Strong-field approximation for the Schrödinger equation

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A perturbation series is derived for the Schrödinger equation where the perturbation is permitted to go to ∞. Such an asymptotic series can be obtained in a representation where the time evolution of the states is due to the unperturbed part of the Hamiltonian of the problem and the time evolution of the observables is determined by the perturbation, contrary to the interaction picture. The equivalence between the series given by such a picture, and an asymptotic perturbation scheme is given. The method is applied to a spin-$\frac{1}{2}$ particle in a two-component magnetic field, one component of which, considered as a perturbation, can be time varying. Choosing a constant perturbation we show the equivalence between the exact solution and the approximate one when a component of the magnetic field is much larger than the other. In this case the limit $t\to\infty$ cannot be taken, as mixed-secular terms appear in the asymptotic series. Taking a linear time-varying dependence for a component of the magnetic field, we get a nonanalytic asymptotic series.

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I. INTRODUCTION

It is well known that a solution series can be derived for the Schrödinger equation in the limit of small perturbations in the framework of the interaction picture [1]. This was the first approach taken by Dirac to solve, in an approximate way, problems where the Hamiltonian depends on time [2–4]. This method has proved successful and is often applied in quantum mechanics and field theory [5] as well. Some difficulties arise if one wants to take the opposite limit, i.e., large perturbations. If we look for an asymptotic-series solution, a standard perturbation approach does not give meaningful results.

This question can be answered, as we are going to show, if we change the time scale of the problem [6]. Then a systematic approach can be made, and an asymptotic series emerges. This way of working is equivalent to defining a representation where the states evolve by a free Hamiltonian and the operators by perturbation, appearing as an interaction picture with the role of the free part of the Hamiltonian and that of the perturbation inverted.

Nonanalytical series can appear, due to the form of the perturbation. In the following we will see an example. The S matrix can still be defined, but a uniform convergence of the series is necessary. This is not always assured; sometimes the exact solution is needed. We will not treat the S-matrix problem in this paper.

The paper is organized as follows. In Sec. II we show the method, first deriving the asymptotic series from the free picture (i.e., the representation defined above) and then, from an asymptotic-perturbation approach, showing in this manner the equivalence. In Sec. III we exploit the case of a spin-$\frac{1}{2}$ particle in a two-component magnetic field with a time-varying component. The equations so obtained are applied to a constant perturbation and a time-varying one with a linear law. The spin motion is also described, obtaining the correction to first order. Section IV gives the conclusions.

II. METHOD

We consider a Hamiltonian that is time independent and write down the Schrödinger equation

$$(H_0+V)\psi=i\hbar\frac{\partial\psi}{\partial t}\ , \tag{1}$$

where the choice of H_0 and V is done as it would be in the interaction picture. Then we put

$$\psi=e^{-(i/\hbar)Vt}\psi_F \tag{2}$$

and substitute in Eq. (1) to obtain

$$H_{0F}\psi_F=i\hbar\frac{\partial\psi_F}{\partial t}\ , \tag{3}$$

with

$$H_{0F}=e^{(i/\hbar)Vt}H_0e^{-(i/\hbar)Vt}\ . \tag{4}$$

The time-evolution operator U is defined so that

$$\psi_F(t)=U(t,t_0)\psi_F(t_0) \tag{5}$$

and

$$H_{0F}U=i\hbar\frac{\partial U}{\partial t}\ , \tag{6}$$

with the initial condition

$$U(t_0,t_0)=I, \tag{7}$$

where I is the identity operator. Equation (6) has the formal solution

$$U(t,t_0)=I-\frac{i}{\hbar}\int_{t_0}^{t}dt_1H_{0F}(t_1)+\left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2H_{0F}(t_1)H_{0F}(t_2)+\cdots\ . \tag{8}$$

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If $T(t,t_0)$ is the time-evolution operator in the Schrödinger picture, the following relation is verified:

$$T(t,t_0)=e^{-(i/\hbar)Vt}U(t,t_0)e^{(i/\hbar)Vt_0} . \tag{9}$$

In this representation we have the result that states evolve because of the free Hamiltonian [Eq. (3)] and that operators evolve because of the perturbation [Eq. (4)]. Equations (8) and (9) give the perturbation series in the Schrödinger picture.

