New U-matrix theory in quantum mechanics

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We have analyzed Dyson's U-matrix theory of solving the Schrödinger equation in the interaction picture and are able to express the U matrix as a dominant term plus an infinite series involving multiple integrals of time. For a certain rather restrictive class of Hamiltonians, our theory is exact for a general time-dependent problem. For other Hamiltonians, we can only obtain approximate expressions for our U matrix and hence the wave function. Treating a time-independent problem as a special case of the time-dependent situation with a sudden-switching process, we have shown that our U matrix is exact. To demonstrate the working procedures of our theory, we apply it to study the well-known time-independent charged harmonic-oscillator problem and the more general harmonic oscillator with a time-dependent driving force. Compared with other methods, our new theory appears to lead to a result which contains more information than others due to the inclusion of noncommutability properties of operators in the operator Schrödinger equation. It has been shown that the classical Feynman path-integral formalism can be deduced from quantum mechanics with the use of the Green's-function operator. It is interesting to note that apart from a step function, the Green's-function operator is the same as that of our $U^{(s)}$ matrix, which is the U matrix obtained within the regime of the Schrödinger picture for a time-independent Hamiltonian, as a special case of our general time-dependent treatment.

I. INTRODUCTION

Dyson proposed the basic U-matrix theory in 1949,[1,2] writing the wave function in terms of a U-matrix within the regime of the interaction picture. The U matrix, however, is expressed as a series of multiple integrals in time, the limits of integration following a time-order sequence. In solving actual problems, one can calculate a few terms in this series, but one does not know exactly how much these terms represent in the whole U matrix. One cannot, in general, handle other terms (for example, a triple integral in the old U-matrix theory) and express the U matrix in a ready, workable form. Gell-Mann and Low[3] applied the U-matrix theory to study the bound states of nucleons. In order to have a solution, they used the Feynman diagram technique to solve for the kernel in the integral equation. In arriving at Gell-Mann and Low's solution, the "adiabatic hypothesis" has been proposed. Snyder[4] has found that for a scattering process, the use of the adiabatic switch-off procedure is unnecessary. This aspect was confirmed in the work of Moses,[5] who, using Friedrick's perturbative approach,[6] has derived expressions for the "outgoing" and "incoming" eigenfunctions and the scattering operator arising from the time-dependent Schrödinger equation. These works can be considered as stages of development of the U-matrix (or S-matrix) theory. In fact, it has long been known that it is difficult to obtain a solution directly from the basic U-matrix theory.

The Green's-function method[7–10] is rather frequently used. In this formalism, we arrive at a number of coupled integral equations for the different Green's functions in general. No exact solutions can be obtained unless we decouple the integral equations. Here approximations have to be taken for such decoupling, and these approximations usually correspond to including only a number of relevant terms in the usual perturbation technique. Often, the approximated Green's-function solutions are presented in a diagrammatic language closely related to the result of perturbation method. Taking for granted that the approximations are good ones, if we know the answers (observables) beforehand from experimental data, the Green's-function method enables us to explore the dominant perturbation terms responsible for the observed physical results.

The perturbation theory[11–13] begins with a noninteracting system, and by adding a perturbation term to the Hamiltonian, one hopes that the correction due to interaction can be expressed as a convergent power series of the interaction strength. The working procedures are very complicated and the validity of this method is rather restrictive. The unitary transformation[14] approach is exact, in principle, and can be simpler than using other methods. However, success of such a method relies on guessing the right transformation; the method is therefore indirect and not workable in many cases. In using the variational approach, one assumes some trial wave function for the system with built-in variational parameters. Taking a variational process, one can obtain an upper bound of the ground-state energy. The accuracy of this method depends on how close the trial wave function is to the exact wave function.

The path-integral method was introduced to study quantum-mechanical problems using the classical least action principle.[15] Later, the path-integral method is bridged to the S-matrix representation in quantum mechanics.[16] A relationship between the U-matrix and a function of the Lagrangian has been established.[17] A more comprehensive development and the application of the path-integral approach to solve quantum-mechanical problems is given in Ref. 18. A comparison between the path-integral formalism and our U-matrix theory is discussed in Sec. VII.

The above-mentioned methods have been used to study single- and many-particle quantum-mechanical problems, directly or indirectly. Recently, Fung, Wong, and co-workers[19–21] have obtained the exact wave function for an interacting many-boson system and a bridge is built between the basis-correlation function formalism (which may be considered to be in the trial wave-function regime) and the Bogoliubov canonical transformation method.

Despite all the efforts stated above, an exact workable method to treat a general time-dependent quantum-mechanical problem still awaits. In this investigation we intend to develop the U-matrix theory for the stated reason. We shall start with the basic formalism of Dyson and express the U matrix as an infinite series. We are able to reduce the order of the multiple integral of the U matrix, isolating what we believe to be the dominant contribution. Using the interaction picture as before, we can then express the approximate time-dependent wave function of a system in terms of the Hamiltonian explicitly. We treat a time-independent problem as a special case of a time-dependent problem. Employing the "sudden-switching" model for turning on the interaction, we shall show that for a time-independent problem our formalism is exact as the U matrix terminates.

In Sec. V, we apply our theory to study the well-known time-independent charged harmonic oscillator. Our result is, of course, identical to the established one.[8] To demonstrate the working procedures of our theory for a time-dependent problem we study in Sec. VI the time-dependent harmonic oscillator[22] with a general driving force, using the same Hamiltonian as in Ref. 23. For this problem we can only calculate our U matrix and hence the wave function in an approximate manner. Peng[23] attempted to solve the problem directly using the Schrödinger equation, and the method is supposed to be exact. Our approximate result is shown to be identical to Peng's, suggesting that our theory leads to result which contains more information than the "exact" one. We discuss the sources of this "surplus" information.

II. BASIC FORMALISM OF THE U-MATRIX THEORY

For a time-dependent quantum-mechanical system with Hamiltonian $\hat{H}(t)$, the Schrödinger equation is

$$i\frac{\partial\Phi(t)}{\partial t}=\hat{H}(t)\Phi(t)\ , \tag{2.1}$$

where $\Phi(t)$ is the wave function of the system and units are chosen such that $\hbar$ is one. We express the Hamiltonian in the following form:

$$\hat{H}(t)=\hat{H}_0+\hat{v}(t)\hat{\eta}(t)\ , \tag{2.2}$$

where the "interaction generating operator" $\hat{\eta}(t)$ has the property

$$\hat{\eta}(t)\Phi(t)=\begin{cases}0 \text{ for } -\infty<t<-b\\ S_W(t)\Phi(t) \text{ for } -b\le t<0\\ \Phi(t) \text{ for } 0\le t<\infty\end{cases} \tag{2.3}$$

where b is a positive number. We can also rewrite Eq. (2.3) in the following form:

$$\hat{\eta}(t)\Phi(t)=S_W(t)\Phi(t)\ , \tag{2.4}$$

where the eigenvalue $S_W(t)$ of the above equation is specified by

$$\begin{aligned}&S_W(-\infty<t<-b)=0\ ,\\ &S_W(-b\le t<0)\ge 0\ ,\\ &S_W(0\le t<\infty)=1\ .\end{aligned} \tag{2.5}$$

Separation of the function $S_W(t)$ into the above three regions means that there is a transient period $-b\le t<0$ for an interaction to take place and the interaction is starting from $t=0$. Gell-Mann proposed that $b\to-\infty$, but we leave b a finite quantity so that both "slow-switching" and sudden-switching processes can be taken care of with our formalism.

We shall call S_W the switching function and it will be seen later that this concept is crucial and will lead to more contributions to the solution of a physical problem.

Keeping in mind relations (2.2) and (2.3), our Schrödinger equation becomes

$$i\frac{\partial\Phi(t)}{\partial t}=[\hat{H}_0+S_W(t)\hat{v}(t)]\Phi(t) . \tag{2.6}$$

In order to express (2.6) in a form consistent with the interaction picture, we make the following transformations:

$$\Psi(t)=e^{i\hat{H}_0 t}\Phi(t) , \tag{2.7a}$$

$$\hat{H}_1(t)=e^{i\hat{H}_0 t}[S_W(t)\hat{v}(t)]e^{-i\hat{H}_0 t}$$

$$=S_W(t)\hat{V}(t) , \tag{2.7b}$$

$$\hat{V}(t)=e^{i\hat{H}_0 t}\hat{v}(t)e^{-i\hat{H}_0 t} \tag{2.7c}$$

so that the interaction Hamiltonian becomes

$$\hat{H}_1(t)=S_W(t)\hat{V}(t) . \tag{2.8}$$

Differentiating Eq. (2.7a), with respect to time, and using Eq. (2.6) and (2.8), we obtain

$$i\frac{\partial\Psi(t)}{\partial t}=S_W(t)\hat{V}(t)\Psi(t)$$

$$=\hat{H}_1(t)\Psi(t) . \tag{2.9}$$

This is, of course, the Schrödinger equation in the interaction picture. Integrating the above equation,

$$\Psi(t)=\Psi(t_0)-i\int_{t_0}^{t}\hat{H}_1(u)\Psi(u)du . \tag{2.10}$$

Carrying out an iterative process, we can relate Ψ and Ψ_0 through a U matrix:

$$\Psi(t)=\hat{U}(t,t_0)\Psi(t_0) , \tag{2.11}$$

where

$$\hat{U}(t,t_0)=1+\sum_{n=1}^{\infty}\hat{U}_n(t,t_0) \tag{2.12}$$

and

$$\hat{U}_n(t,t_0)=(-i)^n\int_{t_0}^{t}du_1\int_{t_0}^{u_1}du_2\cdots\int_{t_0}^{u_{n-1}}du_n\hat{H}_1(u_1)\hat{H}_1(u_2)\cdots H_1(u_n) . \tag{2.13}$$

In view of (2.2) and (2.4), we can express $\Phi(t)$ in terms of $\Phi(t_0)$:

$$\Phi(t)=\hat{S}(t,t_0)\Phi(t_0) , \tag{2.14}$$

where

$$\hat{S}(t,t_0)=e^{-i\hat{H}_0 t}\hat{U}(t,t_0)e^{i\hat{H}_0 t_0} . \tag{2.15}$$

Apart from introducing the switching function S_W as specified by (2.4) and (2.5), the formalism is a standard U-matrix theory in the interaction picture. In the past, one could not express the U matrix in a manageable form. We shall show in Sec. III that we can reduce the order of the multiple integral in (2.13) by two, separating out the dominant term for our U matrix.

