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A general procedure for solving the time-dependent Schrödinger equation

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Abstract

A nonperturbative procedure for solving the time-dependent Schrödinger equation, called the multi-projection approach or phase dynamics of quantum mechanics, is derived and illustrated. With the help of this new procedure, time-dependent quantum systems become generally solvable (if corresponding stationary systems are solvable) and the phase character of quantum mechanics reveals itself very clearly.

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1. Introduction

Solutions of the time-dependent Schrödinger equation have been of considerable interest since quantum mechanics was established. Driven by the need to solve theoretical and practical problems throughout physical fields, such as atomic physics, condensed matter physics and laser–matter interaction physics, perturbative and nonperturbative methods were proposed and developed.

As a relatively essential and somewhat perplexing issue, Dirac's perturbation theory [1], being one of the most successful methods in dealing with time-dependent quantum systems, caused seemingly unnecessary concerns. Discussions and suggestions about its validity kept on appearing for several decades. Kobe examined the gauge issue of the formalism [2]. Forney *et al* proposed a special gauge, called the preferential gauge, to eliminate the gauge uncertainty of related calculations [3–5]. Mercouris *et al* stated that in addition to using the preferential gauge, appropriate phase factors should, sometimes, be introduced in order to make coefficients of wavefunction expansion represent the true transition probabilities [6]. The author of this paper studied the classical version and quantum version of the perturbation theory and also met with nontrivial problems [7, 8].

A nonperturbative procedure for solving the time-dependent Schrödinger equation, called the multi-projection approach or phase dynamics of quantum mechanics, will be derived and

illustrated in this paper. The method is not truly new in the sense that the principles employed are quite elementary and have been elaborated in many textbooks. The objective of this paper is to illustrate that these principles are indeed workable in terms of solving the time-dependent Schrödinger equation and to show that the evolution of a quantum system can be characterized almost entirely by phase dynamics.

The structure of this paper is as follows. Section 2 introduces the new approach, which is based on the assumption that the time-dependent Hamiltonian can be approximated by its stepwise time-varying counterparts. The obtained formalism turns out to bear the phase character of quantum mechanics manifestly. In section 3, we use the proposed approach to deal with several simple cases and the effectiveness of the proposed approach is demonstrated to a large extent. Section 4 rederives the Dirac perturbation theory and answers several related questions. Section 5 concludes the paper.

2. The multi-projection approach

Let us directly enter our major subject: to determine a wavefunction $\Psi(t)$ on the premise that the initial wavefunction $\Psi(t_0)$ and the time-dependent Hamiltonian $H(t)$ are explicitly given.

According to the basic formalism of quantum mechanics, we can formally construct a unitary operator to obtain the dynamical wavefunction $\Psi(t)$ from the initial wavefunction $\Psi(t_0)$, namely, we have

$$\Psi(t) = \exp\left(-\frac{i}{\hbar} \int_{t_0}^t H(\tau) d\tau\right) \Psi(t_0). \quad (1)$$

This formula, albeit listed as one of the four axioms of quantum mechanics in some textbooks [9], was not widely appreciated, whereas its time-ordering perturbative variant, leading finally to the famous S -matrix, found many applications and was highly regarded. This is probably due to the fact that Hamiltonians of a system at different times are not generally commutable and the implication of the Hamiltonian integral in (1) is rather ambiguous.

To bypass the problem related to the noncommutability of the Hamiltonian and to make formula (1) conceptually and mathematically explicable (while invoking no perturbative procedure), we first slice the entire time span from t_0 to t into N intervals as

$$\Delta t_1 = t_1 - t_0 \quad \Delta t_2 = t_2 - t_1, \dots \quad \Delta t_N = t - t_{N-1} \quad (2)$$

where $\Delta t_1, \Delta t_2, \dots, \Delta t_N$ are equal to each other or otherwise. The formal solution (1) now becomes

$$\Psi(t) = \exp\left(-\frac{i}{\hbar} \int_{t_{N-1}}^t H(\tau) d\tau\right) \cdots \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t_1} H(\tau) d\tau\right) \Psi(t_0) \quad (3)$$

or, in terms of the intermediate quantum states,

$$\Psi(t_j) = \exp\left(-\frac{i}{\hbar} \int_{t_{j-1}}^{t_j} H(\tau) d\tau\right) \Psi(t_{j-1}) \quad (j = 1, 2, \dots). \quad (4)$$

