Quantum adiabatic approximation and the geometric phase

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(Received 11 June 1996; revised manuscript received 21 October 1996)

A precise definition of an adiabaticity parameter ν of a time-dependent Hamiltonian is proposed. A variation of the time-dependent perturbation theory is presented which yields a series expansion of the evolution operator $U(\tau)=\Sigma_{\ell} U^{(\ell)}(\tau)$ with $U^{(\ell)}(\tau)$ being at least of the order ν^{ℓ}. In particular, $U^{(0)}(\tau)$ corresponds to the adiabatic approximation and yields Berry's adiabatic phase. It is shown that this series expansion has nothing to do with the $1/\tau$ expansion of $U(\tau)$. It is also shown that the nonadiabatic part of the evolution operator is generated by a transformed Hamiltonian which is off-diagonal in the eigenbasis of the initial Hamiltonian. This suggests the introduction of an adiabatic product expansion for $U(\tau)$ which turns out to yield exact expressions for $U(\tau)$ for a large number of quantum systems. In particular, a simple application of the adiabatic product expansion is used to show that for the Hamiltonian describing the dynamics of a magnetic dipole in an arbitrarily changing magnetic field, there exists another Hamiltonian with the same eigenvectors for which the Schrödinger equation is exactly solvable. Some related issues concerning geometric phases and their physical significance are also discussed. [S1050-2947(97)00303-X]

PACS number(s): 03.65.Bz

I. INTRODUCTION

Since the introduction of the adiabatic geometrical phase by Berry [1], the study of the cyclic evolution of quantum states of nonconservative quantum systems (explicitly, time-dependent Hamiltonians) has attracted much attention. By definition, a pure cyclic state $|\mathcal{N};\tau\rangle\langle\mathcal{N};\tau|$ is an eigenstate of the evolution operator $U(\tau)$, i.e.,

$$U(\tau)=:\sum_{\mathcal{N}} e^{i\beta_{\mathcal{N}}(\tau)}|\mathcal{N};\tau\rangle\langle\mathcal{N};\tau|,\beta_{\mathcal{N}}(\tau)\in[0,2\pi). \quad (1)$$

Therefore, the quantity of main importance in the study of cyclic states and the accompanying phases $\beta_{\mathcal{N}}(\tau)$ is the evolution operator $U(\tau)$. This operator is defined by

$$|\psi(\tau)\rangle=:U(\tau)|\psi(0)\rangle, \quad (2)$$

where $|\psi(\tau)\rangle$ is the solution of the Schrödinger equation. Alternatively, one can define $U(\tau)$ as the solution of

$$\frac{d}{d\tau}U(\tau)=-\frac{i}{\hbar}H(\tau)U(\tau), \quad U(0)=1, \quad (3)$$

where $H=H(\tau)$ stands for the Hamiltonian and $\tau\in[0,\infty)$ parametrizes the time. The solution of Eq. (3) can be implicitly expressed in the form

$$U(\tau):=\mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^{\tau}H(t)dt\right), \quad (4)$$

where $\mathcal{T}$ denotes the time-ordering operator [2].

The purpose of this article is threefold. First, a precise definition of an *adiabaticity parameter* ν is given. This is a parameter that quantifies the rapidity of the time dependence of the Hamiltonian. Next, a series expansion of the evolution operator $U(\tau)$ is proposed whose ℓth term is at least of the order ν^{ℓ}. Finally, an adiabatic product expansion of $U(\tau)$ is introduced. In particular, the adiabatic approximation:

$$U(\tau)\approx\sum_n e^{i\alpha_n(\tau)}|n;\tau\rangle\langle n;0| \quad (5)$$

is recovered as the first term in both the series and the product expansions. In Eq. (5), $|n;t\rangle$ are the instantaneous eigenstate vectors of the Hamiltonian, i.e.,

$$H(t)|n;t\rangle=E_n(t)|n;t\rangle, \quad (6)$$

and

$$\alpha_n(t):=\delta_n(t)+\gamma_n(t),$$

$$\delta_n(t):=-\frac{1}{\hbar}\int_0^t E_n(t')dt',$$

$$\gamma_n(t):=i\int_0^t\left\langle n;t'\left|\frac{d}{dt'}\right|n;t'\right\rangle dt'. \quad (7)$$

If the Hamiltonian is T periodical, i.e., $H(T+t)=H(t)$, then $\alpha_n(T)$, $\delta_n(T)$, and $\gamma_n(T)$ are called *adiabatic total phase angle*, *adiabatic dynamical phase angle*, and *adiabatic geometrical phase* or *Berry phase angle*, respectively [1].

The quantum adiabatic approximation was discovered by Born and Fock in 1928 [4]. The geometric phase effects, which were later noticed by Mead and Truhlar [5] and Berry [1], were not included in the traditional approach of Born and Fock. This approach forms the basis of the discussion of the quantum adiabatic approximation in standard textbooks in quantum mechanics [6,7]. In 1950, a mathematically more rigorous treatment of the adiabatic approximation was given

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by Kato [8] whose results have since been used to improve and generalize the adiabatic approximation, [9–15].

The approach pursued in this article may be viewed as a variation of the traditional adiabatic approximation that includes the geometric phase effects by construction. It also clarifies the possible misconception that the adiabatic approximation of $U(\tau)$ is given by the zeroth order term in its $1/\tau$ expansion, i.e., it is only valid for $\tau\to\infty$. Here I do not mean to imply that there is a widespread misconception in the physics community about the conditions under which the adiabatic approximation is valid. However, it is necessary to emphasize the distinction between the role of the large τ limit used in the proof of the adiabatic theorem [8] and the (sufficient and necessary) conditions under which the adiabatic approximation is valid.

Furthermore, the results presented here provide a convenient framework for a perturbative computation of the nonadiabatic corrections to Berry's adiabatic phase. A perturbative scheme to improve the adiabatic geometric phase has been proposed by Berry [16]. Although the methods used by Berry in [16] are similar to some of those employed here, Berry's scheme does not seem to be related to the present analysis.

Probably the most important implication of the approach pursued in this article is the introduction of an adiabatic product expansion for the evolution operator $U(\tau)$. This expansion provides an alternative generalization of the adiabatic approximation which is nonperturbative in nature. One of the immediate consequences of the adiabatic product expansion is the identification of a large number of exactly solvable quantum systems.

This paper is organized as follows. Sec. II provides a brief discussion of the adiabaticity parameter. Section III includes a thorough treatment of the evolution operator that differs with those of the existing literature [4,8–15]. Section IV reveals the role of time-dependent unitary transformations of the Hilbert space in relating the generator of the nonadiabatic part of the evolution operator to the Hamiltonian. Section V uses these transformations to derive the nonadiabatic geometric phase associated with periodic Hamiltonians. Here the physical significance of the dynamical, geometrical, and total phases is also discussed. Specifically, it is shown that it is the differences of the total phases which enter into the calculation of the physical observables. Section VI demonstrates the application of the adiabatic series expansion for a magnetic dipole in a rotating magnetic field. In particular, the first-order nonadiabatic term in the adiabatic series expansion is explicitly calculated for a nutating magnetic field. Section VII introduces the adiabatic product expansion and gives its general properties. The application of this expansion for a dipole in a changing magnetic field is also demonstrated. In particular, it is shown how this expansion can be used to obtain exactly solvable models. Finally, Sec. VIII includes the concluding remarks.

II. THE ADIABATICITY PARAMETER

Following Berry [1], consider a parameter-dependent Hamiltonian:

$$H[R]=\sum_n E_n[R]|n;R\rangle\langle n;R|, \tag{8}$$

where $R=(R^1,\cdots,R^d)$ are real parameters viewed as the coordinates of a parameter space $\mathcal{M}$, $E_n[R]$ are the real eigenvalues, and $\{|n;R\rangle\}$ is a complete orthonormal set of eigenvectors of $H[R]$. In this case, a time-dependent Hamiltonian $H(t)$ corresponds to a curve $C:[0,\tau]\to\mathcal{M}$ in $\mathcal{M}$:

$$H(t):=H[C(t)]=H[R_C(t)],$$

$$\text{with}\quad C(t)=:(R_C^1(t),\cdots,R_C^d(t))=:R_C(t).$$

Furthermore, suppose that the spectrum of $H[R]$ for all $R\in\mathcal{M}$ is discrete, the energy eigenvalues $E_n[R]$ are nondegenerate, and there is no level crossing, i.e., for every $t\in[0,\tau]$, $E_n[R_C(t)]<E_{n+1}[R_C(t)]$.