Now we show that Eqs. (8) and (9) form an asymptotic series for Eq. (1). In order to accomplish our aims, we introduce a parameter ε and take V to be time dependent, so that we may rewrite Eq. (1) as

$$[H_0+\varepsilon V(t)]\psi=i\hbar\frac{\partial\psi}{\partial t} , \tag{10}$$

and we look for a solution of the form

$$\psi=\psi^{(0)}+\frac{1}{\varepsilon}\psi^{(1)}+\frac{1}{\varepsilon^2}\psi^{(2)}+\cdots . \tag{11}$$

A direct substitution of Eq. (11) in Eq. (10) does not give meaningful results. A way out of this problem is gained by redefining the time scale as

$$\tilde{t}=\varepsilon t , \tag{12}$$

so that

$$(H_0+\varepsilon V)\left[\psi^{(0)}+\frac{1}{\varepsilon}\psi^{(1)}+\frac{1}{\varepsilon^2}\psi^{(2)}+\cdots\right]=i\hbar\varepsilon\frac{\partial}{\partial\tilde{t}}\left[\psi^{(0)}+\frac{1}{\varepsilon}\psi^{(1)}+\frac{1}{\varepsilon^2}\psi^{(2)}+\cdots\right] . \tag{13}$$

By comparing, order by order, the following set of equations is obtained:

$$V\psi^{(0)}=i\hbar\frac{\partial\psi^{(0)}}{\partial\tilde{t}} , \tag{14}$$

$$H_0\psi^{(0)}+V\psi^{(1)}=i\hbar\frac{\partial\psi^{(1)}}{\partial\tilde{t}} , \tag{15}$$

$$H_0\psi^{(1)}+V\psi^{(2)}=i\hbar\frac{\partial\psi^{(2)}}{\partial\tilde{t}} , \tag{16}$$

$$\vdots$$

$$H_0\psi^{(k-1)}+V\psi^{(k)}=i\hbar\frac{\partial\psi^{(k)}}{\partial\tilde{t}} . \tag{17}$$

For the sake of simplicity, we assume that

$$[V(t),V(t')]=0 , \tag{18}$$

so that we can write the formal solution of the set as

$$\psi^{(0)}=T_0(\tilde{t},\tilde{t}_0)\psi(\tilde{t}_0) , \tag{19}$$

$$\psi^{(1)}=-\frac{i}{\hbar}T_0(\tilde{t},\tilde{t}_0)\int_{\tilde{t}_0}^{\tilde{t}}dt_1H_0'(t_1)\psi(\tilde{t}_0) , \tag{20}$$

$$\psi^{(2)}=\left[-\frac{i}{\hbar}\right]^2T_0(\tilde{t},\tilde{t}_0)\times\int_{\tilde{t}_0}^{\tilde{t}}dt_1\int_{\tilde{t}_0}^{t_1}dt_2H_0'(t_1)H_0'(t_2)\psi(\tilde{t}_0) , \tag{21}$$

$$\vdots$$

where

$$T_0(\tilde{t},\tilde{t}_0)=\exp\left[-\frac{i}{\hbar}\int_{\tilde{t}_0}^{\tilde{t}}dt'V\left[\frac{\tilde{t}}{\varepsilon}\right]\right] \tag{22}$$

and

$$H_0'(\tilde{t})=T_0(\tilde{t},\tilde{t}_0)^{-1}H_0T_0(\tilde{t},\tilde{t}_0) . \tag{23}$$

For V independent of time and $\varepsilon=1$, we get complete coincidence with Eqs. (8) and (9). The need for a time-dependent perturbation will be shown in the following.

III. APPLICATIONS

In order to show the properties of this kind of approximation, we derive the wave function for the case of a spin-$\frac{1}{2}$ particle in a magnetic field with two components, one of which is time varying. We take

$$H_0=\sigma_3\Omega_3 \tag{24}$$

and, for the perturbation,

$$V(t)=\sigma_1\Omega_1(t) , \tag{25}$$

where σ_i are the Pauli matrices with $i=1,2,3$.

It easily verified that

$$T_0(\tilde{t},\tilde{t}_0)=I\cos\left[\frac{\theta(\tilde{t})}{2}\right]-i\sigma_1\sin\left[\frac{\theta(\tilde{t})}{2}\right] , \tag{26}$$

where

$$\theta(\tilde{t})=\frac{2}{\hbar}\int_{\tilde{t}_0}^{\tilde{t}}dt'\Omega_1\left[\frac{t'}{\varepsilon}\right] . \tag{27}$$

