar{E}_a(\bar{q}) \; ,$$

or, with a change of notation for the independent variables,

$$\bar{U}(\bar{r},t) = \frac{1}{c}(-e)\int \Delta\tau' c\bar{A}_{low}(\bar{r}',t) \cdot \sum_{a,low} \bar{E}_a(\bar{r}')\bar{E}_a(\bar{r}) \; .$$

We write this equation more succintly as

$$\bar{U} = \frac{1}{c}(-e)\int \Delta\tau' c\bar{A}'_{low} \cdot \sum_{a,low} \bar{E}'_a\bar{E}_a \qquad (263)$$

We use this expression in (203). At the same time we make the changes of notation that we made before. For instance, we use the vector $\bar{\chi}$ instead of its cartesian components χ^j, and we introduce the electronic mass m. Of course, we set V equal to zero, since we are dealing with free electrons. The final result is

$$A_{\substack{a,b \\ appr,quant}} = \int_{t=a}^{b} dt\{\frac{\varepsilon_o}{2}\int\Delta\tau[\frac{\partial}{\partial ct}c\bar{A}_{low}]\cdot[\frac{\partial}{\partial ct}c\bar{A}_{low}] -$$

$$- \frac{\varepsilon_o}{2}\int\Delta\tau[\bar{\nabla}\times c\bar{A}_{low}]\cdot[\bar{\nabla}\times c\bar{A}_{low}] +$$

$$+ \sum_{\substack{electrons \\ \#p}}[[\int\Delta\tau[\frac{i\hbar}{2}(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t} + \bar{\chi}^*\cdot\bar{\nabla}\psi - \bar{\chi}\cdot\bar{\nabla}\psi^*) +$$

$$+ \frac{m}{2}\bar{\chi}^*\cdot\bar{\chi}]_p + \frac{1}{c}(-e)\iint\Delta\tau'\Delta\tau\, c\bar{A}'_{low}\cdot\sum_{a,low}\bar{E}'_a\bar{E}_a\cdot\tfrac{1}{2}(\bar{\chi}^*\psi + \bar{\chi}\psi^*)_p]]\} \tag{264}$$

When we apply the action principle to this action functional, we obtain the following set of equations in the usual manner:

$$i\hbar\bar{\nabla}\psi_p + m\bar{\chi}_p + \psi_p\frac{1}{c}(-e)\int\Delta\tau'\sum_{a,low}\bar{E}_a\bar{E}'_a\cdot c\bar{A}'_{low} = 0\ ,$$

$$i\hbar\frac{\partial\psi_p}{\partial t} + \frac{i\hbar}{2}\bar{\nabla}\cdot\bar{\chi}_p + \frac{1}{2c}(-e)\bar{\chi}_p\cdot\int\Delta\tau'\sum_{a,low}\bar{E}_a\bar{E}'_a\cdot c\bar{A}'_{low} = 0\ ,$$

$$\frac{\partial^2}{(\partial ct)^2}c\bar{A}_{low} + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_{low}) = \frac{1}{\varepsilon_o c}(-e)\sum_{\substack{electrons \\ \#p}}\int\Delta\tau'\sum_{a,low}\bar{E}_a\bar{E}'_a\cdot(\bar{\chi}'^*_p\psi'_p + \bar{\chi}'_p\psi'^*_p) =$$

$$= \frac{1}{\varepsilon_o c}(-e)\rho_{T,low}\sum_{\substack{electrons \\ \#p}}\tfrac{1}{2}(\bar{\chi}^*_p\psi_p + \bar{\chi}_p\psi^*_p)\ .$$

To obtain the last equation we had interchanged the primed and unprimed coordinates in the double integral of (264). Since $c\bar{A}_{low}$ is a superposition of terms comprising only the low transverse modes, we have

$$\int\Delta\tau'\sum_{a,low}\bar{E}_a\bar{E}'_a\cdot c\bar{A}'_{low} = c\bar{A}_{low}\ . \tag{265}$$