III. SERIES EXPANSION OF THE U MATRIX

First, we note that for general operators $\hat{P}$, $\hat{Q}$, it is elementary to prove that

$$e^{\hat{P}}\hat{Q}e^{-\hat{P}}=\hat{Q}+[\hat{P},\hat{Q}]+\frac{1}{2!}[\hat{P},[\hat{P},\hat{Q}]]$$

$$+\frac{1}{3!}[\hat{P},[\hat{P},[\hat{P},\hat{Q}]]]+\cdots$$

$$=\sum_{n=0}^{\infty}\frac{1}{n!}[\hat{P},\hat{Q}]_n , \tag{3.1}$$

where

$$[\hat{P},\hat{Q}]_0=1 ,$$

$$[\hat{P},\hat{Q}]_r=[\hat{P},[\hat{P},[\cdots,[\hat{P},\hat{Q}]]\cdots]] ,$$

where there are r commutator terms. In the same way, we can write the interaction Hamiltonian as

$$\hat{H}_1(t)=S_W(t)\left[\hat{v}(t)+\sum_{r=1}^{\infty}\frac{(it)^r}{r!}\hat{\Gamma}_r(t)\right] , \tag{3.2}$$

where

$$\hat{\Gamma}_r(t)=[\hat{H}_0,\hat{v}(t)]_r . \tag{3.3}$$

We shall call $\hat{\Gamma}_r(t)$ the termination operator on account of property (i) stated below. We shall see later that one important step in solving an actual problem is to study this termination operator. There are several properties of $\hat{\Gamma}_r$ worth noting. They are as follows.

(i) Generally, $\hat{\Gamma}_1(t),\hat{\Gamma}_2(t),\cdots\hat{\Gamma}_\infty(t)\neq 0$. But if for a certain integer j,

$$\hat{\Gamma}_{r=j}(t)=0 \text{ or } C\,, \text{ const}$$

then

$$\hat{\Gamma}_{r>j}(t)=0\,. \tag{3.4}$$

(ii) It follows that

$$[\hat{H}_0+\hat{v}(t),\hat{\Gamma}_r(t)]=\hat{\Gamma}_{r+1}(t)+\hat{\Gamma}_r^{(1)}(t)\,, \tag{3.5}$$

where $\Gamma_r^{(1)}(t)\equiv[\hat{v}(t),\hat{\Gamma}_r(t)]$.

(iii) Then,

$$[\hat{H}(t),\hat{\Gamma}_r(t)]_p=\hat{\Gamma}_{r+p}(t)+S_W(t)\{\hat{\Gamma}_{r+p-1}^{(1)}(t)+[\hat{H}(t),\hat{\Gamma}_{r+p-2}^{(1)}(t)]+[\hat{H}(t),[\hat{H}(t),\hat{\Gamma}_{r+p-3}^{(1)}(t)]]+\cdots$$
$$+[\hat{H}(t),\hat{\Gamma}_r^{(1)}(t)]_{p-1}\}\,. \tag{3.6}$$

(iv) Therefore,

$$[\hat{H}_0,\hat{\Gamma}_r^n]=\sum_{j=0}^{n-1}\hat{\Gamma}_r^j\hat{\Gamma}_{r+1}\hat{\Gamma}_r^{n-(j+1)}\,. \tag{3.7}$$

(v) Finally,

$$\hat{H}_0^n\hat{\Gamma}_r=\hat{\Gamma}_r\hat{H}_0^n+\sum_{j=0}^{n-1}\hat{H}_0^{n-(j+1)}\hat{\Gamma}_{r+1}\hat{H}_0^j\,. \tag{3.8}$$

The proofs are rather elementary and will not be presented here. Since this paper is the first of a series, we shall keep (3.5)—(3.8) here for further use in solving actual problems.

In the process of obtaining a series expression for $\hat{U}$, we first write a recurrence expression for $\hat{U}_n$ based simply on definition (2.13):

$$\hat{U}_n(t,t_0)=-i\int_{t_0}^t\hat{H}_1(u)\hat{U}_{n-1}(u,t_0)du\,,\quad n\geq 1\,. \tag{3.9}$$

For $n=1$,

$$\hat{U}_1(t,t_0)=-i\int_{t_0}^t\hat{H}_1(u)\hat{U}_0(u,t_0)du\,. \tag{3.10}$$

Comparing (2.13) and (3.10), obviously,

$$\hat{U}_0(u,t_0)\equiv 1 \text{ for } t_0\leq u\leq t\,. \tag{3.11}$$

Notice that in (2.12), n starts from 1 and we take $\hat{U}_{-1}=\hat{U}_{-2}=\hat{U}_{-3}=\cdots=0$.

We would note that, in view of (3.2),

$$[\hat{H}_1(t_1),\hat{H}_1(t_2)]=[S_W(t_1)\hat{v}(t_1),S_W(t_2)\hat{v}(t_2)]+S_W(t_1)S_W(t_2)\sum_{r=1}^{\infty}\frac{(it_2)^r}{r!}[\hat{v}(t_1),\hat{\Gamma}_r(t_2)]$$
$$+S_W(t_1)S_W(t_2)\sum_{r=1}^{\infty}\frac{(it_1)^r}{r!}[\hat{\Gamma}_r(t_1),\hat{v}(t_2)]$$
$$+S_W(t_1)S_W(t_2)\sum_{r=1}^{\infty}\sum_{s=1}^{\infty}\frac{(it_1)^r(it_2)^s}{r!s!}[\hat{\Gamma}_r(t_1),\hat{\Gamma}_s(t_2)]\,. \tag{3.12}$$

Using (3.12), one can readily show that

$$\left[\int_{t_0}^t\hat{H}_1(u)du\right]\hat{H}_1(t)=\hat{H}_1(t)\int_{t_0}^t\hat{H}_1(u)du+\hat{A}(t,t_0)\,, \tag{3.13}$$

where

$$\hat{A}(t,t_0)=S_W(t)\left[\left[\int_{t_0}^{t}S_W(u)\hat{v}(u)du\ ,\hat{v}(t)\right]+\sum_{r=1}^{\infty}\frac{(it)^r}{r!}\left[\int_{t_0}^{t}S_W(u)\hat{v}(u)du\ ,\hat{\Gamma}_r(t)\right]\right.$$
$$\left.+\sum_{r=1}^{\infty}\frac{(i)^r}{r!}[\hat{\gamma}_r{}^{(r)}(t,t_0)\ ,\hat{v}(t)]+\sum_{r=1}^{\infty}\sum_{s=1}^{\infty}\frac{(i)^{r+s}}{r!s!}t^s[\hat{\gamma}_r^{(r)}(t,t_0)\ ,\hat{\Gamma}_s(t)]\right] \tag{3.14}$$

with

$$\hat{\gamma}_r^{(p)}(t,t_0)=\int_{t_0}^{t}S_W(u)u^p\hat{\Gamma}_r(u)du\ .$$

Employing (3.9) and (3.13), if we carry out a series of integrations by parts (Appendix A), we obtain

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+i\int_{t_0}^{t}\hat{H}_1(u)\hat{U}_1(u,t_0)\hat{U}_{n-2}(u,t_0)du+\int_{t_0}^{t}\hat{A}(u,t_0)\hat{U}_{n-2}(u,t_0)du\ . \tag{3.15}$$

Based on (3.15), after a rather tricky iterative process (Appendix B), we can express our U matrix as an infinite series

$$\hat{U}(t,t_0)=\hat{\mathscr{U}}(t,t_0)+\hat{\Delta}(t,t_0)\ , \tag{3.16}$$

where

$$\hat{\mathscr{U}}(t,t_0)=\exp\left[-i\int_{t_0}^{t}\hat{H}_1(u)du\right]\ ,$$

$$\hat{\Delta}(t,t_0)=\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)![\hat{U}_1(t,t_0)]^{n-(r+2)}\hat{B}_r(t,t_0)\ , \tag{3.17}$$

and

$$\hat{B}_r(t,t_0)=\sum_{j=0}^{r}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{r-j}(u_{j+1},t_0)\ , \tag{3.18}$$

where $t>u_1>u_2>u_3>\cdots u_r$.

We have thus expressed our U matrix as a series, the first term of which involves only a single integration of $\hat{H}_1(u)$. If we consider the interaction Hamiltonian to be a perturbation to the total Hamiltonian, clearly the rest of the series represents a small contribution to our U matrix. Note that the summation for n runs from two instead of one in (2.12). So far, we cannot readily sum nor terminate the series. However, it is obvious from relation (3.13) that if $\hat{H}_1(u_1)$ and $\hat{H}_1(u_2)$ are commutable for different times u_1, u_2, namely,

$$[\hat{H}_1(u_1),\hat{H}_1(u_2)]=0 \tag{3.19}$$

then $\hat{A}(t,t_0)=0$ leading to $\hat{B}_r(t,t_0)=0$ and our U matrix is simply exactly given by

$$\hat{U}(t,t_0)=\exp\left[-i\int_{t_0}^{t}\hat{H}_1(u)du\right]\ . \tag{3.20}$$

It is not difficult to prove that under the following three sets of conditions $\hat{H}_1(u_1)$ and $\hat{H}_1(u_2)$ are commutable:

case (i),

$$[\hat{H}_0,\hat{v}(u)]=\text{const}\ ,$$

and (3.21)

$$[\hat{v}(u_1),\hat{v}(u_2)]=0\ ;$$

case (ii),

$$[\hat{H}_0,\hat{v}(u)]=\mathscr{C}(u)$$

and (3.22)

$$[\hat{v}(u_1),\hat{v}(u_2)]=0\ ,$$

where $\mathscr{C}(u)$ is a function of u;

case (iii),

$$[\hat{H}_0,\hat{v}(u)]=\beta(u)\hat{v}^n(u)$$

and (3.23)

$$[\hat{v}(u_1),\hat{v}(u_2)]=0\ ,$$

where $\beta(u)$ is a function of u and n is an integer.

