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Improving the Method of Calculating Electronic Properties of Narrow Bandgap Semiconductors

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ABSTRACT

A previously developed code for calculating the mobility of charge carriers in narrow bandgap semiconductors does not predict the correct temperature dependence in all cases. It is thought that this is due to the way the electronic screening of the carriers is treated in the model. The objective of this research is to improve the handling of the screening by going beyond the current first Born approximation. Much of this work is directly related to the alloy semiconductor $Hg_{1-x}Cd_xTe$ which is important for infrared detectors and is a good candidate for microgravity crystal growth. The principal conclusion, so far, is that the major difficulty is probably the treatment of short range screening at higher temperatures.

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1. Introduction

$Hg_{1-x}Cd_xTe$ is a mixed pseudo-binary semiconductor. Its energy gap can be "tuned" from 0.0 to 1.6 eV as x varies from x .17 to x=1 at zero degrees (Dornhaus, Nimtz and B. Schlicht, 1983, p. 148). This variation of band gap with x allows one to optimize for infrared detection (Long and Schmit, 1970, Kruse, 1981). Because of difficulties with producing compositionally uniform crystals due to gravity driven convective effects, $Hg_{1-x}Cd_xTe$ is a good candidate for production in the reduced gravity environment of space (Lehoczky and Szofran, 1981, 1982).

Semiconductors with small gaps tend to have small effective masses and hence high mobilities (Kruse, 1981). The band structure of these materials is now understood from Kane's three level band model and k.p perturbation calculation (Kane, 1957) which leads to non parabolic band structure. See appendix A.5.

Since these semiconductors are polar, scattering by the optical modes is important. The energy of the optical phonons is comparable to the energy of the electrons and hence the electrons are not scattered elastically. This means a relaxation time approximation is not valid (Howard and Sondheimer, 1953; Dingle, 1956) and therefore variational methods are used to solve the Boltzmann equation (Ehrenreich, 1957). The Boltzmann equation must contain all appropriate scattering terms and the narrow band gap means that thermally excited electrons will screen the carriers in certain scattering interactions (Ehrenreich, 1959 - two papers). We attempt to improve the calculation of the scattering by improving the treatment of screening (see Appendix A.1). There are several contributions to the scattering of electrons in $Hg_{1-x}Cd_xTe$ and hence to the determination of electron mobility (Lehoczky, Szofran and Martin, 1980; Lehoczky, Summers, Szofran and Martin, 1982). These include longitudinal - optic phonon interactions (LO), acoustic phonon scattering (ac), ionized impurity scattering (ii), electron hole scattering (eh), compositional disorder scattering (dis) and neutral defect (nd) scattering. Screening is involved in (LO), (ii), and (eh). At temperatures above approximately liquid nitrogen temperatures, LO scattering is easily the most important. See Appendix A.6 for a discussion of the basic interaction term in the Hamiltonian. The LO modes are important rather than the TO modes because it is only the LO modes that have strong electric fields which accompany their vibration

2. Objectives

In alloy semiconductors, such as $Hg_{1-x}Cd_xTe$, there is a strong polar coupling of the carriers to the optic modes. In describing this interaction, one must properly account for the screening by use of a suitable dielectric function (Ziman, 1972; Mahan, 1981; Whitsett et al., 1981, see also appendix A.2). The dielectric function depends on several factors (Lehoczky et al. 1974, Nelson et al, 1978) among which is the Fermi Thomas wave vector or its reciprocal which is essentially the screening length. Previous calculations of electron mobility considering, among other factors, the scattering of carriers by optical phonon modes have yielded electron mobilities which are too high (Lehoczky et al, 1982). We aim to improve these calculations by using the Friedel sum rule and the second Born approximation (Joachain, 1975) for the phase shifts to calculate a better screening length (Stern, 1967; Agarwal and Singh, 1983).

A second objective is to fill in the necessary background material by use of a suitable set of appendices (some reviews are by Zawadski, 1974; Chattopadhyay and Queisser, 1981; Chattopadhyay and Nag, 1974; Nag, 1980; Nag, 1975; Rode, 1975).

It is essential in all our calculations to take into account the fact that the energy bands are non parabolic, although they may still be assumed to be spherically symmetric (Szymanska and Dietl, 1978; Pfeffer and Zawadzki, 1978). The non parabolicity of the band is a major complicating feature.