In order to define a dimensionless adiabaticity parameter, first one defines a *characteristic frequency*:

$$\omega_c(\tau_1,\tau_2):=\text{Sup}\{|A_{mn}(t)|:n\neq m=0,1,\ldots,t\in[\tau_1,\tau_2]\};$$

$$[\tau_1,\tau_2]\subseteq[0,\tau], \tag{9}$$

with Sup denoting supremum (least upper bound) and

$$A_{mn}(t):=\left\langle m;t\left|\frac{d}{dt}\right|n;t\right\rangle \tag{10}$$

$$=\frac{\left\langle m;t\left|\left[\frac{d}{dt}H(t)\right]\right|n;t\right\rangle}{E_n(t)-E_m(t)},\quad \text{for}\quad m\neq n. \tag{11}$$

Then the desired *adiabaticity parameter* is defined according to

$$\nu:=\frac{\hbar\,\omega_c(0,\tau)}{\Delta E}, \tag{12}$$

where ΔE is a convenient energy scale. For example, one can take ΔE to be the first transition energy of the initial Hamiltonian, i.e., $\Delta E:=E_1(0)-E_0(0)$.

The main motivation for this definition is the fact that according to Eqs. (9), (11), and (12), $\omega_c(0,\tau)$ and therefore ν involve time derivatives of the Hamiltonian $H(t)$. The use of $\omega_c(0,\tau)$ in the definition of the adiabaticity parameter will be self-evident once one examines the evolution operator. The role of ΔE is to provide a convenient energy ($\hbar\times$frequency) scale

It must also be emphasized that by definition, ν is a ''global'' quantity that characterizes the time-dependence of the Hamiltonian. In particular, it is neither equal nor proportional to $1/\tau$. Furthermore, note that although $|n;t\rangle$ are only determined up to arbitrary $R_C(t)$-dependent phase factors (gauge transformations along C [2]), $|A_{mn}(t)|$ with $m\neq n$ and therefore $\omega_c(\tau_1,\tau_2)$ and ν are independent of the choice of such phases (they are gauge-invariant quantities). In other words, ν is well defined.

III. COMPUTATION OF $U(\tau)$

Consider the definition of the time-ordered product in (4):

$$U(\tau):=\lim_{N\to\infty}\left[1-\frac{i}{\hbar}H(t_N)\epsilon\right]\cdots\left[1-\frac{i}{\hbar}H(t_k)\epsilon\right]\cdots\left[1-\frac{i}{\hbar}H(t_0)\epsilon\right], \tag{13}$$

where $\epsilon:=\tau/N$ and $t_k:=k\epsilon$, for $k=0,1,\cdots N$. Using the orthonormality and completeness of the energy eigenvectors $|n;t\rangle$, one can compute

$$\begin{aligned}U(\tau)&=\lim_{N\to\infty}\sum_{n_0,\cdots,n_N}\left\{|n_N;t_N\rangle\langle n_N;t_N|\left[1-\frac{i}{\hbar}H(t_N)\epsilon\right]|n_{N-1};t_{N-1}\rangle\langle n_{N-1};t_{N-1}|\cdots|n_k;t_k\rangle\right.\\&\left.\times\langle n_k;t_k|\left[1-\frac{i}{\hbar}H(t_k)\epsilon\right]|n_{k-1};t_{k-1}\rangle\langle n_{k-1};t_{k-1}|\cdots|n_1;t_1\rangle\langle n_1;t_1|\left[1-\frac{i}{\hbar}H(t_0)\epsilon\right]|n_0;t_0\rangle\langle n_0;t_0|\right\},\\&=\lim_{N\to\infty}\sum_{n_0,\cdots,n_N}\left\{\exp\left[-(i/\hbar)\sum_{j=0}^{N}E_{n_j}(t_j)\epsilon\right]\prod_{k=1}^{N}\langle n_k;t_k|n_{k-1};t_{k-1}\rangle\right\}|n_N;t_N\rangle\langle n_0;t_0|.\end{aligned}$$

Introducing

$$\begin{aligned}K_{n_Nn_0}(\tau)&:=\langle n_N;\tau|U(\tau)|n_0;0\rangle\\&=\lim_{N\to\infty}\sum_{n_1,\cdots,n_{N-1}}\exp\left[-(i/\hbar)\sum_{j=1}^{N-1}E_{n_j}(t_j)\epsilon\right]\prod_{k=1}^{N}\langle n_k;t_k|n_{k-1};t_{k-1}\rangle,\end{aligned} \tag{14}$$

one then has

$$U(\tau)=\sum_{mn}K_{mn}(\tau)|m;\tau\rangle\langle n;0|. \tag{15}$$

The computation of the terms in the product in Eq. (14) is straightforward:

$$\begin{aligned}\langle n_k;t_k|n_{k-1};t_{k-1}\rangle&=\delta_{n_kn_{k-1}}-\epsilon\left\langle n_k;t\left|\frac{d}{dt}\right|n_{k-1};t\right\rangle\Big|_{t=t_{k-1}}+\mathcal{O}(\epsilon^2),\\&=e^{-\epsilon A_{n_kn_{k-1}}(t_{k-1})}\delta_{n_kn_{k-1}}+\epsilon\Delta_{n_kn_{k-1}}(t_{k-1})+\mathcal{O}(\epsilon^2),\\&=e^{-\epsilon A_{n_kn_k}(t_k)}[\,\delta_{n_kn_{k-1}}+\epsilon e^{\epsilon A_{n_kn_k}(t_k)}\Delta_{n_kn_{k-1}}(t_k)\,]+\mathcal{O}(\epsilon^2).\end{aligned} \tag{16}$$

Here

$$\Delta_{mn}(t):=(\delta_{mn}-1)A_{mn}(t). \tag{17}$$

Substituting Eq. (16) in Eq. (14), one obtains 2^N terms which can be arranged in the order of the appearance of different powers of ϵ. In this way one finds only N terms of order $\epsilon^0=1$.[1] These will be denoted by $K^{(\ell)}_{mn}(\tau)$:

$$K_{mn}(\tau)=\lim_{N\to\infty}\sum_{\ell=0}^{N}K^{(\ell)}_{mn}(\tau). \tag{18}$$

Performing the algebra, one finds

[1]Note that a sum of N^ℓ terms of order ϵ^ℓ is of order $\epsilon^0=1$.

$$K^{(\ell)}_{n_N n_0}(\tau) := \sum_{n_1 \cdots n_{N-1}} \sum_{t_{i_1} < \cdots < t_{i_\ell} = 0}^{\tau} \epsilon^{\ell} \Bigg[\exp\Bigg(\frac{i}{\hbar} \sum_{j=1}^{N} [-E_{n_j}(t_j) + i\hbar A_{n_j n_j}(t_j)] \epsilon \Bigg) \delta_{n_0 n_1} \cdots \delta_{n_{i_1-2} n_{i_1-1}} e^{\epsilon A_{n_{i_1} n_{i_1}}(t_{i_1})} \Delta_{n_{i_1} n_{i_1-1}}(t_{i_1})$$

$$\times \delta_{n_{i_1} n_{i_1+1}} \cdots \delta_{n_{i_\ell-2} n_{i_\ell-1}} e^{\epsilon A_{n_{i_\ell} n_{i_\ell}}(t_{i_\ell})} \Delta_{n_{i_\ell} n_{i_\ell-1}}(t_{i_\ell}) \delta_{n_{i_\ell} n_{I_\ell+1}} \cdots \delta_{n_{N-1} n_N} \Bigg] + \mathcal{O}(\epsilon), \tag{19}$$

where $\ell = 0,1,\cdots,N$ and $t_k = k\epsilon/N = 0,\epsilon,\cdots,\tau$. In particular,

$$K^{(0)}_{n_N n_0}(\tau) = \Gamma_{n_N}(\tau)\,\delta_{n_N n_0} + \mathcal{O}(\epsilon), \tag{20}$$

$$K^{(1)}_{n_N n_0}(\tau) = -\frac{i}{\hbar}\Gamma_{n_N}(\tau) \sum_{t_i = t_j}^{t_k} \epsilon H'_{n_N n_0}(t_i) + \mathcal{O}(\epsilon),$$

$$= -\frac{i}{\hbar} \sum_m \left[K^{(0)}_{n_N m}(\tau) \sum_{t_i=0}^{\tau} \epsilon H'_{m n_0}(t_i) \right] + \mathcal{O}(\epsilon), \tag{21}$$

where

$$\Gamma_n(t_k) := \exp\Bigg(i/\hbar \sum_{t_j=0}^{t_k} [-E_n(t_j) + i\hbar A_{nn}(t_j)] \epsilon \Bigg), \tag{22}$$

$$H'_{mn}(t_k) := i\hbar \Gamma^*_m(t_k) \Delta_{mn}(t_k) \Gamma_n(t_k), \tag{23}$$

and $\Gamma^*_m(t_k) = 1/\Gamma_m(t_k)$ is the complex conjugate of $\Gamma_m(t_k)$.

