THE GENERAL NECESSARY CONDITION FOR THE VALIDITY OF DIRAC'S TRANSITION PERTURBATION THEORY

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Abstract

For the first time, from the natural requirements for the successive approximation the general necessary condition of validity of the Dirac's method is explicitly established. It is proved that the conception of "the transition probability per unit time" is not valid. The "super-platinium rules" for calculating the transition probability are derived for the arbitrarily strong time-independent perturbation case.

1 Introduction

The problem of calculating the probability of a transition caused by a small perturbation was considered by P.A.M.Dirac in 1926 [1] . The validity condition of the Dirac's theory for the case of the constant in time perturbation is that the acting time must be not too large. In an application of the theory the coupling parameter or the interaction constant often plays a role of the perturbation coefficient. Naturally, it is very valuable to clarify the relationship between the perturbation coefficient and the time range, in which the theory is valid.

In this paper the problem is solved: the general necessary condition of validity is established as a explicit function of the perturbation coefficient. By deriving the exact formulae we show that the conception of "the transition probability per unit time" always is not valid.

2 Theory

Let us now analyze the Dirac's method in detail. For calculating the transition probability one has to solve the Schrödinger equation:

$$\begin{aligned} i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} &= \hat{H}\,\Psi(\vec{r},t) \\ \hat{H} &\equiv \hat{H}_0 + \varepsilon\hat{V}(t) \qquad ; \quad 0 < \varepsilon < 1 \end{aligned} \tag{1}$$

with the initial condition:

$$\Psi(\vec{r},t=0) = \varphi_i(\vec{r}) \tag{2}$$

where

$$\hat{H}_0\,\varphi_n(\vec{r}) \;=\; E_n^{(0)}\,\varphi_n(\vec{r}) \quad . \tag{3}$$

First, consider the discrete spectrum case [1]. The transition probability W_{if} from state φ_i to φ_f is $\mid a_f(t) \mid^2$ where

$$\Psi(\vec{r},t) \;=\; \sum_f a_f(t)\,\varphi_f(\vec{r},t) \quad . \tag{4}$$

The equation defining $a_f(t)$ is [2]:

$$i\hbar\,\dot{a}_f(t) \;=\; \varepsilon \sum_k V_{fk}(t)\,e^{i\omega_{fk}t}\,a_k(t) \tag{5}$$

or in the integral form is :

$$i\hbar\,a_f(t) \;=\; i\hbar\,\delta_{if} \;+\; \varepsilon \int_0^t dt_1 \sum_k V_{fk}(t_1)\,e^{i\omega_{fk}t_1}\,a_k(t_1) \tag{6}$$

where

$$V_{fk}(t) \;\equiv\; \int d^3\vec{r}\,\varphi_f^*(\vec{r})\,\hat{V}(t)\,\varphi_k(\vec{r}) \quad ; \quad \omega_{fk} \equiv \frac{E_f^{(0)} - E_k^{(0)}}{\hbar} \quad . \tag{7}$$

The $a_f(t)$ is expressed in the form [2]:

$$\begin{aligned} a_f(t) \;&=\; a_f^{(0)} + \varepsilon\,a_f^{(1)}(t) + \varepsilon^2\,a_f^{(2)}(t) + \ldots \\ a_f^{(0)} \;&=\; \delta_{if} \\ a_f^{(1)}(0) \;&=\; a_f^{(2)}(0) \;=\; \ldots \;=\; 0 \quad . \end{aligned} \tag{8}$$

