Time-development operator method in quantum mechanics

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We discuss the time-development operator method in quantum mechanics. The equivalence of this method and the usual method of expansion in terms of energy eigenfunctions discussed in textbooks is pointed out. As examples of cases of time-dependent Hamiltonians, we discuss the time development of a Gaussian wave packet for a charged particle subject to a time-dependent electric field using an operator differential equation. We also consider a spin in a time-dependent magnetic field through a time-development operator.
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I. INTRODUCTION

In a publication in this Journal, Robinett[1] has drawn attention to the merits of the time-development operator method for obtaining the quantum mechanical state function at any future time t from the one at $t=0$. The time evolution of a free particle wave packet[2] and the oscillating harmonic oscillator wave packet[3] are some of the possible examples. Reference 1 has dealt with the time-development operator for a particle subject to a uniform and time-independent force. A brief discussion of this operator for the same case has also been presented earlier in this Journal.[4] This problem has also been discussed using the Heisenberg picture.[5] Arrighini *et al.*[6] have considered the same problem and discussed different methods for obtaining the quantum propagator. Holstein[7] has also presented additional methods to calculate the linear potential propagator. Calculations of the propagator for a harmonic oscillator have also been reported in this Journal.[8–10] All these cases involve time-independent Hamiltonians.

It will be useful to consider additional examples involving time-dependent Hamiltonians for illustrating the time-development operator method, which may be suitable for introductory courses in quantum mechanics. Fallieros *et al.*[4] have considered the propagator for a particle subject to a sinusoidal electric field and have briefly discussed the time-development operator for a constant force case. Many years ago Parker[11] presented the time evolution operator for a charged harmonic oscillator in a uniform time-varying electric field.

In the present work we treat the case of a charged particle in a time-varying electric field and obtain the time-development operator and the propagator which are generalizations of the ones given in Refs. 1, 6, and 7. The method used is also applicable for cases with time-independent Hamiltonians. We also treat the problem of a spin in a time-dependent magnetic field.

II. CHARGED PARTICLE IN A TIME-DEPENDENT ELECTRIC FIELD

Before treating this case, a few remarks on the methods of obtaining the future state function from the initial state are in order. The time-developed state function $\psi(x,t)$ at any time t is given in terms of $\psi(x,0)$ (for a system with stationary states $\psi_n(x)$ and energies E_n) by

$$\psi(x,t)=\sum_n \left(\int \psi_n^*(x')\psi(x',0)\,dx' \right)\psi_n(x)e^{-iE_nt/\hbar}. \tag{1}$$

One can also see that Eq. (1) may be written as

$$\psi(x,t)=e^{-iHt/\hbar}\left[\sum_n \left(\int \psi_n^*(x')\psi(x',0)\,dx' \right)\psi_n(x)\right]. \tag{2}$$

Identifying the terms in the rectangular bracket as $\psi(x,0)$ and the exponential term as the time-development operator $U(t)$, one sees the equivalence of the time-development operator method and the usual method of expansion in terms of the energy eigenfunctions. The equivalence is exact for classes of initial state functions $\psi(x,0)$ for which there are no technical difficulties in handling the series

$$\left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}Ht\right)^n\right]\psi(x,0).$$

When there are difficulties arising out of convergence requirements, one has to prefer using Eq. (1) instead of Eq. (2).[12,13] For cases with time-dependent Hamiltonians for which there are no stationary states, one has either to solve directly the time-dependent Schrödinger equation to find $\psi(x,t)$ or use the time-development operator $U(t)$. This operator is now not simply $\exp(-i/\hbar\, Ht)$, but can be formally written as an ordered series of integrals.[14] In view of the merits of the time-development operator method indicated in Ref. 1, it will be useful to find $U(t)$ for such cases in closed form. $U(t)$ is to be obtained by solving the operator differential equation:

$$i\hbar\frac{\partial U(t)}{\partial t}=H(t)U(t) \tag{3}$$

with

$$U(0)=I,$$

the unit operator.

For a particle of charge q and mass m constrained to move in one dimension and subject to an electric field $\epsilon(t)$, the Hamiltonian is

$$H(t)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-q\epsilon(t)x. \tag{4}$$

The general solution of the operator equation of the form in Eq. (3) has been discussed by Wilcox.[15] Following Refs. 11 and 15, we write

$$U(t)=e^{-i/\hbar\, H_0 t}Y(t), \tag{5}$$

where H_0 is the kinetic energy operator (time-independent part). Substituting in Eq. (3), one immediately finds

$$i\hbar\,\frac{\partial Y}{\partial t}=e^{i/\hbar\, H_0 t}H_1 e^{-i/\hbar\, H_0 t}Y(t) \tag{6}$$

with

$$Y(0)=I,$$

where H_1 is the potential energy term (time-dependent part) in Eq. (6). Making use of the operator expansion,[15]

$$e^{A}Be^{-A}=B+[A,B]+\frac{1}{2!}[A,[A,B]]+\cdots, \tag{7}$$

one gets

$$\frac{\partial Y}{\partial t}=A(t)Y(t) \tag{8}$$

with

$$A(t)=-\frac{1}{i\hbar}\left[q\epsilon(t)x+\frac{q\epsilon(t)}{m}tp\right]. \tag{9}$$