We then explore the possibility of replacing the Hamiltonian $H(t)$ by its stepwise time-varying approximation $\hat{H}(t)$, as shown in figure 1. Without losing generality, consider a charged particle in an electromagnetic field, whose Hamiltonian reads

$$H(t) = \frac{1}{2\mu} \left(\mathbf{p} - \frac{Q}{c} \mathbf{A}\right)^2 + \Phi \quad (5)$$

where Φ and \mathbf{A} are the time-dependent scalar and vector potentials, respectively. If $\Phi \neq 0$ and $\mathbf{A} \equiv 0$, the replacement of $H(t)$ with $\hat{H}(t)$ is justified by the observation that the two

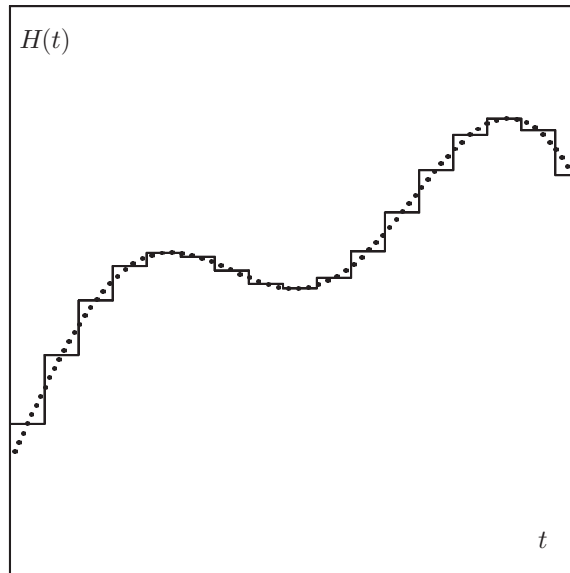


Figure 1. A typical time-dependent Hamiltonian and its stepwise time-varying counterpart.

Hamiltonians represent roughly the same physical system. For the case in which both Φ and \mathbf{A} are nonzero, the situation becomes slightly subtle. As is well-known, the vector potential \mathbf{A} can be separated into two parts: the longitudinal field \mathbf{A}_l and the transverse field \mathbf{A}_t . For a reason that will be made clear in the next paragraph, we accept the gauge in that only the transverse vector potential \mathbf{A}_t and the scalar potential Φ are nonzero. The gauge choice should be allowable in view of the fact that a certain gauge transformation can always make the longitudinal vector field vanish.

The reason why this formulation discriminates against longitudinal vector fields manifests itself in the following consideration. Suppose that an atom is subject to an external electric field $\mathbf{E}(t)$ and the true dynamical wavefunction under the gauge choice $\Phi \neq 0$ and $\mathbf{A}_l = 0$ has been found to be $\Psi(t, \mathbf{r})$. Then, it is well known that the function

$$e^{if(t, \mathbf{r})} \Psi(t, \mathbf{r}) \tag{6}$$

where $f(t, \mathbf{r})$ is an arbitrary function of t and \mathbf{r} , is also the system's wavefunction provided that the gauge in question is allowed to be arbitrary. By noting that a phase factor of the form $e^{if(t, \mathbf{r})}$ can be a nonuniformly continuous function and there are mathematical complications in dealing with nonuniformly continuous function [10, 11], we are convinced that the gauge arbitrariness related to (6) should be excluded. For this to be seen more intuitively, consider simple functions such as e^{ixt} , which oscillates violently as $x \rightarrow \infty$, and great difficulty will arise if we try to differentiate, integrate or expand it.

