Time-dependent Perturbation Theory in Quantum Mechanics

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Abstract: After revealing difficulties of the standard time-dependent perturbation theory in quantum mechanics mainly from the viewpoint of practical calculation, we propose a new quasi-canonical perturbation theory. In the new theory, the dynamics of physical observables, instead of that of coefficients of wave-function expansion, is formulated so that the gauge-invariance and correspondence principles are observed naturally.

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1 Introduction

The standard time-dependent perturbation theory has two versions: one is for classical mechanics (CM) and the other for quantum mechanics (QM). The quantum version, proposed by Dirac at the early stage of QM, has been included as an important content in almost every textbook of QM and employed in many papers throughout various physical fields.

Although the two versions of the theory deal with different dynamical equations, Hamilton’s equations in CM and Schrödinger’s equation in QM, they use the same canonical variable system and the same Hamiltonian-separation technique. In light of the methodology consistency, people believe that the correspondence principle, which states that QM must be consistent with CM in the classical limit ħ → 0, is well observed.

During the last two decades, difficulties related to the canonical perturbation theory in CM revealed themselves. In particular, Littlejohn indicated that with the use of the vector potential the standard theory mixes up the ordering scheme and proposed using the elegant Lie-formalism to obviate the difficulty. In a relatively recent paper, we manifestly showed that the standard perturbation theory in CM encounters gauge difficulties such that in numerical calculations errors larger than expected may involve and in theoretical analyses unphysical formulations may result. By employing quasi-canonical variables (or “pseudo-canonical” variables), we established another perturbation formalism in CM, which suffers from no gauge difficulties and is still cast in terms of “ordinary” Hamiltonian mechanics.

In contrast with the developments in classical mechanics, the quantum version of the perturbation theory has not been challenged in a similar way. A question arises very naturally. How about the correspondence principle if we, on the one hand, revise the classical version of the theory and, on the other
hand, assume that the quantum version of the theory needs no reconsideration?

This paper is devoted to investigating the issue. Sec. 2 briefly recalls the standard time-dependent perturbation theory in QM. In Sec. 3 we illustrate difficulties that the standard quantum perturbation theory involves. The illustration is mainly from the viewpoint of practical calculations. In Sec. 4, a new perturbation theory is introduced by dealing with physical variables in the Heisenberg picture, and the formulation in the Schrödinger picture is given afterwards. In Sec. 5, we give application and discussion of the new theory. Finally, the paper is summarized in Sec. 6.

2 Standard Perturbation Theory

For convenience of the later discussion, we briefly recall the standard time-dependent perturbation theory in QM.

Consider a quantum system whose Hamiltonian $H$ splits into two parts

$$H = H_0 + H_1$$

where the time-independent $H_0$ describes the unperturbed system and the time-dependent $H_1$ represents involved perturbations. It is assumed that the unperturbed system is exactly solvable, and solutions of it can be expressed by

$$\exp(-\frac{i}{\hbar}\varepsilon_n t)\Psi_n(q)$$

(2)

where $\varepsilon_n$ and $\Psi_n(q)$ are the eigenenergy and the eigenfunction. The basic idea of the standard theory lies in expanding the state function of the real system (described by the total Hamiltonian $H$) in terms of the known unperturbed solutions. In other words, one writes the real state function as

$$\Psi(t) = \sum_n C_n \exp(-\frac{i}{\hbar}\varepsilon_n t)\Psi_n,$$

(3)

and then try to determine the dynamics of the coefficients. If the perturbation is absent, the coefficients $C_n$‘s in Eq. (3) are obviously constants. When the perturbation $H_1$ is taken into account, the coefficients are regarded as depending on time only, or, in explicit form, they can be expressed by

$$C_n = C_n(t).$$

(4)