Thus, the set of three equations simplifies to

$$i\hbar\bar{\nabla}\psi_p + m\bar{\chi}_p = -\psi_p\frac{1}{c}(-e)c\bar{A}_{low}\ , \tag{266}$$

$$i\hbar\frac{\partial\psi_p}{\partial t} + \frac{i\hbar}{2}\bar{\nabla}\cdot\bar{\chi}_p = \frac{1}{2c}(-e)\bar{\chi}_p\cdot c\bar{A}_{low}\ , \tag{267}$$

$$\frac{\partial^2}{(\partial ct)^2}c\bar{A}_{low} + \bar{\nabla}\times(\bar{\nabla}\times c\bar{A}_{low}) = \frac{1}{\varepsilon_o c}(-e)\rho_{T,low}\sum_{\substack{electrons \\ \#p}}\tfrac{1}{2}(\bar{\chi}^*_p\psi_p + \bar{\chi}_p\psi^*_p) \tag{268}$$

These three equations are the exact equations of motion for the action functional (264), whereas the set (256) - (262) results from the perturbation calculus. Equation (268) shows that the excitation term for the vector potential is the quantum-mechanical expectation value of the current density, except for the factor $\frac{1}{\epsilon_o c}$. Of course, we must not forget to use the projection operator $P_{T,low}$. Its presence ensures that $c\bar{A}_{low}$ continues to be a linear combination of low transverse modes only, if it started out that way.

If we combine equations (266) and (267) we arrive at the usual form of the Schrödinger equation for electron #p, namely

$$i\hbar \frac{\partial}{\partial t} \psi_p = \frac{1}{2m} (-i\hbar\bar{\nabla} - \frac{1}{c}(-e)c\bar{A}_{low}) \cdot (-i\hbar\bar{\nabla} - \frac{1}{c}(-e)c\bar{A}_{low})\psi_p \ . \qquad (269)$$

In the entire development of this section we have treated each electron as an independent entity, just as we did it for the atoms that were described by (203). In mathematical terms, this means that we regarded the quantum-mechanical functions of the many-electron problem as products of single-electron functions in the manner of equations (194a) - (194c). This is not quite correct because our procedure did not take account of the Pauli exclusion principle, which requires that, instead of products, we should have used determinants. But the pursuit of this matter is probably not worth the effort.

Note #1. Derivation of the Relation $\frac{\partial}{\partial q^i}\bar{J}_j - \frac{\partial}{\partial q^j}\bar{J}_i = \bar{\nabla}\times(\frac{1}{\rho}\bar{J}_i \times \bar{J}_j)$.

We start with the requirement that a tagged element of charge which happens to be at position $\bar{r}$ for the atomic configuration $\{q^i\}$ ought to move with a velocity $\bar{w}$ given by

$$\rho\bar{w} = \bar{J} \ , \qquad (N1,1)$$

where, of course, ρ and $\bar{J}$ are evaluated at $(q^i,\bar{r})$.

Next we consider a particular element which happens to be at the position $\bar{a}(q^i)$ in our home-space when the atomic configuration is $\{q^i\}$. We chose the symbol $\bar{a}$, not $\bar{r}$, because $\bar{r}$ stood for the generic position, which ranges over the whole room that contains the atom and the radiation field, whereas $\bar{a}$ refers to just one discrete and tagged point. Now we evaluate the velocity $\frac{d}{dt}\bar{a}$ of this tagged point. Here we have to be careful with the notation for partial derivatives. We have used the symbol $\frac{\partial}{\partial q^i}$ when the q^i and $\bar{r}$ were the independent variables. But $\bar{a}$ depends only on the q^i, the $\bar{r}$ does not enter. So when only the q^i (not the q^i and $\bar{r}$) are the independent variables, we use the symbol $\frac{\not\partial}{\not\partial q^i}$ ("$\not\partial$ slash") to denote partial derivatives. Then we have

$$\frac{d}{dt}\bar{a} = \frac{\not\partial\bar{a}}{\not\partial q^i}\frac{dq^i}{dt} = \frac{\not\partial\bar{a}}{\not\partial q^i}v^i \ . \qquad (N1,2)$$

