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BRIEF REPORTS

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Magnus approximation in the adiabatic picture

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We describe a simple approximate nonperturbative method for treating time-dependent problems that works well in the intermediate regime far from both the sudden and the adiabatic limits. The method consists of applying the Magnus expansion after transforming to the adiabatic basis defined by the eigenstates of the instantaneous Hamiltonian.

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Problems involving time-dependent Hamiltonians occur in many different areas of physics and are usually treated by perturbation methods. An exact treatment is, however, possible for a very large class of such Hamiltonians in the infinitely fast (sudden) or infinitely slow (adiabatic) limit. The latter has been extensively investigated after Berry [1] and Simon [2] uncovered the remarkable geometric properties of the additional phase present in the formulation of the quantum-adiabatic theorem [3,4] and to which nobody paid attention to before. Many significant contributions reporting on various manifestations of the geometrical phase can be found in Ref. [5].

The adiabatic theorem provides solid ground for accurately calculating small effects due to the finite slowness met in actual physical processes by some approximate method such as perturbation theory [6–8], unitary iteration [9,10], WKB [11,12], or analytic continuation in the complex t plane [13–15]. Rapidly changing Hamiltonians which are close to the sudden limit are also easily handled by several methods. In particular, an efficient nonperturbative approach is provided by the so-called Magnus expansion [16,17]. By contrast, no reliable approximation method seems to be available yet in the intermediate regime far from both extreme situations mentioned above. In this Brief Report we adopt a pragmatic point of view and explore the outcome of a simple procedure which consists in applying the Magnus approach in the adiabatic basis set. The results obtained so far seem most promising. While the sudden limit now is out of reach, the procedure appears to be extremely efficient in both the adiabatic and intermediate regimes.

Before proceeding with this program it is useful to briefly recall the Magnus expansion in its usual setting. Let us consider a finite-dimensional complex vector space referred to a fixed basis set $\{|n\rangle\}$, and a Hermitian Hamilton operator depending smoothly on time through the variable $s = t/T$, where T determines the time scale. The time development of the system is globally contained in the unitary evolution operator $U(s) = U(s,0)$ [occasionally $U(s) = U(s,-\infty)$ is better suited]. The Schrödinger equation satisfied by $U(s)$ reads

$$\dot{U}(s) = \tilde{H}(s)U(s), \qquad U(0) = I, \tag{1}$$

where the dot means the derivative with respect to s and $\tilde{H} = (T/i\hbar)H$ is a dimensionless anti-Hermitian operator. Magnus [16] has derived a *true* exponential solution (i.e., without chronological ordering) $U(s) = \exp[\Omega(s)]$ of Eq. (1) where the anti-Hermitian operator $\Omega(s)$ is given by an infinite nested commutator expansion. The first two terms in this expansion $\Omega(s) = \sum_m \Omega_m(s)$ are

$$\begin{aligned} \Omega_1(s) &= \int_0^s ds' \tilde{H}(s') \ , \\ \Omega_2(s) &= \frac{1}{2}\int_0^s ds' \int_0^{s'} ds'' [\tilde{H}(s'), \tilde{H}(s'')] \ . \end{aligned} \tag{2}$$

Higher terms can be generated recursively [18] but in some special cases the expansion actually stops after a few terms. Since the general term is of order T^m one expects the Magnus method to work well near the sudden limit ($T \to 0$) and very badly in the adiabatic regime ($T \to \infty$). On the other side, unitarity is always trivially satisfied at any order of truncation in the expansion.