The unperturbed Hamiltonian is [Eq. (23)]

$$H_0'(\tilde{t})=\Omega_3\{\sigma_3\cos[\theta(\tilde{t})]+\sigma_2\sin[\theta(\tilde{t})]\} , \tag{28}$$

from which we derive the first three terms of the perturbation series [Eqs. (19)–(21)] that can be cast in the form

$$\psi^{(0)}=\left[I\cos\left[\frac{\theta(\tilde{t})}{2}\right]-i\sigma_1\sin\left[\frac{\theta(\tilde{t})}{2}\right]\right]\psi(\tilde{t}_0) , \tag{29}$$

$$\psi^{(1)}=-\frac{i}{\hbar}\Omega_3\int_{\tilde{t}_0}^{\tilde{t}}dt_1\left[\sigma_3\cos\left[\theta(t_1)-\frac{\theta(\tilde{t})}{2}\right]+\sigma_2\sin\left[\theta(t_1)-\frac{\theta(\tilde{t})}{2}\right]\right]\psi(\tilde{t}_0) , \tag{30}$$

$$\psi^{(2)}=\left[-\frac{i}{\hbar}\Omega_3\right]^2\int_{\tilde{t}_0}^{\tilde{t}}dt_1\int_{\tilde{t}_0}^{t_1}dt_2\left[I\cos\left[\theta(t_1)-\theta(t_2)-\frac{\theta(\tilde{t})}{2}\right]+i\sigma_1\sin\left[\theta(t_1)-\theta(t_2)-\frac{\theta(\tilde{t})}{2}\right]\right]\psi(\tilde{t}_0)\ , \tag{31}$$

$$\vdots$$

It is easily seen from Eq. (29) that a particle in a strong magnetic field undergoes always Rabi flopping in the leading term of this approximation. The time scale of the flopping is determined by the perturbation.

A. Constant perturbation

The aim of this almost trivial example is to show that the correct asymptotic expansion can be obtained by working out the preceding equations in a specific case and comparing them with the exact solution. For this model we take Ω_1 to be time independent in Eq. (25). Choosing $t_0=0$, the solution for this problem is obtained from the time-evolution operator

$$T(t,0)=I\cos\left[\frac{\Omega}{\hbar}t\right]-i\left[\frac{\Omega_3}{\Omega}\sigma_3+\frac{\Omega_1}{\Omega}\sigma_1\right]\sin\left[\frac{\Omega}{\hbar}t\right]\ , \tag{32}$$

with

$$\Omega=(\Omega_1^2+\Omega_3^2)^{1/2}\ . \tag{33}$$

From Eqs. (29)–(31) we get

$$\psi^{(0)}=\left[\cos\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]-i\sigma_1\sin\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]\right]\psi(0)\ , \tag{34}$$

$$\psi^{(1)}=-i\frac{\Omega_3}{\Omega_1}\sigma_3\sin\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]\psi(0)\ , \tag{35}$$

$$\psi^{(2)}=-\frac{\Omega_3^2}{2\hbar\Omega_1}\left\{I\tilde{t}\sin\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]+i\sigma_1\left[\tilde{t}\cos\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]-\frac{\hbar}{\Omega_1}\sin\left[\frac{\Omega_1}{\hbar}\tilde{t}\right]\right]\right\}\psi(0)\ , \tag{36}$$

which agree with Eq. (32) when the approximation $\Omega_3/\Omega_1\ll 1$ is made. This series is of no use for $t\to\infty$, as mixed-secular terms appear. In this limit we need to resort to the exact solution.

B. Linear time-varying perturbation

We consider a perturbation of the form

$$\Omega_1(t)=\alpha t\ . \tag{37}$$

A similar Hamiltonian has been considered in the Landau-Zener theory [7,8] and provides a simple model in some NMR experiments, for example. Here we take the strong-field approximation in order to see the asymptotic development of the wave function.

Taking $t_0=0$, we obtain, from Eqs. (29)–(31),

$$\psi^{(0)}=\left[I\cos\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]-i\sigma_1\sin\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]\right]\psi(0)\ , \tag{38}$$

$$\psi^{(1)}=-i\left[\varepsilon\frac{\Omega_3^2}{\hbar\alpha}\right]^{1/2}[\sigma_2\mathcal{F}_1(\tilde{t})+\sigma_3\mathcal{G}_1(\tilde{t})]\psi(0)\ , \tag{39}$$

$$\psi^{(2)}=-\left[\varepsilon\frac{\Omega_3^2}{\hbar\alpha}\right][I\mathcal{F}_2(\tilde{t})-i\sigma_1\mathcal{G}_2(\tilde{t})]\psi(0)\ , \tag{40}$$

with

$$\mathcal{F}_1(\tilde{t})=S\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\cos\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]-C\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\sin\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]\ , \tag{41}$$

$$\mathcal{G}_1(\tilde{t})=C\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\cos\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]+S\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\sin\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]\ , \tag{42}$$

