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

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The case of a quantum two-level system coupled to a time variable magnetic field is investigated. The Schrodinger equation pertaining to the system is reduced to a second order linear equation in time and its solutions are sought by an integrating factor technique. A differential equation for the integrating factor and, therefrom, a criterion for fields leading to exact solutions are derived. The formalism is capable of giving a wide variety of closed form radio frequency (RF) wave forms for which Schrodinger's equation is exactly solvable.

1. Introduction

Of interest to NMR spectroscopy are solutions of Schrodinger's equation for spin systems with time dependent external coupling. The need for such solutions is hastened with the development of magnetic resonance imaging (MRI). Several approximation methods of perturbative nature and some numerical methods have been developed. The exponential perturbation series of Magnus[1] is good for short time intervals. Its convergence for longer times, however, has been questioned by Salzman.[2] Improvement to Magnus's method is worked out by Popescu and Popescu.[3] Ford[4] has introduced a method of averaging in perturbation theory. Montogomery and Ruijgrok,[5] have developed and used the quantum versions of the classical perturbation techniques of Krylov and Bogolyubov[6] and of Bogolyubov and Mitropolskii.[7] In numerical approaches, McCurdy, Stroud, and Wisinski[8] have extended complex coordinate techniques of scattering theory to time dependent Schrodinger's equation. They use Simon's[9] exterior scaling contour. Sen Gupta[10] explores the relationship between the classical and quantum mechanical problems of precession in magnetic fields. He generates a host of nonequivalent state functions once one is known.

Exact solutions have also been sought. The integrability of Schrodinger's equation for fields of constant direction is well known. For rotating fields the problem is solved by Rabi.[11] Recently Dutta, Ghosh, and Engineer[12] have studied the exact integrability of spin-1/2 systems. By means of an auxiliary function they produce

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exact solutions by standard techniques of Hamiltonian dynamics. Their auxiliary function, however, should satisfy a simplifying differential equation which, in general, they solve by perturbation techniques. Carlson[13] uses inverse scattering techniques to find RF fields capable of producing desired selective excitation profiles. He is successful in giving some closed RF pulses, for which Schrodinger's equation is exactly solvable. He does not, however, give these solutions. In paper 1,[14] we introduced a frame in which an RF field became planar and a second frame in which the field and consequently the Hamiltonian became static. This led to a criterion for a class of fields that Schrodinger's equation for them was exactly solvable.

Here we relax the condition of staticity and arrive at a wider class of exactly solvable problems. In Sec. 2 we consider a spin-1/2 system in an arbitrary time dependent magnetic field. We transform Schrodinger's equation into a frame in which the corresponding field appears planar for all times. In Sec. 3 we choose a frame in which the new wave equation becomes a second order one in time with a diagonalized complex Hamiltonian. In Sec. 4 we consider the integrability of this equation. We arrive at two criteria, one for the integrating factor and the other for the RF field. The class of RF fields found here is much wider than that of paper 1. In Sec. 5 we treat few examples on the way of illustration.

2. Transformation to a Planar Field

Time evolution of a two level (spin-1/2) system in a time dependent magnetic field is given by

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

$$H_i(t) = -\frac{1}{2}\hbar\gamma B_i(t)\,, \tag{1b}$$

where σ's are Pauli matrices, $\psi(t)$ is a two-component spinor, $\gamma =$ gyromagnetic ratio and $B_i(t)$ are the magnetic field components. By a rotation around the y-axis one may write

$$\phi(t) = e^{-\frac{i}{\hbar}\sigma_2\int^t H_2(\tau)d\tau}\psi(t)\,. \tag{2}$$

Substitution in Eq. (1a) gives

$$i\hbar\frac{\partial\phi}{\partial t} = H_{\rm T}(t)[\sigma_3\cos\,\alpha(t) + \sigma_1\sin\alpha(t)]\phi\,, \tag{3a}$$

where

$$H_{\rm T}(t) = (H_1^2 + H_3^2)^{\frac{1}{2}}\,, \tag{3b}$$

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

$$\cos\beta(t) = \frac{H_3}{H_{\rm T}}\,, \quad \sin\beta(t) = \frac{H_1}{H_{\rm T}}\,, \tag{3d}$$

$$\theta(t) = \frac{2}{\hbar}\int^t H_2(\tau)d\tau\,. \tag{3e}$$

By a change of variable t to $\alpha(t)$, we get

$$i\,\frac{\partial\phi}{\partial\alpha} = g(\alpha)[\sigma_3\cos\alpha + \sigma_1\sin\alpha]\phi\,, \tag{4a}$$

$$g(\alpha) = \frac{H_{\mathrm{T}}}{\hbar\dot{\alpha}}\,,\quad \dot{\alpha} = \frac{d\alpha}{dt}\,. \tag{4b}$$