In order to render the Magnus expansion effective in a nonsudden regime we first transform to the "adiabatic" picture by changing from the fixed basis to that defined by the eigenvectors $|n(s)\rangle$ of the instantaneous total

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Hamiltonian $H(s)$. For simplicity we assume the energy spectrum of $H(s)$ to be free from any accidental or systematic, symmetry induced, degeneracies. We can always arrange for the transformation from the fixed basis to the adiabatic one to be generated by a smoothly varying unitary operator $G(s)$ such that $|n(s)\rangle = \sum_m G_{mn}(s)|m\rangle$ [hence $G_{mn}(s) = \langle m|n(s)\rangle$]. This is in the spirit of the adiabatic theorem. We therefore have $G^\dagger(s)H(s)G(s) = E(s) = \mathrm{diag}[E_1(s), E_2(s), \ldots]$ and

$$U(s) = G(s)U_G(s)G^\dagger(0). \tag{3}$$

The equation satisfied by $U_G(s)$ reads

$$\dot{U}_G(s) = \tilde{H}_G(s)U_G(s), \tag{4}$$

where

$$\tilde{H}_G(s) = \tilde{E}(s) - G^\dagger(s)\dot{G}(s) \tag{5}$$

and $\tilde{E}(s)$ is a diagonal matrix with elements $TE_n(s)/i\hbar$. Let us now split up the new Hamiltonian into its diagonal and off-diagonal parts, viz.

$$\tilde{H}_G(s) = \tilde{H}_0(s) + \tilde{H}_1(s), \tag{6}$$

where

$$\tilde{H}_0 = \tilde{E} - (G^\dagger\dot{G})_{\mathrm{d}}, \quad \tilde{H}_1 = -(G^\dagger\dot{G})_{\mathrm{nd}}. \tag{7}$$

At this stage we introduce the generalized Dirac (interaction) picture by writing

$$U_G(s) = \exp\left(\int_0^s ds'\tilde{H}_0(s')\right) U_G^{(I)}(s). \tag{8}$$

The Schrödinger equation for $U_G^{(I)}$ reads

$$\dot{U}_G^{(I)}(s) = \tilde{H}_G^{(I)}(s)U_G^{(I)}(s), \qquad U_G^{(I)}(0) = I, \tag{9}$$

with

$$\tilde{H}_G^{(I)}(s) = \exp\left(-\int_0^s ds'\tilde{H}_0(s')\right) \times \tilde{H}_1(s)\exp\left(\int_0^s ds'\tilde{H}_0(s')\right). \tag{10}$$

Equivalently $U_G^{(I)}$ may be obtained by solving the integral equation

$$U_G^{(I)}(s) = I + \int_0^s ds'\tilde{H}_G^{(I)}(s')U_G^{(I)}(s'). \tag{11}$$

The new Hamiltonian $\tilde{H}_G^{(I)}$ is of course nondiagonal, like $\tilde{H}_1$, but in addition its matrix elements contain some phases increasing linearly with T that arise from the diagonal part $\tilde{H}_0$. In analogy with the well-known Riemann-Lebesgue lemmas [19] this eventually leads to the vanishing of the integral in Eq. (11) when $T \to \infty$, i.e., to the adiabatic theorem (notice the close connection with the semiclassical limit $\hbar \to 0$).

The operator $U_G^{(I)}(s)$ is all one needs for calculating transition probabilities between instantaneous eigenstates. Iteration of Eq. (11) generates the adiabatic perturbation expansion which gives good results when T is large for the reason stated above. To first order one has simply

$$U_G^{(I)}(s) \simeq I + \int_0^s ds'\tilde{H}_G^{(I)}(s'). \tag{12}$$

Alternatively we can integrate Eq. (9) by using the Magnus expansion which has the advantage of preserving unitarity to each order (in this respect Fer's infinite product expansion offers another interesting possibility [20]). The first order approximation then reads

$$U_G^{(I)}(s) \simeq \exp\left(\int_0^s ds'\tilde{H}_G^{(I)}(s')\right). \tag{13}$$