IV. EFFECTS OF SWITCHING PROCESSES ON THE PROPERTIES OF THE U MATRIX

In our formalism, we have introduced a switching function to describe how the interaction is switched on. We have separated the time space into three intervals: the period before the interaction is turned on, the transient period, and the period during which the interaction is "steady." For a time-independent problem, the interaction remains con-

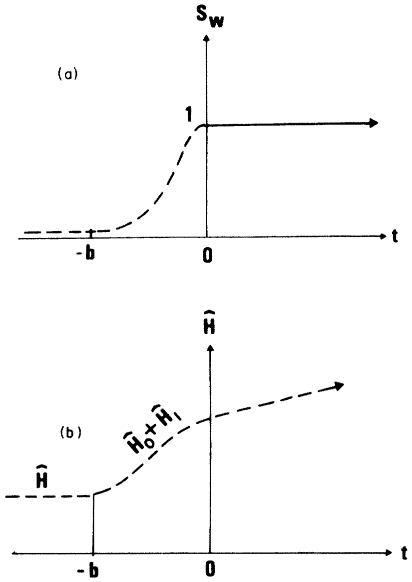

FIG. 1. Schematic representation of a smooth-switching time-dependent problem.

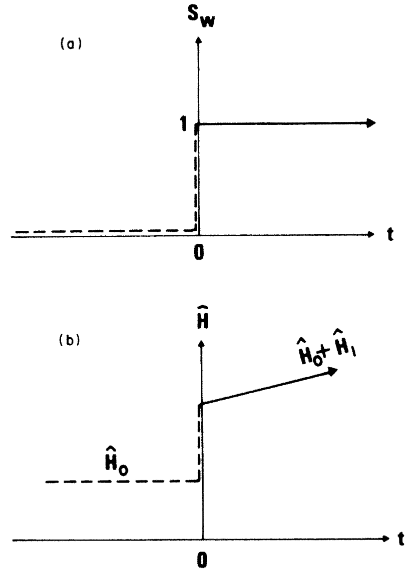

FIG. 2. Schematic representation of the switching function S_W and Hamiltonian $\hat{H}$ in a sudden-switching time-dependent problem.

stant during the last $(0 \leq t \leq \infty)$ period. If the interaction is time dependent in the U matrix, the wave function should be continuous functions of time except at $t=0$. It would be interesting to study some relevant properties of the U matrix based on our proposed properties of S_W as stated in (2.5).

(i) During the interval $-\infty \leq t < -b$, $\hat{H}_1=0$ and $S_W(t)\equiv 0$ and one sees from (2.7) and (3.1) that

$$\hat{\mathscr{U}}(t,t_0)\equiv \exp\left[-i\int_{t_0}^{t}\hat{H}_1(u)du\right] =\exp\left[-i\int_{t_0}^{t}S_W(u)\hat{V}(u)du\right]=1 \quad (4.1)$$

for $-\infty \leq t_0 < t < -b$. As $\hat{H}_1(u)=S_W(u)\hat{V}(u)$ and $S_W(u)=0$, it is obvious from (3.14) that $\hat{A}(t,t_0)=0$ also for this period and $\hat{\Delta}(t,t_0)=0$, giving

$$\hat{U}(t,t_0)=1 \quad \text{for} \quad -\infty \leq t_0 < t < -b \ . \quad (4.2)$$

Therefore

$$\Psi(t)=\Psi(t_0) \ . \quad (4.3)$$

It is easy to find that

$$\Phi(t)=\exp[-i\hat{H}_0(t-t_0)]\Phi(t_0) \ . \quad (4.4)$$

We observe that in the interaction picture, the wave function does not change in time before the interaction occurs (which must be the case), whereas in the Schrödinger picture the wave function at time t is transformed from the basis wave function (at the reference time t_0) by $\exp[-i\hat{H}_0(t-t_0)]$.

(ii) During the interval $-b \leq t \leq 0$, $S_W(t)$ and $\hat{v}(t)$ can, in general, be nonzero. Usually one takes $t=0$ as the reference point to study the time evolution of the wave function and other quantities. If $S_W(t)$ is a continuous function during this period and *across* $t=0$, we can simply shift our time of origin to $t=-b$ to study this time-dependent problem. The situation is represented in Fig. 1 schematically. However, there is certain discontinuity in $\hat{H}=\hat{H}_0+\hat{H}_1$ in this period and we are interested to find that

$$\hat{U}(0,-b)=\exp\left[-i\int_{-b}^{0}S_W(u)\hat{V}(u)du\right] +\hat{\Delta}(0,-b) \ . \quad (4.5)$$

Suppose we have a sudden-switching process across the reference time $t=0$, namely, we consider the case $-b\rightarrow 0^-$. The switching function $S_W(0^-)=0$ but $S_W(0)=1$ (Fig. 2). The U matrix is

$$\hat{U}(0,0^-)=\hat{\mathscr{U}}(0,0^-)+\hat{\Delta}(0,0^-) =\exp\left[-i\left\{\lim_{-b\rightarrow 0-}\left[\int^{0}\hat{V}(u)du-\int_{-b}^{0}\frac{dS_W(u)}{du}\left[\int \hat{V}(u)du\right]du\right]\right\}\right]+\lim_{-b\rightarrow 0-}\hat{\Delta}(0,-b) \quad (4.6)$$

after integration by parts. In our formalism, we require that $-b \to 0$ faster than

$$\frac{dS_W(u)}{du} \to \infty$$

such that the second integral in (4.6) is zero. A similar type of requirement is taken by Gell-Mann's formalism[3] where $-b \to -\infty$. Thus, in our case the dominant contribution is

$$\hat{\mathcal{U}}(0,0^-) = \exp\left[-i\int^0 \hat{V}(u)du\right] . \tag{4.7}$$

A nondivergent and generally nonzero contribution to $\hat{\mathcal{U}}(0,0^-)$ is necessary since in the interaction picture, the Hamiltonian is $\hat{H}_0$ before $t=0$. Starting from $t=0$, there is a sudden change in $\hat{H}$ and there should be a finite but sudden change in both the wave function Ψ and Φ across $t=0$.

On inspection of expression (3.18), we notice that the upper limits of the integrals follow a time-evolution sequence: $t > u_1 > u_2 > u_3 > \cdots > u_r$. As $S_W(u) = 0$ except for $u=0$ and all the u_r's are less than zero, $\hat{B}_r(0,0^-)$ is equal to a product of zeros apart from the integral which has the upper limit 0. Thus

$$\hat{B}_r(0,0^-) = 0$$

and

$$\hat{\Delta}(0,0^-) = 0 . \tag{4.8}$$

Hence, from (4.6),

$$\hat{U}(0,0^-) = \exp\left[-i\int^0 \hat{V}(u)du\right] \tag{4.9}$$

is an exact expression. For this time, one readily sees that

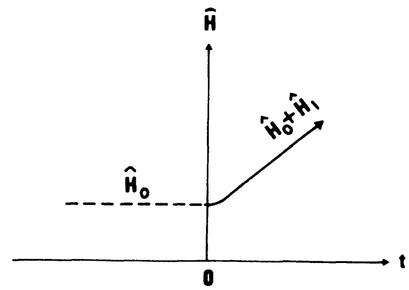

FIG. 3. Variation of the Hamiltonian with time in the situation where the interaction Hamiltonian is zero at $t=0$.

$$\hat{S}(0,0^-) = \exp\left[-i\int^0 \hat{V}(u)du\right] \tag{4.10}$$

also.

We should remark that the above discussion for the sudden-switching process is valid for $\hat{v}(t) \neq 0$ at $t=0$. If $\hat{v}(t) = 0$ at $t=0$ and develops from then on, (4.9) is automatically zero and, in this case, the switching is essentially smooth for $\hat{H}$ is continuous all the way (see Fig. 3).

(iii) During the time interval $0 < t_0 < t \leq \infty$, $S_W(t_0) = S_W(t) \equiv 1$, so that

$$\hat{U}(t,t_0) = \exp\left[-i\int_{t_0}^t \hat{V}(u)du\right] + \hat{\Delta}(t,t_0)\,|_{S_W=1} . \tag{4.11}$$

Bridging the wave function just before interaction to the wave function at time t, we have from (2.15), for a sudden-switching process,

$$\Phi(t) = e^{-i\hat{H}_0 t}\left[\exp\left[-i\int_0^t \hat{V}(u)du\right] + \hat{\Delta}(t,0)\right]\left[\exp\left[-i\int^0 \hat{V}(u)du\right]\right]\Phi(0^-) \tag{4.12a}$$

$$\approx e^{-i\hat{H}_0 t}\exp\left[-i\int_0^t \hat{V}(u)du\right]\exp\left[-i\int^0 \hat{V}(u)du\right]\Phi(0^-) . \tag{4.12b}$$

Generally, $\hat{\Delta}(t,0) \neq 0$.