By substituting Eq. (3) into the Schrödinger equation, using the orthogonality of the eigenfunctions, equations of motion for all individual coefficients are obtained as

$$i\hbar \frac{dC_n}{dt} = \sum_k C_k(H_1)_{nk} \exp(i\omega_{nk}t),$$

(5)
where \( \omega_{nk} = (\varepsilon_n - \varepsilon_k)/\hbar \) and \((H_1)_{nk}\) is the matrix element of the perturbing Hamiltonian \(H_1\) in terms of the eigenfunctions \(\Psi_n\) and \(\Psi_k\). If the initial conditions

\[
C_k(0) = 1 \quad \text{and} \quad C_n(0) = 0 \quad (n \neq k)
\]

are introduced, which means that the system is in the \(k\)-state initially, then (5) yields

\[
C_n(t) \approx -i\bar{\hbar}\int_0^t (H_1)_{nk} \exp(i\omega_{nk}\tau)d\tau \quad (n \neq k).
\]

Note that in obtaining (7) a mathematical approximation method, the method of variation of constant, is applied.

After the perturbation turns off, the system settles down again and the probability of finding the system in the \(n\)-state is

\[
P_{nk} = |C_n(\infty)|^2 = \left|\frac{i}{\bar{\hbar}}\int_0^\infty (H_1)_{nk} \exp(i\omega_{nk}\tau)d\tau\right|^2.
\]

It is quite common in textbooks to consider a microsystem perturbed by an electromagnetic field as a further illustration of the method. For instance, a charged particle in an atomlike system may be described by

\[
H_0 = \frac{1}{2m}p^2 + Q\Phi_0
\]

where \(Q\) is the charge of the particle and \(\Phi_0\) represents the unperturbed field. If an electromagnetic perturbation applies, the perturbing Hamiltonian takes the form

\[
H_1 = -\frac{Q}{mc}A_1 \cdot p + \frac{Q^2}{2mc^2}A_1^2 + Q\Phi_1
\]

where "\(*\)" means an symmetry operation such that for any two operators \(f\) and \(g\), which may be a scalar or a vector, we have (the notation will be used throughout this paper)

\[
f \ast g = \frac{1}{2}(f \cdot g + g \cdot h).
\]

In such notation, (8) becomes

\[
P_{nk} = \left|\frac{i}{\bar{\hbar}}\int_0^{+\infty} \left(-\frac{Q}{mc}A_1 \ast p + Q\Phi_1\right)_{nk} \exp(i\omega_{nk}\tau)d\tau\right|^2,
\]

where the \(A_1^2\)-term has been omitted as a second-order quantity.

### 3 Difficulties of the Standard Theory

The standard perturbation theory outlined in the last section, while seeming stringent and flawless, suffers from difficulties. One of the difficulties has something to do with the gauge transformation.
It is very easy to see that the resultant formula (12) is not gauge-invariant. If the gauge fields $A_1, \Phi_1$ are replaced by

$$A_1 + \nabla f, \quad \Phi_1 - \frac{1}{c} \frac{\partial f}{\partial t},$$

(13)

the expression (13) becomes

$$P_{nk} = \left| \frac{Q}{\hbar} \int_0^\infty \left[ -\frac{1}{mc} (A_1 + \nabla f) \ast \mathbf{p} + Q \left( \Phi_1 - \frac{1}{c} \frac{\partial f}{\partial t} \right) \right] e^{i\omega_n t} dt \right|^2. \quad (14)$$

Apparently, this expression can take any value. Also note that including the $A_1^2$-term in it provides no improvement.

The difficulty was known long ago and many discussions appeared in the literature; but, oddly enough, no consensus has been reached. If different physicists in the community are asked, different answers will be obtained\[9\]. Some suggested that the so-called preferential gauge, in which the vector potential vanishes whenever the electromagnetic perturbation is off, should be employed\[10\]. Others proposed that a certain phase factor should be introduced to the wave function before the whole calculation is applied\[11\]. Furthermore, there are people who assume that the gauge paradox aforementioned is intrinsic for quantum mechanics and can be solved only in quantum field theory; and there are also ones who believe that the gauge trouble is kind of superficial: if higher-order contributions, for instance from the $A_1^2$-term, are carefully taken into account the result will turn out unique and correct.