Notice that the second term $\tilde{H}_1$ in the right-hand side of Eq. (6) is of purely geometric origin, whereas $\tilde{H}_0$ contains both a dynamical part ($\tilde{E}$) and a geometrical part. This corresponds to the now familiar splitting of the phase acquired by a system evolving adiabatically from an eigenstate of the instantaneous Hamiltonian. However the geometrical character here is not related to a parameter space, but rather to the Hilbert space of states (as in the Aharonov-Anandan [21] analysis) and is manifest in the fact that $\tilde{H}_1$ does not depend on the time scale T. It is obvious that the two characters (geometrical and dynamical) are completely mixed up in the adiabatic interaction Hamiltonian $\tilde{H}_G^{(I)}$ and hence in $U_G^{(I)}$. This intermingling is responsible, in particular, for Berry's geometrical factors in the amplitudes of inelastic transitions [15]. Finally we remark that the evolution operator $U_G^{(I)}$ automatically takes into account the specific properties of the basis as a function of time. It furnishes the correct answer irrespective of such conditions as parallel transport or being single valued. Since the diagonal elements of $G^\dagger\dot{G}$ are just the scalar products $\langle n(s)|\dot{n}(s)\rangle$, this is simply a matter of transferring the geometrical phase from $\tilde{H}_0$ to the eigenvectors of the adiabatic basis, or vice versa.

We now specialize the above formalism for the two-state case described by the Hamiltonian

$$H(s) = \boldsymbol{a}(s)\boldsymbol{\sigma}, \tag{14}$$

where $\boldsymbol{a}(s)$ is a real time-dependent vector and $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices. A simple choice for the diagonalizing operator is $G(s) = \hat{\mathbf{b}}(s)\boldsymbol{\sigma}$, with the unit vector $\hat{\mathbf{b}}$ pointing in the direction of $\boldsymbol{b} = \hat{\mathbf{a}} + \hat{\mathbf{k}}$ ($\hat{\mathbf{k}}$ is the unit vector along the z axis). Further one finds

$$\tilde{H}_G(s) = (T/i\hbar)a\sigma_z - i(\hat{\mathbf{b}} \times \dot{\hat{\mathbf{b}}})\boldsymbol{\sigma}, \tag{15}$$

where the first term represents the diagonalized Hamiltonian $\tilde{E}$ and the second term the complete geometrical contribution. Denoting the polar angles of $\mathbf{a}$ by θ, ϕ, the two pieces of $\tilde{H}_G$ defined in Eq. (6) read

$$\tilde{H}_0 = [(T/i\hbar)a + i\mu_z]\sigma_z, \qquad \tilde{H}_1 = i(\mu_x\sigma_x + \mu_y\sigma_y), \tag{16}$$

where the vector $\boldsymbol{\mu} = \boldsymbol{\mu}(s)$ has components

$$\mu_x = (\dot{\phi}/2)\cos\phi\sin\theta + (\dot{\theta}/2)\sin\phi,$$
$$\mu_y = (\dot{\phi}/2)\sin\phi\sin\theta - (\dot{\theta}/2)\cos\phi, \quad (17)$$
$$\mu_z = -(\dot{\phi}/2)(1-\cos\theta) = -\dot{\phi}\sin^2(\theta/2).$$

Thus if ϕ is constant there is no geometrical contribution to $\tilde{H}_0$ and therefore no Berry phase.

More specifically we consider a spin one-half system in a rotating magnetic field that makes an angle θ with the z axis. Equation (14) then holds with $\boldsymbol{a} = (\hbar/2)\gamma\boldsymbol{B}$ yielding the dimensionless Hamiltonian

$$\tilde{H}(s) = -(i\gamma T/2)\boldsymbol{B}(s)\boldsymbol{\sigma}. \quad (18)$$

Here γ is the gyromagnetic ratio, $T = 2\pi/\omega$ is the period of rotation and

$$\boldsymbol{B}(s) = B(\sin\theta\cos 2\pi s, \sin\theta\sin 2\pi s, \cos\theta). \quad (19)$$