3. The Calculation

The background details and the definitions can be found in the appendices. Here we outline the calculation. The idea is to choose a form for the screened potential of a charged impurity and then to use the Friedel sum rule to place a constraint on this potential which involves the screening length. From Appendix A.3, the Friedel sum rule is

$$2/\pi \sum_\ell (2\ell+1) \int_0^\infty \frac{d\delta_\ell}{dE} f(E)\, dE = Z. \tag{1}$$

From Appendix A.4 the phase shifts δ_ℓ can be determined, at least to second order Born approximation accuracy, by

$$\tan \delta_\ell = - \frac{k A_\ell}{1 - B_\ell / A_\ell} , \tag{2}$$

where

$$A_\ell = \int_0^\infty j_\ell^2 (kr)\, U(r)\, r^2 dr , \tag{3}$$

$$B_\ell = \int_0^\infty dr \int_0^\infty dr'\, j_\ell(kr)\, U(r)\, G(r,r')\, U(r')\, j_\ell(kr')\, r^2 r'^2 , \tag{4a}$$

with $U(r) = (2m^*/\hbar^2)\, V(r),$ (4b)

and $V(r)$ is the customary screened Coulomb potential (see Appendix A.1)

$$V(r) = -Za\, e^{-r/L}/r, \tag{5}$$

with L being the screening length.

$$G(r,r') = k\, j_\ell(kr_<)\, \eta_\ell\, (kr_>),$$

with $r_<, r_>$ being the smaller and the larger of r and r' and j_ℓ, η_ℓ are the spherical Bessel functions.

Since $\tan \delta_\ell \cong \delta_\ell$ through second order we can write Eq. (2) as

$$\delta_\ell \cong -k\left[A_\ell + \frac{B_\ell}{1 - B_\ell/A_\ell}\right]. \tag{6}$$

Since $\quad \sum_\ell (2\ell+1)\, j_\ell^2(x) = 1,$

we can easily show

$$\sum_\ell A_\ell (2\ell+1) = -Za\, L^2. \tag{7}$$

If we assume $(kr) \ll 1$ for $r \lesssim L$ where L is the screening length in the spherical Bessel functions of Eqs. (3) and (4) (see Appendix A.7 for a discussion of the validity of our approximations) then we find

$$A_\ell = -Za\, k^{2\ell}\, \frac{2\ell!!}{(2\ell+1)!!}\, L^{2(\ell+1)}, \tag{8}$$

$$B_\ell = -(Za)^2 k^{2\ell} \frac{(2\ell)!}{[(2\ell+1)!!]^2}\, L^{2\ell+3}\, \frac{2}{2^{2(\ell+1)}}. \tag{9}$$

Following Agarwal and Singh (1983) (also see Appendix A.7), we approximate Eq. (6) as

$$\delta_\ell \cong -k\left[A_\ell + \frac{B_0}{1 - B_0/A_0}\, \delta_\ell^0\right]. \tag{10}$$

The screening length in the first Born approximation is $L_{(1)}$ where

$$L_{(1)}^{-2} = \left\{ 2b\pi\hbar^2 \int_0^\infty \left(-\frac{\partial f}{\partial E}\right) \rho(E)\, dE \right\}, \quad b = a/m^* \tag{11}$$

(see e.q. Szymanska and Dietl, 1978) This expression is good even for non parabolic bands (See Appendix A.8 for different ways of expressing the density of states). We find

$$(L/L_{(1)})^2 = 1 - \frac{aZL}{2}, \tag{12}$$

where m^* has been treated as constant in the factor multiplying δ_ℓ^0 in Eq. (2).

Eq. (12) is readily solved with the following results

$$(L/L_{(1)}) = \sqrt{1 + A^2} - A,$$

which gives with A = $\frac{aZ}{4} L_{(1)}$

the following numbers.

A	$L/L_{(1)}$
-1	2.41
-.5	1.62
0	1
.5	.62
1	.41

4. Conclusions and Recommendations

The results of the previous section were derived with the following approximations applied to the correction term to the first Born approximation [$B_\ell/(1-B_\ell/A_\ell)$ of Eq. (6)]

a. A constant effective mass can be used beyond the first Born approximation,
b. $kL<<1$ where L is the screening length
c. need only the $\ell = 0$ term.