Though the situation is confusing and opinions are diverse, most in the community seem to lose interest in the subject. Related discussions disappear from the central circulation and only people in the “pedagogical field” still make fuss on it. However, we happen to have a different opinion. In our view, since the derivation of the standard perturbation theory, outlined in Sec. 2, seems quite stringent, the gauge problem aforementioned must be rather fundamental. The more stringent the derivation seems, the more fundamental the problem must be. In one of our recent paper\[12\], motivated partly by the desire of clarifying the gauge issue involved, we challenge the general validity of the principle of superposition.

In this paper we confine ourselves to the perturbation theory. For this reason, we will, in what follows, examine the performance of the theory mainly in terms of practical calculations.

Consider an atomlike system whose quantum state is specified by the quantum numbers $n, l, m$, which are the energy, azimuthal and magnetic quantum numbers respectively. (No spin is considered.) Suppose that the system is perturbed by a magnetic “pulse”

$$B_1 = \epsilon T(t) e_z,$$

(15)
where $T(t)$ is a function whose time-dependence is

$$T(t) = \begin{cases} 
1 & (0 \leq t \leq t_1) \\
0 & \text{(otherwise)}.
\end{cases} \quad (16)$$

We may let the related vector potential take the form

$$A_1 = e T(t) \left(-\frac{y}{2} e_x + \frac{x}{2} e_y\right), \quad (17)$$

which is used commonly and also conforms to the preferential gauge. In terms of classical mechanics such perturbation will definitely affect the state of the system (linearly as well as nonlinearly). If the Schrödinger equation could be solved exactly, the result should be qualitatively the same.

However, the perturbation theory in QM tells us a different story. The perturbing Hamiltonian is, according to (10),

$$H_1 = -\frac{eQT(t)}{2mc} (xp_y - yp_x) + \frac{e^2Q^2T^2(t)}{8mc}(x^2 + y^2). \quad (18)$$

Ignoring the $\epsilon^2$-order nonlinear term, we arrive at

$$\langle n, l, m | H_1 | n', l', m' \rangle \propto \delta_{nn'}\delta_{ll'}\delta_{mm'}.$$ \quad (19)

This means that, linearly speaking, the transition probability from one state to another state is zero!

If we wish to try a numerical calculation, in an attempt to include the nonlinear effects for instance, we will encounter even greater, also more fundamental, difficulties. The formal integration of (13) is

$$C_k(\Delta t) = C_k(0) - \left(-\frac{\hbar}{\bar{\hbar}}\sum_{k'} C_{k'}(0)(H_1)_{kk'} \bar{\Delta} t \right)$$

$$C_k(2\Delta t) = C_k(\Delta t) - \left(-\frac{\hbar}{\bar{\hbar}}\sum_{k'} C_{k'}(\Delta t)(H_1)_{kk'} e^{i\omega_{kk'} \Delta t} \bar{\Delta} t \right)$$

$$\ldots \ldots , \quad (20)$$

where $k$ represents a set of the quantum number $n, l, m$. Suppose that the system is initially described by

$$C_k(0) = 1, \quad C_{k'}(0) = 0 \ (k' \neq k). \quad (21)$$

The first equation of (20) becomes

$$C_k(\Delta t) = 1 - \frac{i}{\bar{\hbar}}(H_1)_{kk} \Delta t. \quad (22)$$

Since the perturbing Hamiltonian $H_1 = H - H_0$ is a self-adjoint operator, $(H_1)_{kk}$ must be a real number. Expressions (13) and (13) show further that the real number in our example is nonzero. All these lead us to

$$|C_k(\Delta t)|^2 > 1, \quad (23)$$
which is not acceptable if we take it for granted that the Schrödinger equation preserves the unity of the total probability.

With the discussion above, we are convinced that there are sufficient practical reasons for that the existing perturbation theory in QM needs to be reconsidered.

4 Quasi-Canonical Perturbation Theory

Before presenting our new perturbation theory, we wish to offer a philosophical reason why we have to give up the existing perturbation theory. Coefficients of wave-function expansion, whose true values are not observable, do not serve as appropriate “objects” for a perturbation theory of the variation-of-constant type. Non-observable quantities are not bound up with the physical inertia of a quantum system; while the system undergoes only a small practical change, they may overreact and get prompt and large variation. (For instance, a phase factor depending on time and space nontrivially may involve instantly.)