The exact solution of Eq. (1) is readily worked out by substituting $U = \exp(-i\pi s\sigma_z)U_R$. As a result the system is referred to a rotating frame in which the magnetic field and hence the Hamiltonian are constant, so that U_R may be written at once [22]. From $U_R(s)$ one obtains the spin-flip probability

$$P_{\rm ex} = (\gamma BT/2)^2\sin^2\theta\sin^2\lambda s/\lambda^2, \quad (20)$$

where $\lambda^2 = (\gamma BT/2)^2 - \pi\gamma BT\cos\theta + \pi^2$. This refers to the spin projection on the z axis and the corresponding states are not eigenvectors of the Hamiltonian. Notice that such transitions occur even in the adiabatic regime, defined by the condition $BT \gg 1$.

Changing for the adiabatic basis via the operator $G(s) = \hat{\mathbf{b}}(s)\boldsymbol{\sigma}$ with $\boldsymbol{b} = \hat{\mathbf{B}} + \hat{\mathbf{k}}$ leads to

$$\tilde{H}_G(s) = i\varphi\sigma_z + i\pi\sin\theta(\sigma_x\cos 2\pi s + \sigma_y\sin 2\pi s), \quad (21)$$

where

$$\varphi = -\gamma BT/2 - \pi(1-\cos\theta). \quad (22)$$

With regard to the time structure, the new Hamiltonian is quite similar to the original one: its diagonal part $\tilde{H}_0 = i\varphi\sigma_z$ does not depend on time, while the off-diagonal part $\tilde{H}_1$ displays the same periodicity. The essential difference lies in the relative magnitude of these two terms: in $\tilde{H}$ they were both large (of order BT); in $\tilde{H}_G$ the first is still of order BT, whereas the second does not depend on B and T any more.

Because of the similarity between $\tilde{H}_G$ and $\tilde{H}$ the Schrödinger equation for U_G can also be solved exactly by transforming the system to a rotating frame as explained above. The analytical expression obtained in this way reads

$$U_G(s) = \exp(-i\pi s\sigma_z)\exp\{i[\beta\sigma_z + (\pi\sin\theta)\sigma_x]s\}, \quad (23)$$

where $\beta = \varphi + \pi$. From the matrix form of the second exponential operator one further obtains the transition probability

$$P'_{\rm ex}(s) = \pi^2\sin^2\theta\sin^2\lambda s/\lambda^2, \quad (24)$$

where λ is the same as in Eq. (20). This formula was first derived by Rabi [23] and Schwinger [24]. It refers to transitions between the two eigenstates of the Hamiltonian that belong, respectively, to spin projections $\pm 1/2$ along the rotating magnetic field $\boldsymbol{B}(s)$. Accordingly, the probability $P'_{\rm ex}$ vanishes in the adiabatic limit.

In order to apply our approximation procedures, we start by integrating the diagonal part $\tilde{H}_0$ of $\tilde{H}_G$. To zero order, we substitute $U_G^{(I)} \simeq I$ in Eq. (8) and get the diagonal evolution operator of the adiabatic approximation (no transitions):

$$U_G(s) \simeq \exp(i\varphi s\sigma_z). \quad (25)$$

For $s = 1$ (one period) this gives

$$U_G(1) \simeq \exp\{-i[\gamma BT/2 + \pi(1-\cos\theta)]\sigma_z\}, \quad (26)$$

where the usual expressions for the dynamical and geometrical (Berry) phases are clearly recognized.