Under the understanding indicated above, we define the stepwise varying Hamiltonian $\hat{H}(t)$ as

$$\hat{H}_j \equiv \frac{1}{\Delta t_j} \int_{t_{j-1}}^{t_j} H(t) dt \quad (\text{for } t_{j-1} < t < t_j) \tag{7}$$

or, in a much simpler way, $\hat{H}_j \equiv H(\hat{t}_j)$ in that $\hat{t}_j = (t_{j-1} + t_j)/2$. Now, during each of the time intervals expressed by (2), the newly defined Hamiltonian \hat{H}_j is independent of time and the typical intermediate state in (4) becomes

$$\Psi(t_j) \approx e^{-\frac{i}{\hbar} \hat{H}_j \Delta t_j} \Psi(t_{j-1}) \tag{8}$$

which implies that formula (1) makes sense in the form

$$\Psi(t) = \lim_{N \rightarrow \infty} e^{-\frac{i}{\hbar} \hat{H}_N \Delta t_N} \dots e^{-\frac{i}{\hbar} \hat{H}_2 \Delta t_2} e^{-\frac{i}{\hbar} \hat{H}_1 \Delta t_1} \Psi(t_0). \quad (9)$$

For the Hilbert space related to \hat{H}_j (each \hat{H}_j defines a Hilbert space and there are N Hilbert spaces), we have

$$\hat{H}_j \Psi_n^j(\mathbf{r}) = E_n^j \Psi_n^j(\mathbf{r}) \quad (10)$$

where E_n^j and Ψ_n^j are the n th eigenenergy and n th normalized eigenfunction during $t_j < t < t_{j-1}$. After the wavefunction $\Psi(t_{j-1})$ is known, the wavefunction $\Psi(t_j)$ can be expressed by

$$\Psi(t_j) = \sum C_n^j e^{-iE_n^j \Delta t_j / \hbar} \Psi_n^j(\mathbf{r}) \quad (11)$$

where C_n^j is determined by a projection

$$C_n^j = \int \Psi(t_{j-1}) W_n^{j*}(\mathbf{r}) d\mathbf{r}. \quad (12)$$

It has been assumed, for simplicity, that the system has discrete eigenstates only. (If this is not the case, we may employ the box normalization and get a similar formulation.) In the Dirac notation, equations (11) and (12) become

$$|\Psi(t_j)\rangle = \sum_n e^{-i\omega_n^j \Delta t_j} |t_j, n\rangle \langle t_j, n | \Psi(t_{j-1})\rangle \quad (13)$$

where $\omega_n^j = E_n^j / \hbar$. Equation (13) shows that for a short time interval a dynamical system and its corresponding stationary system evolve in almost the same way. If the initial wavefunction $\Psi(t_{j-1})$ is expanded in terms of the eigenfunctions during Δt_{j-1}

$$|\Psi(t_{j-1})\rangle = \sum_l C_l |t_{j-1}, l\rangle \quad (14)$$

equation (13) can be rewritten as

$$|\Psi(t_j)\rangle = \sum_n C_n |t_j, n\rangle \quad \text{with} \quad C_n = e^{-i\omega_n^j \Delta t_j} \sum_l C_l \langle t_j, n | t_{j-1}, l\rangle. \quad (15)$$

Equations (14) and (15) are particularly useful for determining the wavefunction step by step in numerical work. As for the final wavefunction, we obtain

$$|\Psi(t)\rangle = \sum_{k, \dots, l, n} e^{-i\Theta_{k, \dots, l, n}} |t_N, k\rangle \langle t_N, k | \dots |t_2, l\rangle \langle t_2, l | t_1, n\rangle \langle t_1, n | \Psi(t_0)\rangle \quad (16)$$

where

$$\exp(-i\Theta_{k, \dots, l, n}) = \exp[-i(\omega_k^N \Delta t_N + \dots + \omega_l^2 \Delta t_2 + \omega_n^1 \Delta t_1)]. \quad (17)$$

Expressions (16) and (17) are directly explicable in the sense that the multiprojection component $|t_N, k\rangle \dots \langle t_2, l | t_1, n\rangle \langle t_1, n | \Psi(t_0)\rangle$, as a part of the initial wavefunction, indeed 'passes through' the energy states labelled n, l, \dots, k in the defined time-division sequence and should 'naturally' get the phase factor (17). Noting $\sum_n |t_j, n\rangle \langle t_j, n| \equiv 1$, we find another interesting and important fact that if all phase factors of the form $e^{-i\Theta}$ disappeared from (16), the wavefunction would not change at all.