Furthermore, for every $\ell > 1$, one can express $K^{(\ell)}_{mn}(\tau)$ in terms of $K^{(0)}_{mn}(\tau)$ and $H'_{mn}(t_i)$, namely,

$$K^{(\ell)}_{m m_\ell}(\tau) = \left(\frac{-i}{\hbar} \right)^{\ell} \sum_{t_{i_1} < \cdots < t_{i_\ell} = 0}^{\tau} \epsilon^{\ell} \sum_{m_0 \cdots m_{\ell-1}} K^{(0)}_{m m_0}(\tau)$$

$$\times \left[\prod_{a=1}^{\ell} H'_{m_{a-1} m_a}(t_{i_a}) \right] + \mathcal{O}(\epsilon),$$

$$= \frac{1}{\ell!} \left(\frac{-i}{\hbar} \right)^{\ell} \sum_{m_0 \cdots m_{\ell-1}} K^{(0)}_{m m_0}(\tau)$$

$$\times \sum_{t_{i_1} \cdots t_{i_\ell} = 0}^{\tau} \epsilon^{\ell} \mathcal{T} \left[\prod_{a=1}^{\ell} H'_{m_{a-1} m_a}(t_{i_a}) \right] + \mathcal{O}(\epsilon). \tag{24}$$

Therefore, if one defines

$$U^{(\ell)}(\tau) := \lim_{N \to \infty} \sum_{mn} K^{(\ell)}_{mn}(\tau) |m;\tau\rangle\langle n;0|, \tag{25}$$

$$H'(t) := \lim_{N \to \infty} \sum_{mn} H'_{mn}(t) |m;0\rangle\langle n;0|,$$

$$= i\hbar \sum_{mn} e^{-i[\alpha_m(t) - \alpha_n(t)]} \Delta_{mn}(t) |m;0\rangle\langle n;0|,$$

$$= -i\hbar \sum_{m \neq n} e^{-i[\alpha_m(t) - \alpha_n(t)]} A_{mn}(t) |m;0\rangle\langle n;0|, \tag{26}$$

then

$$U(\tau) = \sum_{\ell=0}^{\infty} U^{(\ell)}(\tau) = U^{(0)}(\tau) [\mathcal{T} e^{-(i/\hbar)\int_0^\tau dt H'(t)}], \tag{27}$$

where by taking $N \to \infty$ the sums of the form $\Sigma_{t_i = t}^{t'} \epsilon f(t_i)$ have been promoted to the integrals $\int_t^{t'} dt f(t)$. In particular, one has

$$U^{(0)}(\tau) = \sum_n e^{i\alpha_n(\tau)} |n;\tau\rangle\langle n;0|, \tag{28}$$

$$U^{(1)}(\tau) = U^{(0)}(\tau) \left[\frac{-i}{\hbar} \int_0^\tau dt H'(t) \right]. \tag{29}$$

By construction, $U^{(0)}(\tau)$ yields $U(\tau)$ in the adiabatic approximation (5).Therefore, adiabatic approximation is valid only if one can neglect $\int_o^\tau dt H'(t)$ in Eq. (27). It is not difficult to observe that this condition is fulfilled if the adiabaticity parameter ν as defined by Eq. (12) is negligible. In fact, for every t_1 and t_2 satisfying $0 \leq t_1 \leq t_2 \leq \tau$, one has

$$\left| \langle m;0| \int_{t_1}^{t_2} dt H'(t) |n;0\rangle \right| \leq \int_{t_1}^{t_2} dt |\langle m;0|H'(t)|n;0\rangle|$$

$$\leq \hbar \int_{t_1}^{t_2} dt |A_{mn}(t)| \leq \Delta\tau \Delta E \nu, \tag{30}$$

where $\Delta\tau := \tau_2 - \tau_1$ with $[\tau_1, \tau_2] \subseteq [0,\tau]$ is the time interval over which ω_c is nonvanishing, i.e., τ_1 and τ_2 and therefore $\Delta\tau$ are defined by the condition

$$\omega_c(\tau'_1, \tau'_2) = 0 \text{ if and only if } \tau'_2 < \tau_1 \text{ or } \tau'_1 > \tau_2. \tag{31}$$

Note that usually $\Delta\tau$ is a finite time interval whereas τ may be infinite (arbitrarily large). A case for which $\Delta\tau = \tau$ is when the Hamiltonian depends periodically on time. In this case, however, the physically interesting features of the evo-

lution is given by $\Delta\tau=\tau\ll T$, where T is the period of the Hamiltonian. Particularly interesting is the case $\tau=T$.

In general, $\Delta\tau$ may become arbitrarily large, in which case Eq. (30) is a trivial statement. However, even in this case ν plays a most important role. In fact, one can argue that in general the following relation holds:

$$U(\tau)=\sum_{\ell=0}^{N-1} U^{(\ell)}(\tau)+\mathcal{O}(\nu^N). \tag{32}$$

In particular, the adiabatic approximation is valid if and only if $\nu\ll 1$. In order to establish Eq. (32), it is sufficient[2] to show that $U^{(1)}(\tau)$ and therefore $\int dt H'(t)$ are at least of order ν. This is, however, self-evident, since one knows that if $\nu=0$, then $U(\tau)=U^{(0)}(\tau)$. Consequently, in a ν expansion of $U(\tau)$, $U^{(1)}(\tau)$ is necessarily of order ν or higher.

An alternative way of expressing Eq. (32) is to define $\tilde{U}^{(\ell)}(\tau):=U^{(\ell)}(\tau)/\nu^{\ell}$ and $\tilde{H}'(\tau):=H'(\tau)/\nu$ and write $U(\tau)$ in the form

$$U(\tau)=\sum_{\ell=0}^{\infty} \tilde{U}^{(\ell)}(\tau)\nu^{\ell}=U^{(0)}(\tau)[\mathcal{T}e^{-(i\nu/\hbar)\int_0^\tau dt\tilde{H}'(t)}]. \tag{33}$$

This equation must not, however, be viewed as a true power series expansion of $U(\tau)$ in ν, for $\tilde{U}^{(\ell)}(\tau)$ may in general depend on ν.

A simple consequence of Eq. (33) is the fact that the essential ingredient that determines $U(\tau)$ beyond the adiabatic approximation is not τ, but (τ_1,τ_2) of Eq. (31) and ν. For physically realistic nonperiodic Hamiltonians, the latter quantities take finite values, whereas the duration τ of the evolution of the system may be arbitrarily large. For a quantum system with a periodic Hamiltonian $H(t)=H(t+T)$, the physically interesting case is when $\tau_2=\tau\ll T$. In this case, ν may or may not be determined by T. This is because, in general, the parameters $R_C^\mu(t)$ of the Hamiltonian have different periods. These are necessarily of the form $T_\mu=T/z_\mu$, respectively, where z_μ is a positive integer. Clearly, $\omega_c(0,\tau)$ and consequently ν will depend on the largest value of z_μ. Therefore, in general the statement that ''the adiabatic approximation is valid if the period of the Hamiltonian is large,'' is false. The only case where ν depends on T and the preceding statement is valid is the case where the energy eigenstates are time dependent and either there is effectively one changing parameter or $T_\mu=T$ for all μ. Typical examples of these two cases are a spin in a precessing magnetic field [2] and a spin in a precessing and nutating magnetic field with equal precession and nutation periods, respectively.