But according to (N1,1) we should have

$$\frac{d}{dt}\bar{a} = \frac{1}{\rho(q^j,\bar{a}(q^j))}\bar{J}(q^j,\bar{a}(q^j)) = \frac{1}{\rho(q^j,\bar{a}(q^j))}\bar{J}_i(q^j,\bar{a}(q^j))v^i \ , \qquad (N1,3)$$

where we indicated, how the ρ and $\bar{J}_i$ depend on the n configurational coordinates q^j. This dependence is not only explicit, as indicated by the first q^j in $(q^j,\bar{a}(q^j))$, but also implicit by way of the position $\bar{r} = \bar{a}(q^j)$, as indicated by the second q^j in $(q^j,\bar{a}(q^j))$. On comparing (N1,1) with (N1,3) and remembering that the v^i might be any arbitrary set of configurational velocity components we obtain

$$\frac{\partial \bar{a}}{\partial q^i} = \frac{1}{\rho(q^j, \bar{a}(q^j))} \bar{J}_i(q^j, \bar{a}(q^j)) \ . \qquad (N1,4)$$

Now we take the partial derivative of this equation with respect to q^j, i.e. we take $\frac{\partial}{\partial q^j}$, (not $\frac{\partial}{\partial q^j}$). Here we must remember that the dependence on the q^j is not only explicit, but also implicit. In order to make the ensuing equation less cumbersome to write, we leave out the symbol $(q^j, \bar{a}(q^j))$ for the independent variables. We obtain

$$\frac{\partial}{\partial q^j} \frac{\partial \bar{a}}{\partial q^i} = \frac{\partial}{\partial q^j} \left(\frac{1}{\rho} \bar{J}_i\right) + \frac{\partial \bar{a}}{\partial q^j} \cdot \bar{\nabla} \left(\frac{1}{\rho} \bar{J}_i\right) \ .$$

We express the $\frac{\partial \bar{a}}{\partial q^j}$ an the right-hand side with the aid of (N1,4) written for the index j instead of i. We then get

$$\frac{\partial}{\partial q^j} \frac{\partial \bar{a}}{\partial q^i} = \frac{\partial}{\partial q^j} \left(\frac{1}{\rho} \bar{J}_i\right) + \frac{1}{\rho} \bar{J}_j \cdot \bar{\nabla} \left(\frac{1}{\rho} \bar{J}_i\right) \qquad (N1,5a)$$

Similarly (Interchange i and j).

$$\frac{\partial}{\partial q^i} \frac{\partial \bar{a}}{\partial q^j} = \frac{\partial}{\partial q^i} \left(\frac{1}{\rho} \bar{J}_j\right) + \frac{1}{\rho} \bar{J}_i \cdot \bar{\nabla} \left(\frac{1}{\rho} \bar{J}_j\right) \ . \qquad (N1,5b)$$

According to the principle of gene-identity the position $\bar{a}$ of the tagged particle is a function of the atomic configuration $\{q^i\}$ alone. A necessary and sufficient condition for this is that the two mixed partial derivatives on the left-hand sides of (N1, 5a of b) have the same value. Equating the two right-hand sides yields

$$\frac{\partial}{\partial q^j} \left(\frac{1}{\rho} \bar{J}_i\right) + \frac{1}{\rho} \bar{J}_j \cdot \bar{\nabla} \left(\frac{1}{\rho} \bar{J}_i\right) = \frac{\partial}{\partial q^i} \left(\frac{1}{\rho} \bar{J}_j\right) + \frac{1}{\rho} \bar{J}_i \cdot \bar{\nabla} \left(\frac{1}{\rho} \bar{J}_j\right) \ . \qquad (N1,6)$$