Operator equations of the form of Eq. (8) also occur in the Heisenberg and interaction pictures in quantum mechanics. We look for the solution of Eq. (8) in the following form;

$$Y(t)=e^{\alpha(t)i\hbar+\beta(t)x+\gamma(t)p} \tag{10}$$

where α, β, and γ are to be determined.

On using the special case of the Zassenhaus formula,[15]

$$e^{A+B}=e^{A}e^{B}e^{-1/2[A,B]}, \tag{11}$$

where A and B are two noncommuting operators, each commuting with their commutator, one gets

$$Y(t)=e^{i\hbar\,[\alpha(t)-1/2\beta(t)\gamma(t)]}e^{\beta(t)x}e^{\gamma(t)p}. \tag{12}$$

Substituting $Y(t)$ given in Eq. (12) in Eq. (8) and premultiplying by Y^{-1}, one gets

$$i\hbar\,(\dot\alpha-1/2\dot\beta\gamma-1/2\beta\dot\gamma)+\left[\dot\beta+\frac{q\epsilon(t)}{i\hbar}\right]Y^{-1}xY + \dot\gamma p+\frac{q\epsilon(t)t}{i\hbar m}Y^{-1}pY=0, \tag{13}$$

where the dot indicates differentiation with respect to t. Again using the expansion in Eq. (7) and after some simplification, one gets

$$\beta(t)=-\frac{q}{i\hbar}\int_0^t\epsilon(t')dt', \tag{14}$$

$$\gamma(t)=-\frac{q}{i\hbar m}\int_0^t t'\epsilon(t')dt', \tag{15}$$

$$\alpha(t)=-\frac{1}{2i\hbar}\left[\frac{q}{m}\int_0^t\epsilon(t')t'\beta(t')dt' -q\int_0^t\epsilon(t')\gamma(t')dt'\right] \tag{16}$$

$$=\frac{q^2}{2\hbar^2 m}\int_0^t dt'\int_0^{t'}dt''\epsilon(t')\epsilon(t'')(t'-t''). \tag{17}$$

At this point our results may be compared with those of Parker,[11] who investigated a harmonic oscillator subject to a time-varying electric field. Our results in Eqs. (14)–(17) are the same as those of Parker in the limit as the oscillator frequency $\omega\to 0$ in his work. Parker, however, made use of the Magnus expansion,[15] which involves commutators of operators at different times, instead of the simpler Zassenhaus formula used by us.

The time-development operator is now given by

$$U(t)=e^{-i/\hbar\, p^2 t/2m}e^{i\hbar\,[\alpha(t)-1/2\beta(t)\gamma(t)]}e^{\beta(t)x}e^{\gamma(t)p} \tag{18}$$

with α, β, and γ as given above. Using the Baker–Campbell–Hausdorff formula[15] for any two operators A and B,

$$e^{A}e^{B}=e^{A+B+1/2[A,B]+1/12[A,[A,B]]+1/12[B,[A,B]]+\cdots}, \tag{18a}$$

we can recast $U(t)$ in a more convenient form,

$$U(t)=e^{i\hbar\,[\alpha(t)-1/2\beta(t)\gamma(t)]}e^{\beta(t)x}e^{-itp^2/2\hbar m}e^{[\gamma(t)-\beta(t)t/m]p}. \tag{19}$$

We consider Eq. (19) as a generalized form for $U(t)$ discussed in Refs. 1, 6, and 7. If $\epsilon(t)$ is independent of time, one can easily evaluate α, β, and γ and obtain

$$U(t)=e^{i/\hbar\, q\epsilon tx}e^{-itp^2/2\hbar m}e^{-iq\epsilon t^2 p/2\hbar m}e^{-iq^2\epsilon^2 t^3/6\hbar m}, \tag{20}$$

which agrees with that obtained in Refs. 1, 6, and 7.