Another useful observation is that in the eigenbasis $\{|n;0\rangle\}$ of $H(0)$, $H'(t)$ has no diagonal matrix elements, i.e.,

$$\langle m;0|H'(t)|n;0\rangle=\begin{cases} 0 & \text{for} \quad m=n \\ i\hbar\,\dfrac{\langle m;t|[(d/dt)H(t)]|n;t\rangle}{E_m(t)-E_n(t)}e^{-i[\alpha_m(t)-\alpha_n(t)]} & \text{for} \quad m\neq n. \end{cases} \tag{34}$$

Here, use is made of Eqs. (26) and (11). This equation also implies that the matrix elements $\langle m;\tau|U^{(\ell)}(\tau)|n;0\rangle$ are directly related to $|n-m|^{-\ell}$, i.e., the main contribution to $U^{(\ell)}(\tau)$ comes from the nearest energy levels.

IV. RELATION BETWEEN $H'(t)$ AND $H(t)$

Consider Eq. (26). Since the $m=n$ term is missing in the sum in Eq. (26), one can express $H'(t)$ in the form

$$H'(t)=-i\hbar\sum_{m\neq n}[\langle m;t|e^{-i\alpha_m(t)}]\frac{d}{dt}[e^{i\alpha_n(t)}|n;t\rangle]\times|m;0\rangle\langle n;0|. \tag{35}$$

This equation, together with the definition of $U^{(0)}(t)$, leads to

$$H'(t)=U^{(0)\dagger}(t)H(t)U^{(0)}(t)-i\hbar U^{(0)\dagger}(t)\frac{d}{dt}U^{(0)}(t). \tag{36}$$

The resemblance of this equation to the gauge transformations of the gauge potential in non-Abelian gauge theories (connections on principal fiber bundles) is remarkable [17]. Moreover, a simple calculation shows that

$$U^{(0)\dagger}(t)H(t)U^{(0)}(t)=\sum_n E_n(t)|n;0\rangle\langle n;0|, \tag{37}$$

$$H'(t)=-i\hbar\sum_{n\neq m}\langle m;0|U^{(0)\dagger}(t)\frac{d}{dt}U^{(0)}\times(t)|n;0\rangle|m;0\rangle\langle n;0|. \tag{38}$$

Therefore, the role of the first term on the right-hand side of Eq. (36) is to cancel the diagonal matrix elements of the second term.

Eqs. (36) and (38) signify the importance of the adiabatic approximation in the determination of the nonadiabatic corrections $U^{(\ell)}(\tau)$ $(\ell>0)$ to $U^{(0)}(\tau)$ and consequently the exact evolution operator $U(\tau)$.

[2]This is because $U^{(\ell)}(\tau)$ involves ℓ copies of $H'(\tau)$ in its integrand.

In order to fully appreciate the meaning of Eq. (36), one should recall the effect of a general time-dependent unitary transformation of the Hilbert space $\mathcal{H}$. Let $\mathcal{U}(t):\mathcal{H}\rightarrow\mathcal{H}$ be such a transformation and suppose that the transformed state vectors

$$|\check{\psi}(t)\rangle := \mathcal{U}(t)|\psi(t)\rangle \tag{39}$$

satisfy the following Schrödinger equation:

$$i\hbar\frac{d}{dt}|\check{\psi}(t)\rangle = \check{H}(t)|\check{\psi}(t)\rangle. \tag{40}$$

Then, requiring $|\psi(t)\rangle$ to satisfy the Schrödinger equation defined by the original Hamiltonian $H(t)$, one finds

$$\check{H}(t) = \mathcal{U}(t)H(t)\mathcal{U}^{\dagger}(t) - i\hbar\mathcal{U}(t)\frac{d}{dt}\mathcal{U}^{\dagger}(t). \tag{41}$$

Therefore, Eq. (36) is a particular example of Eq. (41) with $\mathcal{U}(t)=U^{(0)\dagger}(t)$ and $\check{H}(t)=H'(t)$. In other words, the nonadiabatic effects are given by a transformed Hamiltonian $H'(t)$ where the transformation is performed by the inverse of the adiabatically approximate evolution operator, i.e., $U^{(0)\dagger}(t)$.

Transformation (39) may be used to yield an exact solution of the Schrödinger equation, if one can find a $\mathcal{U}(t)$ that makes the transformed Schrödinger equation (40) easily solvable. The Rabi-Ramsey-Schwinger method [18] is a special case of this approach, where one uses the symmetry of the problem to find a unitary transformation $\mathcal{U}(t)$ which renders $\check{H}$ time independent.[3] This is, in general, possible for cranked Hamiltonians with a fixed cranking direction [19,20].

V. TIME-DEPENDENT UNITARY TRANSFORMATIONS AND THE GEOMETRIC PHASE

There is another significant application of time-dependent unitary transformations of the Hilbert space when the Hamiltonian is T periodic. In this case, one knows from the Floquet theory [21] that the evolution operator is given by $U(\tau)=Z(\tau)\exp[-i\tau\widetilde{H}/\hbar]$, where $Z(\tau)$ is a T-periodic unitary operator with $Z(T)=Z(0)=1$ and $\widetilde{H}$ is a time-independent Hermitian operator. Then by definition the cyclic states $|\mathcal{N};T\rangle\langle\mathcal{N};T|$ at $\tau=T$ are given by the eigenstates of $\widetilde{H}$ and the associated total phase angles are $\beta_{\mathcal{N}}(T)=-T\langle\mathcal{N};T|\widetilde{H}|\mathcal{N};T\rangle/\hbar$. Next, consider choosing $\mathcal{U}(t)$ of Eq. (39) to be $Z^{\dagger}(t)$ and $|\psi(0)\rangle=|\check{\psi}(0)\rangle=|\mathcal{N};T\rangle$. Then by virtue of Eq. (41), one has

$$\begin{aligned}\beta_{\mathcal{N}}(T) &= -\frac{T}{\hbar}\langle\psi(0)|\widetilde{H}|\psi(0)\rangle = T\Big[-\frac{1}{\hbar}\langle\psi(t)|H(t)|\psi(t)\rangle \\ &\quad + i\Big\langle\psi(0)\Big|Z^{\dagger}(t)\frac{d}{dt}Z(t)\Big|\psi(0)\Big\rangle\Big], \\ &= \Delta_{\mathcal{N}}(T)+\Gamma_{\mathcal{N}}(T),\end{aligned} \tag{42}$$

$$\Delta_{\mathcal{N}}(\tau) := -\frac{1}{\hbar}\int_0^{\tau}dt\langle\psi(t)|H(t)|\psi(t)\rangle, \tag{43}$$

$$\Gamma_{\mathcal{N}}(\tau) := i\int_0^{\tau}dt\Big\langle\phi_{\mathcal{N}}(t)\Big|\frac{d}{dt}\Big|\phi_{\mathcal{N}}(t)\Big\rangle, \tag{44}$$

where $|\phi(t)\rangle := Z(t)|\psi(0)\rangle$.[4] The phase angles $\Delta_{\mathcal{N}}(\tau)$ and $\Gamma_{\mathcal{N}}(\tau)$ were first introduced by Aharonov and Anandan [22] and called the *dynamical* and *geometrical* phase angles.[5] They generalize their adiabatic counterparts, which were previously discovered by Berry [1]. Clearly, for $\nu\ll 1$, one has $|\mathcal{N};T\rangle\approx|n;0\rangle$, $\Delta_{\mathcal{N}}(T)\approx\delta_n(T)$, and $\Gamma_{\mathcal{N}}(T)\approx\gamma_n(T)$.

Next, consider the general case. If $\mathcal{U}(t)$ is also assumed to leave the original energy eigenstates invariant, i.e., if $\check{H}(t)$ has the same eigenstates as $H(t)$, then one can show that $\mathcal{U}(t)$ and $\check{H}(t)$ must be of the form

$$\mathcal{U}(t) = e^{if(t)}\mathcal{U}_0, \tag{45}$$

$$H(t)\rightarrow\check{H}(t) = H(t) - \hbar\frac{df(t)}{dt}1, \tag{46}$$

where $f=f(t)$ is a real-valued function, $\mathcal{U}_0$ is a constant unitary transformation, and 1 is the identity operator on $\mathcal{H}$. Note that transformation (39) with $\mathcal{U}(t)$ given by Eq. (45) leaves all the observables invariant. It shifts the energy eigenvalues

$$E_n(t)\rightarrow E_n'(t) = E_n(t) - \hbar\frac{df(t)}{dt}, \tag{47}$$

but does not affect the observable transition energies $E_n(t)-E_m(t)$. Therefore, one can identify a physical system with the equivalence class of all the quantum systems which are related by transformations of the form (39,45).