We believe that, as stressed in Ref. 7 and 8, in applying a perturbation method of the variation-of-constant type the two following requirements should be fulfilled: (i) Without perturbations, the defined variables, as “objects” of the perturbation theory, are true invariants. (ii) With perturbations involved, the defined variables remain essentially physical. Actually, failure to meet the two requirements has been the source of many errors and much confusion.

For the reasons aforementioned, our theory will mainly be concerned with the dynamics of quantum observables. We shall mainly work in the Heisenberg picture, where the wave function does not change and the dynamics of physical quantities can be examined directly. Obviously, the features of the Heisenberg picture will serve our purpose extremely well. In this section, operators are conventionally defined in the Heisenberg picture. If necessary, the bar notation will be put on the head of an operator that is defined in the Schrödinger picture. The unitary operator $e^{iS(t,q)}$ is reserved to relate the two picture such that for an operator $u$ we have $u = e^{-iS}ue^{iS}$.

We now consider one motion invariant of a quantum system $L(q, v)$. The use of $L(q, p)$ is avoided, since such operator may represent an unphysical quantity after the time-dependent vector potential gets involved. Note that the operator $L(q, v)$ can be constructed out of two basic operators

$$q, p_0 \equiv q, mv + \frac{Q}{c}A_0,$$

(24)

where $q, p_0$ are canonical variables in, and only in, the unperturbed system. (In this sense the new theory may be regarded as a quasi-canonical one.) And, as almost always in quantum mechanics, $L$ is assumed to be a polynomial of its basic operators $q$ and $p_0$. In our discussion we do not consider a quantity that contain the third power of $q$ and $p_0$. 

6
Since we have assumed $L$ to be a motion invariant in the unperturbed system, there must be
\[
\frac{dL}{dt} = \left( \frac{\partial L}{\partial t} \right)_{q, p_0} + \{L, H_0\}_{q, p_0} = 0, \tag{25}
\]
where
\[
H_0 = \frac{m}{2} v^2 + Q\Phi_0. \tag{26}
\]
For the later use, we rewrite (25) in terms of physical quantities. Trivially, the first term in the right-hand side of (25) is
\[
\left( \frac{\partial L}{\partial t} \right)_{q, p_0} = 0. \tag{27}
\]
For an arbitrary operator $G(q)$, we have
\[
\{L(v), G(q)\}_{q, p_0} = \frac{1}{m} \frac{\partial L}{\partial v_i} * \frac{\partial G}{\partial q_i}. \tag{28}
\]
Therefore, we get
\[
\{L, Q\Phi_0\}_{q, p_0} = \frac{Q}{m} \frac{\partial L}{\partial v_i} * E_{0i}. \tag{29}
\]
The calculation of the term $\{L, mv^2/2\}$ is a bit more complex. First, we have
\[
\{L, \frac{1}{2}mv^2\}_{q, p_0} = m \{L, v_j\}_{q, p_0} * v_j; \tag{30}
\]
in which,
\[
m \{L, v_j\}_{q, p_0} = \{L, p_j - \frac{Q}{c} A_{0j}\}_{q, p_0}. \tag{31}
\]
By further calculations,
\[
\{L, -\frac{Q}{c} A_{0j}\}_{q, p_0} = \frac{Q}{mc} \frac{\partial L}{\partial v_i} * \frac{\partial A_{0j}}{\partial q_i}. \tag{32}
\]
and
\[
\{L, p_j\}_{q, p_0} = \frac{\partial L}{\partial q_j} - \frac{Q}{mc} \frac{\partial L}{\partial v_i} * \frac{\partial A_{0i}}{\partial q_j}. \tag{33}
\]
Finally, we obtain
\[
\{L, H_0\}_{q, p_0} = \frac{\partial L}{\partial q_j} * v_j + \frac{Q}{m} \frac{\partial L}{\partial v_i} * E_{0i} + \frac{Q\epsilon_{ijl}}{mc} \frac{\partial L}{\partial v_i} * B_{0l} * v_j = 0, \tag{34}
\]
where $\epsilon_{ijl}$ is the antisymmetric Kronecker symbol.
After a perturbation is applied, we have the equation of motion in the Heisenberg picture as

