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EXACT SOLUTIONS OF SCHRODINGER'S EQUATION FOR SPIN SYSTEMS IN A CLASS OF TIME-DEPENDENT MAGNETIC FIELDS*

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A spin system in a time variable magnetic field is considered. For certain fields there exists a frame in which the Hamiltonian becomes static. The criterion for such fields is derived. The unitary transformation that accomplishes this task is obtained and the underlying Schrodinger equation is solved exactly.

1. Introduction

Of interest in problems of NMR spectroscopy are solutions of Schrodinger's equation for a spin system in time-dependent magnetic fields. Exact solutions however, are available only for rotating fields (Rabi[1]) and fields of constant directions. On the other hand, several approximation methods, mainly of perturbation nature, have been developed. As early as 1954, Magnus[2] introduced time-evolution operators as exponential functions of certain anti-Hermitian operators. He then expanded the exponent as infinite series such that the nth term of the expansion was of nth order in the perturbation Hamiltonian. Magnus' expansion has a good prediction power for short time intervals. For larger intervals, however, its convergence has been questioned by Salzman.[3] Recently, Popescu and Popescu[4] have improved Magnus' method by dividing the time interval into smaller intervals and have increased the convergence of the exponential perturbation technique. Ford[5] has developed a method of averaging in which the slowly and rapidly varying terms in the expansion of a wave function are treated differently. The method has applicability for certain class of time-dependent fields. A significant number of investigators, notable among them Montogomery and Ruijgrok,[6] have developed quantum versions of the well reputed perturbation techniques of Krylov,[7] of Bogolyubov and Mitropolskii,[8] and of Frieman[9] for classical systems.

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In this paper we consider a spin $\frac{1}{2}$ particle in an initially unspecified magnetic field. In Sec. 2 we transform the Schrodinger equation into a frame in which the magnetic field appears planar for all times. In Sec. 3 we look for those unitary transformations that render the associated Hamiltonian time-independent. In the process a criterion for fields apt to become static emerges. Once this is achieved the Schrodinger equation becomes exactly solvable. In Sec. 4 we obtain the exact solution of Schrodinger's equation for such fields. In Sec. 5 we work out three examples in detail.

2. Transformation of Schrodinger's Equation to a Plane-form Field

Schrodinger's equation for a spin $\frac{1}{2}$ particle in an arbitrary magnetic field may be written as

$$i\hbar\,\frac{\partial\psi}{\partial t} = H_i(t)\sigma_i\psi\,, \quad i = 1,\,2,\,3\,. \tag{1}$$

where σ_i's are Pauli matrices, $H_i(t)$'s are proportional to field components and $\psi(t)$ is a two-component spinor.

By means of the unitary transformation

$$\psi(t) = e^{\frac{-i}{\hbar}\sigma_3\int_0^t H_3(\tau)d\tau}\phi(t)\,, \tag{2}$$

Eq. (1) transform into

$$i\hbar\,\frac{\partial\phi}{\partial t} = H_T(t)[\sigma_1\cos\alpha(t) + \sigma_2\sin_\alpha(t)]\phi\,, \tag{3a}$$

where

$$H_T(t) = (H_1^2 + H_2^2)^{\frac{1}{2}}\,, \tag{3b}$$

$$\alpha(t) = \beta(t) - \gamma(t)\,, \tag{3c}$$

$$\cos\beta(t) = \frac{H_1}{H_T}\,, \quad \sin\beta(t) = \frac{H_2}{H_T}\,, \tag{3d}$$

$$\gamma(t) = \frac{2}{\hbar}\int_0^t H_3(\tau)d\tau\,. \tag{3e}$$

Changing the variable t to $\alpha(t)$, Eq. (3a) becomes

$$i\hbar\,\frac{\partial\phi}{\partial\alpha} = \frac{H_T}{\dot\alpha}\,(\sigma_1\cos\alpha + \sigma_2\sin\alpha)\phi = \mathcal{H}(\alpha)\phi\,, \tag{4a}$$

where the second equality defines

$$\mathcal{H}(\alpha) = \mathcal{H}_1(\alpha)\sigma_1 + \mathcal{H}_2(\alpha)\sigma_2\,. \tag{4b}$$

The transformation from t to α is possible if and only if α is a monotonically increasing or decreasing function of t. It will be shown that this indeed is the case for the fields of our interest. The Hamiltonian of Eq. (4b) is seemingly that of a particle in a planar field. For $(H_T/\dot{\alpha}) =$ constant, the equation is of Rabi type and is immediately solvable. We shall however, come back to this point from a much wider point of view.