In a real calculation, the major approximation of this method is that the real Hamiltonian is replaced by its stepwise time-varying counterparts. This can be made more plausible by comparing this approach with the influential path-integral approach [12, 13]. In doing that, the following similarities between the two can be observed rather directly. (i) As far as the

numerical computation is concerned, both approaches have to invoke their discrete forms. (ii) In terms of their finite discrete forms, both approaches are approximate, but nonperturbative, theories. (iii) Both approaches assume that as the stepwise time-varying approximation of the Hamiltonian, or that of the corresponding Lagrangian, approaches the real one, convergent and correct results will be obtained. (iv) In both approaches, taking on the zero- \mathcal{A}_I gauge is actually necessary.

In this formalism, the system's energy within any specific time interval can be calculated with the help of the intermediate Hamiltonian and the intermediate wavefunction. In the sense of taking the limit, the result represents the true dynamical energy of the system.

Before concluding this section, it seems in order to point out that the proposed approach offers a different view on quantum dynamics. The Dirac perturbation theory leads us to imagine how a nonstationary system makes a transition from one eigenstate to another. Whereas this theory states that the wavefunction of a nonstationary system experiences no other change than that each of the multiprojection components acquires its own phase factor. (For a stationary system, the same thing takes place except that the involved projection is a single-step one.) To be consistent with the spirit of enlightening discussions about Berry's phase [14], the obtained formalism may therefore be called the phase dynamics of quantum mechanics.

3. Applications

The discussion in the last section has shown that the key tasks in this approach are (i) to find, in a numerical or analytical way, eigenfunctions for each of the Hilbert spaces associated with intermediate Hamiltonians; (ii) to project the wavefunction from one Hilbert space onto the next Hilbert space and (iii) to multiply each of projection components by an appropriate phase factor. The following examples illustrate that for many realistic problems the work that needs to be done is less complicated and less laborious than it appears to be. (There have been worries about treating too many Hilbert spaces.)

Firstly, we study an artificial case which can be solved exactly by the method proposed. Consider a harmonic oscillator disturbed for a time $0 < t < T$ and having the Hamiltonian

$$H(t) = \frac{p^2}{2} + \frac{S(t)}{2}x^2 \quad (18)$$

with $S(t)$ being a stepwise function

$$S(t) = \begin{cases} 1 & (t \leq 0) \\ \xi & (0 < t < T) \\ 1 & (t \geq T) \end{cases} \quad (19)$$

where $\xi \neq 1$ stands for a positive constant. For convenience of discussion, we denote the n th eigenfunction of the oscillator at any time t by $|n, S(t)\rangle$ and the initial wavefunction of the system by $|0\rangle$. From (14) and (15), the system's wavefunction during $0 < t < T$ takes the form

$$\Psi(t) = \sum_n e^{-iE_{n,\xi}t} |n, \xi\rangle \langle n, \xi | 0 \rangle \quad (20)$$

where $E_{n,\xi} = \omega_\xi(n + 1/2)$ with $\omega_\xi = \sqrt{\xi}$ ($\hbar = 1$). After $t = T$,

$$\Psi(t) = \sum_{n,m} e^{-iE_{n,\xi}T - iE_{m,1}(t-T)} |m, 1\rangle \langle m, 1 | n, \xi \rangle \langle n, \xi | 0 \rangle. \quad (21)$$

An interesting fact observed is that if $T = 4\pi/\omega_\xi$, the wavefunction after $t = T$ expressed by (21) becomes, due to $e^{-iE_{n,\xi}T} = 1$ and $\sum_n |n, \xi\rangle \langle n, \xi| = 1$,

$$\Psi(t) = \sum_m e^{-iE_{m,1}(t-T)} |m, 1\rangle \langle m, 1 | 0 \rangle \quad (22)$$

as if the system has been completely frozen during $0 < t < T$, which is somewhat similar to the phenomena predicted by the quantum Zeno effect [15, 16]. On the other hand, the phase character involved can manifest itself more vividly if we assume that the system is initially in the ground state and let T still be equal to $4\pi/\omega_\xi$. Such a system will, after $t = T$, return to the same ground eigenstate, and the only effect of the disturbance is to produce an additional phase factor $\exp(iE_{0,1}T) = \exp(i2\pi/\sqrt{\xi})$. (Note that if the disturbance were not applied at all, namely $\xi = 1$ in the process, the wavefunction would otherwise acquire a phase factor $\exp(-iE_{0,1}T)$ during the same time $0 < t < T$.)