This equation may be brought into a form that will be more useful to us later on, namely into the form shown in the title of this note. We multiply (N1,6) by ρ and differentiate out the products. At the same time we replace $-\frac{\partial \rho}{\partial q^j}$ and $-\frac{\partial \rho}{\partial q^i}$ by $\bar{\nabla} \cdot \bar{J}_j$ and $\bar{\nabla} \cdot \bar{J}_i$ respectively, according to equation (7)

of the appendix. We then obtain

$$\frac{1}{\rho}\bar{J}_i\bar{\nabla}\cdot\bar{J}_j + \frac{\partial}{\partial q^j}\bar{J}_i + \frac{1}{\rho}\bar{J}_j\cdot\bar{\nabla}\bar{J}_i + \bar{J}_j\times(\bar{\nabla}\frac{1}{\rho})\bar{J}_i =$$

$$= \frac{1}{\rho}\bar{J}_j\bar{\nabla}\cdot\bar{J}_i + \frac{\partial}{\partial q^i}\bar{J}_j + \frac{1}{\rho}\bar{J}_i\cdot\bar{\nabla}\bar{J}_j + \bar{J}_i\cdot(\bar{\nabla}\frac{1}{\rho})\bar{J}_j ,$$

or after rearranging,

$$\frac{\partial}{\partial q^i}\bar{J}_j - \frac{\partial}{\partial q^j}\bar{J}_i = (\bar{\nabla}\frac{1}{\rho})\times(\bar{J}_i\times\bar{J}_j) + \frac{1}{\rho}\bar{\nabla}\times(\bar{J}_i\times\bar{J}_j) .$$

The two terms on the right may be combined. Thus finally

$$\frac{\partial}{\partial q^i}\bar{J}_j - \frac{\partial}{\partial q^j}\bar{J}_i = \bar{\nabla}\times(\frac{1}{\rho}\bar{J}_i\times\bar{J}_j) . \qquad (N1,7)$$

And this is the equation shown in the title.

Equation (N1,7) must hold wherever there is an element of charge that may be tagged, i.e. at all points $\bar{r}$ of the home-space where the charge density ρ does not vanish. But wherever the charge density ρ (and then also $\bar{J}_i$ and $\bar{J}_j$) is zero, the equation is fulfilled by default. It simply states "0 = 0". Thus (N1,7) is fulfilled everywhere.

The reader who is satisfied with this proof may stop right here. Others, however, might feel more comfortable if they saw a second and different proof. In this second proof, we use the same set of independent variables, namely the q^i and $\bar{r}$, that was used in the main text of the appendix. So there is no need for employing the slash-derivatives $\frac{\not\partial}{\not\partial q^i}$. Instead of tagging just one element of charge, as we did before, we tag all elements at once. Since the charge elements form a continuous distribution, we have to employ a triplet $\{\xi^1,\xi^2,\xi^3\}$ of quantities to tag each particular element. For instance, for the ξ^α (Greek indices range from 1 to 3, whereas latin indices range from 1 to n.) we might

use the cartesian coordinates of the element when it was placed according to some arbitrarily chosen fiducial configuration of the atom. We then have to deal with the three functions $\xi^\alpha(q^i,\bar{r})$. They tell us which tagged element is at some chosen location $\bar{r}$ for the atomic configuration $\{q^i\}$.

The principle of gene-identity allows us to evaluate the velocity $\bar{w}(q^i,\bar{r})$ of an element of charge. We know that the ξ^α-tags of an element never change when the element is in motion. Thus the material time derivatives $\frac{d\xi^\alpha}{dt}$ (taken as we move with the element) must vanish. But

$$\frac{d}{dt}\,\xi^\alpha = \frac{\partial}{\partial t}\,\xi^\alpha + \bar{w}\cdot(\bar{\nabla}\xi^\alpha)\ , \qquad (N1,8)$$

where $\frac{\partial}{\partial t}\,\xi^\alpha$ is the local time derivative (taken at fixed position $\bar{r}$), given by

$$\frac{\partial}{\partial t}\,\xi^\alpha = \frac{dq^i}{dt}\,\frac{\partial\xi^\alpha}{\partial q^i} = v^i\,\frac{\partial\xi^\alpha}{\partial q^i}\ . \qquad (N1,9)$$