3. Transformation of Hamiltonian (4b) into a Static One

Let us suppose there exists a unitary operator $U(\alpha)$, which transforms $\mathcal{H}(\alpha)$ into an α-independent $\mathcal{H}'$. Thus,

$$\mathcal{H}' = U(\alpha)\mathcal{H}(\alpha)U^\dagger(\alpha)\,, \quad \mathcal{H}(\alpha) = U^\dagger \mathcal{H}' U\,. \tag{5}$$

Differentiating with respect to α gives

$$\frac{\partial \mathcal{H}}{\partial \alpha} = \frac{\partial U^\dagger}{\partial \alpha}\mathcal{H}' U + U^\dagger \mathcal{H}' \frac{\partial U}{\partial \alpha}\,. \tag{6}$$

From $UU^\dagger = 1$, one has $(\partial U/\partial \alpha)U^\dagger = -U(\partial U^\dagger/\partial\alpha)$. Eliminating $(\partial U^\dagger/\partial\alpha)$ in favour of $(\partial U/\partial\alpha)$ and substituting for $\mathcal{H}'$ in terms of $\mathcal{H}$ gives

$$\frac{\partial \mathcal{H}}{\partial \alpha} = i[\Omega(\alpha), \mathcal{H}(\alpha)]\,, \tag{7}$$

where we have used the notation

$$\Omega(\alpha) = iU^\dagger \frac{\partial U}{\partial \alpha} \quad \text{or} \quad \frac{\partial U}{\partial \alpha} = -iU\Omega\,. \tag{8}$$

For a given $\mathcal{H}$, Eq. (7) may be solvable for $\Omega(t)$. Equation (8) will then be a differential equation for $U(t)$.

Criterion for the existence of static hamiltonian

The Hamiltonian of Eq. (4b) is an expansion in Pauli matrices. The same could be assumed for $\Omega(\alpha)$,

$$\Omega(\alpha) = \Omega_i(\alpha)\sigma_i\,, \quad i = 1, 2, 3\,. \tag{9}$$

where $\Omega(\alpha)$'s are as yet unknown functions of α. Substituting Eqs. (4b) and (9) in Eq. (7) and using the commutation rules $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$, $\epsilon_{ijk} =$ Levi-Civita symbol, gives

$$\frac{\partial \mathcal{H}_i}{\partial \alpha} = 2\epsilon_{ijk}\mathcal{H}_j\Omega_k\,. \tag{10}$$

Multiplying Eq. (10) by $\mathcal{H}_i$ and summing over i gives

$$\mathcal{H}_i \frac{\partial H_i}{\partial \alpha} = 2\epsilon_{ijk}\mathcal{H}_i\mathcal{H}_j\Omega_k = 0\,, \tag{11a}$$

or

$$\mathcal{H}_i\mathcal{H}_i = \mathcal{H}_1^2 + \mathcal{H}_2^2 = \text{const.} = K^2\,. \tag{11b}$$

Substituting for $\mathcal{H}_i$ from the defining Eq. (4b) and using Eq. (11b) gives

$$H_T = K\dot{\alpha}\,. \tag{12}$$

Considering the fact that H_T is the magnitude of the magnetic field in the xy-plane and is non-negative, the monotonically increasing or decreasing nature of α with time becomes evident.

With the definitions of Eqs. (4b)–(4d), Eq. (12) becomes

$$\frac{2}{\hbar}\,H_3(t) = \frac{d}{dt}\cos^{-1}\frac{H_1}{H_T} - \frac{1}{K}\,H_T\,. \tag{13}$$

Equation (13) is a relation between the three components of the magnetic field. It is the criterion for the integrability of Schrodinger's equation. To elucidate the point let us consider the simple case of NMR fields $\mathbf{B}$: $[B_1\cos\omega t,\ B_1\sin\omega t,\ B_3(t)]$ where B_1 is constant. Equation (13) requires B_3 also to be constant. As a second example consider $\mathbf{B}$: $[af(t),\ bf(t),\ B_3(t)]$ which is a field whose projection in the xy-plane has a constant direction. From Eq. (13) one obtains $B_3(t) \propto f(t)$ that is the whole field has to have a constant direction in space. As the last example, consider $\mathbf{B}$: $[at,\ b,\ B_3(t)]$ where a, b are constant. Solving Eq. (13) for $B_3(t)$ gives $B_3(t) = -ab/(b^2+a^2t^2) = (1/K)(b^2+a^2t^2)^{1/2}$. The following section is devoted to derivation of $\Omega(t)$ and $U(t)$ for the field satisfying the criterion (13).

4. Solution of Schrodinger's Equation

Equation (10) is three-algebraic equation for Ω_k. Equation (11b), however, shows that they are not independent. Hence, one may choose any one of Ω_k's arbitrarily. In the following we choose Ω_2 equal to zero and solve Eq. (12) for Ω. Thus,

$$\Omega(\alpha) = \frac{1}{2\mathcal{H}_2}\left(\frac{\partial\mathcal{H}_1}{\partial\alpha}\right)\sigma_3 = -\frac{1}{2}\,\sigma_3\,. \tag{14}$$