The transformation from t to $\alpha(t)$ should be single valued and nonsingular. This requires α to be a monotonically increasing or decreasing function of t and $\dot{\alpha} \neq 0$. As we shall see shortly, this imposes a constraint on the RF fields. Equation (4a) has the form of Schrodinger's equation for a particle in a planar field. Choosing $g(\alpha)$ = constant specifies a class of fields for which the wave equation is of Rabi type and is exactly solvable.[14] The case of variable $g(\alpha)$ is treated below.

3. Transformation of Equation (4a) into a Second Order One

By means of the unitary transformation

$$\chi = e^{\frac{i}{2}\sigma_2\alpha}\phi = \left(\mathbf{I}\cos\frac{\alpha}{2} + i\sigma_2\sin\frac{\alpha}{2}\right)\phi\,, \tag{5}$$

Eq. (4a) transforms into

$$i\,\frac{\partial\chi}{\partial\alpha} = \left[\sigma_3 g(\alpha) - \frac{1}{2}\sigma_2\right]\chi\,, \tag{6}$$

where $\mathbf{I}$ is the unit matrix. Taking another α-derivative of Eq. (6), eliminating $\partial\chi/\partial\alpha$ by Eq. (6) itself, and noting that $\sigma_i^2 = 1$, $\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k$, gives

$$-\chi_{\alpha\alpha} + V(\alpha)\chi = \frac{1}{4}\chi\,, \tag{7a}$$

$$V(\alpha) = -(g^2\mathbf{I} + i\sigma_3 g_\alpha)\,, \tag{7b}$$

where a subscript α denotes a derivative with respect to α. Equation (7a) consists of two uncoupled linear differential equations of second order one for each component of spinor χ. The two equations are complex conjugates of each other. Each of them has the form of Schrodinger's equation in which the eigenvalue is 1/4, α plays the role of a one dimensional space coordinate, and the potential $V(\alpha)$, given by Eq. (7b), is complex. If desired, these equations can be solved by approximation methods. In the following, however, we aim at their exact solutions.

4. Integrability of Equation (7a)

Let

$$\eta = e^{i\sigma_3\int^\alpha g(x)dx}\chi\,. \tag{8}$$

Equation (7a) becomes

$$\eta_{\alpha\alpha} - 2i\sigma_3 g(\alpha)\eta_\alpha + \frac{1}{4}\eta = 0\,. \tag{9a}$$

Let us denote the upper and lower components of the spinor η by η^1 and η^2, respectively. The equation for η^1 is

$$\eta^1_{\alpha\alpha} - 2ig(\alpha)\eta^1_\alpha + \frac{1}{4}\eta^1 = 0. \tag{9b}$$

The equation for η^2 is the complex conjugate of that of η^1. Thus, $\eta^2 = \eta^{1*}$. Assume $P(\alpha)$ is an integrating factor for Eq. (9a). That is, the expression

$$P(\alpha)[\eta^1_{\alpha\alpha} - 2ig(\alpha)\eta^1_\alpha + \frac{1}{4}\eta^1],$$

is an exact differential in α of the form

$$\frac{d}{d\alpha}\left[P\eta^1_\alpha + \frac{1}{4}(\textstyle\int^\alpha P\,dx)\eta^1\right] = 0. \tag{10}$$

Comparing Eq. (10) with Eq. (9b) gives

$$-2ig(\alpha) = \frac{P_\alpha + \frac{1}{4}\int^\alpha P\,dx}{P}. \tag{11}$$

Equation (10) gives

$$P\eta^1_\alpha + \frac{1}{4}(\textstyle\int^\alpha P\,dx)\eta^1 = C_1 = \text{constant}. \tag{12}$$

