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Classical Limit of the Probability Density for a Perturbed Change in the Hamiltonian†

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Abstract

The stationary perturbation series is derived from the time-dependent perturbation series up to any order by using a formula derived from the theory of divergent series. The probability density of the perturbed state turns out as the evolution of the density operator of the pure unperturbed initial state as $\hbar \to 0$. This result, for $\hbar \to 0$, indicates that the particle moves in the classical trajectory with the Hamiltonian $H = H_0 + V$ immediately after V is turned on, if it is in the trajectory of H_0 initially. This confirms the classical dynamics. Further, the adiabatic theorem is introduced in order to get the same conclusion for arbitrary finite potential V.

1. *Introduction*

Earlier in this volume (p. 1), we concluded that the ψ-function in quantum mechanics (de Broglie, 1960, 1964) with the probability interpretation does have a particle behaviour (trajectory picture) as $\hbar \to 0$. A theorem was obtained

$$\lim_{t\to\infty} \exp \frac{H(p,q) - \epsilon(n)}{i\hbar} t = \sum_r |\phi_n^{(r)}\rangle\langle\phi_n^{(r)}| \tag{1.1}$$

where $H(p,q)$ is the Hamiltonian of the system and $\phi_n^{(r)}$ its eigenstate with possible degeneracy r corresponding to the eigenvalue $\epsilon(n)$. Further, it was claimed there that the mathematics of divergent series is necessary if a consistent theory of quantum physics with classical physics is expected to exist. Especially, the correctness of the following function was emphasised

$$\begin{aligned} \delta(x,y) &= \lim_{t\to\infty} \exp[i(x-y)t] \\ &= \begin{cases} 1 & x = y \\ 0 & x \neq y \end{cases} \end{aligned} \tag{1.2}$$

In this paper, the perturbation problem is considered, using

$$H = H_0 + V \tag{1.3}$$

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If (1.1) is considered as an evolution operator for H for an infinite time interval, then the time-dependent perturbation series goes to the stationary Rayleigh–Schrödinger (abbreviated as RS hereafter) perturbation series by using (1.2). Similar treatments, but with different bases, have been done by Gell-Mann & Low (1951), Schönberg (1951) and Bates (1961). Since the time interval goes infinitely long, the adiabatic theorem (abbreviated as AT hereafter) should be obeyed (Born & Fock, 1928; Kato, 1950; Messiah, 1961). We claim in Section 2 that in the classical limit $\hbar \to 0$ the system, having an initial unperturbed state, goes to the perturbed state (i.e. it obeys the Hamiltonian H) immediately after V is turned on. This conclusion verifies the classical dynamics as a limit of quantum mechanics if the Hamiltonian of the system is changing by a small amount V.

In Section 3 we express the AT in a form related to (1.1). Then we verify that the above conclusion is also correct for a classical dynamical system in a change of H_0 to $H = H_0 + V$ for an arbitrary V as a limit of the quantum mechanical results *with* probability interpretation and $\hbar \to 0$.

2. *Transient Approach to the Perturbation Theory in Quantum Mechanics and in Its Classical Limit*

In this section, (1.1) is used as an evolution operator and the perturbed state is obtained when (1.1) operates on the unperturbed initial state. Using the probability interpretation, we conclude that in quantum mechanics we need an infinite time interval to arrive at the eigenstate of H from an eigenstate of H_0 as the adiabatic theorem requires, but in its classical limit, the classical trajectory according to H is arrived at promptly after V is turned on, just as given in the classical dynamics.

Denoting ψ_i the eigenstate of H_0

$$H_0 \psi_i = E_i \psi_i$$

and assuming that it is a non-degenerate case, (1.1) implies the perturbed state

$$\phi_n \langle \phi_n | \psi_i \rangle = \left(\lim_{t \to \infty} \exp \frac{H - \epsilon(n)}{i\hbar} t \right) \psi_i \tag{2.1}$$

where, on the right-hand side, ψ_i may be considered as an initial state at $t = 0$. As proved in Appendix A below, by using the well-known time-dependent perturbation formula

$$U(t, t_0) = P \exp (i\hbar)^{-1} \int_{t_0}^{t} dt'\, V'(t') \tag{2.2}$$

where $V'(t) \equiv \exp(-H_0 t/i\hbar) V \exp(H_0 t/i\hbar)$ and P is the time-ordered product. We obtain, $\phi_n = \phi_i$, the stationary RS perturbed state up to any orders as may be calculated from (2.2), and $\langle \phi_i | \psi_i \rangle$ may be put as unity, as usual. Further, in Appendix B (both Appendix A and Appendix B contain material first presented in Su, 1968), the eigenvalue $\epsilon(n) = \epsilon(i)$

in (2.1) for $\phi_n = \phi_i$ is exactly the perturbed energy in RS perturbation theory. Consequently, the quantum-mechanical proof above implies that the perturbed state can be obtained from the unperturbed state via an infinite time transiency after V is turned on. This confirms the adiabatic theorem requirement (Born & Fock, 1928; Kato, 1950; Messiah, 1961).