V. CHARGED HARMONIC OSCILLATOR

The charged harmonic-oscillator problem has been studied using the displacement transformation method[8] and the Green's-function approach.[23] We take this problem as an example for demonstrating some working procedures of our method. The Hamiltonian of this system in the time-independent situation is well known:

$$\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}) + \lambda(\hat{a}^\dagger + \hat{a}) = \hat{H}_0 + \hat{H}_1 , \tag{5.1a}$$

where

$$\hat{H}_0 = \omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}) ,$$

$$\hat{v}(t) = \hat{H}_1 = \lambda(\hat{a}^\dagger + \hat{a}) , \tag{5.1b}$$

and ω and λ are constants. In this case the termination operators are [see (3.3)]

$$\hat{\Gamma}_1 = \lambda\omega(\hat{a}^\dagger - \hat{a}) ,$$

$$\hat{\Gamma}_2 = \lambda\omega^2(\hat{a}^\dagger + \hat{a}) , \tag{5.2}$$

$$\vdots$$

$$\hat{\Gamma}_r = \lambda\omega^r[\hat{a}^\dagger + (-1)^r\hat{a}] .$$

Leaving the problem as a time-dependent one for the time being, from (3.2) and (5.2),

$$\hat{H}_1(t)=S_W(t)\left[\hat{v}(t)+\sum_{r=1}^{\infty}\frac{(it)^r}{r!}\hat{\Gamma}_r(t)\right]$$

$$=\lambda S_W(t)(e^{i\omega t}\hat{a}^\dagger+e^{-i\omega t}\hat{a})\ . \qquad (5.3)$$

Since this is a time-independent problem, we consider our solutions at $t=0$. Based on (4.10), we need to calculate

$$\hat{U}(0,0^-)=\exp\left[-i\int^0\hat{V}(u)du\right]$$

$$=\exp\left[\frac{\lambda}{\omega}(\hat{a}-\hat{a}^\dagger)\right]\ , \qquad (5.4)$$

taking into account relation (5.3). We will need to calculate $(\hat{H}_0+\hat{H}_1)\hat{U}(0,0^-)$. First, we need to put (5.4) in a proper order of $\hat{a}^\dagger$ and $\hat{a}$. In Appendix C we have shown that for operators $\hat{P},\hat{Q}$,

$$\exp\{\tau[\alpha(\tau)\hat{P}+\beta(\tau)\hat{Q}]\}$$
$$=\{\exp[\tau\alpha(\tau)\hat{P}]\}\{\exp[\tau\beta(\tau)\hat{Q}]\}\hat{K}(\tau)\ , \qquad (5.5a)$$

where

$$\hat{K}(\tau)=\exp\left[\int_0^\tau\hat{\mathscr{Y}}(u)du\right]+\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)!\left[\int_0^\tau\hat{\mathscr{Y}}(u)du\right]^{n-(r+2)}\hat{\mathscr{B}}_r(\tau,0) \qquad (5.5b)$$

with

$$\hat{\mathscr{Y}}(\tau)=[\alpha(\tau)+\tau\alpha'(\tau)]\sum_{r=1}^{\infty}\frac{[\tau\beta(\tau)]^r}{r!}\hat{R}_r \qquad (5.5c)$$

and

$$\hat{\mathscr{B}}_r(\tau,0)\sum_{j=0}^{r}\int_0^\tau dt_1\hat{\mathscr{Y}}(t_1)\int_0^{t_1}dt_2\hat{\mathscr{Y}}(t_2)\cdots\int_0^{t_j}dt_{j+1}\left[\int_0^{t_{j+1}}[\hat{\mathscr{Y}}(t),\hat{\mathscr{Y}}(t_{j+1})]dt\right]\hat{Y}_{r-j}(t_{j+1},0) \qquad (5.5d)$$

with

$$\hat{Y}_n(\tau,0)=\int_0^\tau dt_1\hat{\mathscr{Y}}(t_1)\int_0^{t_1}dt_2\hat{\mathscr{Y}}(t_2)\cdots\int_0^{t_{n-1}}dt_n\hat{\mathscr{Y}}(t_n)\ , \qquad (5.5e)$$
$$\hat{R}_r=[\hat{Q},\hat{P}]_r\ ,$$

while the prime symbol indicates differentiation with respect to τ. Applying (5.5) to (5.4), one finds that

$$\hat{U}(0,0^-)=\exp\left[-\frac{1}{2}\left[\frac{\lambda}{\omega}\right]^2\right]\exp\left[\frac{\lambda}{\omega}\hat{a}\right]\exp\left[-\frac{\lambda}{\omega}\hat{a}^\dagger\right] \qquad (5.6)$$

and

$$\hat{H}\hat{U}(0,0^-)=\exp\left[-\frac{1}{2}\left[\frac{\lambda}{\omega}\right]^2\right]\exp\left[\frac{\lambda}{\omega}\hat{a}\right]\exp\left[-\frac{\lambda}{\omega}\hat{a}^\dagger\right]\left[\omega\left[\hat{a}^\dagger\hat{a}-\frac{\lambda}{\omega}(\hat{a}^\dagger+\hat{a})+\frac{\lambda^2}{\omega^2}\right]+\lambda(\hat{a}^\dagger+\hat{a})+\tfrac{1}{2}\omega-\frac{2\lambda^2}{\omega}\right]$$

$$=\hat{U}(0,0^-)\left[\omega(\hat{a}^\dagger\hat{a}+\tfrac{1}{2})-\frac{\lambda^2}{\omega}\right]\ . \qquad (5.7)$$

Now we are in a position to calculate the ground-state energy, using (2.15) and (5.7), the fact that $\hat{H}_0$ and $\hat{a}^\dagger\hat{a}$ are commutable, and $\hat{U}^*\hat{U}=1$:

$$\langle E\rangle=\langle\Phi(0)\,|\,\hat{H}\,|\,\Phi(0)\rangle$$
$$=\lim_{-b\to0-}[\langle\Phi(-b)\,|\,\hat{S}^*(0,-b)\hat{H}\hat{S}(0,-b)\,|\,\Phi(-b)\rangle]$$
$$=\lim_{-b\to0-}[\langle\Phi(-b)\,|\,e^{i\hat{H}_0^*b}\hat{U}^*(0,-b)\hat{H}\hat{U}(0,-b)e^{-i\hat{H}_0b}\,|\,\Phi(-b)\rangle]$$
$$=\omega(n+\tfrac{1}{2})-\frac{\lambda^2}{\omega}\ , \qquad (5.8)$$

where

$$\hat{a}^\dagger \hat{a} \mid \Phi(-b)\rangle = n \mid \Phi(-b)\rangle \ .$$

Using our direct method, we have obtained the exact wave function and ground-state energy for a charged harmonic oscillator. Our result is identical, of course, to the exact solutions using other methods (see, e.g., work listed in Ref. 8).

VI. TIME-DEPENDENT QUANTUM HARMONIC OSCILLATOR

In this example we shall study a time-dependent quantum harmonic-oscillator problem with our new method. This problem has, of course, been studied by a number of workers (see, e.g., Refs. 23–25). For convenience in comparison, we follow the form of the Hamiltonian used by Peng[23]

$$\hat{H} = \frac{1}{2m} P^2 + \frac{1}{2}\left[K - \frac{C^2}{4m}\right] X^2 - X f(t) e^{Ct/2m} \ , \tag{6.1}$$

where m is the mass, X and P are, respectively, spatial coordinate and momentum, $f(t)$ the time-dependent driving force, and C,K are constants. Using operator notation,

$$\hat{H}_0 = \omega(\hat{a}^\dagger \hat{a} + \tfrac{1}{2}) \ ,$$

$$\hat{v}(t) = \lambda(t)(\hat{a}^\dagger + \hat{a}) \ ,$$

where (6.2)

$$\lambda(t) = -\left[\frac{1}{2m\omega}\right]^{1/2} f(t) e^{Ct/2m} \ .$$

We shall use our sudden-switching model to describe the appearance of the driving force, the explicit form of which is yet to be specified. There are, however, two general cases for which $f(t)$ must satisfy, as discussed in Sec. IV:

$$t<0 \ , \ f(t)=0 \ ,$$
$$t\geq 0 \ , \ f(t)\neq 0 \ , \tag{6.3a}$$
$$t\leq 0 \ , \ f(t)=0 \ ,$$
$$t>0 \ , \ f(t)\neq 0 \ . \tag{6.3b}$$

The switching function then satisfies

$$S_W(t)=0 \ \text{ for } \ -b\leq t<0$$
$$S_W(t)=1 \ \text{ for } \ 0\leq t\leq \infty \tag{6.4}$$
$$\frac{dS_W(t)}{dt}=0 \ \text{ except at } \ t=0 \ .$$

Using (6.2), our termination operators are

$$\hat{\Gamma}_1(t) = \omega\lambda(t)(\hat{a}^\dagger - \hat{a}) \ ,$$
$$\hat{\Gamma}_2(t) = \omega^2\lambda(t)(\hat{a}^\dagger + \hat{a}) \ , \tag{6.5}$$
$$\vdots$$
$$\hat{\Gamma}_r(t) = \omega^r\lambda(t)[\hat{a}^\dagger + (-1)^r \hat{a}]$$

so that

$$\hat{V}(t) = \hat{v}(t) + \sum_{r=1}^{\infty} \frac{(it)^r}{r!}\hat{\Gamma}_r(t)$$
$$= \lambda(t)(e^{i\omega t}\hat{a}^\dagger + e^{-i\omega t}\hat{a}) \ . \tag{6.6}$$

Now we can write the interaction Hamiltonian as

$$\hat{H}_1(t) = S_W(t)\hat{V}(t)$$
$$= \lambda(t) S_W(t)(e^{i\omega t}\hat{a}^\dagger + e^{-i\omega t}\hat{a}) \ . \tag{6.7}$$

We separate our time interval into two parts, $(0^-,0)$ and $(0,t)$ so that the U matrix is

$$\hat{U}(t,0^-) = \hat{U}(t,0)\hat{U}(0,0^-) = [\hat{\mathscr{U}}(t,0) + \hat{\Delta}(t,0)]\hat{U}(0,0^-)$$
$$\approx \hat{\mathscr{U}}(t,0)\hat{U}(0,0^-) = \exp\left[-i\int_0^t \hat{V}(u)du\right]\exp\left[-i\int^0 \hat{V}(u)du\right] \ . \tag{6.8}$$

In view of (6.6) we get

$$\hat{U}(0,0^-) = \exp[-i(G^\dagger \hat{a}^\dagger + G\hat{a})] \ , \tag{6.9}$$

where

$$G^\dagger = \int^0 \lambda(u) e^{i\omega u} du \ ,$$
$$G = \int^0 \lambda(u) e^{-i\omega u} du \ , \tag{6.10}$$

and

$$\hat{\mathscr{U}}(t,0)=\exp[-i(G_t^\dagger\hat{a}^\dagger+G_t\hat{a})] , \tag{6.11}$$

where

$$G_t^\dagger=\int_0^t \lambda(u)e^{i\omega u}du , \quad G_t=\int_0^t \lambda(u)e^{-i\omega u}du . \tag{6.12}$$