The next move is to build up the adiabatic interaction Hamiltonian of Eq. (10), which results in

$$\tilde{H}_G^{(I)}(s) = i\pi\sin\theta(\sigma_x\cos 2\beta s + \sigma_y\sin 2\beta s). \quad (27)$$

With this form, time integration is easily performed even in the higher orders of perturbation theory or of the Magnus expansion $\Omega = \sum_m \Omega_m$. Thus, up to third order, the perturbative approach leads to transition probabilities

$$P'_{p1} = P'_{p2} = q_1^2, \quad P'_{p3} = q_1^2[1 + (\pi\sin\theta/\beta)^2 g(s)]^2, \quad (28)$$

where $q_1 = \pi\sin\theta\sin\beta s/\beta$ and

$$g(s) = \frac{1}{2}(\beta s\cot\beta s - 1). \quad (29)$$

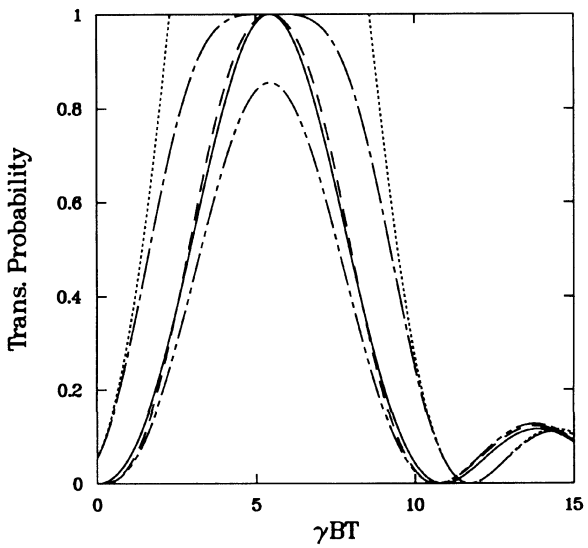

FIG. 1. Transition probability for a spin one-half system in a rotating magnetic field after one period as a function of γBT for $\theta = \pi/6$ (in the adiabatic picture). Solid line is the exact result; dash-dotted line denotes first-order Magnus approximation; dashed line denotes third-order Magnus approximation; dotted line denotes first-order perturbation theory; dash-double dotted line denotes third-order perturbation theory.

Similarly, the Magnus expansion to third order reads

$$\Omega_1 + \Omega_2 + \Omega_3 = i\boldsymbol{q}\boldsymbol{\sigma}, \tag{30}$$

where $\boldsymbol{q} = \boldsymbol{q}(s)$ has components

$$\begin{aligned} q_x &= (\pi \sin\theta/\beta) \sin\beta s \cos\beta s\,[1 + (\pi \sin\theta/\beta)^2 f(s)], \\ q_y &= (\pi \sin\theta/\beta) \sin^2\beta s\,[1 + (\pi \sin\theta/\beta)^2 f(s)], \\ q_z &= (\pi \sin\theta/\beta)^2 (\beta s - \sin\beta s \cos\beta s)/2, \end{aligned} \tag{31}$$

and $f(s) = g(s) + \frac{1}{6}\sin^2\beta s$. The corresponding approximate evolution operator is

$$U_G^{(I)}(s) \simeq \exp[i\boldsymbol{q}(s)\boldsymbol{\sigma}]. \tag{32}$$

This further yields for the transition probabilities to first and third order the following expressions:

$$P'_{M1}(s) = \sin^2 q_1, \quad P'_{M3}(s) = (q_x^2 + q_y^2)\sin^2 q/q^2, \tag{33}$$

where $q^2 = q_x^2 + q_y^2 + q_z^2$ and q_1, q_x, q_y, q_z have been defined above.

In Fig. 1 we compare all these approximations with the exact result of Eq. (24) for $s = 1$ (one complete rotation of the field) and $\theta = \pi/6$. The rapid numerical convergence of the Magnus expansion is quite remarkable. By contrast, it may be seen that with high-order perturbation theory, improvement is achieved only for the very small transition probabilities, in particular in the adiabatic regime. A similar situation prevails for other exactly solvable models [25].

We conclude with the hope that the arguments presented in this Brief Report offer sufficiently convincing evidence of the power of the Magnus expansion as a tool for approximately solving the time-dependent Schrödinger equation even farther away from the sudden limit.

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