A simple consequence of this observation is that unlike the dynamical phase angle (43), the geometric phase angle (44) is a physical quantity [2]. This statement, however, requires a clarification. One can easily see that Eq. (46) changes the dynamical phase angle $\Delta_{\mathcal{N}}(\tau)$. It does, nevertheless, leave the difference of two dynamical phase angles and consequently two total phase angles invariant. Therefore, the dynamical phase angle also carries physically significant information about the evolving system. In fact, a close look at

[3]For a recent review of the application of this method to a spin system in a precessing magnetic field, see Ref. [2].

[4]Note that the expression in the bracket in Eq. (42) is independent of t. This is the reason why the sum of the integrals in Eqs. (43) and (44) leads to a simple multiplicative factor of T.

[5]Note that in general the Hamiltonian need not be periodic and the Floquet theory does not apply. However, even in this case one can define $|\phi_{\mathcal{N}}(t)\rangle$ and Eqs. (42)–(44) are valid. See [22,2] for more details.

the experimental results of the detection of the geometric phase [23] clearly shows that the measurable quantities are related to the differences of total phase angles. This is usually overshadowed by the fact that in the best studied system, namely the two-level spin ($j=1/2$) system in a precessing magnetic field [1], the conventional choice of the Hamiltonian (48) leads to two cyclic states whose total phase angles differ by a minus sign. Therefore, their difference is twice one of them and it appears that the experiments detect a total phase. In reality however, the experiments always detect the differences between total phase angles, a quantity which is invariant under Eq. (46). This can be easily seen if one uses a complete orthonormal set of cyclic states $\{|\mathcal{N};\tau\rangle\}$ to compute the expectation values

$$\begin{aligned}\langle X(\tau)\rangle :&= \langle\psi(\tau)|X(0)|\psi(\tau)\rangle \\ &= \langle\psi(0)|U^{\dagger}(\tau)X(0)U(\tau)|\psi(0)\rangle, \\ &= \sum_{\mathcal{N},\mathcal{N}'} \langle\psi(0)|\mathcal{N};\tau\rangle\langle\mathcal{N};\tau|U^{\dagger}(\tau)X(0)U(\tau)|\mathcal{N}',\tau\rangle \\ &\quad\times\langle\mathcal{N}';\tau|\psi(0)\rangle \\ &= \sum_{\mathcal{N},\mathcal{N}'} e^{-i[\beta_{\mathcal{N}}(\tau)-\beta'_{\mathcal{N}}(\tau)]}\langle\psi(0)|\mathcal{N};\tau\rangle \\ &\quad\times\langle\mathcal{N};\tau|X(0)|\mathcal{N}',\tau\rangle\langle\mathcal{N}';\tau|\psi(0)\rangle,\end{aligned}$$

where $X(0)$ is an observable and in the last equality use is made of Eq. (1).

Incidentally, it is not too difficult to see that by definition, the adiabaticity parameter ν (12), the operator $H'(t)$ of Eq. (26), and consequently all the nonadiabatic corrections $U^{(\ell)}(\tau)$ (with $\ell\geq 1$) to $U^{(0)}(\tau)$ are invariant under the transformation (45). Therefore, all of these quantities signify physically measurable effects.

VI. APPLICATION TO A MAGNETIC DIPOLE IN A ROTATING MAGNETIC FIELD

In this section, the utility of the expansion (27) is demonstrated for the quantum system consisting of a magnetic dipole moment subject to a magnetic field with changing direction.

The Hamiltonian[6] of this system is given by

$$H(\theta,\varphi)=b\vec{R}(\theta,\varphi)\cdot\vec{J}=b(\sin\theta\cos\varphi J^1+\sin\theta\sin\varphi J^2+\cos\theta J^3), \tag{48}$$

where b is the Larmor frequency, θ and φ are the azimuthal and polar angles in spherical coordinates, respectively, and $\vec{J}$ is the angular momentum operator with components J^{μ}, $\mu=1,2,3$. Clearly, the parameter manifold is the two-dimensional sphere S^2 and the time-dependence of the Hamiltonian is described by a curve $C:[0,\tau]\rightarrow S^2$. Without loss of generality, one can choose a coordinate system in which C does not pass through the south pole. This allows one to work with a single coordinate patch of S^2 that excludes the south pole.

In this patch one has [2]

$$E_n(\theta,\varphi)=E_n(0,0)=b\hbar n \quad \text{with } n=0,\pm\tfrac{1}{2},\pm 1,\pm\tfrac{3}{2},\ldots, \tag{49}$$

$$|n;(\theta,\varphi)\rangle = e^{-(i\varphi/\hbar)J^3}e^{-(i\theta/\hbar)J^2}e^{(i\varphi/\hbar)J^3}|n;(0,0)\rangle, \qquad \theta\in[0,\pi),\varphi\in[0,2\pi). \tag{50}$$

By definition, $|n;(0,0)\rangle$ are the eigenvectors of $H(\theta=0,\varphi=0)=bJ^3$, i.e.,

$$J^3|n;(0,0)\rangle=\hbar n|n;(0,0)\rangle.$$

In order to compute the operators $U^{(0)}(\tau)$ and $H'(\tau)$, one first calculates

$$A_{mn}(t)=A^{(mn)}_{\theta}\dot{\theta}(t)+A^{(mn)}_{\varphi}\dot{\varphi}(t) \tag{51}$$

$$A^{(mn)}_{\theta}:=\left\langle m;(\theta,\varphi)\left|\frac{\partial}{\partial\theta}\right|n;(\theta,\varphi)\right\rangle = \frac{i}{\hbar}[\sin\varphi\langle J^1_{mn}\rangle_0-\cos\varphi\langle J^2_{mn}\rangle_0], \tag{52}$$

$$\begin{aligned}A^{(mn)}_{\varphi}:&=\left\langle m;(\theta,\varphi)\left|\frac{\partial}{\partial\varphi}\right|n;(\theta,\varphi)\right\rangle \\ &= i\left[m(1-\cos\theta)\delta_{mn}+\frac{1}{\hbar}\sin\theta(\cos\varphi\langle J^1_{mn}\rangle_0+\sin\varphi\langle J^2_{mn}\rangle_0)\right],\end{aligned} \tag{53}$$

where $\langle J^{\mu}_{mn}\rangle_0:=\langle m;(0,0)|J^{\mu}|n;(0,0)\rangle$, $(\theta(t),\varphi(t))=C(t)$ and the dot stands for d/dt. In the derivation of Eqs. (52) and (53) use is made of the following identities:

$$e^{-(i\varphi/\hbar)J^3}J^2e^{(i\varphi/\hbar)J^3}=-\sin\varphi J^1+\cos\varphi J^2,$$

$$e^{(i\theta/\hbar)J^2}J^3e^{-(i\theta/\hbar)J^2}=\cos\theta J^3-\sin\theta J^1,$$

$$e^{-(i\varphi/\hbar)J^3}J^1e^{(i\varphi/\hbar)J^3}=\cos\varphi J^1+\sin\varphi J^2.$$

The next step is the calculation of the phase angles $\alpha_n(t)$ of Eq. (7). These are given by

$$\alpha_n(t)=\delta_n(t)+\gamma_n(t), \quad \delta_n(t)=-btn,$$

$$\gamma_n(t)=-n\gamma(t), \tag{54}$$

where

$$\gamma(t):=\int_0^t dt'(1-\cos\theta)\dot{\varphi}=\int_0^{\varphi(t)}(1-\cos\theta)d\varphi. \tag{55}$$

In (55), $\varphi(0)$ is set to zero and in the second integral φ is used to parametrize the curve C, i.e., $\theta=\theta(\varphi)$.