We have discussed this approximation in A.7. In Appendix A.9 we note that improvements are not so easy and it is not clear our results are valid at higher temperatures.

The major comment to make about this result is that it disagrees with that of Agarwal and Singh (1983) who in my notation get

$$
\begin{aligned}
(L/L_{(1)})^2 &= (1-LaZ)^{-1} \\
&\cong 1+LaZ. \qquad (13)
\end{aligned}
$$

Both Eq. (12) (my result) and Eq. (13) assume $|LaZ|<<1$. It should be noted that my result differs qualitatively from Agarwal and Singh. They predict corrections to the first Born approximation increase L (for donors, Z>0) whereas I predict they decrease L. The literature seems to be divided as to which qualitative effect to expect (D. Chattopadhyay and H.J. Queisser, 1981). It should be mentioned that a decrease in L would mean more screening, less scattering and hence higher mobility - the opposite result from what we expected.

We can also obtain the results of Agarwal and Singh if we use their expression for the second Born approximation but this expression does not appear to agree with standard sources (Joachain, 1975).

It remains to be seen whether better treatment of corrections to the first Born approximation would lower the mobilities and yield better agreement with experiment. This would be the first thing we would recommend investigating as our low energy approximation are suspect at higher temperatures. As shown in Appendix A.9, going beyond $\ell = 0$ in the correction term quickly yielded equations that must be solved numerically for L.

Also if we drop the assumption that $kL<<1$, then the integrals may still be doable, but they certainly are not convenient.

Experimentally the calculations of the mobility are off by a factor of perhaps 2. If the corrections to the first Born approximation were enough to bring agreement with experiment it is likely that we would have cause to suspect the convergence of our procedure.

Our recommendations would stress the positive aspects of the calculation which has already been done. The calculation is so complex that it is remarkable that qualitative and in some cases perhaps quantitative agreement with experiment can be achieved. It would appear that a review of the whole calculation is in order. It could be that the lack of agreement with experiment might not reflect just one error but perhaps several, none of them particularly serious by themselves.

The error at high temperature should mean that close in scattering is overscreened by this model. Whatever the approach it seems this basic problem should be fixed. We also need to take into account that in general more than one type of carrier can contribute to electric current and to screening. There is also the troublesome problem of antiscreening which can occur in polar optic mode scattering when the electrons don't move fast enough to "follow the charge motion due to lattice waves (Ehrenreich, 1959).

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Appendix A.1
Screening

We present here the basic ideas (Ziman, 1972) without putting in the details. A key idea we wish to mention is the difference between screening by free electrons and by band electrons which are described by Bloch Wave functions.

For a free electron gas (with a uniform positive background) the applied potential can be written

$$V(\vec{r},t) = \iint V(\vec{q},\omega)\, e^{i(\vec{q}\cdot\vec{r}+\omega t)}\, d\vec{q}\, d\omega\,, \tag{A.1.1}$$

with $\vec{r}$ being the space coordinate, t the time, $\vec{q}$ and ω are the usual wave vector and frequency. The Fourier components of the effective potential is then $V(\vec{q},\omega)$ divided by the dielectric function.

The Lindhard or Random Phase Approximation dielectric function is the Fourier component of the displacement vector divided by the Fourier component of the electric field and it comes out;

$$\epsilon(\vec{q},\omega) = 1 - \frac{4\pi e^2}{V q^2}\sum_{\vec{q},\sigma} \frac{f(\vec{k}) - f(\overrightarrow{k+q})}{E_{\vec{k}} - E_{\vec{k}+\vec{q}} + \hbar\omega - i\delta}\,, \tag{A.1.2}$$

where f is the Fermi Function and $E_{\vec{k}}$ is the electron energy at wave vector $\vec{k}$.

It is particularly interesting to examine this for the static case ($\omega = 0$) when $\vec{q}$ is near zero. For then (assuming one band)

$$E_{\vec{k}} - E_{\overrightarrow{k+q}} \cong -\vec{q}\cdot\vec{\nabla}_k E_{\vec{k}}\,, \tag{A.1.3}$$

$$f(\vec{k}) - f(\overrightarrow{k+q}) \cong -\vec{q}\cdot\vec{\nabla}_{\vec{k}} E_{\vec{k}} \left(\frac{\partial f}{\partial E_{\vec{k}}}\right). \tag{A.1.4}$$

The static dielectric constant then comes out

$$\epsilon(\vec{q},0) = 1 + k_{TF}^2 / q^2, \tag{A.1.5}$$

where k_{TF} is the Thomas-Fermi screening wave vector and it is given by

$$k_{TF}^2 = 4\pi e^2 \int \left(-\frac{\partial f}{\partial E}\right) \rho(E)\, dE, \tag{A.1.6}$$

where $\rho(E)$ is the density of states including spin.