C and S being the Fresnel integrals defined by

$$C(ax)=\int_0^{ax}dz\cos(z^2)\ , \tag{43}$$

$$S(ax)=\int_0^{ax}dz\sin(z^2)\ , \tag{44}$$

where a is a generic constant. Moreover, we have

$$\mathcal{F}_2(\tilde{t})=\mathcal{J}_1\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\cos\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]-\mathcal{J}_2\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\sin\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]\ , \tag{45}$$

$$\mathcal{G}_2(\tilde{t})=\mathcal{J}_2\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\cos\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]+\mathcal{J}_1\left[\left[\frac{\alpha}{\varepsilon\hbar}\right]^{1/2}\tilde{t}\right]\sin\left[\frac{\alpha\tilde{t}^2}{2\varepsilon\hbar}\right]\ , \tag{46}$$

with the functions $\mathcal{J}_1$ and $\mathcal{J}_2$ defined as

$$\mathcal{J}_1(ax)=\int_0^{ax}dz\,[C(z)\cos(z^2)+S(z)\sin(z^2)]\ , \tag{47}$$

$$\mathcal{J}_2(ax)=\int_0^{ax}dz\,[S(z)\cos(z^2)-C(z)\sin(z^2)]\ . \tag{48}$$

Two considerations are in order. First, it is easily verified that the limit $t\to\infty$ is meaningful for C, S, $\mathcal{J}_1$, and $\mathcal{J}_2$. Second, the series for the wave function is not analytical as the development parameter goes like $1/\alpha^{1/2}$ and we have a series

$$\psi \sim \psi^{(0)} + \left[\frac{\Omega_3^2}{\hbar\alpha}\right]^{1/2} \psi^{(1)} + \left[\frac{\Omega_3^2}{\hbar\alpha}\right] \psi^{(2)} + \cdots . \quad (49)$$

A last note should be done on the development parameter that appears to be the same as the one characterizing the transition probability in Landau-Zener theory [9]. The experimental implementation of Hamiltonians of this kind is described in Ref. [9].

C. Motion of spin in a strong magnetic field

The method outlined here provides some insights into the physics of spin motion in a strong magnetic field. In order to make the discussion clear, we choose $t_0 = 0$, $\varepsilon = 1$, and take

$$\psi(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} . \quad (50)$$

From Eq. (29), it is easily realized that

$$\langle \sigma_1 \rangle = 0 , \quad (51)$$

$$\langle \sigma_2 \rangle = -\sin\theta , \quad (52)$$

and

$$\langle \sigma_3 \rangle = \cos\theta , \quad (53)$$

showing that, at order 0, the component of the spin along the perturbation is 0, while the other two components describe a circle of unity radius on a plane orthogonal to the first. This should be expected from Eq. (14) as the unperturbed part of the Hamiltonian plays no role.

The first-order term gives

$$\langle \sigma_1 \rangle = \frac{2\Omega_3}{\hbar} \int_0^t dt' \sin[\theta(t')] , \quad (54)$$

while for the other two components, we have higher-order corrections. So we get $\langle \sigma_1 \rangle \neq 0$ and varying in time. Such a small secular effect could be revealed in some NMR experiments.

IV. CONCLUSIONS

We showed that the Schrödinger equation may have an asymptotic-series solution that describes situations with a strong perturbation applied to a quantum system. Such a perturbation series derives also from a picture defined as the interaction picture where the roles of the free Hamiltonian and the perturbation are reversed. The direct application to a spin-$\frac{1}{2}$ particle in a magnetic field has shown that the series could not be uniformly convergent and, depending on the form of the perturbation, also not analytical in the development parameter. In this paper we gave just an example of the applicability of this approximation, but great utility should be expected in the analysis of quantum analogs of chaotic classical Hamiltonians where it is known that strong perturbations come into play and that the standard perturbation theory is of no use. This question is definitely open. The same could be said whenever standard perturbation theory breaks down. If some useful generalization to field theory could be found, an analysis of the asymptotic behavior of the S matrix with strong-coupling constants could be done.

[1] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), pp. 472ff.
[2] P. A. M. Dirac, Proc. R. Soc. London A **112**, 661 (1926).
[3] P. A. M. Dirac, Proc. R. Soc. London A **113**, 621 (1927).
[4] P. A. M. Dirac, Proc. R. Soc. London A **114**, 243 (1927).
[5] T. D. Lee, *Particle Physics and Introduction to Field Theory* (Harwood Academic, New York, 1990), Chap. 5.
[6] J. Kevorkian and J. D. Cole, *Perturbation Methods in Applied Mathematics* (Springer-Verlag, New York, 1985), Chaps. 1 and 2.
[7] N. Rosen and C. Zener, Phys. Rev. **40**, 502 (1932).
[8] C. Zener, Proc. R. Soc. London A **137**, 696 (1932).
[9] J. W. Zwanziger, S. P. Rucker, and G. C. Chingas, Phys. Rev. A **43**, 3232 (1991).