Now, we turn our attention to the anharmonic quantum oscillator that is of a certain significance in studying the early inflationary universe. Due to the complexity of the subject, various related models and considerations appeared in the literature, which are much beyond the scope of this paper. The discussion here, brief and quite primitive in many senses, is almost entirely motivated to show that whenever the Hamiltonian in a consideration is time-dependent, there is a possibility of applying the proposed method.

According to the ‘slow rollover’ scenario of the early universe [17–20], the phase transition can be thought of as one where at very high temperature the potential has a minimum at $\phi = 0$, which becomes unstable as the temperature decreases, with the stable minima moving to a new larger value of $\phi = \pm\sigma$. In the one-dimensional quantum model to simulate the process, the wavefunction initially takes the form of a Gaussian, which is maintained by a harmonic oscillator potential (as explicitly indicated in [18]) and then the wavefunction evolves under a potential that becomes a symmetry-breaking one with minima moving from the central point to new places $x = \pm a$. In this paper, we consider a particle whose Hamiltonian takes the form ($\hbar = 1$)

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) \quad \text{with} \quad V(x) = \lambda_0 + \lambda_2 x^2 + \lambda_4 x^4 \quad (23)$$

where the values of λ_i vary with time in such a way that $V(x)$ makes the following transformation:

$$\frac{1}{2}x^2 \rightarrow \frac{0.01}{24}(x^2 - 5^2)^2. \quad (24)$$

Before dealing with this time-dependent problem fully, let us treat the corresponding stationary systems first. As an illustrative case, it is useful to examine the stationary ‘oscillator’ whose potential is $0.01(x^2 - 5^2)^2/24$. To deal with this system numerically, we replace the potential with a new one having the step shape shown in figure 2, where every spatial step $(\Delta x)_i = x_i - x_{i-1}$ takes the unit value 1 and the average potential within $(\Delta x)_i$ is $U_i = 0.01(\bar{x}_i^2 - 5^2)^2/24$ with $\bar{x}_i = (x_{i-1} + x_i)/2$. After adopting these treatments, it becomes quite easy to get the eigenenergies and eigenfunctions of the system in a semi-analytical way. When the n th eigenenergy ε_n is larger than or equal to the local potential U_i , the analytical form of the wavefunction within the spatial segment Δx_i takes the form

$$\Psi_i(x) = A \cos(k_i x) + B \sin(k_i x) \quad (25)$$

where $k_i = \sqrt{|\varepsilon_n - U_i|}$ and, similarly, when ε_n is smaller than U_i ,

$$\Psi_i(x) = A \exp(k_i x) + B \exp(-k_i x). \quad (26)$$

The numerical value of ε_n in (25) and (26) can be determined by the wavefunction continuity between different $(\Delta x)_i$ and by letting the wavefunction vanish for large x . A simple code written for that purpose yields the energies of eigenstates with even parity as follows:

$$\begin{array}{cccccc} 0.128\ 978 & 0.309\ 293 & 0.571\ 582 & 0.941\ 175 & 1.376\ 138 \\ 1.862\ 994 & 2.393\ 802 & 2.963\ 328 & 3.565\ 216 & 4.208\ 901. \end{array}$$

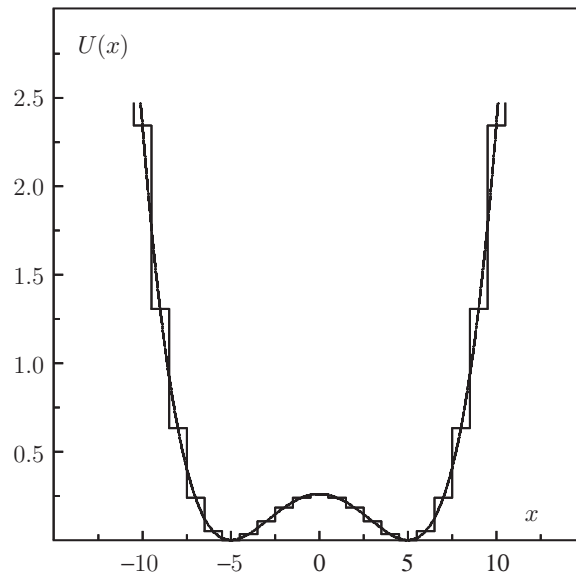


Figure 2. The potential of the anharmonic oscillator and its numerically solvable approximation.