Using Appendix C, we can show that

$$\hat{U}(0,0^-)=e^{Z_0}e^{-iG^\dagger\hat{a}^\dagger}e^{-iG\hat{a}} , \tag{6.13}$$

$$\hat{\mathscr{U}}(t,0)=e^{Z}e^{-iG_t^\dagger\hat{a}^\dagger}e^{-iG_t\hat{a}} , \tag{6.14}$$

where

$$Z_0=-\tfrac{1}{2}G^\dagger G+\tfrac{1}{2}\int d\tau\left[\frac{\partial G^\dagger}{\partial\tau}G-G^\dagger\frac{\partial G}{\partial\tau}\right]\tau^2 ,$$

$$Z=-\tfrac{1}{2}G_t^\dagger G_t+\tfrac{1}{2}\int d\tau\left[\frac{\partial G_t^\dagger}{\partial\tau}G_t-G_t^\dagger\frac{\partial G_t}{\partial\tau}\right]\tau^2 ,$$

$$\tau=-i . \tag{6.15}$$

Taking the approximation stated in (6.8), the wave function at time t is

$$\Phi(t)=\hat{S}(t,0^-)\Phi(0^-) \tag{6.16a}$$

with

$$\hat{S}(t,0^-)=e^{Z_0+Z}e^{-i\hat{H}_0t}e^{-iG_t^\dagger\hat{a}^\dagger}e^{-iG_t\hat{a}}\times e^{-iG^\dagger\hat{a}^\dagger}e^{-iG\hat{a}} . \tag{6.16b}$$

At $t=0^-$, the Hamiltonian is $\hat{H}_0$, so that

$$\Phi(0^-)=\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0,0^-\rangle ,$$

where n is the number of states, as represented by the number of quantum particles in the system. Using (6.13), therefore,

$$\begin{aligned}\Phi(0)=\hat{U}(0,0^-)\Phi(0^-)&=e^{Z_0}e^{-iG^\dagger\hat{a}^\dagger}e^{-iG\hat{a}}\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0,0^-\rangle\\
&=\frac{1}{\sqrt{n!}}e^{Z_0}\sum_{p=0}^{\infty}\frac{(-iG^\dagger)^p}{p!}(\hat{a}^\dagger)^p(\hat{a}^\dagger-iG)^n e^{-iG\hat{a}}|0,0^-\rangle\\
&=\frac{1}{\sqrt{n!}}e^{Z_0}\sum_{p=0}^{\infty}\frac{(-iG^\dagger)^p}{p!}\sum_{j=0}^{n}(-iG)^{n-j}C_j^n(\hat{a}^\dagger)^{j+p}|0,0^-\rangle ,\end{aligned} \tag{6.17}$$

where C_j^n is the usual permutation coefficient. Let $j+p=s$ and, operating $(\hat{a}^\dagger)^s$ on $|0,0^-\rangle$, we can write (6.17) as

$$\Phi(0)=\sum_s \alpha_s|s,0^-\rangle , \tag{6.18}$$

where α_s is a complicated algebraic function involving $G^\dagger,G$ and the ways of counting when an operator acts on a state. At this moment, there is no point to waste space in writing out an expression for α_s. We note, however, that α_s must satisfy the normalization condition

$$\langle\Phi(0)|\Phi(0)\rangle=\sum_s\alpha_s^*\alpha_s=1 .$$

Using (6.14) and (6.18) we can find $\Phi(t)$:

$$\begin{aligned}\Phi(t)&=e^{Z}e^{-i\hat{H}_0t}e^{-iG_t^\dagger\hat{a}^\dagger}e^{-iG_t\hat{a}}\sum_{s=0}^{\infty}\alpha_s\frac{(\hat{a}^\dagger)^s}{\sqrt{s!}}|0,0^-\rangle\\
&=e^{Z}e^{-i\hat{H}_0t}\sum_{p=0}^{\infty}\sum_{s=0}^{\infty}\frac{\alpha_s}{\sqrt{s!}}\frac{(-iG_t^\dagger)^p}{p!}\sum_{j=0}^{s}(-iG_t)^{s-j}C_j^s(\hat{a}^\dagger)^{p+j}|0,0^-\rangle .\end{aligned} \tag{6.19}$$

Setting $q=p+j$, as before,

$$\begin{aligned}\Phi(t)&=\sum_{p=0}^{\infty}\sum_{s=0}^{\infty}\sum_{j=0}^{s}\frac{\alpha_s}{\sqrt{s!}}\frac{(-iG_t^\dagger)^p}{p!}e^{Z}(-iG_t)^{s-j}C_j^s\sqrt{q}!\exp[-i\omega(q+\tfrac{1}{2})t]|q,0^-\rangle\\
&=\sum_{q=0}^{\infty}\sum_{s=0}^{\infty}\sum_{j=0}^{s}\frac{\alpha_s}{\sqrt{s!}}\mathscr{I}_{q,j}\exp[-i\omega(q+\tfrac{1}{2})t]|q,0^-\rangle ,\end{aligned} \tag{6.20}$$

where $\mathscr{I}_{q,j}$ is a complicated algebraic function, as before.

So far we have used the approximated form for our U matrix: $\hat{U}=\hat{\mathscr{U}}+\hat{\Delta}\simeq\hat{\mathscr{U}}$. If we take the exact form, we have found after a very lengthy process of calculation that the wave function appears exactly in the same form as given by (6.18), with $\mathscr{I}_{q,j}$ replaced by $\mathscr{I}_{q,j}+\Omega_{q,j}$. The detail of the working procedure is elementary but too lengthy to be presented here. In order to compare our result with Peng's, we calculate the average displacement:

$$\langle X(t)\rangle=\langle\Phi(t)\,|\,\hat{X}\,|\,\Phi(t)\rangle$$
$$=\langle\Phi(t)\,|\left[\frac{1}{2m\omega}\right]^{1/2}e^{-Ct/2m}\times(\hat{a}^{\dagger}+\hat{a})\,|\,\Phi(t)\rangle\ . \tag{6.21}$$

In order to compare our results with Peng's we also use the first line of expression (6.19) for $\Phi(t)$ [instead of (6.20)] and express it as

$$\Phi(t)=e^{Z}e^{-i\hat{H}_0t}e^{-iG_t^{\dagger}\hat{a}^{\dagger}}e^{-iG_t\hat{a}}\sum_s\alpha_s\,|\,s,0^-\rangle$$
$$=e^{Z}\hat{P}\hat{Q}e^{-i\hat{H}_0t}\sum_s\alpha_s\,|\,s,0^-\rangle\ , \tag{6.22}$$

where

$$\hat{P}=e^{-iG_t^{\dagger}}e^{-i\omega t}\hat{a}^{\dagger}\ ,$$
$$\hat{Q}=e^{-iG_t}e^{i\omega t}\hat{a}\ . \tag{6.23}$$

Then

$$\langle X(t)\rangle=\langle v,0^-\,|\sum_s\sum_v\alpha_v^*\alpha_s\left[\frac{1}{2m\omega}\right]^{1/2}e^{-Ct/2m}\times e^{i\hat{H}_0t}\hat{Q}^*\hat{P}^*(\hat{a}^{\dagger}+\hat{a})\hat{P}\hat{Q}e^{-i\hat{H}_0t}\,|\,s,0^-\rangle\ . \tag{6.24}$$

Noticing that

$$(\hat{a}^{\dagger}+\hat{a})\hat{P}=\hat{P}(\hat{a}^{\dagger}+\hat{a}-iG_t^{\dagger}e^{-i\omega t})\ ,$$
$$(\hat{a}^{\dagger}+\hat{a})\hat{Q}=\hat{Q}(\hat{a}^{\dagger}+\hat{a}+iG_te^{i\omega t})\ ,$$
$$(\hat{a}^{\dagger}+\hat{a})\hat{P}\hat{Q}=\hat{P}\hat{Q}(\hat{a}^{\dagger}+\hat{a}+iG_te^{i\omega t}-iG_t^{\dagger}e^{-i\omega t})\ ,$$
$$e^{i\hat{H}_0t}\hat{a}^{\dagger}e^{-i\hat{H}_0t}=e^{i\omega t}\hat{a}^{\dagger}\ ,$$
$$e^{i\hat{H}_0t}\hat{a}e^{-i\hat{H}_0t}=e^{-i\omega t}\hat{a}\ , \tag{6.25}$$

we arrive at, from (6.24),

$$\langle X(t)\rangle=\left[\frac{1}{2m\omega}\right]^{1/2}e^{-Ct/2m}\left[e^{i\omega t}\sum_s\alpha_{s+1}^*\sqrt{s+1}\alpha_s+e^{-i\omega t}\sum_s\alpha_{s-1}^*\sqrt{s}\,\alpha_s\right]+\left[\frac{1}{m\omega}\right]\int_0^t\exp[-C(t-u)/2m]f(u)\sin[\omega(t-u)]du\ . \tag{6.26}$$

Our approximate result is seen to be identical to that found in Ref. 23, where the method has been supposed to be exact. Our other contribution, of course, comes from the series $\hat{\Delta}(t,t_0)$. Let us now just write out the first few terms for $\hat{\Delta}(t,t_0)$. First, we recall that

$$\hat{\Delta}(t,t_0)=\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)![\hat{U}_1(t,t_0)]^{n-(r+2)}\hat{B}_r(t,t_0)\ ,$$

where

$$\hat{B}_r(t,t_0)=\sum_{j=0}^{r}(-i)^j\int_{t_0}^{t}\hat{H}_1(u_1)du_1\int_{t_0}^{u_1}\hat{H}_1(u_2)du_2\cdots\int_{t_0}^{u_j}\hat{A}(u_{j+1},t_0)du_{j+1}\hat{U}_{r-j}(u_{j+1},t_0)\ .$$

We have shown that $\hat{\Delta}(0,0^-)=0$, so we need to calculate $\hat{\Delta}(t,0)$ only. With the use of the fact that $U_0(t,t_0)=1$ (see Sec. II),

$$\hat{B}_0(t,0)=\int_0^t\hat{A}(u_1,0)du_1=i2\int_0^t\lambda(u_1)du_1\int_0^{u_1}\lambda(u_2)\sin[\omega(u_1-u_2)]du_2\ , \tag{6.27}$$

since in this case

$$\hat{A}(t,0)=\int_0^t[\hat{H}_1(u),\hat{H}_1(t)]du=i2\lambda(t)\int_0^t\lambda(u)\sin[\omega(t-u)]du\ . \tag{6.28}$$

Also,

$$\hat{U}_1(t,0)=-i\int_0^t \hat{H}_1(u)du=-i(G_t^\dagger\hat{a}^\dagger+G_t\hat{a}) \tag{6.29}$$

and

$$\hat{B}_1(t,0)=2\left[\int_0^t du_1\left[\lambda(u_1)\int_0^{u_1}du_2\lambda(u_2)\sin[\omega(u_1-u_2)]\int_0^{u_1}du_3\lambda(u_3)(e^{i\omega u_3}\hat{a}^\dagger+e^{-i\omega u_3}\hat{a})\right.\right.$$
$$+\int_0^t du_1\lambda(u_1)(e^{i\omega u_1}\hat{a}^\dagger+e^{-i\omega u_1}\hat{a})$$
$$\left.\left.\times\int_0^{u_1}du_3\lambda(u_3)\int_0^{u_3}du_2\lambda(u_2)\sin[\omega(u_3-u_2)]\right]\right]. \tag{6.30}$$

Using the above expressions for $\hat{B}_0$, $\hat{U}_1$, and $\hat{B}_1$, we can calculate the first three terms of $\hat{\Delta}(t,0)$:

$$\hat{\Delta}(t,0)=\tfrac{1}{2}\hat{B}_0(t,0)+\tfrac{1}{3}[\hat{U}_1(t,0)\hat{B}_0(t,0)+2!\hat{B}_1(t,0)]+\cdots . \tag{6.31}$$

Generally, $\hat{B}_0$, $\hat{U}_1$, and $\hat{B}_1$ are not zero, so there is finite contribution to the U matrix due to noncommutability properties of the operators in the Schrödinger equation.