At this stage we have to make the first remark. It is natural that the successive approximation will make sense only if the following question is answered: What ε-order is the contribution of the neglected part less than ? It is evident that $a_f^{(n)}(t)$ takes part in the transition probability:

$$W_{if} \;=\; \mid a_f^{(0)} \mid^2 + \varepsilon\,(\,a_f^{(0)} a_f^{(1)*} + a_f^{(0)*} a_f^{(1)}\,) \;+\; \varepsilon^2\,(\,a_f^{(0)} a_f^{(2)*} + a_f^{(0)*} a_f^{(2)} + \mid a_f^{(1)} \mid^2) \;+\; \ldots \tag{9}$$

at terms containing ε^p with $p \geq n$. After n steps have been carried out, in order that the contribution of the neglected part is less than $\varepsilon^{(n-1)}$, $\mid a_f^{(n)}(t) \mid$ must be of zero-order of ε. Consequently, the numerical value $\mid F^{(n)}(t) \mid_N$ of a time-dependent part $F^{(n)}(t)$ of $a_f^{(n)}(t)$ must be less than ε^{-1}. Inserting (8) into (6) one gets:

$$\begin{aligned} &i\hbar(\,\delta_{mi} + \varepsilon a_m^{(1)}(t) + \varepsilon^2\,a_m^{(2)}(t) + \ldots) \;= \\ &\qquad i\hbar\,\delta_{mi} \;+\; \varepsilon \sum_k \int_0^t dt_1\,V_{mk}(t_1)\,e^{i\omega_{mk}t_1}\,(\,\delta_{ki} + \varepsilon a_k^{(1)}(t_1) + \varepsilon^2\,a_k^{(2)}(t_1) + \ldots) \quad . \end{aligned} \tag{10}$$

Considering $\varepsilon\,\hat{V}$ as a small quantity of the first order of ε ($i.e$ $\hat{V}$ as a zero-order quantity) and " equating terms of the same order " [1], one gets[1]

$$\begin{aligned} i\hbar\,\varepsilon\,a_m^{(1)}(t) \;&=\; \varepsilon \int_0^t dt_1\,V_{mi}(t_1)\,e^{i\omega_{mi}t_1} \\ i\hbar\,\varepsilon^p\,a_m^{(p)}(t) \;&=\; \varepsilon^p \sum_k \int_0^t dt_1\,V_{mk}(t_1)\,e^{i\omega_{mk}t_1}\,a_k^{(p-1)}(t_1) \quad . \end{aligned} \tag{11}$$

[1] From mathematical point of view the group scale $\{\varepsilon^n\}$ with n being integers is chosen for comparing the terms.

In all of these expressions, the summations are extended over all the eigenfunctions of $\hat{H}_0$.

At this stage we have to make the following remarks: 1.Each side of Eq.(10) has infinite number of terms; the set (11) has infinite number of the equations. 2.Because of the term value is changed in time, the term order may be changed. Therefore "equating terms of the same order " is not always equivalent to " equating terms containing the factor ε of the same order ", in geting (11) one has made actually the latter. 3.For separating (10) into (11) by doing so the following conditions are necessary:

i) The modulus of both sides in every equation of set (11) must be of the same order.

ii) The modulus of the right-hand sides in different equations of set (11) must be of different order, *i.e.* in Eq.(10) the modulus of the terms containing the factor ε of different order must be of different one. Therefore at any time $\mid F^{(n)}(t) \mid_N$ must not change their order relation determined by one between their factors $\{\varepsilon^n\}$. This means that

$$\mid F^{(n)}(t) \mid_N < \varepsilon^{-1} \quad \text{for any } n. \tag{12}$$

This condition is in similar but rather deep sence as discussed by Bogoliubov and Mitropolski [3].

Consider now the case when $\hat{V}$ is time-independent. Denoting by I the set of all of the states of energy E_i, *etc*, from Eq.(11) we obtain ($i_\alpha \in I$; $m \notin I$):