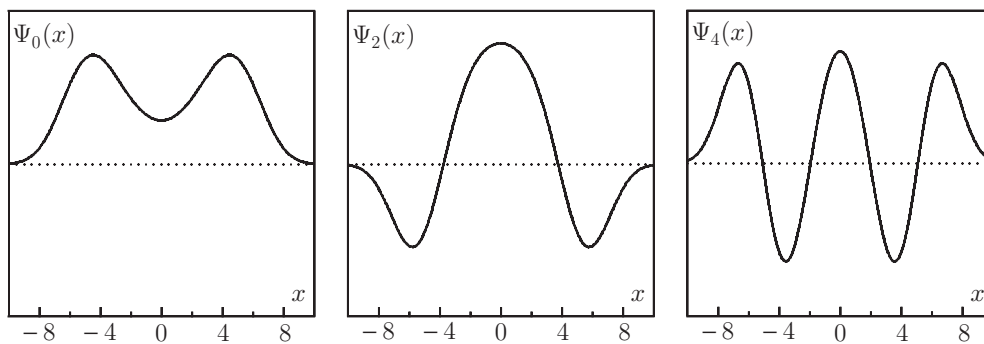


Figure 3. The three lowest even-parity eigenstates of the anharmonic oscillator.

The corresponding eigenfunctions take rather interesting forms. In figure 3, the ground eigenfunction and the two lowest excited eigenfunctions are depicted. Note that for this partially upside-down oscillator, the ground eigenfunction has two maxima.

We now let the parameters λ_i in (23) vary within the time span $\Delta t = 15$. Our numerical calculations show that the final wavefunction is rather insensitive to the concrete pattern of how these parameters vary as long as the potential $V(x, t)$ completes the transformation expressed by (24) for a sufficiently long time. (Here, $\Delta t = 15$ can be considered long enough.) Nonetheless, our typical numerical work was done by setting the parameters in the following way. In the first time stage $0 < t < 5$, λ_2 and λ_4 vary linearly so that the potential is transformed from $x^2/2$ to $0.01x^4/24$; in the second time stage $5 < t < 15$, λ_0 and λ_2 vary linearly so that the potential is transformed from $0.01x^4/24$ to $0.01(x^2 - 5^2)^2/24$. The initial wavefunction takes the Gaussian

$$\Psi(0) = \left(\frac{1}{\pi}\right)^{1/4} \exp\left(-\frac{x^2}{2}\right) \tag{27}$$

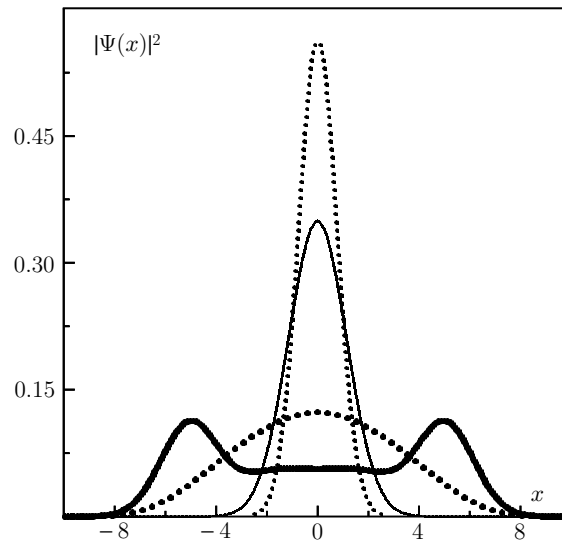


Figure 4. The probability density of the quantum system at different times. The thin dotted and solid lines represent the wavefunctions at $t = 0$ and $t = 5$, respectively; and the thick dotted and solid lines the ones at $t = 10$ and $t = 15$.