Eqations (51)–(55) together with Eqs. (28) and (26) yield

[6]As discussed in the preceding section, the choice of a Hamiltonian is not unique, i.e., one can add a multiple of the identity operator to Eq. (3.1) without having any physical consequences.

$$U^{(0)}(\tau)=\sum_n e^{-i[b\tau+\gamma(\tau)]n}|n;\tau\rangle\langle n;0|, \tag{56}$$

$$H'(t)=\sum_{m\neq n}[H_1'^{mn}(t)\langle J^1_{mn}\rangle_0+H_2'^{mn}(t)\langle J^2_{mn}\rangle_0]|m;0\rangle\langle n;0|, \tag{57}$$

where

$$H_1'^{mn}(t):=e^{i[bt+\gamma](m-n)}(\sin\varphi\dot\theta+\sin\theta\cos\varphi\dot\varphi), \tag{58}$$

$$H_2'^{mn}(t):=e^{i[bt+\gamma](m-n)}(-\cos\varphi\dot\theta+\sin\theta\sin\varphi\dot\varphi). \tag{59}$$

In order to further ease the computation of $H'(\tau)$, one can make the additional assumption that the energy eigenstates have definite total angular momentum, i.e.,

$$|\vec J|^2|n,(\theta,\varphi)\rangle=j(j+1)|n,(\theta,\varphi)\rangle,$$
$$n=-j,-j+1,\ldots,j. \tag{60}$$

This assumption is too restrictive for the applications in molecular physics, where one encounters systems with cylinderical symmetry rather than spherical symmetry [2]. For a magnetic dipole in a classical environment, however, one can safely make this assumption. In this case, one can use the well known relations [24]

$$J^\pm:=J^1\pm iJ^2,\quad J^\pm|n;(0,0)\rangle=\hbar C_{\pm n}|n\pm1;(0,0)\rangle,$$
$$C_m:=\sqrt{(j-m)(j+m+1)}, \tag{61}$$

to compute $\langle J^1_{mn}\rangle_0$ and $\langle J^2_{mn}\rangle_0$. This leads to

$$\langle J^1_{mn}\rangle_0=\frac{\hbar}{2}(C_n\delta_{mn+1}+C_{-n}\delta_{mn-1}),\langle J^2_{mn}\rangle_0$$
$$=\frac{-i\hbar}{2}(C_n\delta_{mn+1}-C_{-n}\delta_{mn-1}). \tag{62}$$

Substituting Eqs. (62) and carrying out the necessary algebra, one has

$$A^{(mn)}_\theta=\frac{1}{2}(e^{i\varphi}C_m\delta_{mn-1}-e^{-i\varphi}C_n\delta_{m-1\,n}), \tag{63}$$

$$A^{(mn)}_\varphi=i[m(1-\cos\theta)\delta_{mn}+\tfrac{1}{2}\sin\theta(e^{i\varphi}C_m\delta_{mn-1}+e^{-i\varphi}C_n\delta_{m-1\,n})], \tag{64}$$

$$\begin{aligned}H'(t)&=\frac{\hbar}{2}\left[h'(t)\sum_n C_n|n+1;0\rangle\langle n;0|+h'^*(t)\sum_n C_n|n-1;0\rangle\langle n;0|\right]\\&=\frac{\hbar}{2}\Big[h'(t)e^{-i(\theta_0/\hbar)J^2}\sum_n C_n|n+1;(0,0)\rangle\langle n;(0,0)|e^{i(\theta_0/\hbar)J^2}\\&\quad+h'^*(t)e^{-i(\theta_0/\hbar)J^2}\sum_n C_n|n-1;(0,0)\rangle\langle n;(0,0)|e^{i\theta_0/\hbar J^2}\Big]\\&=\frac{1}{2}[h'(t)e^{-i(\theta_0/\hbar)J^2}J^+e^{i(\theta_0/\hbar)J^2}+h'^*(t)e^{-i(\theta_0/\hbar)J^2}J^-e^{i(\theta_0/\hbar)J^2}]\\&=\mathrm{Re}[h'(t)](\cos\theta_0J^1-\sin\theta_0J^3)-\mathrm{Im}[h'(t)]J^2,\end{aligned} \tag{65}$$

where

$$h'(t):=e^{i[bt+\gamma-\varphi]}(i\dot\theta+\sin\theta\dot\varphi), \tag{66}$$

$\theta_0:=\theta(0)$, and Re and Im stand for the real part and ($-i$ times) the imaginary part of the argument. Furthermore, in the derivation of Eq. (65) use is made of Eqs. (57), (50), (61), $\varphi(0)=0$, and the identities

$$e^{-i(\theta_0/\hbar)J^2}J^\pm e^{i(\theta_0/\hbar)J^2}=e^{-i(\theta_0/\hbar)J^2}J^1e^{i(\theta_0/\hbar)J^2}\pm iJ^2$$
$$=\cos\theta_0J^1-\sin\theta_0J^3\pm iJ^2. \tag{67}$$

Next, consider the case in which the magnetic field performs a simultaneous precession and nutation, i.e.,

$$C:\quad \varphi=\omega t,\quad \cos\theta=\cos\theta_0+\eta\sin(l\omega t). \tag{68}$$

Here, ω is the frequency of precession and $|l|\omega$ and η are the frequency and amplitude of the nutation, respectively. Clearly $0\leqslant\eta<1\pm\cos\theta_0$ and l is an integer.

The computation of γ is straightforward:

$$\gamma(t)=(1-\cos\theta_0)\omega t-\frac{\eta}{l}[1-\cos(l\omega t)]. \tag{69}$$

Hence, for $\tau=T:=2\pi/\omega$, one recovers Berry's result:

$$\gamma_n(T)=-2\pi n(1-\cos\theta_0)=-n\Omega(C), \tag{70}$$

where $\Omega(C)$ is the solid angle subtended by the curve C. A simple consequence of (70) is that the adiabatic approximation does not detect the effects of the nutation. In fact, one has

$$U^{(0)}(T)=\sum_n e^{-i[bT+2\pi(1-\cos\theta_0)]n}|n;0\rangle\langle n;0| =e^{-i(\theta_0/\hbar)J^2}e^{-(i/\hbar)[bT+2\pi(1-\cos\theta_0)]J^3}e^{i(\theta_0/\hbar)J^2}. \tag{71}$$

The first nonadiabatic correction $U^{(1)}(T)$ to (71) is obtained by integrating $H'(t)$ of Eq. (65). This involves the evaluation of

$$I(T):=\int_0^T h'(t)dt=\int_0^T dt e^{i[bt+\gamma-\varphi]}(i\dot\theta+\sin\theta\dot\varphi). \tag{72}$$

In order to give a closed expression for this integral and subsequently $U^{(1)}(T)$, one can expand the integrand in powers of η. This leads to a lengthy calculation which results in

$$\mathrm{Re}[I(T)]=\zeta\left\{\sin\theta_0\sin(2\pi/\zeta)+\left[\left(\frac{1-\cos(2\pi/\zeta)}{1-(l\zeta)^2}\right)\times\left(\frac{1}{\sin\theta_0}+\cot\theta_0\zeta-\sin\theta_0\zeta^2\right)\right]l\eta+\left[\frac{2\cos\theta_0\sin(2\pi/\zeta)\zeta}{\sin^3\theta_0[1-4(l\zeta)^2]}\right](l\eta)^2\right\}+\mathcal{O}(l\eta^2), \tag{73}$$

$$\mathrm{Im}[I(T)]=\zeta\left\{\sin\theta_0[1-\cos(2\pi/\zeta)]+\left[\left(-\frac{1}{\sin\theta_0}-\cot\theta_0\zeta+\sin\theta_0\zeta^2\right)\left(\frac{\sin(2\pi/\zeta)}{1-(l\zeta)^2}\right)\right]l\eta+\left[\frac{2\cos\theta_0[1-\cos(2\pi/\zeta)]\zeta}{\sin^3\theta_0[1-4(l\zeta)^2]}\right](l\eta)^2\right\}+\mathcal{O}(l\eta^2), \tag{74}$$

where $\zeta:=\omega/(b-\omega\cos\theta_0)$. In terms of $\mathrm{Re}[I(T)]$ and $\mathrm{Im}[I(T)]$, $U^{(1)}(T)$ is expressed in the form

$$U^{(1)}(T)=-\frac{i}{\hbar}U^{(0)}(T)\{\mathrm{Re}[I(T)](\cos\theta_0J^1-\sin\theta_0J^3)-\mathrm{Im}[I(T)]J^2\} =-\frac{i}{\hbar}e^{-(i\theta_0/\hbar)J^2}e^{-(i/\hbar)[bT+2\pi(1-\cos\theta_0)]J^3}\times\{\mathrm{Re}[I(T)]J^1-\mathrm{Im}[I(T)]J^2\}e^{i(\theta_0/\hbar)J^2}. \tag{75}$$