\[
\frac{dL}{dt} = \left( \frac{\partial L}{\partial t} \right)_{q, p} + \{L, H\}_{q, p} = \left( \frac{\partial L}{\partial t} \right)_{q, p} + \{L, Q\Phi_1\}_{q, p} + \{L, H_0\}_{q, p}.
\]

(35)

In obtaining the equation above we have used \(H = H_0 + Q\Phi_1\), where \(H_0\) is defined by (26) instead of (9). (see Ref. 7 for more analysis about this point.)

We cannot let the last term in (35) vanish simply because (34). The Poisson brackets in (35) are defined under the system of \((q, p)\), which takes on the noncommutation relations

\[
\{q_i, p_j\} = \delta_{ij}, \quad \{p_i, p_j\} = 0,
\]

(36)

while the Poisson bracket in (34) is under the system of \((q, p_0)\), which takes on the noncommutation relations

\[
\{q_i, p_{0j}\} = \delta_{ij}, \quad \{p_{0i}, p_{0j}\} = 0.
\]

(37)

To make use of (34), we should rewrite (35) in terms of observable quantities. By a direct calculation, we obtain

\[
\left( \frac{\partial L}{\partial t} \right)_{q, p} = \frac{1}{m} \frac{\partial L}{\partial v_i} * \left\{ \frac{-Q}{c} \frac{\partial A_{1i}}{\partial t} \right\},
\]

(38)

and

\[
\{L, Q\Phi_0\}_{q, p} = \frac{Q}{m} \frac{\partial L}{\partial v_i} * E_{0i},
\]

(39)

with

\[
\{L, Q\Phi_1\}_{q, p} = \frac{Q}{m} \frac{\partial L}{\partial v_i} * (-\nabla_i \Phi_1).
\]

(40)

The treatment of

\[
\{L, \frac{mv^2}{2}\}_{q, p} = m \{L, v_i\}_{q, p} * v_i
\]

(41)

is similar to that of (30). The velocity operator is in the situation

\[
v = \frac{1}{m} (p - \frac{Q}{c} A_0 - \frac{Q}{c} A_1).
\]

(42)

Therefore,

\[
\{L, \frac{mv^2}{2}\}_{q, p} = \frac{\partial L}{\partial q_i} * v_i + \frac{Q}{mc} \frac{\partial L}{\partial v_i} * (B_{0i} + B_{1i}) * v_j = 0.
\]

(43)
It follows from (38)-(43)

$$\frac{dL}{dt} = \frac{\partial L}{\partial q_j} \ast v_j + \frac{Q}{m} \frac{\partial L}{\partial v_i} \ast E_{0i} + \frac{Q \epsilon_{ijl}}{mc} \frac{\partial L}{\partial v_i} \ast B_{0l} \ast v_j$$

$$+ \frac{Q}{m} \frac{\partial L}{\partial v_i} \ast E_{1i} + \frac{Q \epsilon_{ijl}}{mc} \frac{\partial L}{\partial v_i} \ast B_{1l} \ast v_j.$$  \hspace{1cm} (44)

This equation can be regarded as the equation of motion for an observable in quantum mechanics.

If the system is perturbed only after (and at) the time $t$, (44) becomes, by virtue of (34),

$$\frac{dL}{dt}(t) = \left. \frac{Q}{m} \frac{\partial L}{\partial v_i} \ast E_{1i} + \frac{Q \epsilon_{ijl}}{mc} \frac{\partial L}{\partial v_i} \ast B_{1l} \ast v_j, \right|_{t}$$ \hspace{1cm} (45)

where all the operators are those of the unperturbed system in the Heisenberg picture. In particular, $v = (-i/\hbar) \nabla - (Q/c)A_0$. If desired, this equation can be written in terms of Poisson Bracket

$$\dot{L} = Q\{ L, \Phi_1 \} + \{ q, L \} \ast \frac{Q}{c} \frac{\partial A_1}{\partial t}$$

$$+ \frac{Q}{c} \left( \{ L, q \} \ast \{ A_1, H_0 \} - \{ L, A_1 \} \ast \{ q, H_0 \} \right),$$ \hspace{1cm} (46)

where all the Poisson bracket is defined under the $q, p_0$-system. A comparison with the similar equation in Ref. 7 tells us that we can get (46) simply by using the correspondence principle of Poisson bracket.