The significance of k_{TF} is not hard to find. If we have a bare Coulomb potential energy

$$V(\vec{r}) = e^2/r, \tag{A.1.7}$$

then its Fourier transform is

$$V(q) = 4\pi e^2/q^2, \tag{A.1.8}$$

and the effective Fourier transform of the screened Coulomb potential is

$$U(q) = \frac{V(q)}{\epsilon(q,0)} = \frac{4\pi e^2}{q^2 + k_{TF}^2}. \tag{A.1.9}$$

By inversion, we can then show that this leads to the following effective potential energy

$$U(r) = \frac{e^2}{r} e^{-k_{TF} r}. \tag{A.1.10}$$

Many authors have shown for Bloch Wave functions referred to band n, that

$$\epsilon(\vec{q},\omega) = 1 - \frac{4\pi e^2}{Vq^2} \sum_{\vec{k},n,n'} \frac{|\langle \vec{k},n| e^{-i\vec{q}\cdot\vec{r}} |\vec{k+q},n'\rangle|^2 (f_{\vec{k}+\vec{q},n'} - f_{\vec{k},n})}{E_{\vec{k+q},n'} - E_{\vec{k},n} + \hbar\omega - i\alpha}. \tag{A.1.11}$$

For non parabolic but still spherical energy surfaces the Fermi-Thomas wave vector is still given by Eq. (A.1.6) (Szymanska and Dietl, 1978) with

$$\rho(\epsilon) = (k^2/\pi^2) \frac{dk}{d\epsilon}, \tag{A.1.12}$$

(see Appendix A.8).

Appendix A.2
Dielectric Function

We have already discussed the dielectric function and given an expression for a semiconductor. Here we want to summarize the results for the band structure of $Hg_{1-x}Cd_xTe$. Similar material is discussed by Whitsell (1981).

It is usual to start by dividing the dielectric constant into two parts, one part from the ionic lattice via its polarizability (lat) and the other part from the electrons (el) due to inter and intra band effects.

$$\epsilon(\vec{q},\omega) = \epsilon_{lat}(\vec{q},\omega) + \epsilon_{el}(\vec{q},\omega) \tag{A.2.1}$$

The lattice part shows two mode behavior, but can be analyzed with no particular difficulty and reference can be made to the literature. The electronic part is rather complicted but has been well summarized by Lehoczky, Broerman, Nelson and Whitsett (1974), Nelson, Broerman, Summers and Whitsett (1978) and Lehoczky, Szofran and Martin (1980). The later paper gives a summary of how screening and the Thomas-Fermi cruve vectors enter into the longitudinal-optical phonon scattering and in ionizing impurity and electron-hole scattering. Generally speaking we write,

$$\begin{aligned}\epsilon(\vec{q},\omega) &= \epsilon_b + \frac{k(q)}{q^2}k_{TF}^2 = \epsilon_b\left(1 + \frac{k_{TF}^2}{\epsilon_b}\frac{f(q)}{q^2}\right)\\ &= \epsilon_b\left(1 + \frac{f(q)}{L^2 q^2}\right),\end{aligned} \tag{A.2.2}$$

where ϵ_b and f(q), are chosen appropriately according to the scattering mechanism (and notice with $\epsilon_b \neq 1$ we have $\epsilon_b L^{-2} = k_{TF}^2$) and, depending on the circumstances, more complicated frequency dependent forms may be necessary.

Appendix A.3
Friedel Sum Rule

The Friedel sum rule relates phase shifts δ_ℓ (see Joachain, 1975 for a definition of phase shifts) of partial waves of angular momentum ℓ scattered from a spherically symmetric potential to the charge of the scattering center. At large distances, the scattering center is screened and so the charge of this center also equals the magnitude of the charge of the total number of electrons which are attracted to or repelled from it.