Table 1. The time behaviour of the wavefunction in the computational work.

t	C_0	C_2	$\sum E_n C_n ^2$
≤ 0	$1.000\,000 + 0.000\,000\,i$	$0.000\,000 + 0.000\,000\,i$	0.539 847
$0+$	$0.999\,959 + 0.000\,000\,i$	$0.009\,051 + 0.000\,000\,i$	0.525 441
τ_0+	$0.965\,423 - 0.259\,403\,i$	$0.015\,378 - 0.013\,603\,i$	0.496 332
$2\tau_0+$	$0.872\,307 - 0.487\,367\,i$	$0.474\,626 - 0.036\,187\,i$	0.466 001
\dots	\dots	\dots	\dots
$30\tau_0+$	$-0.265\,492 - 0.772\,048\,i$	$-0.498\,776 + 0.287\,855\,i$	0.190 124

which is the ground state of the potential $x^2/2$. Under these conditions, the wavefunction is found to evolve as in table 1,

in which the entire time has been sliced into 30 intervals and C_i are given in terms of intermediate Hilbert space. For lack of space, C_4, C_6, \dots, C_{18} and $\sum_{i=0}^9 |C_{2i}|^2 \approx 1$ have not been listed in the table. Figure 4 shows that the probability density of the system ‘rolls’ down to its final minima gradually and the rolldown takes place mainly during the time $10 < t < 15$.

Another observation has been made in the computation: if the entire time span is shortened by half, while leaving the potential to complete the transformation expressed by (24), the final probability density will not have enough time to ‘roll down’ from the central point.

4. Rederivation of the Dirac perturbation theory

In this section, we rederive the Dirac perturbation theory. The purpose of doing so is twofold. One is to illustrate the analytical ability of this approach, and the other is to further answer questions concerning the Dirac perturbation theory.

To obtain an analytical formalism, which is presumably the same as the standard one, we accept the following assumptions. (i) The quantum system of interest is initially in the n th

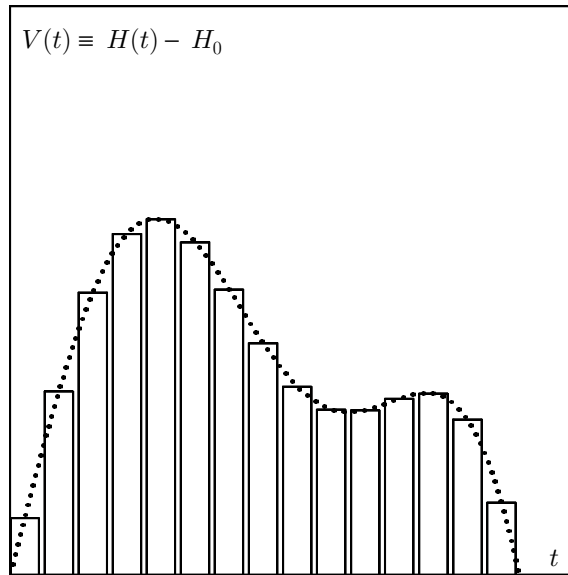


Figure 5. A perturbation and its pulse-like approximation.

eigenstate of H_0 , the perturbation applies at the initial time $t = 0$ and vanishes completely at the final time $t = T$. (ii) The perturbation can be approximated by a series of pulses whose values rise sharply and then vanish sharply and completely, as illustrated in figure 5. That is, we take on the conception that the pulse-like perturbation gives the same physical effects as the real perturbation does. (iii) The leading term of the wavefunction, namely, the value and the phase factor of the n th eigenstate, will not be seriously disturbed. (iv) The other nonleading terms, produced by pulses of the disturbance, will not be seriously disturbed by pulses coming later on. With these assumptions accepted, the derivation here, which can be regarded as an application of the ‘sudden approximation’ due to Pauli [21, 22], holds.

Consider one specific pulse of the perturbation that exists between t' and $t' + \Delta t'$. The leading term of the wavefunction at $t = t'$ is $e^{-i\omega_n t'} |n\rangle$, at $t = T$ it becomes, under the disturbance of the pulse,

$$\begin{aligned}
 e^{-i\omega_n t'} |n\rangle &\rightarrow \sum_k e^{-i\omega_n t'} e^{-i\omega_k \Delta t'} \langle k|n\rangle |k\rangle \\
 &\rightarrow \sum_{k,m} e^{-i\omega_n t'} e^{-i\omega_k \Delta t'} e^{-i\omega_m (T-t'-\Delta t')} \langle m|k\rangle \langle k|n\rangle |m\rangle
 \end{aligned}
 \tag{28}$$