**Figure 1**

![Diagram](image)

Now, we assume that the perturbation makes its effect in a step-like fashion, shown in Fig. 1. At the beginning of each step, the system is considered as being in the unperturbed state and thus the variation of the observable after the step is

$$\Delta L \approx \left\langle \frac{dL}{dt} \right\rangle \Delta t,$$ \hspace{1cm} (47)

where

$$\left\langle \frac{dL}{dt} \right\rangle = \left\langle 0 \left| e^{-\frac{i}{\hbar}H_0} \left[ Q \left( \frac{\partial L}{\partial v_i} \ast E_{1i} + \frac{\epsilon_{ijl}}{c} \frac{\partial L}{\partial v_i} \ast B_{1l} \ast v_j \right) \right] e^{\frac{i}{\hbar}H_0} \right| 0 \right\rangle,$$ \hspace{1cm} (48)
in which \(|0\rangle\) stands for the initial state of the system at \(t = 0\).

As for the average expectation value of \(L\) at \(t = T\), we have

\[
\langle L(T) \rangle = L(0) + \int_0^T \left\langle \frac{dL}{dt} \right\rangle dt,
\]

where \(\langle dL/dt \rangle\) is defined by (48).

In view of the fact that motion invariants can form a complete set for a quantum system, it is, up to this point, appropriate to say that our time-dependent perturbation theory in quantum mechanics has been formulated completely.

5 Application and discussion

By Comparing (45), (46) and (49) with counterparts in Ref. 7, we find that the correspondence principle, as well as the gauge-invariance principle, are well observed.

It can easily be verified that if this new perturbation theory is applied in calculating effects of the magnetic “pulse” in Sec. 4 it will yield a much more reasonable nonzero result.

As a theoretical application, we use the new perturbation theory to prove the ineffectiveness of the magnetic force in terms of changing energy. We define the energy of a quantum particle as

\[
\epsilon = \frac{mv^2}{2} + \Phi_0.
\]

Eq. (45) tells us that

\[
\left( \frac{d\epsilon}{dt} \right)_e = \frac{Q}{m} \frac{\partial \epsilon}{\partial v_i} E_{1i}, \quad \left( \frac{d\epsilon}{dt} \right)_m = \frac{Q\epsilon_{ijl}}{mc} \frac{\partial \epsilon}{\partial v_i} B_{1l} v_j,
\]

where \((dL/dt)_{e,m}\) represent the contributions from the electric field and the magnetic force respectively. It is obvious that

\[
\epsilon_{ijl} v_i \ast B_{1l} \ast v_j \equiv 0.
\]

we obtain

\[
\left( \frac{d\epsilon}{dt} \right)_m = 0.
\]

Note that the proof is not possible for the existing perturbation theory, in which effects of the electric force and the magnetic force cannot be separated.

After obtaining the perturbation theory presented above, one could not help using it to further formulate the transition probability \(P_{nk}\), which seemed to be the ultimate goal of such a theory. Unfortunately, the effort failed. In what follows, we include the unsuccessful formulation to show that determining
the transition probability is beyond the scope of a perturbation theory of the variation-of-constant type.