The Friedel sum rule as customarily written (Ziman, 1978) is

$$Z = 2/\pi \sum_\ell (2\ell+1)\, \delta_\ell (k_F) \;, \qquad \text{(A.3.1)}$$

where k_F is the Fermi wave vector and Z is the charge of the scattering center (in units of the magnitude of the electron charge).

For the conduction electrons in a semiconductor we write (Stern, 1967);

$$Z = 2/\pi \sum_\ell (2\ell+1) \int_0^\infty f(\epsilon)\, \frac{d\delta_\ell}{d\epsilon}\, d\epsilon \,, \qquad \text{(A.3.2)}$$

where $f(\epsilon)$ is the Fermi function. Assuming a sharp Fermi surface, the first equation follows from the second.

The usual form for the screening length (Eq. A.1.6) can be derived from the Friedel sum rule and the first Born approximation. The Friedel sum rule is thought to be exact (Mahan 1981, p. 236).

Appendix A.4
The First and Second Born Approximation

Here we are concerned with the Born series for the phase shifts of partial waves. The development of the appropriate mathematics can be obtained from standard references such as Joachain (1975). The equations we need are

$$\tan\delta_\ell = -k\int_0^\infty j_\ell(kr)\,U(r)\,R_\ell(k,r)\,r^2\,dr, \qquad \text{(A.4.1)}$$

and

$$R_\ell(k,r) = j_\ell(kr) + \int_0^\infty G_\ell(r,r')\,U(r')\,R_\ell(k,r')\,r'^2\,dr', \qquad \text{(A.4.2)}$$

$$G_\ell(r,r') = k\,j_\ell(kr_<)\,\eta_\ell(kr_>), \qquad \text{(A.4.3)}$$

where $r_>$ and $r_<$ are the greater and lesser of r and r′ respectively and j_ℓ, η_ℓ are the spherical Bessel and Neuman functions.

One iteration yields the first Born approximation for the phase shifts

$$\tan\delta_\ell^{(1)} = -kA_\ell, \qquad \text{(A.4.4)}$$

(see Eq. 2).

Two iterations yield the second Born approximation

$$\tan\delta_\ell^{(2)} = \tan\delta_\ell^{(1)} - kB_\ell, \qquad \text{(A.4.5)}$$

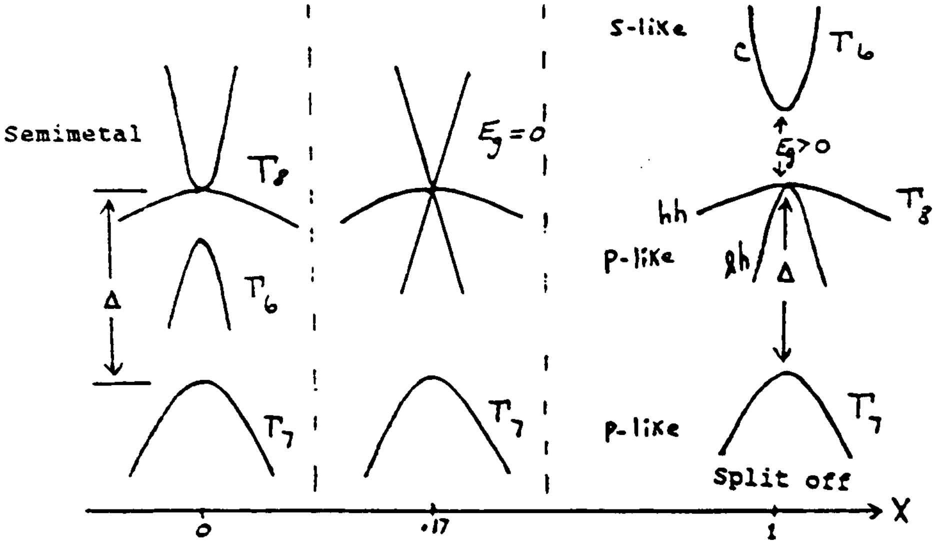
(see Eq. 4).

Variational methods can yield even better approximations (Joachain, ch. 10, 1975). The following agrees with the Born series through second order.

$$\frac{\tan\delta_\ell}{k} = -k\,\frac{A_\ell^2}{A_\ell - B_\ell} \qquad \text{(A.4.6)}$$

Appendix A.5
Band Structure of $Hg_{1-x}Cd_xTe$
The Three Level Model

It is customary to neglect the bands not shown.