$$\begin{aligned}
a_{i_\alpha}^{(1)}(t) &= (-\frac{i}{\hbar})\, V_{i_\alpha i}\, t \\
a_m^{(1)}(t) &= (-\frac{i}{\hbar})\, V_{mi}\, \frac{e^{i\omega_{mi}t} - 1}{i\omega_{mi}} \\
a_{i_\alpha}^{(2)}(t) &= \left(-\frac{i}{\hbar}\right)^2 \left\{ (\sum_{i_\beta \in I} V_{i_\alpha i_\beta} V_{i_\beta i})\, \frac{t^2}{2} + \sum_{n \notin I} V_{i_\alpha n} V_{ni} \left[\frac{t}{i\omega_{ni}} + \frac{(e^{i\omega_{ni}t} - 1)}{\omega_{ni}^2} \right] \right\} \\
a_m^{(2)}(t) &= \left(-\frac{i}{\hbar}\right)^2 \left\{ \sum_{n \notin (M \cup I)} V_{mn} V_{ni} \frac{1}{i\omega_{ni}} \left[\frac{e^{i\omega_{mi}t} - 1}{i\omega_{mi}} - \frac{e^{i\omega_{mn}t} - 1}{i\omega_{mn}} \right] \right. \\
&\quad \left. + \sum_{i_\alpha \in I} V_{mi_\alpha} V_{i_\alpha i} \left[t \frac{e^{i\omega_{mi}t}}{i\omega_{mi}} - \frac{e^{i\omega_{mi}t} - 1}{(i\omega_{mi})^2} \right] + \sum_{m_\beta \in M} V_{mm_\beta} V_{m_\beta i} \frac{1}{i\omega_{mi}} \left[\frac{e^{i\omega_{mi}t} - 1}{i\omega_{mi}} - t \right] \right\}
\end{aligned} \tag{13}$$

It should be noted that in the expression of $a_m^{(3)}$; $m \notin I$ the terms in which the two summation indexes get equal values (*i.e.* the terms with $V_{mk}V_{kk}V_{kj}$, $k \notin J$, $k notin M$) also contain the factor t, *etc.* This means that $a_f^{(n)}(t) with\ n \geq 2$, always contain the secular terms [3].

The general form of $F^{(n)}(t)$ is

$$F^{(n)}(t) = \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} dt_1 \ldots dt_n \ \exp\{i(\gamma_1 t_1 + \ldots + \gamma_n t_n)\}. \tag{14}$$

where γ_n is real for any n. It is easy to see [4] that

$$\mid F^{(n)}(t) \mid \leq \frac{t^n}{n!} \tag{15}$$

The maximal value of $\mid F^{(n)}(t) \mid$ corresponds to the transition , in which the final and all of the intermediate states have the same energy as the initial one. Hence the general necessary condition

of validity (Eq.(12)) leads to (τ denotes the numerical value of t)

$$\tau < \tau_l \equiv \min\left\{(n!\varepsilon^{-1})^{\frac{1}{n}}\right\} \qquad n = 1,2,\ldots\infty \ , \tag{16}$$

i.e. the action time of the time-independent perturbation must be less than the limiting value, which is an explicit function of the perturbation coefficient. For example, when $\varepsilon = \frac{1}{137}$ in the system of units with $\hbar = c = 1$ we get $t_l < 2.4 \times 10^{-10} sec$. Hence the time range,in which the Dirac's method is valid,is ultra-short.

The condition (16) is quite general, purely mathematical and independent of the fact whether the perturbation is turned on suddenly or adiabatically. The time $t = 0$ is namely the moment, from which the perturbation could be considered as constant in time.

In the continuous spectrum case, by repeating the formalism just developed above, it is not difficult to obtain directly the same condition.

This condition is also the necessary one of validity for an arbitrarily time-dependent perturbation case because the time-independent perturbation case is its particular one.

It must be emphasized that when the group scale $\{\varepsilon^n\}$ was chosen it is necessary to use the notions "small of some order of ε", "large of some order of ε^{-1}" *etc.* instead of the uncertain notions as "not too small and not too large", "large enough", "sufficiently small" [1,2,5].In using the Dirac's results it is necessary to justify the existence of the validity range instead of leaning on such very uncertain statement:" There is no difficulty in satisfying both these conditions simultaneously provided the perturbing energy V is sufficiently small" [1].