The requirement that $\frac{d}{dt}\,\xi^\alpha$ be zero yields

$$\bar{w}\cdot(\bar{\nabla}\xi^\alpha) = -\,v^i\,\frac{\partial\xi^\alpha}{\partial q^i}\ . \qquad (N1,10)$$

Equations (N1,10) are a system of 3 scalar equations (one for each $\alpha = 1, 2, 3$) for the velocity vector $\bar{w}$. Hence $\bar{w}$ is determined. If we were to solve these equations (but we are not going to solve them) we would find that $\bar{w}$ is a linear function of the n velocity components v^i. Thus we can write

$$\bar{w} = v^i\bar{w}_i(q^j,\bar{r})\ , \qquad (N1,11)$$

where the n functions $\bar{w}_i(q^j,\bar{r})$ depend only on the atomic configuration $\{q^j\}$and the position $\bar{r}$. On combining (N1,10) and (N1,11) we obtain

$$v^i\bar{w}_i\cdot\bar{\nabla}\xi^\alpha = -\,v^i\,\frac{\partial\xi^\alpha}{\partial q^i}\ .$$

But this equation must hold for any choice of the configurational velocity components v^i. Thus we obtain

$$\frac{\partial \xi^\alpha}{\partial q^i} = - \bar{w}_i \cdot \bar{\nabla} \xi^\alpha \ . \qquad \text{(N1,12)}$$

We differentiate this equation with respect to q^j and obtain

$$\frac{\partial}{\partial q^j} \frac{\partial \xi^\alpha}{\partial q^i} = - \frac{\partial \bar{w}_i}{\partial q^j} \cdot \bar{\nabla} \xi^\alpha - \bar{w}_i \cdot \bar{\nabla} \frac{\partial \xi^\alpha}{\partial q^j} \ ,$$

where we have interchanged $\bar{\nabla}$ and $\frac{\partial}{\partial q^j}$. We replace the $\frac{\partial \xi^\alpha}{\partial q^j}$ on the right-hand side by $- \bar{w}_j \cdot \bar{\nabla} \xi^\alpha$, according to equation (N1,12), written for the index j instead of i. Thus

$$\frac{\partial}{\partial q^j} \frac{\partial \xi^\alpha}{\partial q^i} = - \frac{\partial \bar{w}_i}{\partial q^j} \cdot \bar{\nabla} \xi^\alpha + \bar{w}_i \cdot \bar{\nabla} (\bar{w}_j \cdot \bar{\nabla} \xi^\alpha) \ ,$$

or, on differentiating out the product in the last term,

$$\frac{\partial}{\partial q^j} \frac{\partial \xi^\alpha}{\partial q^i} = - \frac{\partial \bar{w}_i}{\partial q^j} \cdot \bar{\nabla} \xi^\alpha + \bar{w}_i \cdot (\bar{\nabla} \bar{w}_j) \cdot \bar{\nabla} \xi^\alpha + \bar{w}_i \cdot (\bar{\nabla} \bar{\nabla} \xi^\alpha) \cdot \bar{w}_j \ . \qquad \text{(N1,13a)}$$

Similarly (Interchange i and j),

$$\frac{\partial}{\partial q^i} \frac{\partial \xi^\alpha}{\partial q^j} = - \frac{\partial \bar{w}_j}{\partial q^i} \cdot \bar{\nabla} \xi^\alpha + \bar{w}_j \cdot (\bar{\nabla} \bar{w}_i) \cdot \bar{\nabla} \xi^\alpha + \bar{w}_j \cdot (\bar{\nabla} \bar{\nabla} \xi^\alpha) \cdot \bar{w}_i \ . \qquad \text{(N1,13b)}$$