The first step of the formulation is to define a unitary operator as
\[ e^{is} = e^{is} e^{-i\frac{H_0}{\hbar}t}, \]
where \( s(t) \) is a self-adjoint operator. This is possible because the product of \( e^{is} \) and \( e^{-i\frac{H_0}{\hbar}t} \) must be unitary and a unitary operator can be expressed as an exponential of a self-adjoint operator. We then assume that \( s \) is so small that
\[ e^{is} = 1 + is + \cdots. \]

With this expression, we have the relation
\[ L(T) = e^{-i\frac{H_0}{\hbar}T} e^{-is(T)} L(0) e^{is(T)} e^{i\frac{H_0}{\hbar}T} \approx L(0) + ie^{-i\frac{H_0}{\hbar}T} [L(0) s(T) - s(T) L(0)] e^{i\frac{H_0}{\hbar}T}, \]
where the higher-order terms of \( s \) have been omitted. Comparing (56) with (49) yields
\[ s_{kk'}(T) = \frac{e^{i(\omega_{k'} - \omega_k)t}}{i(L_k - L_{k'})} \int_0^T Q \left( \frac{\partial L}{\partial v_i} * E_{1k} + \frac{\epsilon_{ijl}}{c} \frac{\partial L}{\partial v_i} * B_{1l} * v_j \right)_{kk'} e^{i(\omega_k - \omega_{k'})t} dt, \]
where \( L_k \neq L_{k'} \) and \((-)_{kk'}\) is the matrix element of \((-)\). If the system is initially in the \( k \)-state, the probability of finding it in the \( k' \)-state is \( \langle k | e^{i\frac{H_0}{\hbar}T} e^{-is(T)} e^{-i\frac{H_0}{\hbar}T} | k' \rangle \approx | s_{kk'}(T) |^2. \)

Expressions (57) and (58) can indeed yield correct results sometimes. Interested readers may use it to study the forced oscillator and compare the result with the exact solution in textbooks.

However, if we use the formula to calculate transition of an atom, inconsistency emerges. To see it, note that the subscript \( k \) and \( k' \) actually represents a set of quantum eigenvalues, which, for instance, are the energy \( \varepsilon \), the square of azimuthal angular momentum \( \zeta \) and the \( z \)-component of angular momentum \( \zeta \). (We do not use \( L^2 \) and \( L_z \), since \( L \) has been used to represent a general invariant.) Note that (58) may take different values if we apply it to different motion invariants. For (58) to be uniquely defined, we have to, at least, show
\[ | s_{\varepsilon k'}(T) | = | s_{\zeta k'}(T) | \]
where
\[ s_{\varepsilon k'}(T) = \frac{e^{i(\omega_{k'} - \omega_k)t}}{i(\varepsilon_k - \varepsilon_{k'})} \int_0^T Q \left( \frac{\partial \varepsilon}{\partial v_i} * E_{1k} + \frac{\epsilon_{ijl}}{c} \frac{\partial \varepsilon}{\partial v_i} * B_{1l} * v_j \right)_{kk'} e^{i(\omega_k - \omega_{k'})t} dt. \]
\[ s_{\zeta}(T) = \frac{e^{i(\omega_{k'} - \omega_k)T}}{i(\zeta_k - \zeta_{k'})}, \]
\[
\int_0^T \frac{Q}{m} \left( \frac{\partial \zeta}{\partial v_i} \ast E_{it} + \frac{\epsilon_{ijl}}{c} \frac{\partial \zeta}{\partial v_i} \ast B_{lt} \ast v_j \right)_{kk'} e^{i(\omega_{k'} - \omega_k)t} dt.
\]

It is easy to see that, except for a uniform electric perturbation, (59) does not hold.

By inspection of the derivation of (57), we find that the operator \( s(t, q) \) in (54) depends on both the time and the space, and the stringent legitimacy of expanding it into (55) is not there. (This is similar to what happens to the wave-function expansion\[12\].)

As we believe, to determine the value of \( P_{kk'} \) in general cases we have to deal with the Schrödinger equation directly.

6 Brief summary

In this paper, we have showed that the existing time-dependent perturbation theory in QM, like its counterpart in CM, suffers from difficulties and needs to be reconsidered. By investigating the dynamics of physical invariants, instead of the dynamics of coefficients of wave-function expansion, we have formulated a new time-dependent perturbation theory, in which the gauge-invariance principle and the correspondence principle are well observed.

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