In obtaining the second equality, Eqs. (4) and (12) have been used. Substituting Eq. (14) in Eq. (8) and solving for $U(\alpha)$ gives

$$U(\alpha) = e^{\frac{i}{2}\alpha\sigma_3} = \mathcal{I}\cos\frac{\alpha}{2} + i\sigma_3\sin\frac{\alpha}{2}\,, \tag{15}$$

where $\mathcal{I}$ is the unit matrix. Transforming Eq. (4a) by $U(\alpha)$ after some algebra one obtains

$$i\hbar\,\frac{\partial\phi'}{\partial\alpha} = \left(K\sigma_1 - \frac{\hbar}{2}\,\sigma_3\right)\phi'\,, \tag{16a}$$

$$\phi' = U\phi\,. \tag{16b}$$

To obtain the solution of the original Schrodinger's Eq. (1), one takes the following steps. One solves Eq. (16a) for ϕ' with a given initial value $\phi'(0) = \phi(0) = \psi(0)$, gets ϕ from Eqs. (16b) and (15), and $\psi(t)$ from Eq. (2). The final result, using Eqs. (3c)–(3e), becomes

$$\psi(t) = e^{\frac{-i}{2}\beta(t)\sigma_3} e^{\frac{-i}{2}\alpha(t)(\frac{2K}{\hbar}\sigma_1 - \sigma_3)}\psi(0). \tag{17}$$

This completes our discussion of the exactly solvable spin-$\frac{1}{2}$ problems in variable magnetic fields. The case of higher spins are also worked and will be presented elsewhere. In the next section we give two examples on the way of illustration.

5. Examples

Three cases are treated here. 1) The standard rotating magnetic field of NMR and a reproduction of Rabi's solution. 2) Damped rotating field. 3) A planar field with constant component in one direction. The last one is only of academic value and is intended to show the range of applicability of the method.

5.1. *Rotating field, B* : $(B_1 \cos\ \omega t,\ B_1 \sin\omega t,\ B_0)$

With B_1 and B_0 constant, the field satisfies the criterion (13). By Eq. (12) α is proportional to t. From Eqs. (13), (12) and (3d), one obtains $K = (\hbar/2)[\omega_1/(\omega - \omega_0)]$, $\alpha(t) = (\omega - \omega_0)t$ and $\beta(t) = \omega t$. Equation (17) immediately gives

$$\psi(t) = e^{\frac{-i}{2}\omega t\sigma_3} e^{\frac{-i}{2}[\omega_1\sigma_1 + (\omega_0 - \omega)\sigma_3]t}\psi(0), \tag{18}$$

where $\omega_1 = \gamma\beta_1$, $\omega_0 = \gamma B_0$ and $\gamma =$ gyromagnetic ratio. This is Rabi's solution.

5.2. *Damped rotating field, B* : $[B_1 e^{-\lambda t}\cos\omega t,\ B_1 e^{-\lambda t}\sin\omega t,\ B_0 + \left(\frac{\omega}{\gamma} - B_0\right)(1 - e^{-\lambda t})]$

With λ constant, this field satisfies the criterion (13), which in the case of $\lambda \to 0$ becomes Rotating field. As with Rotating field (5.1), we have, $k = (\hbar/2)\,[\omega_1/(\omega - \omega_0)]$, $\alpha(t) = (1 - e^{-\lambda t}/\lambda)(\omega - \omega_0)$ and $\beta(t) = \omega t$. From Eq. (17) we obtain

$$\psi(t) = e^{\frac{-i}{2}\omega t\sigma_3} e^{\frac{-i}{2}\frac{1 - e^{-\lambda t}}{\lambda}[\omega_1\sigma_1 + (\omega_0 - \omega)\sigma_3]}\psi(0). \tag{19}$$

As an application, we may calculate the probability that a spin which is up at time $t = 0$ will be down at time t. This probability is:

$$\begin{aligned} P\left(-\frac{1}{2}, \frac{1}{2}\right) &= \left|(0,\,1)e^{\frac{-i}{2}\omega t\sigma_3} e^{\frac{-i}{2}\frac{1 - e^{-\lambda t}}{\lambda}[\omega_1\sigma_1 + (\omega_0 - \omega)\sigma_3]}\begin{pmatrix}1\\0\end{pmatrix}\right|^2 \\ &= \frac{\omega_1^2}{\omega_1^2 + (\omega - \omega_0)^2}\sin^2\frac{1 - e^{-\lambda t}}{2\lambda}[\omega_1^2 + (\omega - \omega_0)^2]^{\frac{1}{2}}. \end{aligned} \tag{20}$$

In the limit of $\lambda \to 0$ we obtain the Rabi result.

5.3. *B(t)* : $B[f(t),\,1,\,0]$

This is a field with a constant y component and a variable and, as yet, unknown x component, $Bf(t)$. Substituting the field in Eq. (13) gives $f(t) = -at/(1 - a^2t^2)^{1/2}$

where a is an arbitrary but nonzero constant and $0 < t < a^{-1}$. Substituting this field in Eq. (17) and using Eqs. (3d) and (12) gives

$$\psi(t) = e^{\frac{-i}{2}(\sin^{-1} at)\sigma_3} e^{\frac{-i}{2}(\sin^{-1} at)(\frac{\omega}{a}\sigma_1 - \sigma_3)} \psi(0) , \tag{21}$$

where $\omega = \gamma B$.

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