Now consider the evolution

$$\exp\frac{H(p,q)-\epsilon(i)}{i\hbar}t\,|\psi_i(t=0)\rangle\langle\psi_i(t=0)|\exp\frac{H(p,q)-\epsilon(i)}{-i\hbar}t \tag{2.3}$$

As expressed in $\{\exp(iW/\hbar)|q\rangle\}$-representation (Su, 1971) with $W(q,t)$ in the 'energy representation' (not in $\{q\}$-representation as it was above), it becomes

$$\begin{aligned}
&\lim_{\substack{\hbar\to 0\\ t\neq 0}}\left(\exp\frac{H[p+(\partial W/\partial q'),q']-\epsilon(i)}{i\hbar}t\right)\exp\frac{i(W(q,t)-W(q',t))}{\hbar}\times\\
&\qquad\times\langle q',t=0|\psi_i\rangle\langle\psi_i|q,t=0\rangle\exp\frac{H[p+(\partial W/\partial q),q]-\epsilon(i)}{-i\hbar}t\\
&=\delta\left(H\left(\frac{\partial W}{\partial q'},q'\right),\epsilon(i)\right)\delta\left(H_0\left(\frac{\partial W}{\partial q'},q'\right),-\frac{\partial W}{\partial t}=E_i\right)_{t=0}\times\\
&\qquad\times\delta(q'-q)\,\delta\left(H\left(\frac{\partial W}{\partial q},q\right),\epsilon(i)\right)\\
&=\exp\frac{\epsilon(i)\,t}{i\hbar}\langle q'|\phi_i\rangle\langle\phi_i|q\rangle\exp\frac{\epsilon(i)\,t}{-i\hbar}
\end{aligned}\tag{2.4}$$

from (2.1), we express a classical trajectory of a particle at $q' = q$ moving according to the Hamilton–Jacobi equation

$$H\left(\frac{\partial W}{\partial q'},q'\right)=\epsilon(i) \tag{2.5}$$

and with the initial conditions at $t = 0$ for $q' = q_0 = q$ and for the W function

$$H_0\left(\frac{\partial W(q_0,t=0)}{\partial q},q_0\right)=E_i \tag{2.6}$$

This situation is exactly what is expected in the classical dynamics, i.e. once V is turned on, almost immediately the particle moves according to the equation of motion (2.5), instead of $H_0 = E_i$.

Comparing (2.1) and (2.3), we have solved the perturbation problem both in quantum mechanics and its classical correspondence. In the former case, $t \to \infty$ is needed and in the latter, as $\hbar \to 0$ and t equals any value not equal to zero. Furthermore, the energy values are also noted as, from (2.5) and (2.6),

$$\epsilon(i) = E_i + V(q_0)$$

if $V = V(q)$ for simplicity. The classical initial condition in this classical correspondence does have the peculiar features that if both $\epsilon(i)$ and E_i are quantum mechanical values, special or restricted values of q_0 or $V(q_0)$ are needed.

3. *Wave Function at $t \sim \infty$*

As the time $t \to \infty$ is required in Section 2, the adiabatic theorem should be brought in. For the reason below, we consider the time-dependent Hamiltonian of the system

$$\begin{aligned} H &= H_0 & t &< 0 \\ &= H(t) & 0 &\leqslant t < T_1 \\ &= H_1 & T_1 &\leqslant t \leqslant T_2 \end{aligned} \tag{3.1}$$

satisfying all the conditions on the Hamiltonian as required in AT. In (3.1), H_0 and H_1 are time-independent. Let us denote

$$H_0 \psi_i = E_i \psi_i$$
$$H_1 \phi_i = \epsilon(i) \phi_i$$

then the AT gives the time-dependent wave function $\Psi_i(t)$ with

$$\Psi_i(0) = \psi_i, \qquad \lim_{T_2 \to \infty} \Psi_i(t) = \phi_i \exp \frac{\epsilon(i)\, t}{i\hbar} \tag{3.2}$$