As a first use of Eq. (19), we consider the spreading of a Guassian wave packet, which at time $t=0$ has the form

$$\psi(x,0)=\left[\frac{1}{2\pi\lambda^2}\right]^{1/4}e^{-(x-\bar{x})^2/4\lambda^2}. \tag{21}$$

With $U(t)$ given in Eq. (19) we find

$$\psi(x,t)=e^{i\hbar\,[\alpha(t)-1/2\beta(t)\gamma(t)+\beta^2 t/2m]}e^{\beta(t)x} \times e^{-itp^2/2\hbar m}\left[\frac{1}{2\pi\lambda^2}\right]^{1/4} \times e^{-[x+\hbar/i\,\gamma(t)-\hbar/i\,\beta(t)t/m-\bar{x}]^2/4\lambda^2}, \tag{22}$$

where we have used the familiar result

$$e^{b\,d/dx}f(x)=f(x+b). \tag{23}$$

Using the relation[2]

$$\frac{\partial^2}{\partial x^2}\left[\frac{1}{\sqrt{\lambda^2}}e^{-x^2/4\lambda^2}\right]=\frac{\partial}{\partial(\lambda^2)}\left[\frac{1}{\sqrt{\lambda^2}}e^{-x^2/4\lambda^2}\right], \tag{24}$$

we immediately get

$$\psi(x,t)=e^{i\hbar\,[\alpha(t)-1/2\beta(t)\gamma(t)+\beta^2 t/2m]}$$
$$\times e^{\beta(t)x}\left(\frac{\lambda^2}{2\pi}\right)^{1/4}\frac{1}{\sqrt{(\lambda^2+i\hbar\, t/2m)}}$$
$$\times e^{-[x+\hbar/i\gamma-\hbar/i\beta t/m-\bar{x}]^2/4(\lambda^2+i\hbar\, t/2m)}. \tag{25}$$

It is easy to see that the peak position has been shifted to $\bar{x}-q(I_2-tI_1)/m$, where I_1 and I_2 are the integrals in β and γ, respectively, in Eqs. (14) and (15). The shift depends on the electric field and the half-width has become

$$2\lambda\left(1+\frac{\hbar^2 t^2}{4\lambda^4 m}\right)^{1/2},$$

which is independent of the electric field.

Equation (19) can also be used to obtain the quantum mechanical propagator for the present problem:

$$K(x,x',t)=e^{i\hbar[\alpha(t)-1/2\beta(t)\gamma(t)+\beta^2 t/2m]}e^{\beta(t)x}$$
$$\times\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\, e^{-itp^2/2m\hbar}$$
$$\times e^{[\gamma(t)-\beta(t)t/m]p}e^{i/\hbar p(x-x')}. \tag{26}$$

The integral may be easily evaluated and one gets

$$K(x,x',t)=(m/2\pi i\hbar t)^{1/2}e^{i/\hbar(m(x-x')^2)/2t}$$
$$\times e^{i\hbar[\alpha(t)+1/2\beta(t)\gamma(t)-m\gamma^2(t)/2t]}$$
$$\times e^{m\gamma(t)x/t}e^{-mx'/t[\gamma(t)-t\beta(t)]^2}. \tag{27}$$

This again is a generalized form and reduces to the one given in Refs. 1, 6, and 7 when $\epsilon(t)$ is independent of time. It may be noted that the method adopted in our work can also be used when H is independent of time with suitable splitting of H as H_0+H_1. For example, if ϵ is independent of t, H_0 and H_1 could be the same as we had chosen, except now H_1 is also independent of time. Consequently Eq. (8) may be immediately integrated and the subsequent algebra will also be simpler.

III. TIME-DEVELOPMENT OPERATOR FOR A SPIN IN A TIME-DEPENDENT MAGNETIC FIELD

As yet another example involving a time-dependent Hamiltonian, we consider a particle of spin $\mathbf{J}$ (in units of $\hbar$) subject to a magnetic field $\mathbf{B}=(B_1\cos\omega t, B_1\sin\omega t, B_0)$, which corresponds to a static field $\mathbf{B}_0$ along the z direction and a field of amplitude B_1 rotating in the $X-Y$ plane with an angular frequency ω. Such a situation is of interest in magnetic resonance. The Hamiltonian of the system is

$$H(t)=-\gamma B_0 J_z-\gamma B_1(J_x\cos\omega t+J_y\sin\omega t), \tag{28}$$

where γ is a constant. Some textbooks[16] suggest that for the above time-dependent problem one should directly try to solve the time-dependent Schrödinger equation instead of finding $U(t)$. We wish to show how the time-development operator method can be used for the present problem.