In particular, consider the special case, $\theta_0=\pi/2$. Then $\zeta=\omega/b$ and Eqs. (71), and (73)–(75) reduce to

$$U^{(0)}(T)=e^{-i(\pi/2\hbar)J^2}e^{-(i/\hbar)(bT+2\pi)J^3}e^{i(\pi/2\hbar)J^2} =e^{-i2\pi j}e^{-i(\pi/2\hbar)J^2}e^{-(i/\hbar)bTJ^3}e^{i(\pi/2\hbar)J^2}, \tag{76}$$

$$\mathrm{Re}[I(T)]=\zeta\left\{\sin(2\pi/\zeta)+\left[\left(\frac{1-\zeta^2}{1-(l\zeta)^2}\right)\times[1-\cos(2\pi/\zeta)]\right]l\eta\right\}+\mathcal{O}(l\eta^2), \tag{77}$$

$$\mathrm{Im}[I(T)]=\zeta\left\{1-\cos(2\pi/\zeta)+\left[\left(-\frac{1-\zeta^2}{1-(l\zeta)^2}\right)\sin(2\pi/\zeta)\right]l\eta\right\}+\mathcal{O}(l\eta^2), \tag{78}$$

$$U^{(1)}(T)=-\frac{i}{\hbar}e^{-i2\pi j}e^{-i(\pi/2\hbar)J^2}e^{-(i/\hbar)bTJ^3}\{\mathrm{Re}[I(T)]J^1-\mathrm{Im}[I(T)]J^2\}e^{i(\pi/2\hbar)J^2}. \tag{79}$$

The adiabaticity parameter ν of Eq. (12) can also be easily calculated in this case:

$$\nu=c\sqrt{1+(l\eta)^2}\zeta+\mathcal{O}(l\eta^2), \tag{80}$$

where $c:=C_{-j}/2=\sqrt{j(j+1/2)}$. The appearance of ζ in this expression, is an indication of the fact that the leading order term in $U^{(1)}(T)$ is of order ν. In fact, for the two extreme cases, $l\eta\ll1$ and $l\eta\gg1$ [with $l\eta^2\ll1$ so that one can neglect $\mathcal{O}(l\eta^2)$] this is manifestly seen.

As indicated by Eqs. (76)–(79), the nutation of the direction of the magnetic field only contributes to the nonadiabatic part of the evolution operator.

VII. ADIABATIC PRODUCT EXPANSION

Consider writing Eq. (27) in the form

$$U(\tau)=U^{(0)}(\tau)U'(\tau),\quad U'(\tau):=\mathcal{T}e^{-(i/\hbar)\int_0^\tau dtH'(t)}. \tag{81}$$

In view of the analysis of Sec. IV, the operator $U'(\tau)$ is the time-evolution operator for the transformed Hamiltonian $H'(\tau)$, where the transformation is performed using the adjoint of the adiabatically approximate time-evolution operator, i.e., $U^{(0)\dagger}(\tau)$. Since $H'(\tau)$ serves as the Hamiltonian of the system in the transformed frame, one can repeat the analysis of Secs. III and IV to obtain yet another transformed Hamiltonian $H''(\tau)$. Clearly, this is done by separating the adiabatic part $U'^{(0)}(\tau)$ of the evolution operator $U'(\tau)$ and use its adjoint $U'^{(0)\dagger}(\tau)$ to transform the Hilbert space. Repeating this process leads to the product expansion

$$U(\tau)=\prod_{i=0}^{\infty}\mathcal{U}^{(i)}(\tau), \tag{82}$$

where $\mathcal{U}^{(i)}(\tau)$ is the adiabatically approximate part of the evolution operator obtained in the ith step of the above iterative construction.

Let us denote by $H^{(N)}(\tau)$ the transformed Hamiltonian obtained in the Nth step of this construction. Then if the adiabatic approximation happens to be exact in the Nth step,

i.e., the adiabaticity parameter $\nu^{(N)}$ associated with $H^{(N)}(\tau)$ vanishes, the adiabatic product expansion (82) terminates and one has an exact expression for the original evolution operator, namely,

$$U(\tau)=\prod_{i=0}^{N}\mathcal{U}^{(i)}(\tau). \tag{83}$$

In general, $\nu^{(N)}$ may not vanish for any N and Eq. (83) may not hold exactly. But one can still use this equation as an approximation. This is indeed a product generalization of the adiabatic approximation. It reduces to the ordinary adiabatic approximation (5) for $N=0$.

Product and series generalizations of the adiabatic approximation are quite different in the sense that the former may terminate after a finite number of iterations N. This property may indeed be used to identify some previously unknown exactly solvable Schrödinger equations. The utility of the adiabatic product expansion in the identification of exactly solvable models stems from the fact that unlike the series expansion, it is essentially nonperturbative. In principle, the value of the initial adiabaticity parameter ν does not determine whether the product expansion (82) would terminate.

Although at present there is no simple procedure to control the convergence property of the adiabatic product expansion, except computing all $\nu^{(N)}$'s for $N=0,1,2,\ldots$, one can artificially demand its termination by enforcing $\nu^{(N)}=0$ for some small values of N and try to see if this condition would lead to any interesting results. In the remainder of this section, I shall demonstrate the consequences of this condition for a magnetic dipole in an arbitrarily changing (not necessarily rotating) magnetic field.

The Hamiltonian for this system is given by Eq. (48), where the parameter b may also be time dependent. In order to distinguish the two cases $b=$ const. and $b\neq$ const., I shall replace b by $br(t)$ in Eq. (48) where $r=r(t)$ denotes the radial spherical coordinate. Excluding the origin $r=0$ at which the Hamiltonian vanishes, one has $\mathbb{R}^3-\{0\}$ as the parameter space. Clearly, the eigenvalues of $H[R]$ with $R=(r,\theta,\varphi)\in\mathbb{R}^3-\{0\}$ are nondegenerate.

The calculations of the energy eigenvalues and eigenvectors are essentially the same as those presented in Sec. VI. It is not difficult to see that eigenvectors $|n;(r,\theta,\varphi)\rangle$ are independent of r. In fact the r dependence of the Hamiltonian only affects its eigenvalues, which are now scaled by r. Following the same type of lengthy calculations as in Sec. VI, one can show that

$$\begin{aligned}H^{(1)}(t):=H'(t)=\Omega(t)\Big\{&\Big(\cos^2\frac{\theta_0}{2}\cos\sigma(t)-\sin^2\frac{\theta_0}{2}\cos[2\varphi_0+\sigma(t)]\Big)J^1\\&+\Big(-\cos^2\frac{\theta_0}{2}\sin\sigma(t)-\sin^2\frac{\theta_0}{2}\sin[2\varphi_0+\sigma(t)]\Big)J^2+[-\sin\theta_0\cos\sigma(t)]J^3\Big\}\end{aligned} \tag{84}$$

$$=br^{(1)}(t)[\sin\theta^{(1)}(t)\cos\varphi^{(1)}(t)J^1+\sin\theta^{(1)}(t)\sin\varphi^{(1)}(t)J^2+\cos\theta^{(1)}(t)J^3], \tag{85}$$

where I have introduced

$$\Omega(t):=\sqrt{\dot\theta^2+\sin^2\theta\dot\varphi^2},\quad \sigma(t)=-\alpha-\varphi+\xi,$$

$$\alpha(t):=\delta(t)+\gamma(t), \tag{86}$$

$$\delta(t):=-b\int_0^t r(t')dt', \tag{87}$$

$$\gamma(t):=-\int_0^t[1-\cos\theta(t')]\dot\varphi(t')dt',$$

$$\cos\xi:=\frac{\sin\theta\dot\varphi}{\Omega},\quad \sin\xi:=\frac{\dot\theta}{\Omega}, \tag{88}$$

$$\theta_0:=\theta(t=0),\quad \varphi_0:=\varphi(t=0),$$

$$r^{(1)}(t):=\frac{\Omega(t)\Delta(t)}{b}, \tag{89}$$

$$\Delta(t):=\sqrt{1+\sin\varphi_0\sin^2\theta_0\sin[\varphi_0+2\sigma(t)]},$$

$$\theta^{(1)}(t):=\cos^{-1}\Big[-\frac{\sin\theta_0\cos\sigma(t)}{\Delta(t)}\Big], \tag{90}$$

$$\varphi^{(1)}(t):=\tan^{-1}\Big[\frac{\sin\sigma(t)+\tan^2(\theta_0/2)\sin[2\varphi_0+\sigma(t)]}{-\cos\sigma(t)+\tan^2(\theta_0/2)\cos[2\varphi_0+\sigma(t)]}\Big]. \tag{91}$$