Equation (12) is a first order equation. Once P is known, its solution is

$$\eta^1 = U(\alpha)\left(C_1\int^\alpha \frac{U^{-1}(x)}{P(x)}\,dx + C_2\right), \tag{13a}$$

$$U(\alpha) = e^{-\int^\alpha \frac{\int^x P(y)dy}{4P(x)}\,dx}, \tag{13b}$$

where C_1 and C_2 are to be determined from initial values. The transformation from Eqs. (7) to Eqs. (9) has an exceedingly simplifying feature. Because the only α-dependent coefficient in Eqs. (9) is that of η_α. The integrating factor method gives all possible exact solutions without any loss.

The integrating factor $P(\alpha)$ is, in general, complex. Let

$$\int^\alpha P(x)dx = S(\alpha)e^{if(\alpha)}. \tag{14}$$

From Eq. (4a), however, $g(\alpha)$ is real. Therefore, substituting Eq. (14) in Eq. (11) and separating the real and imaginary part of the resulting expression gives

$$(1 + 4f_\alpha^2)S^2 + 4S_\alpha^2 = K^2 = \text{constant}, \tag{15a}$$

$$g(\alpha) = -f_\alpha + \left[2S_\alpha^2\frac{d}{d\alpha}\left(\frac{Sf_\alpha}{S_\alpha}\right) - \frac{K^2}{2}f_\alpha\right]/(S^2 - K^2). \tag{15b}$$

The remaining task is the following:

- For an arbitrary choice of S and K, one solves Eq. (15a) for $f(\alpha)$ and then Eq. (14) for $\int^{\alpha} P(x)dx$ and $P(\alpha)$.
- One substitutes the results in Eq. (15b) and obtains $g(\alpha)$.
- One assigns an arbitrary single-valued and continuous function of time to $\alpha(t)$ and uses Eq. (4b) to get $H_{\mathrm{T}}(t)$.
- One chooses $\theta(t)$ arbitrarily and uses Eq. (3e) to obtain the y-component of the field.
- Finally one employs Eq. (3d) to obtain the other components of RF fields.

The freedom of choices in first, second and fourth steps enables one to produce enormously wide classes of RF fields.

The solution of original Eq. (1a) for $\psi(t)$ as obtained from Eqs. (2), (3c), (5), (8) and (13) is

$$\psi(t) = e^{-\frac{i}{2}\sigma_2\beta(t)} e^{-i\sigma_3\int^{\alpha} g\,dx} \begin{bmatrix} U(\alpha)\left(C_1\int^{\alpha}\frac{U(x)^{-1}}{P(x)}\,dx + C_2\right) \\ U^*(\alpha)\left(C_1^*\int^{\alpha}\frac{U(x)^{*-1}}{P^*(x)}\,dx + C_2^*\right)\end{bmatrix}, \tag{16}$$

where C_1 and C_2 are specified by initial conditions. Equation (16) is the complete and exact solution.

5. Examples

To create integrable RF field we choose $\int^{\alpha} P\,dx = S(\alpha)e^{if(\alpha)}$ arbitrarily and proceed through the steps outlined in the closing paragraphs of Sec. 4.

5.1. *Cases of* $S(\alpha)e^{if(\alpha)} = ae^{ib\alpha}$

Substituting this in Eq. (15b) we find $g(\alpha) = C =$ constant. The state function for this case as obtained from Eq. (6) or (16) is

$$\psi(t) = e^{\frac{-i}{2}\beta(t)\sigma_2} e^{\frac{-i}{2}\alpha(t)(2C\sigma_3-\sigma_2)}\psi(0)\,. \tag{17}$$

Many field configurations can be constructed by the arbitrary choice of β and α. For example, the choice of $\alpha = (\omega - \omega_0)t$, $\beta = \omega t$ and $C = \omega_1/2(\omega_0 - \omega)$ leads through Eqs. (3) and (1b) to the rotating field,

$$\mathbf{B} : (B_1 \sin \omega t,\, B_0,\, B_1 \cos \omega t)\,, \tag{18}$$

where $\omega_0 = \gamma B_0$ and $\omega_1 = \gamma B_1$. Further examples in this category can be found in paper 1.