As we see from AT, (3.2) is valid for $t \sim \infty$. Using (1.1) and (3.2), we get

$$\lim_{T_2 \to \infty} \Psi_i(t) = N \exp \frac{\epsilon(i)\, t}{i\hbar} \left(\lim_{t \to \infty} \exp \frac{H_1 - \epsilon(i)}{i\hbar}\, t \right) \psi_i \tag{3.3}$$

where the normalisation constant

$$N = (\langle \phi_i | \psi_i \rangle)^{-1}$$

may be put as unity if we adopt the usual convention. Formally, (3.3) gives a function $\lim \Psi_i(t)$ for $t \sim \infty$ as a result of the following rules. For $0 \leqslant t < \infty$

$$\Psi_i(t) = \exp \frac{H_1\, t}{i\hbar} \psi_i \tag{3.4}$$

as its evolution with the Hamiltonian H_1 (not H)! But at $t \to \infty$ a factor

$$1 = \exp \frac{\epsilon(i)\, t}{i\hbar} \exp \frac{-\epsilon(i)\, t}{i\hbar}$$

should be inserted in order to keep a time-dependent factor $\exp[\epsilon(i)\, t / i\hbar]$, thus $t \to \infty$ only in one of the two.

There may be such a real, physical situation corresponding to (3.4). If we can have the condition

$$U(T_1, 0) \psi_i = \exp \frac{H_1 T_1}{i\hbar} \psi_i \tag{3.5}$$

for the Hamiltonian H in (3.1) on the left-hand side of (3.5), then the system after $t = T_1$ is described by (3.4) and this formal description of (3.3) is physically meaningful. One special and exact example of (3.5) is for the case with the limit $T_1 \to 0$. AT implies

$$U(T_1, 0) \to 1$$

and (3.5) is certainly valid. This example can be stated as follows. For the case in which H has a sudden 'adiabatic change' at $t = 0$ from H_0 to H_1, $\Psi_i(t)$ should tend to a particular way, as given in (3.3).

A particular case of this example is for the perturbation theory with the perturbed Hamiltonian $H_1 = H_0 + V$. If the change from H_0 to H_1 at $t = 0$ is in an 'adiabatic change', then the perturbation theory in Section 2 confirms the above theory.

Similar to the classical correspondence in Section 2, for a well-behaved H such as given in (3.1) with $T_1 \to 0$, (3.2) and (3.3) give

$$\phi_i = N\left(\lim_{t\to\infty} \exp\frac{H - \epsilon(i)}{i\hbar}\, t\right)\psi_i$$

Considering the evolution processes with the probability interpretation

$$\exp\frac{H - \epsilon(i)}{i\hbar}\, t\,|\psi_i(t=0)\rangle\,\langle\psi_i(t=0)|\exp\frac{H - \epsilon(i)}{-i\hbar}\, t$$

and using the $\{\exp[iW(q,t)/\hbar]|q\rangle\}$-representation (Su, 1971) we have

$$\begin{aligned}
&\lim_{\substack{\hbar\to 0\\ t\neq 0}} \langle q'|\left(\exp\frac{-iW(q',t)}{\hbar}\right)\exp\frac{H-\epsilon(i)}{i\hbar}\, t\,|\psi_i(t=0)\rangle \times \\
&\qquad \times \langle\psi_i(t=0)|\left(\exp\frac{H-\epsilon(i)}{-i\hbar}\, t\right)\exp\frac{iW(q,t)}{\hbar}\,|q\rangle \\
&= \lim_{\substack{\hbar\to 0\\ t>0}} \langle q'|\left(\exp\frac{-iW(q',t)}{\hbar}\right)\exp\frac{H_1-\epsilon(i)}{i\hbar}\, t\,|\psi_i(t=0)\rangle \times \\
&\qquad \times \langle\psi_i(t=0)|\left(\exp\frac{H_1-\epsilon(i)}{-i\hbar}\, t\right)\exp\frac{iW(q,t)}{\hbar}\,|q\rangle \\
&= \delta\left(H_1\left(\frac{\partial W}{\partial q'}, q'\right), \epsilon(i)\right)\delta\left(H_0\left(\frac{\partial W}{\partial q'}, q'\right), -\frac{\partial W}{\partial t} = E_i\right)_{t=0} \times \\
&\qquad \times \delta(q'-q)\,\delta\left(H_1\left(\frac{\partial W}{\partial q}, q\right), \epsilon(i)\right) \\
&= \langle q'|\phi_i\rangle \exp\frac{\epsilon(i)\, t}{i\hbar}\langle\phi_i|q\rangle\exp\frac{-\epsilon(i)\, t}{i\hbar}\,|N|^2
\end{aligned}$$

Exactly the same conclusion as given in Section 2 can be obtained; namely the classical trajectory for $H_1 = H_0 + V$ is followed immediately after V is turned on. Now here we have V arbitrary, not necessarily small. Thus the conclusion obtained in Section 2 is generally valid for all cases provided that the transition from H_0 to H_1 is well behaved as given in (3.1) with $T_1 \to 0$.