VII. CONCLUSION

In this investigation we have developed the previous U-matrix theory in the interaction picture. We would like to remark on the following main features of our study.

(1) Previously, the U matrix was expressed as a multiple integral of the interaction Hamiltonian, governed by a proper time sequence. It is difficult to handle this multiple integral and one can hardly obtain a workable, explicit wave function using the basic formalism. We are able to derive the U matrix as an infinite series. The first term is simply represented by

$$\exp\left[-i\int_{t_0}^t \hat{H}_1(u)du\right],$$

which is identical to solving the operator equation $i\partial\hat{U}/\partial t=\hat{H}_1(t)\hat{U}$ without considering the commutability properties of the operators involved in $\hat{U}$ and $\hat{H}_1(t)$. The other terms of the $\hat{U}$ series are multiple integrals of the interaction Hamiltonian $\hat{H}_1(u)$. If $\hat{H}_1$ represents a small perturbation to the original Hamiltonian $\hat{H}_0$, the rest of the $\hat{U}$ series may be considered as a perturbation to the solution using the first term of $\hat{U}$ alone. In that case, our approximated wave function is a good representation of the system, and is simply given by

$$\Phi(t)=\exp(-i\hat{H}_0t)\exp\left[-i\int_{t_0}^t \hat{H}_1(u)du\right]$$
$$\times\exp(i\hat{H}_0t_0)\Phi(t_0).$$

For a class of Hamiltonians such that either set of the conditions (3.21)–(3.23) is satisfied, the operator function $\hat{A}$ and hence $\hat{B}_r$ is zero. In that case the perturbation $\hat{\Delta}(t,t_0)$ to $\hat{U}(t,t_0)$ is zero also [see (3.16)]. For this class of Hamiltonians again the solution for $\hat{U}(t,t_0)$ is exact. The above-mentioned class of Hamiltonians may not be exclusive, in general. It would therefore be worthwhile to study what types of Hamiltonians would lead to exact solution for the $\hat{U}$ matrix. Such research is in progress.

(2) We have used a switching function S_W to describe how the interaction Hamiltonian is turned on. The interaction can be turned on from $t=-b$ (b is a positive number). From $t=0$ onwards, the interaction becomes effective. If $-b\to 0^-$, we have either (i) a sudden-switching process or (ii) a gradual switching process. In the former case $\hat{H}_1(t)\neq 0$ at $t=0$, while in the latter case $\hat{H}_1(t)=0$ at $t=0$. In case (ii), the main contribution to U is given by

$$\hat{U}(t,t_0)=\exp\left[-i\int_{t_0}^t \hat{V}(u)du\right],$$

where $t_0=0$. In case (i), however, the dominant contribution to $\hat{U}(t,t_0)$ is

$$\hat{U}(t,t_0)=\exp\left[-i\int_{t_0}^t \hat{V}(u)du\right]$$
$$\times\exp\left[-i\int^0 \hat{V}(u)du\right].$$

The second factor

$$\exp\left[-i\int^0 \hat{V}(u)du\right]$$

on the right-hand side describes the sudden finite change in the Hamiltonian across $t=0$. In short, $\hat{U}(0,0^-)=1$ for case (ii) and $\hat{U}(0,0^-)\neq 1$ for case (i).

(3) We have treated the time-independent problem as a special case of the time-dependent solution of the Schrödinger equation in the interaction picture, evaluated at $t=0$. According to our sudden-switching model, the matrix $\hat{U}(0,0^-)$ across

the "time origin" $t=0$ must not be equal to 1, in the sense that it must contain information about the change in Hamiltonian. Based on our discussion in Sec. III, the $\hat{U}$ matrix for the time-independent problem is exactly given by

$$\hat{U}(0,0^-)=\exp\left[-i\int_{0^-}^{0}\hat{H}_1(u)du\right]$$
$$=\exp\left[-\int^{0}\hat{V}(u)du\right].$$

This result is equivalent to the solution of the equation

$$-i\partial U/\partial t=\hat{H}_1(u)\hat{U},$$

without taking into account the noncommutability of the operators in $\hat{H}_1(u)$ and $\hat{U}$. It is true that as the time interval tends to zero as a limit (for a time-independent problem), one observes that it is necessary that the operators in $\hat{H}_1(u)$ and $\hat{U}$ commute. The validity of our result has been checked in Sec. V, with the well-known charged harmonic-oscillator example. In fact, one can easily apply our theory to study other standard time-dependent problems, obtaining results which are identical to those found by other exact methods.

(4) We have applied our theory to study the time-dependent harmonic-oscillator problem and compared our result (the averaged displacement) with that obtained from the Schrödinger equation which is supposed to be exact. We have used an approximated U matrix $\hat{U}=\hat{\mathscr{U}}+\hat{\Delta}\simeq\hat{\mathscr{U}}$ in our treatment and all the terms obtained by Peng are identical to the major part of our result. If we include the contribution of $\hat{\Delta}$ to $\hat{U}$ in our treatment, we should of course obtain more information. This feature has been discussed in (1).

(5) The recent development of the deduction of the path-integral formalism[18] is based on writing the Schrödinger equation in the form

$$\left[\hat{H}-i\frac{\partial}{\partial t}\right]\hat{G}(t,t_0)=-i\hat{1}\delta(t-t_0), \tag{7.1}$$

where $\hat{1}$ is a unit matrix, and the wave function at time t is obtained by operating the Green's-function operator $\hat{G}(t,t_0)$ on the initial wave function $\Phi(t_0)$.

$$\Phi(t)=\hat{G}(t,t_0)\Phi(t_0). \tag{7.2}$$

For a time independent $\hat{H}$, an operator solution to (7.1) according to Ref. 15, is

$$\hat{G}(t,t_0)=\Theta(t-t_0)\exp[-i\hat{H}(t-t_0)], \tag{7.3}$$

where Θ is a step function, taking $\hbar=1$. To compare this formalism with our new theory, suppose we solve the Schrödinger operator equation in the Schrödinger picture with our method; we would arrive at

$$\Phi(t)=\hat{U}^{(s)}(t,t_0)\Phi(t_0) \tag{7.4}$$

in which

$$\hat{U}^{(s)}(t,t_0)=\exp\left[-i\int_{t_0}^{t}\hat{H}(u)du\right]+\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)![\hat{U}_1^{(s)}(t,t_0)]^{n-(r+2)}\hat{B}_r^{(s)}(t,t_0), \tag{7.5}$$

where the superscript (s) stands for the result obtained via the Schrödinger picture rather than the interaction picture which has been used throughout our paper. In (7.5),

$$\hat{B}_r^{(s)}(t,t_0)=\sum_{j=0}^{r}(-i)^j\int_t^t du_1\hat{H}(u_1)\int_{t_0}^{u_1}du_2\hat{H}(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}^{(s)}(u_{j+1},t_0)\hat{U}_{r-j}^{(s)}(u_{j+1},t_0), \tag{7.6}$$

$$\hat{U}_n^{(s)}(t,t_0)=-i\int_{t_0}^{t}du_1\hat{H}(u_1)U_{n-1}^{(s)}(u_1,t_0), \tag{7.7}$$

$$\hat{A}^{(s)}(t,t_0)=\int_{t_0}^{t}[\hat{H}(u),\hat{H}(t)]du. \tag{7.8}$$

For a time-independent Hamiltonian, we can write

$$\hat{H}(t)=S_W(t)\hat{H}, \tag{7.9}$$

where H is not a function of time and $S_W(t)$ is a switching function (if we use a gradual switching function, instead of a sudden-switching model, the Hamiltonian is then changed basically to a time-dependent one before reaching $t=t_0$), satisfying

$$S_W(t)=\begin{cases}1 & \text{for } t_0\le t<\infty\\ 0 & \text{for } t<t_0\end{cases} \tag{7.10}$$

(this is known as the sudden-switching model in our paper). In fact, $S_W(t)$ plays the role in a manner similar to Θ in (7.3).

Substituting (7.9) into (7.8) we arrive at the special case

$$A^{(s)}(t,t_0)=0$$

leading to $B_r^{(s)}(t,t_0)=0$ in (7.6), so that the series in (7.5) is accordingly zero, giving

$$U^{(s)}(t,t_0)=\exp\left[-i\int_{t_0}^{t}\hat{H}(u)du\right]$$
$$=\exp[-i\hat{H}(t-t_0)] \qquad (7.11)$$

using (7.10). Relation (7.11) is identical to (7.3), apart from the step function Θ, meaning that, for a time-independent Hamiltonian, our U matrix is similar to the Green's-function operator in the path-integral formalism. It is interesting, however, to note that the usual meaning of a step function is that

$$\Theta(t<t_0)=0$$
and $\qquad (7.12)$
$$\Theta(t\geq t_0)=1\ .$$

Using (7.12), $\Phi(t<t_0)=0$ in (7.2) (namely, in view of the path-integral approach), whereas $\Phi(t<t_0)=\Phi(t_0)$ in our approach. In other words, our wave function is continuous across t_0 and Φ in (7.2) has a discontinuity at t_0.