Band Structure of $Hg_{1-x}Cd_xTe$ as a function of x

The $\vec{k} \cdot \vec{p}$ Hamiltonian is solved with this model (Kane, 1957) near the Γ point ($k = 0$). The equation describing the conduction band (c), the light hole (lh) band and the split off band is

$$E^3 + (\Delta - E_g) E^2 - (E_g \Delta + P^2 k^2) E - \frac{2}{3} \Delta P^2 k^2 = 0, \qquad \text{(A.5.1)}$$

where P is a momentum matrix element. The heavy hole (hh) band is described by a simple parabolic band. The spin-orbit interaction mixes mixed spin functions and the $\vec{k} \cdot \vec{p}$ interaction mixes s and p functions. The dispersion relations are non parabolic and the electron effective masses are typically small.

Whitsett (1981) gives a two and a half page summary of Kane's band theory and discusses the band structure of the similar compound $Hg_{1-x}Cd_xSe$. For $x > x_0 \cong .17$ (the cross over point) the band structure is like InSb. Γ_6 and the light hole part of Γ_8 are coupled by the $\vec{k}\cdot\vec{p}$ interaction and this "inverts" them. For $x < x_6$, Γ_6 becomes a valence band and $\Gamma_8(\ell h)$ becomes a conduction band. The degeneracy of these two below x_o causes the energy gap to vanish.

Appendix A.6
The Fröhlich Hamitonian

In $Hg_{1-x}Cd_{x}Te$, at not too low temperatures, the scattering of current carriers by polar longitudinal optic phonons is particularly important. The Fröhlich Hamitonian describes this interaction. As given by Mahan (1981, p. 487) it is

$$\begin{aligned} H = \sum_{p} \frac{p^2}{2m} c_p^{+} c_p + \sum \hbar \omega_q a_q^{+} a_q \\ + \sum_{qp} f(q)\, C_{p+q}^{+} c_p \left(a_q + a_{-q}^{+} \right) , \end{aligned} \tag{A.6.1}$$

where c_p^{+}, c_p, a_q^{+}, a_q are the customary creation and annilation operators for electrons and phonons and f(q) which is proportional to the effective charge for interaction (Ehrenreich, 1956) is defined by Mahan. This coupling is not effective for transverse modes because these do not create strong electric fields. It is usual to approximate ω_q by two modes (for HgTe and CdTe).

In order to discuss screening properly, one needs to add to this Hamiltonian electron-electron interactions. Screening affects the way the lattice interacts and so it affects the phonon energies. Screening also affects the electron-phonon interactions (Enhrenreich, 1959). Screening is included by insertion of the correct dielectric function (Zawadski, 1974, Lehoczky et al, 1974, Whisett, 1981 p. 98).

Appendix A.7
Approximations

We first give an order of magnitude estimate for the quantity LaZ which we have assumed to be small.

If $L = 1A$

$Z = 1$

$$a = \frac{2m^*}{\hbar^2} \frac{e^2}{4\pi\varepsilon_0} \quad (MKS)$$

$m^* = .025m_e$

then we find

$LaZ = .1$

Although L might be larger, we also should correct the above by dividing by a static dielectric constant so the estimate may not be too far off. If the electron has an energy of 1 electronvolt and a mass as given above we estimate (on a parabolic band assumption) that

$$k \cong 8 \times 10^8 \ m^{-1},$$

thus if L is 1Å then

$$kL = .08.$$

The following simple argument picks out what ℓ's should be important. If b is the impact parameter we expect

$$kb \sim \ell.$$

Now if b>L then there should be no scattering for those values of ℓ for which

$$b = \ell/k > L.$$

Thus if $kL < 1,$

we would only expect the $\ell = 0$ terms to be important.

Joachain (1975 p. 172) notes that at zero energy ($k = 0$) the Born series converges if

$$\int_0^\infty r\,|U(r)|\,dr < 1 \quad , \quad (\text{for } \ell = 0). \tag{A.7.1}$$

Substituting and evaluating the integrals we find this requires

$$L a \bar{z} < 1.$$

Thus our basic approximations would appear to be O.K. provided kL and $La\bar{z}$ are both small, which would at least be true at low temperature.