Finally, $\lim(T_2 \to \infty)\Psi_i'(t)$ depends on H_1 and ψ_i only. No explicit form of $H(t)$ in (3.1) is needed. Quantum mechanically, if only the final state and the initial state is measurable, the adiabatic transient $H(t)$ is immaterial.

Appendix A

Perturbed Wave Function

Equations (2.1) and (2.2) give, in the Schrödinger picture,

$$\begin{aligned}
\phi_n\langle\phi_n|\psi_i\rangle &= \lim_{t\to\infty}\left(\exp -\frac{\epsilon(n)-E_i}{i\hbar}t\right)\exp\frac{Ht}{i\hbar}\exp -\frac{H_0 t}{i\hbar}\psi_i \\
&= \lim_{t\to\infty}\left(\exp -\frac{\epsilon(n)-E_i}{i\hbar}t\right)U(0,-t)\psi_i \qquad\qquad (A.1)\\
&= \lim_{t\to\infty}\exp -\frac{\epsilon(n)-E_i}{i\hbar}t\left(P\exp(i\hbar)^{-1}\int_{-t}^{0} V'(t')\,dt'\right)\psi_i \\
&\equiv \lim_{t\to\infty}\left(\exp -\frac{\epsilon(n)-E_i}{i\hbar}t\sum_j c^{(j)}\psi_i\right)
\end{aligned}$$

where the operators

$$c^{(j)} \equiv (j!(i\hbar)^j)^{-1}\int_{-t}^{0} dt_1\cdots\int_{-t}^{0} dt_j P(V'(t_1)\cdots V'(t_j)) \qquad (A.2)$$

Let us calculate the matrix element of $c^{(j)}$ in the approximation that t is a large quantity with the rules

(i) $t \to \infty$ except the terms t^n

(ii) t^n is kept as a function of t unchanged (A.3)

(iii) if there is a multiple integral, $t \to \infty$ properly in every integral

Then the matrix elements of $c^{(j)}$ in the unperturbed state $\{\psi_i\}$-representation

$$c_{mi}^{(j)} \equiv \langle\psi_m|c^{(j)}|\psi_i\rangle \qquad (A.4)$$

are calculated as

$$c_{mi}^{(0)} = \delta_{mi}$$

$$\begin{cases} c_{mi}^{(1)} = \dfrac{V_{mi}}{E_i - E_m} & (m \neq i) \\ c_{ii}^{(1)} = \dfrac{V_{ii}}{i\hbar} \end{cases}$$

$$\begin{cases} c_{mi}^{(2)} = \displaystyle\sum_{n\neq i} \frac{V_{mn} V_{ni}}{(E_i - E_m)(E_i - E_n)} - \frac{V_{mi} V_{ii}}{(E_i - E_m)^2} + \frac{V_{mi}}{E_i - E_m} c_{ii}^{(1)} \qquad (m \neq i) \\ c_{ii}^{(2)} \equiv \langle \psi_i | \dfrac{1}{(i\hbar)^2} \dfrac{1}{2!} \displaystyle\int_{-t}^{0} dt_1 \int_{-t}^{t_1} dt_2\, V'(t_1)\, V'(t_2) | \psi_i \rangle \end{cases}$$

$$= \sum_{n\neq i} \frac{V_{in} V_{ni}}{E_i - E_n} \frac{t}{i\hbar} + \frac{1}{2!} c_{ii}^{(1)2} \qquad \text{etc.} \tag{A.5}$$

in which (1.2) has been used frequently. It is noted that in comparing the result of (A.5) with the ordinary RS perturbation series, the perturbed state in the RS theory is

$$\phi_i' \equiv \sum_m \psi_m \sum_j c_{mi}^{(j)}(t=0) \tag{A.6}$$

This formula expresses the perturbed state up to any orders of the perturbation. It may be noted here that the matrix element $c_{ii}^{(2)}$ in (A.5) is defined for the usual perturbation theory condition