5.2. *Cases of* $S(\alpha)e^{if(\alpha)} = (\sin\alpha/2)e^{2i\ln\tan\alpha/4}$, $K = \sqrt{5}$

This expression already satisfies Eq. (15a). Substituting in Eq. (15b) gives $g(\alpha) = -1/(2\sin\alpha/2)$. The state function for this case, as given by Eq. (16), is

$$\psi(t) = e^{\frac{-i}{2}\sigma_2\beta(t)} e^{i\sigma_3\ln\tan\alpha/4} \begin{bmatrix} (2i + \cos\frac{\alpha}{2})\,(C_1h(\alpha) + C_2) \\ (-2i + \cos\frac{\alpha}{2})\,(C_1^*h^*(\alpha) + C_2^*)\end{bmatrix}, \tag{19}$$

where

$$h(\alpha) = \int^{\alpha} \frac{e^{-2i \ln \tan \frac{x}{4}}}{\left(2i + \cos \frac{x}{2}\right)^2}\, dx\,.$$

Again a rich variety of RF field can be accomodated in this class. For example choosing $\alpha = -2\sin^{-1}(1 + \lambda^2 t^2)^{-1/2}$ and $\beta = 0$, Eqs. (3) give the following time decaying pulses.

$$\mathbf{B} : \left(0, \frac{B}{1 + \lambda^2 t^2}, \frac{B}{2\sqrt{1 + \lambda^2 t^2}}\right), \tag{20}$$

where $B = 2\lambda/\gamma$.

A case of common interest is a magnetic field consisting of two parts: a static component directed along the z-axis, and a time varying component along the y-direction, say. For this purpose one may choose $\alpha = -\theta = 2\sin^{-1} U(t)$, where $U(t)$ is as yet unspecific. Using Eqs. (3b)–(3e) and the constancy of the z-component of the field we obtain $U(t) = (\cosh \omega t/2)^{-1}$. The corresponding field becomes

$$\mathbf{B} : \left(0, \frac{B}{\cosh \omega t/2}, B\right), \tag{21}$$

where $\omega = \gamma B$. This is the field that Carlson[13] obtains by his inverse scattering technique.

5.3. *Cases of* $S(\alpha)e^{if(\alpha)} = (\sin\alpha/2\sqrt{2})e^{-i \ln \sin \alpha/2\sqrt{2}})$, $K = 1$

In Eq. (15a) we choose $S(\alpha) = \sin(\alpha/2\sqrt{2})$, $K = 1$ and obtain $f(\alpha) = -\ln \sin(\alpha/2\sqrt{2})$. Substituting this in Eq. (15b) gives $g(\alpha) = (1/2\sqrt{2})\cot(\alpha/\sqrt{2})$. From Eq. (16) the state of system is

$$\psi(t) = e^{-\frac{i}{2}\sigma_2\beta(t)} e^{-\frac{i}{2}\sigma_3 \ln \sin \alpha/\sqrt{2}} \begin{bmatrix} \left(\cos \frac{\alpha}{\sqrt{2}}\right) e^{i \ln \cos \frac{\alpha}{2}} (C_1 h(\alpha) + C_2) \\ \left(\cos \frac{\alpha}{\sqrt{2}}\right) e^{-i \ln \cos \frac{\alpha}{\sqrt{2}}} (C_1^* h^*(\alpha) + C_2^*) \end{bmatrix}, \tag{22}$$

where

$$h(\alpha) = \int^{\alpha} \frac{e^{i \ln \tan \frac{x}{2\sqrt{2}}}}{\cos^2 \frac{x}{2\sqrt{2}}}\, dx\,.$$

We recall that two of the variables α, β, and θ are arbitrary. The choice of $\alpha = \sqrt{2}\cot^{-1} e^{-\lambda t}$ and $\theta = \omega t - \alpha$ gives an oscillating and decaying RF field with three components,

$$\mathbf{B} : \left(\frac{B_1 e^{-\lambda t}}{\cosh \lambda t} \sin \omega t, \frac{\sqrt{2}\, B_1}{\cosh \lambda t} - B, \frac{B_1 e^{-\lambda t}}{\cosh \lambda t} \cos \omega t\right), \tag{23}$$

where $\lambda = 2\gamma B_1$ and $\omega = \gamma B$.

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