(6) We have been able to express the U matrix as an infinite series, the first term of which, we believe, represents the dominant contribution. The rest of the series, again, consists of a series of complicated multiple integrals. Using the same techniques as presented in Appendix B, it might be possible to "isolate" another term which is of second importance to the U matrix. Such a step looks much more complicated than the first step we have taken and awaits for further careful analysis. Apart from a rather restrictive class of Hamiltonians specified in (3.21)–(3.23), we have not been able to solve the general time-dependent problem exactly, but we believe to have already moved one step towards obtaining a more accurate wave function (than what we have done so far in this investigation) expressed as a convergent series.

APPENDIX A

We wish to prove the relation

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+i\int_{t_0}^{t}du\,\hat{H}_1(u)\hat{U}_1(u,t_0)\hat{U}_{n-2}(u,t_0)+\int_{t_0}^{t}du\,\hat{A}(u,t_0)\hat{U}_{n-2}(u,t_0)\ . \qquad (A1)$$

First, we start with (3.9), namely,

$$\hat{U}_n(t,t_0)=-i\int_{t_0}^{t}du\,\hat{H}_1(u)\hat{U}_{n-1}(u,t_0) \qquad (A2)$$

and note that

$$\int\frac{d\hat{F}}{du}\hat{f}\,du=\hat{F}\hat{f}-\int\hat{F}\frac{d\hat{f}}{du}du\ ,$$

then making the substitution $\hat{H}_1^{(u)}=d\hat{F}/du$, $\hat{F}=\int du\,\hat{H}_1(u)$, $\hat{f}(u,t_0)=\hat{U}_{n-1}(u,t_0)$, and

$$d\hat{f}/du=d\hat{U}_{n-1}(u,t_0)/du=-i\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\ ,$$

we obtain

$$\hat{U}_n(t,t_0)=-i\left\{\left[\left[\int du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(u,t_0)]\right]\Bigg|_{t_0}^{t}+i\int_{t_0}^{t}du\left[\int du\,\hat{H}_1(u)\right]\hat{H}_1(u)\hat{U}_{n-z}(u,t_0)\right\}$$
$$=-i\left[\left[\int^{t}du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]-\left[\int^{t_0}du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t_0,t_0)]+i\int_{t_0}^{t}du\left[\int du\,\hat{H}_1(u)\right]\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\right]\ . \qquad (A3)$$

Based on (A2), obviously $\hat{U}_{n-1}(t_0,t_0)=0$; therefore,

$$\hat{U}_n(t,t_0)=-i\left[\left[\int^t du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]+i\int_{t_0}^t du\left[\int du\,\hat{H}_1(u)\right]\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\right]$$

$$=-i\left[\left[\int^t du\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]-\left[\int^{t_0} du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]\right.$$

$$\left.+\left[\int^{t_0} du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]+i\int_{t_0}^t du\left[\int du\,\hat{H}_1(u)\right]\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\right]$$

$$=\left[-i\int_{t_0}^t du\,\hat{H}_1(u)\right][\hat{U}_{n-1}(t,t_0)]$$

$$+\int_{t_0}^t du\left[\left[\int du\,\hat{H}_1(u)\right]-\left[\int^{t_0} du\,\hat{H}_1(u)\right]\right]\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\,. \tag{A4}$$

As $\hat{U}_1(t,t_0)=-i\int_{t_0}^t du\,\hat{H}_1(u)$,

$$\int_{t_0}^t du\,\hat{H}_1(u)=\left[\int^t du\,\hat{H}_1(u)\right]-\left[\int^{t_0} du\,\hat{H}_1(u)\right],$$

expression (A4) becomes

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+\int_{t_0}^t du\left[\int_{t_0}^u dv\,\hat{H}_1(v)\right]\hat{H}_1(u)\hat{U}_{n-2}(u,t_0)\,. \tag{A5}$$

Using (3.13), expression (A5) becomes

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+\int_{t_0}^t du\left[\hat{H}_1(u)\int_{t_0}^u dv\,\hat{H}_1(v)+\hat{A}(u,t_0)\right]\hat{U}_{n-2}(u,t_0)$$

$$=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+i\int_{t_0}^t du\,\hat{H}_1(u)\left[-i\int_{t_0}^u dv\,\hat{H}_1(v)\right]\hat{U}_{n-2}(u,t_0)+\int_{t_0}^t du\,\hat{A}(u,t_0)\hat{U}_{n-2}(u,t_0)$$

$$=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+i\int_{t_0}^t du\,\hat{H}_1(u)\hat{U}_1(u,t_0)\hat{U}_{n-2}(u,t_0)+\int_{t_0}^t du\,\hat{A}(u,t_0)\hat{U}_{n-2}(u,t_0)\,. \tag{A6}$$

APPENDIX B

We start from

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+i\int_{t_0}^t du_1\hat{H}_1(u_1)\hat{U}_1(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)+\int_{t_0}^t du_1\hat{A}(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)\,. \tag{B1}$$

Replacing n by $n-1$,

$$\hat{U}_1(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)=\hat{U}_{n-1}(u_1,t_0)-i\int_{t_0}^{u_1} du_2\hat{H}_1(u_2)\hat{U}_1(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)$$

$$-\int_{t_0}^{u_1} du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)\,. \tag{B2}$$

Substitute (B2) back to (B1),

$$\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)$$

$$+i\int_{t_0}^t du_1\hat{H}_1(u_1)\left[\hat{U}_{n-1}(u_1,t_0)-i\int_{t_0}^{u_1} du_2\hat{H}_1(u_2)\hat{U}_1(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)\right.$$

$$\left.-\int_{t_0}^{u_1} du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)\right]$$

$$+\int_{t_0}^t du_1\hat{A}(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)\,. \tag{B3}$$

As

$$i\int_{t_0}^t du_1\hat{H}_1(u_1)\hat{U}_{n-1}(u_1,t_0)=-\hat{U}_n(t,t_0)$$

[from (3.9)], obviously (B3) can be written as

$$2\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)+\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\hat{U}_1(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)$$
$$-i\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)+\int_{t_0}^{t}du_1\hat{A}(u,t_0)\hat{U}_{n-2}(u_1,t_0)\ . \quad \text{(B4)}$$

Replacing n by $n-2$ in (B1), we have

$$\hat{U}_1(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)=\hat{U}_{n-2}(u_2,t_0)-i\int_{t_0}^{u_2}du_3\hat{H}_1(u_3)\hat{U}_1(u_3,t_0)\hat{U}_{n-4}(u_3,t_0)$$
$$-\int_{t_0}^{u_2}du_3\hat{A}(u_3,t_0)\hat{U}_{n-4}(u_3,t_0)\ . \quad \text{(B5)}$$

Substituting (B5) to (B4), and after simple rearrangements,

$$3\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)$$
$$-i\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\int_{t_0}^{u_2}du_3\hat{H}_1(u_3)\hat{U}_1(u_3,t_0)\hat{U}_{n-4}(u_3,t_0)$$
$$-\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\int_{t_0}^{u_2}du_3\hat{A}(u_3,t_0)\hat{U}_{n-4}(u_3,t_0)$$
$$-i\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)+\int_{t_0}^{t}du_1\hat{A}(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)\ . \quad \text{(B6)}$$

We can repeat the above iterative process by letting $n=n-3,n-4,\ldots$, in relation (B1) and substitute the result to equations similar to (B6), obtaining

$$4\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)$$
$$-(-i)^4\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\int_{t_0}^{u_2}du_3\hat{H}_1(u_3)\int_{t_0}^{u_3}du_4\hat{H}_1(u_4)\hat{U}_1(u_4,t_0)\,\hat{U}_{n-5}(u_4,t_0)$$
$$+(-i)^3\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\int_{t_0}^{u_2}du_3\hat{H}_1(u_3)\int_{t_0}^{u_3}du_4\hat{A}(u_4,t_0)\hat{U}_{n-5}(u_4,t_0)$$
$$+(-i)^2\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\int_{t_0}^{u_2}du_3\hat{A}(u_3,t_0)\hat{U}_{n-4}(u_3,t_0)$$
$$+(-i)\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)$$
$$+\int_{t_0}^{t}du_1\hat{A}(u_1,t_0)\hat{U}_{n-2}(u_1,t_0) \quad \text{(B7)}$$

and then

$$(n-1)\hat{U}_n(t,t_0)=\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)$$
$$-(-i)^{n-1}\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-2}}du_{n-1}\hat{H}_1(u_{n-1})\hat{U}_1(u_{n-1},t_0)$$
$$\times\hat{U}_{n-(n-1+1)}(u_{n-1},t_0)$$
$$+(-i)^{n-2}\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-2}}du_{n-1}\hat{A}(u_{n-1},t_0)$$
$$\times\hat{U}_{n-n}(u_{n-1},t_0)$$
$$+(-i)^{n-3}\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-3}}du_{n-2}\hat{A}(u_{n-2},t_0)\hat{U}_{n-(n-1)}$$
$$\times(u_{n-2},t_0)+\cdots$$
$$+(-i)\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{A}(u_2,t_0)\hat{U}_{n-3}(u_2,t_0)$$
$$+\int_{t_0}^{t}du_1\hat{A}(u_1,t_0)\hat{U}_{n-2}(u_1,t_0)\ . \quad \text{(B8)}$$

Using the boundary condition (3.11) $U_0(u_{n-1},t_0)=1$, we obtain from (B8) after simple rearrangement

$$\begin{aligned}(-i)^{n-1}&\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-2}}du_{n-1}\hat{H}_1(u_{n-1})\hat{U}_1(u_{n-1},t_0)\hat{U}_{n-(n-1+1)}(u_{n-1},t_0)\\&=(-i)^{n-1}\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-2}}du_{n-1}\hat{H}_1(u_{n-1})\hat{U}_1(u_{n-1},t_0)\\&=(-i)^{n}\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_{n-2}}du_{n-1}\hat{H}_1(u_{n-1})\int_{t_0}^{u_{n-1}}du_n\hat{H}_1(u_n)\\&=\hat{U}_n(t,t_0)\;.\end{aligned}\tag{B9}$$