Now we subtract (N1, 13b) from (N1, 13a). The terms on the left-hand side will cancel, because mixed partial derivatives do not depend on the order. Also the last terms on the right-hand side will cancel, because $\bar{\nabla} \bar{\nabla} \xi^\alpha$ is a symmetric tensor. Thus, after rearranging and factoring out the common term $\cdot \bar{\nabla} \xi^\alpha$,

$$\{ \frac{\partial}{\partial q^i} \bar{w}_j + \bar{w}_i \cdot \bar{\nabla} \bar{w}_j - \frac{\partial}{\partial q^j} \bar{w}_i - \bar{w}_j \cdot \bar{\nabla} \bar{w}_i \} \cdot \bar{\nabla} \xi^\alpha = 0 \ .$$

This single printed equation really stands for three equations, one for each $\alpha = 1, 2, 3$. But the three vectors $\bar{\nabla} \xi^\alpha$ are linearly independent. Thus the expression in the parenthesis must vanish, and we obtain

$$\frac{\partial}{\partial q^j} \bar{w}_i + \bar{w}_j \cdot \bar{\nabla} \bar{w}_i = \frac{\partial}{\partial q^i} \bar{w}_j + \bar{w}_i \cdot \bar{\nabla} \bar{w}_j \ . \qquad \text{(N1,14)}$$

From the equations (N1,1), (N1,11), and (5) of the appendix, repeated here for convenience,

$$\rho\bar{w} = \bar{J} \ , \qquad (N1,1)$$

$$\bar{w} = v^i \bar{w}_i \ , \qquad (N1,11)$$

$$\bar{J} = v^i \bar{J}_i \ , \qquad (5)$$

we conclude that

$$\rho\bar{w}_i v^i = \bar{J}_i v^i \ .$$

But this equation must hold for any choice of the configurational velocity components v^i, so that

$$\bar{w}_i = \frac{1}{\rho} \bar{J}_i \ . \qquad (N1,15)$$

Inserting this into (N1,14) yields

$$\frac{\partial}{\partial q^j}\left(\frac{1}{\rho}\bar{J}_i\right) + \frac{1}{\rho}\bar{J}_j \cdot \bar{\nabla}\left(\frac{1}{\rho}\bar{J}_i\right) = \frac{\partial}{\partial q^i}\left(\frac{1}{\rho}\bar{J}_j\right) + \frac{1}{\rho}\bar{J}_i \cdot \bar{\nabla}\left(\frac{1}{\rho}\bar{J}_i\right) \qquad (N1,16)$$

But this equation is the same as (N1, 6), from which the desired relation (N1,7) follows by means of purely algebraic manipulations.

Note #2. Vectorial Derivation of the Equations

$$\delta\bar{J} = \frac{\partial}{\partial t}(\rho\delta\bar{r}) + \bar{\nabla} \times (\delta\bar{r} \times \bar{J}) \text{ and } \delta\rho = -\bar{\nabla} \cdot (\rho\delta\bar{r}) .$$

One may always express the charge density ρ and the current density $\bar{J}$ in terms of three scalar functions $\alpha(\bar{r},t)$, $\beta(\bar{r},t)$, $\gamma(\bar{r},t)$ of the position $\bar{r}$ and the time t. These expressions are

$$\rho = \bar{\nabla}\alpha \cdot \bar{\nabla}\beta \times \bar{\nabla}\gamma , \tag{N2,1}$$

and

$$\bar{J} = -\frac{\partial\alpha}{\partial t}\bar{\nabla}\beta \times \bar{\nabla}\gamma - \frac{\partial\beta}{\partial t}\bar{\nabla}\gamma \times \bar{\nabla}\alpha - \frac{\partial\gamma}{\partial t}\bar{\nabla}\alpha \times \bar{\nabla}\beta . \tag{N2,2}$$

One can readily verify that the continuity equation

$$\frac{\partial\rho}{\partial t} + \bar{\nabla} \cdot \bar{J} = 0 . \tag{N2,3}$$

is automatically satisfied. The triple $\{\alpha,\beta,\gamma\}$ may be regarded as a tag for an individual element of charge.