where $|m\rangle$ stand for eigenfunctions defined by the Hamiltonian H_0 and $|k\rangle$ eigenfunctions defined by the intermediate Hamiltonian within the pulse. Note that in (28), before t' and after $t' + \Delta t'$ all the phase factors evolve regularly as if the other pulses do not exist. (This is a conditional assumption as has been indicated.) Since $\Delta t'$ is short, the following approximation is acceptable:

$$\sum_k \langle m|k\rangle e^{-i(\omega_k - \omega_m)\Delta t'} \langle k|n\rangle \approx \langle m|1 - \frac{i}{\hbar}[H(t') - H_0]\Delta t'|n\rangle
 \tag{29}$$

thus, the m th coefficient of the wavefunction at $t = T$ is

$$b_m = -\frac{i}{\hbar} \Delta t' \langle m|V|n\rangle e^{-i(\omega_n - \omega_m)t'} e^{-i\omega_m T} \quad (m \neq n)
 \tag{30}$$

where $V \equiv H(t') - H_0$. Taking contributions from all pulses into account, we obtain at $t = T$

$$b_m = -\frac{i}{\hbar} e^{-i\omega_m T} \int_0^T V_{mn} e^{-i(\omega_n - \omega_m)t'} dt' \quad (m \neq n). \quad (31)$$

Except for the phase factor $\exp(-i\omega_m T)$, the above formula is consistent with the well-known one.

The present derivation, called the sudden-approximation (SA) derivation, is quite different from the textbook derivation. On the ‘positive side’, it confirms the validity of (31) without differentiating or integrating the wavefunction expansion term by term. On the ‘negative side’, it reveals several factors restricting the use of the perturbation theory. To be more specific about such factors, the following mention should be made. (i) If the final Hamiltonian $H(t > T)$ is not the same as the initial Hamiltonian $H(t_0)$, this formalism will mistakenly assume that there are ever-lasting ‘perturbation pulses’ and yield misleading predictions. (ii) If the phase factors of the wavefunction, including all those related to relevant eigenstates, are severely disturbed, the formalism will not be accurate. (iii) The formulation holds only under the gauge in that no longitudinal vector field exists, which, together with $H(t > T) = H(t_0)$, can be interpreted as the preferential gauge [3–5].

Before leaving this subject, we wish to comment on the common belief that a dynamical wavefunction can formally be represented by a series of the form

$$\sum_n C_n(t) e^{-i\omega_n t} \Psi_n(\mathbf{r}) \quad \text{or} \quad \sum_n C_n(t) \Psi_n(\mathbf{r}) \quad (32)$$

in which ω_n and $\Psi_n(\mathbf{r})$ are, by convention, related to the initial Hamiltonian.

In our view, expansion (32), though holding its significance at any fixed instant, should not be utilized to obtain solutions for the time-dependent Schrödinger equation. Mathematically speaking, (32) is not a uniformly convergent series and it is not legitimate to differentiate or integrate such series term by term [8]. Physically speaking, after a dynamical system leaves its initial state, the eigenfunctions and eigenfrequencies associated with the initial Hamiltonian become out of date. If we still use them at later times, some coefficients of the series have to adjust themselves violently, so violently that they cannot be determined in a practical way.

The above discussion implies, in a different perspective, that formulating successive, but discrete, states of a quantum system is a rather good alternative. Interestingly enough, the path-integral approach and Berry’s phase studies have taken approaches of this type for a long time [23].

5. Summary

A nonperturbative procedure, called the multiprojection approach or phase dynamics of quantum mechanics, has been proposed, which in a way unifies treatments of different quantum systems: stationary and nonstationary, weakly-disturbed and strongly-disturbed. Considering that knowledge about stationary systems has long been accumulated and many systems with strong fields need to be studied, such a unification seems desirable.

The similarities between the multi-projection approach and the path-integral approach also suggest that the proposed method may find applications in a variety of quantum fields.

It has been shown that a system’s dynamics can be described by the process in which each multiprojection component of the wavefunction acquires its own phase factor. This ‘state transition’ picture is quite different from that of the standard theory. The standard picture, usually associated with the initial Hilbert space and paying much less attention to the disturbance of phase factors, is useful only if several conditions are simultaneously satisfied,

which in general include: the final Hamiltonian is the same as the initial Hamiltonian, the perturbation is relatively small and the action time of the perturbation is relatively short.

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