$$\langle \phi_i' | \psi_i \rangle = 1 \tag{A.7}$$

[or equivalently $\langle \phi_i | \psi_i \rangle = 1$, cf. (A.8) below]. If we want to maintain the unitarity of $U(0,-t) = \sum c^{(j)}$, we need to define

$$c_{ii}^{(2)\prime} \equiv \langle \psi_i | \frac{1}{(i\hbar)^2} \frac{1}{2!} \int_{-t} dt_1 \int_{-t} dt_2 P(V'(t_1)\, V'(t_2)) | \psi_i \rangle$$

$$= -\sum_{n\neq i} \frac{V_{in} V_{ni}}{2(E_i - E_n)^2} + c_{ii}^{(2)}$$

The perturbed state ϕ_i' in (A.6) thus obtained satisfies the unitarity (Schiff, 1955).

Substituting the perturbed energy values from (B.1) below, we get for (A.1) with (A.5)

$$\phi_i \langle \phi_i | \psi_i \rangle = \lim_{t\to\infty} \exp - \frac{\epsilon(i) - E_i}{i\hbar} t \sum_m \psi_m \sum_j c_{mi}^{(j)}$$

After substituting in (A.6), (A.7) and (B.1)

$$\phi_i = \lim_{t\to\infty} \exp \frac{\epsilon(i) - E_i}{-i\hbar} t \left(1 + \frac{E^{(1)}t}{i\hbar} + \frac{1}{2!}\left(\frac{E^{(1)}t}{i\hbar}\right)^2 + \cdots + \frac{E^{(2)}t}{i\hbar} + \cdots\right)\phi_i'$$
$$= \phi_i'$$

apart from a possible unimportant phase factor. Therefore the state ϕ_i above is exactly the perturbed state in the RS theory.

Appendix B

Perturbed Energy

With the rules (A.3), (A.1) can be applied to get the energy eigenvalue

$$\epsilon(i) = \langle\psi_i|(\sum c^{(j)})^{-1} H \sum c^{(j)}|\psi_i\rangle$$
$$\equiv \sum_\alpha E^{(\alpha)}$$

where $\epsilon(i)$ is resolved into the powers of V^α. Define

$$(\sum c^{(j)})^{-1} \equiv \sum c^{-1(j)}.$$

Using $(\sum c^{(j)})^{-1}(\sum c^{(j)}) = 1$, we have

$$\begin{aligned}
c^{-1(0)} &= 1\\
c^{-1(1)} &= -c^{(1)}\\
c^{-1(2)} &= -c^{(2)} + (c^{(1)})^2\\
c^{-1(3)} &= -c^{(3)} + c^{(1)}c^{(2)} + (c^{(2)} - (c^{(1)})^2)c^{(1)}\\
c^{-1(4)} &= -c^{(4)} + c^{(1)}c^{(3)} + c^{(3)}c^{(1)} - c^{(1)}c^{(2)}c^{(1)} -\\
&\quad -c^{(2)}(c^{(1)})^2 + (c^{(1)})^4 + (c^{(2)})^2 - (c^{(1)})^2 c^{(2)} \qquad \text{etc.}
\end{aligned}$$

Thus we have

$$(\sum c^{(j)})^{-1} H \sum c^{(j)} = H + \sum_{\alpha=1}^{\infty} \sum_j e^{(j)}[H, c^{(\alpha-j)}]$$

where

$$\begin{aligned}
c^{(-n)} &= 0 \qquad (n > 0)\\
e^{(-n)} &= 0\\
e^{(0)} &= 1\\
e^{(1)} &= -c^{(1)}\\
e^{(2)} &= -c^{(2)} + (c^{(1)})^2\\
e^{(3)} &= -c^{(3)} + c^{(2)}c^{(1)} + c^{(1)}c^{(2)} - (c^{(1)})^3 \qquad \text{etc.}
\end{aligned}$$

Hence

$$\epsilon(i) = \sum_\alpha E^{(\alpha)} = \langle\psi_i|\left\{H + \sum_{\alpha=1}^{\infty}\sum_j e^{(j)}[H, c^{(\alpha-j)}]\right\}|\psi_i\rangle$$

or

$$
\begin{aligned}
E^{(0)} &= E_i \\
E^{(1)} &= V_{ii} \\
E^{(2)} &= \sum_{n \neq i} \frac{V_{in} V_{ni}}{E_i - E_n} \qquad \text{etc.}
\end{aligned}
\tag{B.1}
$$

which are exactly the values for the perturbed energy in the RS theory.

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