Sometimes one may wish to express ρ and $\bar{J}$ in terms of several triples $\{\alpha_n,\beta_n,\gamma_n\}$, as in

$$\rho = \sum_n \bar{\nabla}\alpha_n \cdot \bar{\nabla}\beta_n \times \bar{\nabla}\gamma_n , \tag{N2,4}$$

and

$$\bar{J} = \sum_n \{ -\frac{\partial\alpha_n}{\partial t}\bar{\nabla}\beta_n \times \bar{\nabla}\gamma_n - \frac{\partial\beta_n}{\partial t}\bar{\nabla}\gamma_n \times \bar{\nabla}\alpha_n - \frac{\partial\gamma_n}{\partial t}\bar{\nabla}\alpha_n \times \bar{\nabla}\beta_n \}. \tag{N2,5}$$

However, one such triple suffices. At any rate, our derivations will employ only linear operations. Thus what is true for one triple will also hold for the more general expressions (N2,4) and (N2,5). Therefore, we stay with the simpler forms (N2,1) and (N2,2).

Now let us subject the three functions α, β, γ to the variations $\delta\alpha$, $\delta\beta$, $\delta\gamma$. The resulting variations $\delta\rho$ and $\delta\bar{J}$ of ρ and $\bar{J}$ are then given by

$$\delta\rho = (\bar{\nabla}\delta\alpha) \cdot \bar{\nabla}\beta \times \nabla\gamma + (\bar{\nabla}\delta\beta) \cdot \bar{\nabla}\gamma \times \bar{\nabla}\alpha + (\bar{\nabla}\delta\gamma) \cdot \bar{\nabla}\alpha \times \nabla\beta$$

and

$$\delta\bar{J} = -\left(\frac{\partial}{\partial t}\ \delta\alpha\right) \cdot \bar{\nabla}\beta \times \bar{\nabla}\gamma - \frac{\partial\alpha}{\partial t}(\bar{\nabla}\delta\beta) \times \bar{\nabla}\gamma - \frac{\partial\alpha}{\partial t}\bar{\nabla}\beta \times (\bar{\nabla}\delta\gamma) -$$

$$- \left(\frac{\partial}{\partial t}\delta\beta\right) \cdot \bar{\nabla}\gamma \times \bar{\nabla}\alpha - \frac{\partial\beta}{\partial t}(\bar{\nabla}\delta\gamma) \times \bar{\nabla}\alpha - \frac{\partial\beta}{\partial t}\bar{\nabla}\gamma \times (\bar{\nabla}\delta\alpha) -$$

$$- \left(\frac{\partial}{\partial t}\delta\gamma\right) \cdot \bar{\nabla}\alpha \times \bar{\nabla}\beta - \frac{\partial\gamma}{\partial t}(\bar{\nabla}\delta\alpha) \times \bar{\nabla}\beta - \frac{\partial\delta}{\partial t}\bar{\nabla}\alpha \times (\bar{\nabla}\delta\beta) .$$

By means of a straightforward, though tedious, calculation one shows that the preceding two equations may be written in the following form.

$$\delta\rho = \bar{\nabla} \cdot [\delta\alpha\ \bar{\nabla}\beta \times \bar{\nabla}\gamma + \delta\beta\ \bar{\nabla}\gamma \times \nabla\alpha + \delta\gamma\ \bar{\nabla}\alpha \times \bar{\nabla}\beta] , \qquad (N2,6)$$

and

$$\delta\bar{J} = -\frac{\partial}{\partial t}[\delta\alpha\ \bar{\nabla}\beta \times \bar{\nabla}\gamma + \delta\beta\ \bar{\nabla}\gamma \times \bar{\nabla}\alpha + \delta\gamma\ \bar{\nabla}\alpha \times \bar{\nabla}\beta] +$$

$$+ \bar{\nabla} \times [\delta\alpha\left(\frac{\partial\beta}{\partial t}\bar{\nabla}\gamma - \frac{\partial\gamma}{\partial t}\bar{\nabla}\beta\right) + \delta\beta\left(\frac{\partial\gamma}{\partial t}\bar{\nabla}\alpha - \frac{\partial\alpha}{\partial t}\bar{\nabla}\gamma\right) + \delta\gamma\left(\frac{\partial\alpha}{\partial t}\bar{\nabla}\beta - \frac{\partial\beta}{\partial t}\bar{\nabla}\alpha\right)] . \qquad (N2,7)$$