Following the method adopted in Sec. II, we look for the solution of Eq. (3) with H now given in Eq. (28) in the form

$$U(t)=e^{-iJ_z\omega t}Y(t) \tag{29}$$

and obtain by substituting U in Eq. (3),

$$(\omega_0-\omega)J_zY(t)+i\frac{\partial Y}{\partial t}=e^{iJ_z\omega t}\omega_1(J_x\cos\omega t$$
$$+J_y\sin\omega t)e^{-iJ_z\omega t}Y(t), \tag{30}$$

where we have written $-\gamma B_0=\omega_0$ and $-\gamma B_1=\omega_1$. Using the expansion formula in Eq. (7) and the familiar commutation relations for the spin operators, $\mathbf{J}\times\mathbf{J}=i\mathbf{J}$ we get

$$\frac{\partial Y}{\partial t}=-i[\omega_1 J_x+(\omega_0-\omega)J_z]Y(t), \tag{31}$$

which can be immediately integrated to obtain $Y(t)$. Thus one gets

$$U(t)=e^{-iJ_z\omega t}e^{-i\mathbf{J}\cdot\hat{n}\lambda t} \tag{32}$$

where

$$\hat{n}=\frac{\omega_1\hat{x}+(\omega_0-\omega)\hat{z}}{\lambda}$$

with $\hat{x}$ and $\hat{z}$ being the unit vectors along the x and z directions and $\lambda=(\omega_1^2+(\omega_0-\omega)^2)^{1/2}$. The operator $U(t)$ may also be obtained by going to a rotating coordinate system.[17] The operator of the form $e^{-i\mathbf{J}\cdot\hat{n}\lambda t}$ in Eq. (32) is a rotation operator which will mix all spin states and the problem of obtaining the spin-flip probability is slightly more involved.[18] For the special case of a spin 1/2 particle, it turns out that we have a simple expansion of the exponential operator now involving the Pauli spin operator $\boldsymbol{\sigma}$. For this case, one has

$$U(t)=e^{-1/2\sigma_z\omega t}\left[\cos\frac{\lambda t}{2}-i\sin\left(\frac{\lambda t}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}\right], \tag{33}$$

which is obtained by expanding $e^{-1/2(\boldsymbol{\sigma}\cdot\hat{n})\lambda t}$ and using the result $(\boldsymbol{\sigma}\cdot\hat{n})^2=I$. $U(t)$ can also be written down using the following result (which can be simply proved);

$$e^{bA}=\frac{\lambda_2 e^{b\lambda_1}-\lambda_1 e^{b\lambda_2}}{\lambda_2-\lambda_1}+\frac{e^{b\lambda_1}-e^{b\lambda_2}}{\lambda_1-\lambda_2}A, \tag{34}$$

where λ_1 and λ_2 are the distinct eigenvalues of the operator A which can be represented by a 2×2 matrix and b is a scalar.

Supposing the initial spin state $\chi(0)$ is given by $\binom{1}{0}$ (the ''spin-up'' spinor), one gets

$$\chi(t)=e^{-i\omega t/2}\left[\cos\frac{\lambda t}{2}-\frac{i(\omega_0-\omega)}{\lambda}\sin\frac{\lambda t}{2}\right]\begin{pmatrix}1\\0\end{pmatrix}$$
$$-e^{i\omega t/2}\left[\frac{i\omega_1}{\lambda}\sin\frac{\lambda t}{2}\right]\begin{pmatrix}0\\1\end{pmatrix}. \tag{35}$$

Equation (35) gives the well known ''spin-flip'' probability

$$\frac{\omega_1^2}{\lambda^2}\sin^2\left(\frac{\lambda t}{2}\right).$$

The spin-flip probability shows a peak at $\omega=\omega_0$ which is the condition for ''spin resonance.''

IV. SUMMARY

We have drawn attention to the equivalence of the time-development operator method and the method of expansion in terms of energy eigenfunctions for obtaining $\Psi(x,t)$ from

$\Psi(x,0)$ when the Hamiltonian is time independent. We have shown how the time-development operator may be obtained for a charged particle in a time-dependent electric field and hence the propagator for the problem. The results are generalizations of the ones for the case of a particle in a time-independent electric field discussed in this Journal. The well-known problem of a spin in time-dependent magnetic field is also treated through the time-development operator method.

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EARLY VACUUM PHYSICS

Dear Uncle Robert, I enclose receipt signed. I forgot to dispatch it as I was sent for to London, to be ready to explain to the Queen why Otto von Guericke devoted himself to the discovery of nothing, and to show her the two hemispheres in which he kept it, and the picture of the 16 horses who could not separate the hemispheres, and how after 200 years W. Crookes has come much nearer to nothing and has sealed it up in a glass globe for public inspection.* Her Majesty however let us off very easily and did not make much ado about nothing, as she had much heavy work cut out for her all the rest of the day . . .

*As the editors note: ''This is a reference to the Loan Exhibition of Scientific Apparatus, held in London in 1876. Queen Victoria visited the exhibition where Maxwell presented 'Molecular Physics' and explained the operation of various pieces of apparatus.''

James Clerk Maxwell, letter to Robert Cay, 15 May 1876, reprinted in Elizabeth Garber, Stephen G. Brush, and C. W. F. Everitt, editors, *Maxwell on Heat and Statistical Mechanics: On ''Avoiding All Personal Enquiries'' of Molecules* (Lehigh University Press, Bethlehem, PA, 1995), p. 404.