Appendix A.8
Density of States and Screening Length

If $\rho(\epsilon)$ is the density of states per unit volume, several authors give the screening length as

$$L_{(1)}^{-2} = k_{TF}^{2}/\epsilon_b , \tag{A.8.1}$$

where a background dielectric constant ϵ_b is included and Eq. A.1.6 gives k_{TF} (with A.1.12). As we have seen, this can also be called the screening length in the 1st Born approximation. This expression is still valid for non parabolic bands provided they are spherical.

Now

$$\rho(\epsilon)d\epsilon = \frac{2}{(2\pi)^3} 4\pi k^2 dk, \tag{A.8.2}$$

for spherical energy surfaces using the usual factor of $(2\pi)^{-3}$ for the number of states per unit volume in real and $\underset{\sim}{k}$ space and the factor of 2 comes from spin. This implies

$$\rho(E) = \frac{k^2}{\pi^2}\frac{dk}{dE}. \tag{A.8.3}$$

Sometimes the momentum effective mass (m*) is used. For m*,

$$m^* v = \hbar k$$

$$v = \frac{1}{\hbar}\frac{dE}{dk}$$

so

$$\rho(E) = \frac{k m^*}{\hbar^2 \pi^2}. \tag{A.8.4}$$

Appendix A.9
Better Approximations

If we are to make better approximations we must eliminate the three approximations we made; namely,

(a) m* in V(r) a constant for corrections to the first Born approximation

(b) kL<<1

(c) only need ℓ = 0 term.

We first indicate what happens when we relax (a) and (c). It is convenient to redo the derivation a bit to see how things fit together.

We assume a $\propto$ m* is not a constant. In order to get agreement with previous results for the screening length, m* is interpreted as the momentum effective mass as in Eq. A.8.4. If we assume

$$\delta_\ell f(E) \Big|_0^\infty = 0,$$

the Friedel sum rule can be written

$$2/\pi \sum_\ell (2\ell+1) \int_0^\infty \delta_\ell \left(-\frac{\partial f}{\partial E}\right) dE = Z. \qquad (A.9.1)$$

With A_ℓ and B_ℓ defined as previously

$$\delta_\ell = -k\left[\int_0^\infty j_\ell^2(kr)\,U(r)\,r^2 dr + B_\ell\left(1 - B_\ell/A_\ell\right)^{-1}\right], \qquad (A.9.2)$$

If we let a = m*b where now m* is considered a function of k, putting the expression for δ_ℓ into the Friedel sum rule and using

$$j_\ell(z) = \frac{z^\ell}{(2\ell+1)!!} \qquad (A.9.3a)$$

and

$$\eta_\ell(z) = -\frac{(2\ell-1)!!}{z^{\ell+1}} \qquad (A.9.3b)$$

as long as $|Z| << 1$, we find

$$\frac{L^2}{L_{(1)}^2} = 1 - \frac{2Zb^2}{\pi}\sum_{\ell}\left[2^{-(2\ell+1)}(2\ell)!!/(2\ell+1)!!\right]L^{2\ell+3}\int\frac{k^{2\ell+1}m^{*2}\left(-\frac{\partial f}{\partial \epsilon}\right)d\epsilon}{1-\frac{bZ}{2\ell+1}2^{-(2\ell+1)}m^{*}L}, \qquad \text{(A.9.4)}$$

where as before $L_{(1)}$ is the screening length in the first Born approximation. This is obviously not a simple equation to solve.

To see what happens if we do not assume $kL<<1$, it is instructive to evaluate A_0.

$$A_0 = \int_0^\infty j_0^2\, U(r)\, r^2 dr$$

$$= -\int_0^\infty \frac{\sin^2(kr)}{(kr)}(Za)\, r e^{-r/L}\, dr. \qquad \text{(A.9.5)}$$

We easily obtain

$$A_0 = -\frac{Za}{k}\left[\frac{1}{4}\ln\left(1+4k^2L^2\right)\right]. \qquad \text{(A.9.6)}$$

If kL<<1 we obtain,

$$A_0 = -(LaZ)L\left[1-2\ (kL)^2\right], \qquad \text{(A.9.7)}$$

which goes over to our previous results when $(kL)^2$ is negligible compared to 1. Similar results can be obtained for B_0, but they do not appear to be particularly transparent.