So far we left the variations $\delta\alpha$, $\delta\beta$, $\delta\gamma$ unspecified. But now we shall introduce specific variations related to shifts $\delta\bar{r}$, δt in the event space, i.e. the four dimensional space of position $\bar{r}$ and time t. We shift the three function patterns α, β, γ by $\delta\bar{r}$ and δt. The variations $\delta\bar{r}$ and δt may still depend on the event $\bar{r},t$. Then, for each fixed $(\bar{r},t)$, the variations $\delta\alpha$, $\delta\beta$, $\delta\gamma$ are given by

$$\begin{aligned}
\delta\alpha &= -\delta t\,\frac{\partial\alpha}{\partial t} - \delta\bar{r} \cdot \bar{\nabla}\alpha , \\
\delta\beta &= -\delta t\,\frac{\partial\beta}{\partial t} - \delta\bar{r} \cdot \bar{\nabla}\beta , \qquad (N2,8) \\
\delta\gamma &= -\delta t\,\frac{\partial\gamma}{\partial t} - \delta\bar{r} \cdot \bar{\nabla}\gamma .
\end{aligned}$$

Note the minus signs, which come about in the following way. Since we shifted the functional pattern α, we know that the new α at the shifted event $\bar{r} + \delta\bar{r}$, $t + \delta t$ is equal to the old α at the original event. Thus we have

$$(\alpha + \delta\alpha)(\bar{r} + \delta\bar{r},\ t + \delta t) = \alpha(\bar{r},t)$$

On expanding the left-hand side by Taylor's theorem and retaining only the zero-order and first order terms, we obtain

$$\alpha(\bar{r},t) + \delta t\,\frac{\partial\alpha}{\partial t} + \delta\bar{r}\cdot\bar{\nabla}\alpha + \delta\alpha = \alpha(\bar{r},t)$$

On cancelling $\alpha(\bar{r},t)$, we obtain the first equation of (N2,8). The other two equations result in a similar way.

We insert the expressions (N2,8) into (N2,6) and (N2,7) and use equations (N2,1) and (N2,2). With the aid of the relation

$$(\bar{\nabla}\alpha)(\bar{\nabla}\beta\times\bar{\nabla}\gamma) + (\bar{\nabla}\beta)(\bar{\nabla}\gamma\times\bar{\nabla}\alpha) + (\bar{\nabla}\gamma)(\bar{\nabla}\alpha\times\bar{\nabla}\beta) = (\bar{\nabla}\alpha\cdot\bar{\nabla}\beta\times\bar{\nabla}\gamma)\,\bar{\bar{I}}\ , \qquad \text{(N2,9)}$$

where $\bar{\bar{I}}$ is the unit tensor (or idemfactor), we have

$$\delta\alpha\ \bar{\nabla}\beta\times\bar{\nabla}\gamma + \delta\beta\ \bar{\nabla}\gamma\times\bar{\nabla}\alpha + \delta\gamma\ \bar{\nabla}\alpha\times\bar{\nabla}\beta = -\rho\delta\bar{r} + \bar{J}\delta t \qquad \text{(N2,10)}$$

In the expression behind the curl sign $\bar{\nabla}\times$ of (N2,7), the terms in δt will cancel, while the terms in $\delta\bar{r}$ combine to $\delta\bar{r}\times\bar{J}$. Altogether then, we obtain

$$\delta\rho = -\bar{\nabla}\cdot(\rho\delta\bar{r} - \bar{J}\delta t) \qquad \text{(N2,11)}$$

$$\delta\bar{J} = \frac{\partial}{\partial t}(\rho\delta\bar{r} - \bar{J}\delta t) + \bar{\nabla}\times(\delta\bar{r}\times\bar{J}) \qquad \text{(N2,12)}$$

In the special case $\delta t = 0$ (no shift in the time direction), we obtain the equations in the title of this note.