Substituting (B9) to (B8),

$$\begin{aligned}n\hat{U}_n(t,t_0)=&\hat{U}_1(t,t_0)\hat{U}_{n-1}(t,t_0)\\&+\sum_{j=0}^{n-2}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{2}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{n-(j+2)}(u_{j+1},t_0)\;.\end{aligned}\tag{B10}$$

Replacing n by $n-1$ in (B10) and resetting the result back into (B10)

$$\begin{aligned}\hat{U}_n(t,t_0)=&\frac{1}{n(n-1)}\hat{U}_1^2(t,t_0)\hat{U}_{n-2}(t,t_0)\\&+\frac{1}{n(n-1)}\hat{U}_1(t,t_0)\\&\times\sum_{j=0}^{n-3}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{n-(j+3)}(t,t_0)\\&+\frac{1}{n}\sum_{j=0}^{n-2}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\,\hat{U}_{n-(j+2)}(u_{j+1},t_0)\;.\end{aligned}\tag{B11}$$

With the use of (B10) again, replacing n by $n-2$, and substituting the result back into (B11)

$$\begin{aligned}\hat{U}_n(t,t_0)=&\frac{1}{n(n-1)(n-2)}\hat{U}_1^3(t,t_0)\hat{U}_{n-3}(t,t_0)\\&+\frac{1}{n(n-1)(n-2)}\hat{U}_1^2(t,t_0)\\&\times\sum_{j=0}^{n-4}(-i)^j\int_{t_0}^{t}du_1\hat{H}(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\\&\qquad\times\int_{t_0}^{u_2}du_3\hat{H}_1(u_3)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\,\hat{U}_{n-(j+4)}(u_{j+1},t_0)\\&+\frac{1}{n(n-1)}\hat{U}_1(t,t_0)\sum_{j=0}^{n-3}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\\&\qquad\times\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{n-(j+3)}(u_{j+1},t_0)\\&+\frac{1}{n}\sum_{j=0}^{n-2}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{n-(j+2)}(u_{j+1},t_0)\;,\end{aligned}\tag{B12}$$

where $t>u_1>u_2>u_3>\cdots>t_0$.

We can continue this process until we have expressed the high-order operator $\hat{U}_{n-3}(t,t_0)$ in terms of $\hat{U}_1(t,t_0)$ (as a first linear term plus others), arriving at

$$\hat{U}_n(t,t_0)=\frac{1}{n!}\hat{U}_1^{n-1}(t,t_0)\hat{U}_{n-(n-1)}(t,t_0)+\frac{1}{n(n-1)\cdots[n-(n-2)]}\hat{U}_1^{n-2}(t,t_0)\hat{B}_{n-(n-2+2)}(t,t_0)$$
$$+\frac{1}{n(n-1)\cdots[n-(n-3)]}\hat{U}_1^{n-3}(t,t_0)\hat{B}_{n-(n-3+2)}(t,t_0)+\cdots+\frac{1}{n(n-1)}\hat{U}_1(t,t_0)\hat{B}_{n-3}(t,t_0)$$
$$+\frac{1}{n}\hat{B}_{n-2}(t,t_0)\ , \tag{B13}$$

where

$$\hat{B}_r(t,t_0)=\sum_{j=0}^{r}(-i)^j\int_{t_0}^{t}du_1\hat{H}_1(u_1)\int_{t_0}^{u_1}du_2\hat{H}_1(u_2)\cdots\int_{t_0}^{u_j}du_{j+1}\hat{A}(u_{j+1},t_0)\hat{U}_{r-j}(u_{j+1},t_0)\ ,$$
$$t>u_1>u_2>u_3\cdots>u_r\ . \tag{B14}$$

Obviously, (B13) can be written as

$$\hat{U}_n(t,t_0)=\frac{1}{n!}\hat{U}_1^n(t,t_0)+\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)![\hat{U}_1(t,t_0)]^{n-(r+2)}\hat{B}_r(t,t_0)\ . \tag{B15}$$

APPENDIX C

We shall show some properties of the operator function in (C1), relevant to calculations presented in Secs. V and VI. Suppose we express

$$\exp\{\tau[\alpha(\tau)\hat{P}+\beta(\tau)\hat{Q}]\}$$
$$=\exp[\tau\alpha(\tau)\hat{P}]\hat{K}(\tau)\exp[\tau\beta(\tau)\hat{Q}]$$
$$=\hat{K}(\tau)\exp[\tau\alpha(\tau)\hat{P}]\exp[\tau\beta(\tau)\hat{Q}]$$
$$=\exp[\tau\alpha(\tau)\hat{P}]\exp[\tau\beta(\tau)\hat{Q}]\hat{K}(\tau)\ , \tag{C1}$$

where the operator function $\hat{K}(\tau)$ is assumed to satisfy the commutation rules

$$[\hat{K}(\tau),\hat{P}]=[\hat{K}(\tau),\hat{Q}]=0\ . \tag{C2}$$

We want to find the explicit form of $\hat{K}(\tau)$. From inspection of (C1), we know that

$$\hat{K}(\tau)=\exp[-\tau\alpha(\tau)\hat{P}]$$
$$\times\exp\{\tau[\alpha(\tau)\hat{P}+\beta(\tau)\hat{Q}]\}$$
$$\times\exp[-\tau\beta(\tau)\hat{Q}]\ . \tag{C3}$$

Obviously, when $\tau=0$, $\hat{K}(0)=1$. Differentiating (C3), and after a simple process of rearrangement,

$$\frac{d\hat{K}(\tau)}{d\tau}=\hat{K}(\tau)[\alpha(\tau)+\tau\alpha'(\tau)]\times\sum_{r=1}^{\infty}\frac{[\tau\beta(\tau)]^r}{r!}\hat{R}_r\ , \tag{C4}$$

where the prime symbol signifies differentiation with respect to τ, and

$$\hat{R}_r=[\hat{Q},\hat{P}]_r\ . \tag{C5}$$

Let

$$\hat{\mathscr{Y}}(\tau)=[\alpha(\tau)+\tau\alpha'(\tau)]\sum_{r=1}^{\infty}\frac{[\tau\beta(\tau)]^r}{r!}\hat{R}_r\ .$$

Solving for $\hat{K}(\tau)$ in (C4),

$$\hat{K}(\tau)=\hat{K}(0)\left[1+\sum_{n=1}^{\infty}\hat{Y}_n(\tau,0)\right] \tag{C6}$$

in which

$$\hat{Y}_n(\tau,0)=\int_0^{\tau}dt_1\hat{\mathscr{Y}}(t_1)\int_0^{t_1}dt_2\hat{\mathscr{Y}}(t_2)\cdots\int_0^{t_{n-1}}dt_n\hat{\mathscr{Y}}(t_n)\ . \tag{C7}$$

It is easy to see that $\hat{K}(0)=1$, and we can readily arrange (C6) in the following form:

$$\hat{K}(\tau)=\exp\left[\int_0^{\tau}\hat{\mathscr{Y}}(u)du\right]+\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)!\left[\int_0^{\tau}\hat{\mathscr{Y}}(u)du\right]^{n-(r+2)}\hat{\mathscr{B}}_r(\tau,0)\ , \tag{C8}$$

where

$$\hat{\mathscr{B}}_r(\tau,0)=\sum_{j=0}^{r}\int_0^{\tau}dt_1\hat{\mathscr{Y}}(t_1)\int_0^{t_1}dt_2\hat{\mathscr{Y}}(t_2)\cdots\int_0^{t_j}dt_{j+1}\left[\int_0^{t_{j+1}}[\hat{\mathscr{Y}}(t),\hat{\mathscr{Y}}(t_{j+1})]dt\right]\hat{Y}_{r-j}(t_{j+1},0)\ . \tag{C9}$$

[1]F. J. Dyson, Phys. Rev. 75, 1736 (1949).
[2]A. S. Davydov, *Quantum Mechanics* (Pergamon, New York, 1969).
[3]M. Gell-Mann and F. Low, Phys. Rev. 95, 1300 (1954).
[4]H. S. Snyder, Phys. Rev. 83, 1154 (1951).
[5]H. E. Moses, Nuovo Cimento 1, 103 (1955).
[6]K. O. Friedrichs, Comm. Pure Appl. Math. 1, 361 (1948).
[7]A. Abrikosov, L. Gorkov, and I. Dzyaloshinski, *Quantum Field Theoretical Methods in Statistical Physics* (Pergamon, London, 1965).
[8]G. D. Mahan, Many-Particle Physics (Plenum, New York, 1981), Chaps. 2, 3, and 6.
[9]T. T. Matsubara, Prog. Theor. Phys. 14, 351 (1955).
[10]D. ter Haar, *Lectures on Selected Topics in Statistical Mechanics* (Pergamon, New York, 1977), Chap. 2.
[11]G. C. Wick, Phys. Rev. 80, 268 (1950).
[12]K. A. Brueckner, Phys. Rev. 100, 36 (1955).
[13]N. M. Hugenholtz and L. Van Hove, Physica (Utrecht) 24, 363 (1958).
[14]N. N. Bogoliubov, *A New Method in the Theory of Superconductivity* (Consultants Bureau, New York, 1959).
[15]R. P. Feynmann and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1964).
[16]C. L. Hammer, J. E. Shrauner, and B. DeFacio, Phys. Rev. D 18, 373 (1978).
[17]C. L. Hammer, J. E. Shrauner, and B. DeFacio, Phys. Rev. D 19, 667 (1979).
[18]L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley-Interscience, New York, 1981).
[19]K. W. Wong and P. C. W. Fung, Nuovo Cimento B 25, 595 (1975).
[20]P. C. W. Fung, H. K. Tsang, and K. W. Wong, Nuovo Cimento B 28, 313 (1975).
[21]K. W. Wong, P. C. W. Fung, and C. C. Lau, Phys. Rev. A 22, 1272 (1980).
[22]P. G. L. Leach, J. Math. Phys. 18, 1608 (1977).
[23]H. W. Peng, Acta Phys. Sin. 29, 1084 (1980).
[24]L. F. Landovitz, Phys. Rev. A 11, 67 (1975).
[25]D. C. Khandekar and S. V. Lawande, J. Math. Phys. 20, 1870 (1979).