Note that the transformed Hamiltonian $H^{(1)}$ is obtained from the original Hamiltonian H by replacing the original coordinates (r,θ,φ) with the transformed coordinates $(r^{(1)},\theta^{(1)},\varphi^{(1)})$. Next one defines $(r^{(2)},\theta^{(2)},\varphi^{(2)})$ by replacing (r,θ,φ) in Eqs. (86) – (91) with $(r^{(1)},\theta^{(1)},\varphi^{(1)})$, and replaces $(r^{(1)},\theta^{(1)},\varphi^{(1)})$ with $(r^{(2)},\theta^{(2)},\varphi^{(2)})$ in Eq. (85) to obtain the transformed Hamiltonian $H^{(2)}$. Continuing this simple iterative procedure one can compute all the transformed Hamiltonians $H^{(N)}(t)$.

Next let us impose the condition $\nu^{(1)}=0$ or, alternatively, $H^{(2)}(t)=0$ or $r^{(2)}(t)=0$. This condition results in the following exact expression for the evolution operator:

$$U(\tau)=\mathcal{U}^{(0)}(\tau)\mathcal{U}^{(1)}(\tau). \tag{92}$$

The condition $r^{(2)}(t)=0$ can easily be fulfilled if one demands that $\dot{\sigma}(t)=0$. In order to see this, note that $r^{(2)}$ is proportional to $\Omega^{(1)}:=\sqrt{(\dot{\theta}^{(1)})^2+\sin^2\theta^{(1)}(\dot{\varphi}^{(1)})^2}$ and that both $\dot{\theta}^{(1)}$ and $\dot{\varphi}^{(1)}$ are proportional to $\dot{\sigma}$. Thus, $\dot{\sigma}=0$ implies $r^{(2)}=0$. Furthermore, one can easily check that $\dot{\sigma}$ is linear in r. This allows one to express the condition $\dot{\sigma}=0$ in the form

$$r(t)=r_*(t):=\frac{1}{b}\left[\cos\theta\dot{\varphi}-\frac{d/dt(\dot{\theta}/\sin\theta\dot{\varphi})}{1+(\dot{\theta}/\sin\theta\dot{\varphi})^2}\right]$$
$$=\frac{\dot{\varphi}}{b}\left[\cos\theta-\frac{(d/d\varphi)(\theta'/\sin\theta)}{1+(\theta'/\sin\theta)^2}\right], \tag{93}$$

where $\theta'=d\theta/d\varphi$. It is this relation between the coordinate functions that guarantees the exact expression (92) for the evolution operator. In fact, one can check by direct computation of $\mathcal{U}^{(0)}(\tau)$ and $\mathcal{U}^{(1)}(\tau)$ that Eq. (93) is a sufficient condition for $U(\tau)=\mathcal{U}^{(0)}(\tau)\mathcal{U}^{(1)}(\tau)$ to satisfy the Schrödinger equation (3).

Surprisingly, Eq. (93) only restricts the magnitude of the magnetic field and leaves its direction to vary arbitrarily. Therefore, since the instantaneous eigenvectors of the Hamiltonian are independent of the magnitude of the magnetic field, *for any arbitrarily changing Hamiltonian* $H[r(t),\theta(t),\varphi(t)]$ *(magnetic field) there is another Hamiltonian* $H_*[r_*(t),\theta(t),\varphi(t)]$ *(magnetic field) with the same time-dependent eigenvectors (direction) but possibly different eigenvalues (magnitude) for which the Schrödinger equation (3) is exactly solvable.* The physical justification of this remarkable result is still obscure for the author. Its mathematical origin may be traced back to the simple derivation of Eq. (16) which in turn led to the separation of the adiabatic part of the time-evolution operator $U^{(0)}(\tau)$ – that included the geometric phase effects – from its nonadiabatic part. The capability of the adiabatic product expansion to give rise to such a wide class of previously unnoticed exactly solvable models may be attributed to its nonperturbative nature.

Finally, let me conclude this section by noting that the apparent positivity restriction on r does not pose any difficulty for the above argument. This is because for the time intervals during which $r_*(t)$ is negative one can obtain the exact expression for the evolution operator of the time-reversed system. By virtue of the appearance of $\dot{\varphi}$ on the right-hand side of Eq. (93), for the time-reversed system r_* is positive. The evolution operator for the original system is then obtained from the time-reversed one by inverting (taking the adjoint of) the latter. The only source of possible difficulty is the cases where r_* vanishes for extended periods of time.

VIII. SUMMARY AND CONCLUSION

In this article, I have tried to address some of the basic issues regarding the meaning of the adiabatic approximation and the implications of their resolution to the phenomenon of the geometric phase. A precise definition of an adiabaticity parameter, although being rather unimportant in practice, provides an objective criterion for the applicability of the adiabatic approximation. In particular, it shows that in general there is no direct relation between the validity of the adiabatic approximation and the length of the duration of the evolution or the period of a periodic Hamiltonian. For example, for the system described by Eqs. (48) and (68), consider the case in which both the period T and the nutation parameter $l\eta$ are large but in such a way that ν as given by Eq. (80) is also large. Then clearly the adiabatic approximation is not valid. A simple example of a periodic system with an arbitrarily small period for which the adiabatic approximation is valid exactly is a system with constant energy eigenstates but time-dependent energy eigenvalues. A typical example of such a system is a magnetic dipole in a magnetic field whose magnitude is rapidly changing but whose direction is fixed. Clearly, in this case, the adiabaticity parameter ν vanishes identically and the adiabatic approximation is valid exactly. In fact the limit $\tau\to\infty$ considered in the proof of the adiabatic theorem [8] is used to mean that the time period during which the Hamiltonian changes appreciably is very large. This condition is only a sufficient condition for the validity of the adiabatic approximation, whereas $\nu\to 0$ is both necessary and sufficient.

I have also given two iterative expansions of the evolution operator $U(\tau)$. The first one is an adiabatic series expansion that provides a perturbative generalization of the adiabatic approximation. I have shown how one can separate the adiabatic and nonadiabatic parts of $U(\tau)$ and yield the nonadiabatic part as a time-ordered exponential defined by a Hermitian operator $H'(t)$. In a basis that diagonalizes the initial Hamiltonian, $H'(t)$ is off-diagonal. Moreover, the dominant contribution to this operator and consequently to the nonadiabatic part of the evolution operator comes from the nearest energy levels. Particularly interesting is to view $H'(t)$ as a transformed Hamiltonian. This corresponds to a time-dependent unitary transformation of the state vectors which undoes the adiabatic part of the evolution operator. A logical consequence of this observation is an adiabatic product expansion.

I have also presented a brief review of the general time-dependent unitary transformations of the state vectors and a simple application of such a transformation which yields a splitting of the total phase of a cyclic state into its dynamical and geometric parts for a periodically changing Hamiltonian. I have discussed the physically equivalent quantum systems and showed that the physical observables only depend on the differences of the total phase angles of cyclic states.

Next I have applied the adiabatic series expansion to study the dynamics of a magnetic dipole subject to a rotating magnetic field. In particular, I have given an explicit derivation of the formula for the transformed Hamiltonian $H'(t)$ for the general case and studied the case of a precessing and nutating magnetic field in detail.

Finally, I have presented the basic properties and a simple application of the adiabatic product expansion. The preliminary results indicate that this expansion and the corresponding generalized adiabatic approximation have quite surprising consequences. For instance, for the dipole system they

lead to the identification of previously unknown exactly solvable Schrödinger equations. The adiabatic product expansion has also potential applications in the exact calculation of non-Abelian holonomy elements and in particular Wilson loop integrals.

ACKNOWLEDGMENTS

I would like to thank Bahman Darian and Rouzbeh Allahverdi for interesting discussions, and acknowledge the support of the Killam Foundation of Canada.

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