Now we prove that the conception of "the transition probability per unit time" is not valid. In the time-independent perturbation case the perturbed Hamiltonian has also certain eigenvalues and the full set of the normalized stationary eigenfunctions

$$\hat{H} \mid q\rangle = E_q \mid q\rangle \ . \tag{17}$$

The initial condition (2) means that at $t = 0$ the system state $\mid t\rangle$ is $\mid i\rangle_0$ where $\langle \vec{r} \mid i\rangle_0 \equiv \varphi_i(\vec{r})$

$$\mid t = 0\rangle = \mid i\rangle_0 = \sum_q \mid q\rangle\langle q \mid i\rangle_0 \tag{18}$$

At time t the system state is:

$$\mid t\rangle = \sum_q \mid q\rangle e^{-iE_q t}\langle q \mid i\rangle_0 \ . \tag{19}$$

The probability W_{if} of a transition to $\mid f\rangle_0$ is:

$$W_{if} \equiv \mid {}_0\langle f \mid t\rangle \mid^2 = \left| \sum_q {}_0\langle f \mid q\rangle e^{-iE_q t}\langle q \mid i\rangle_0 \right|^2 \ . \tag{20}$$

The probability W_i of the transitions to the final states $\mid f'\rangle_0$ in the region $\triangle f_0$ [2] is:

$$\begin{aligned} W_i &= \int_{\triangle f_0} df' \left| \sum_q \langle q \mid i\rangle_0 e^{-iE_q t}\, {}_0\langle f' \mid q\rangle \right|^2 \\ &= \sum_{qq'} {}_0\langle i \mid q'\rangle\langle q \mid i\rangle_0 e^{-it(E_q - E_{q'})} \int_{\triangle f_0} df' {}_0\langle f' \mid q\rangle\langle q' \mid f'\rangle_0 \end{aligned} \tag{21}$$

It must be emphasized that these results are exact. They show that even when the perturbation is "sufficiently small"and the time t is "not too small and not too large" [1,2,5], the transition probabilities W_{if} and W_i are not proportional to t, *i.e.* it is impossible to define the conception of "the transition probability per unit time". Moreover, when t approachs infinity because of these exact results are always definite, any approximation, in which W_i, W_{if} are proportional to t, *i.e.* approach infinity, is not valid even qualitatively. In fact, this conception and the Fermi's "golden rule" [2,6] are only the consequences of the approximation used by Dirac without justifying the existence of a validity region.

The right way is the following. When Eq.(17) is one of the well-known exactly solved eigenvalue problems in Quantum Mechanics and when by using the dynamical symmetries and the integrals of the motion [7] we can solve exactly the time-dependent Schrödinger equation, the formulae (20) and (21) give the exact results immediately. When it is not so fortunate, it is possible to use the perturbation method for the eigenvalue problem [1,2,5,6] carefully (*i.e.* it is necessary to verify the validity condition at every step) for solving Eq.(17) and then to calculate the transition probability following formula (20) or (21) up to the necessary accuracy. Therefore, it is interesting to call them "the super-platinium rules".

This means that the method of expansion in power of small parameter is possible for the eigenvalue problem but is very bad for solving the time-dependent Schrödinger equation, which is in a similar situation with the one of the analyzed in [3] equations concerned with the secular terms.

The conception of "the transition probability per unit time" is not valid for the particular case and therefore, is not valid for the general case of the time-dependent perturbation either.

Since the nonrelativistic case is a particular one of the relativistic case when the particle velocity is very much less than the light velocity, this conception is not valid in the relativistic case either, consequently, in Quantum field theory,in which there are many self-inconsistences.

Thus, the carelessness of the genius laureates of Nobel prices have the negative influence on the development of the modern physics.

With a honesty and a courage of the scientist we have to see directly to the truth and together reconstruct the current physics without Dirac's conception of "the transition probability per unit time".

The author would like to thank Profs. V.I.Manko, G.C.Ghirardi and E.C.G.Sudarshan for their support.

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