Magnetic resonance in an elliptic magnetic field

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Abstract

The behaviour of a particle with a spin 1/2 and a dipole magnetic moment in a time-varying magnetic field in the form $(h_0 \text{cn}(\omega t, k), h_0 \text{sn}(\omega t, k), H_0 \text{dn}(\omega t, k))$, where $\omega$ is the driving field frequency, $t$ is the time, $h_0$ and $H_0$ are the field amplitudes, $\text{cn}$, $\text{sn}$, $\text{dn}$ are Jacobi elliptic functions, $k$ is the modulus of the elliptic functions has been considered. The variation parameter $k$ from zero to 1 gives rise to a wide set of functions from trigonometric shapes to exponential pulse shapes modulating the field. The problem was reduced to the solution of general Heun’ equation. The exact solution of the wave function was found at resonance for any $k$. It has been shown that the transition probability in this case does not depend on $k$. The present study may be useful for analysis interference experiments, improving magnetic spectrometers and the field of quantum computing.

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1 Introduction

Rabi [1] studied the temporal dynamics of a particle featuring a dipole magnetic moment $\frac{1}{2}$ in a constant magnetic field $H_0$, directed along the $z$-axis, and another varying magnetic field $H_x = h_0 \cos \omega t$, $H_y = h_0 \sin \omega t$ rotating with a frequency $\omega$ perpendicular to $H_0$ ($H_0$, $h_0$ are the amplitudes). There are several methods of modulating magnetic fields while studying the phenomenon of magnetic resonance [2]. This work focuses on the temporal evolution of a particle with a dipole magnetic moment in a distorted magnetic field described by $\vec{H}(t) = (h_0 \text{cn}(\omega t, k), h_0 \text{sn}(\omega t, k), H_0 \text{dn}(\omega t, k))$. Such field modulation under a changing modulus $k$ of the elliptic functions from zero to unity describes an entire class of field shapes from trigonometric [1] to pulsed exponential [3, 4].

The Schrödinger equation of a wave function $\Psi(t)$ that describes the dynamics of a particle featuring a spin of $\frac{1}{2}$ and a magnetic moment in a time-varying magnetic field $\vec{H}(t)$ is given

$$i\hbar \partial_t \Psi(t) = \frac{g \mu_0}{2} \vec{\sigma} \vec{H}(t) \Psi(t),$$

where $g$ is the Lande factor, $\mu_0$ is the Bohr magneton, and the Pauli matrices are

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) = \left( \begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{array} \right).$$

The solution to the Schrödinger equation could be found by expanding in eigenfunctions of matrix $\sigma_z$

$$\Psi(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Psi_1(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Psi_2(t).$$

Functions $\Psi_1(t)$ and $\Psi_2(t)$ describe the probability amplitudes without a spin flip and with one, respectively, and by definition obey the normalization restriction

$$|\Psi_1(t)|^2 + |\Psi_2(t)|^2 = 1$$

and are assumed to be defined at the initial time $t$.

Considering the condition (2), Eq. (1) takes form

$$i\partial_t \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix} = \begin{pmatrix} H \text{dn}(\omega t, k) & h(\text{cn}(\omega t, k) + i\text{sn}(\omega t, k)) \\ h(\text{cn}(\omega t, k) - i\text{sn}(\omega t, k)) & -H \text{dn}(\omega t, k) \end{pmatrix} \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix},$$

$$H = \frac{g \mu_0 H_0}{2\hbar}, \quad h = \frac{g \mu_0 h_0}{2\hbar}.$$
2 Independence of resonance on modulus $k$

Let us turn to a dimensionless independent variable $\tau = \omega t$ and substitute the dependent variables:

$$
\begin{pmatrix}
\Psi_1(\tau) \\
\Psi_2(\tau)
\end{pmatrix} =
\begin{pmatrix}
f & 0 \\
0 & f^*
\end{pmatrix}
\begin{pmatrix}
\varphi_1(\tau) \\
\varphi_2(\tau)
\end{pmatrix},
$$

(6)

where

$$
f = \sqrt{cn\tau - isn\tau} = \sqrt{\frac{1 + cn\tau}{2}} - isign \left( \sqrt{1 - \frac{cn\tau^2}{2}} \right).
$$

(7)

The system in (4) takes on a different form through change in (6)

$$
i\partial_{\tau} \begin{pmatrix}
\varphi_1(\tau) \\
\varphi_2(\tau)
\end{pmatrix} =
\begin{pmatrix}
\hat{\omega}dn\tau & \frac{\Delta}{\omega} \\
\frac{\Delta}{\omega} & -\hat{\omega}dn\tau
\end{pmatrix}
\begin{pmatrix}
\varphi_1(\tau) \\
\varphi_2(\tau)
\end{pmatrix},
$$

(8)

in which detuning $\Delta$ is

$$
\Delta = H - \frac{\omega}{2}.
$$

(9)

The system in (8) may become similar to one studied by Shirley [5] through a time independent orthogonal transformation $\begin{pmatrix}\sqrt{2} & \sqrt{2} \\
\sqrt{2} & -\sqrt{2}\end{pmatrix}$.

Let us note the mechanical-geometrical analog of the system in (8) while presenting the unknown functions as $\varphi_1(\tau) = x + iy$, $\varphi_2(\tau) = u + iv$, where $x$, $y$, $u$, $v$ are real functions that are defined at the initial time and satisfy a non-linear system of differential equations with constant coefficients:

$$
x^2 + y^2 + u^2 + v^2 = 1,
$$

(10)

$$
v\partial_{\tau} x - u\partial_{\tau} y + y\partial_{\tau} u - x\partial_{\tau} v = \frac{h}{\omega},
$$

(11)

$$
(\partial_{\tau} x)^2 + (\partial_{\tau} y)^2 + (\partial_{\tau} u)^2 + (\partial_{\tau} v)^2 + \frac{\Delta^2 k^2}{\omega^2}sn^2(\tau, k) = \frac{h^2 + \Delta^2}{\omega^2},
$$

(12)

$$
y\partial_{\tau} x - x\partial_{\tau} y + u\partial_{\tau} v - v\partial_{\tau} u = \frac{\Delta}{\omega}dn(\tau, k),
$$

(13)
which describe the motion of a 4-vector \((x, y, u, v)\) along the spherical surface (10) under two conservation restrictions (11), (12).

The equation which is required to determine function \(\varphi_2(\tau)\) could be found from the system (8)

\[
\partial_{\tau\tau}\varphi_2(\tau) + \left(\frac{i}{\omega} \Delta k^2 sn^2 n_\tau - \frac{\Delta^2}{\omega^2} k^2 sn^2 \tau + \frac{\Omega^2_R}{\omega^2}\right) \varphi_2(\tau) = 0,
\]

where

\[
\Omega^2_R = h^2 + \Delta^2,
\]

and is presented as a generalized Lame equation in the Jacobi form.

Eq. (14) shows that the real \(u\) and the imaginary \(v\) components of function \(\varphi_2(\tau)\) define a gyroscopic system with a parametric excitation of its intrinsic frequency \(\frac{h}{\omega}\) [6].

Let \(f_1(\tau)\) and \(f_2(\tau)\) become a fundamental system that defines a general solution to Eq. (14)

\[
\varphi_2(\tau) = Af_1(\tau) + Bf_2(\tau),
\]

where \(A, B\) are arbitrary constants. The solution of the Cauchy problem (1) could be expressed through functions \(f_1(\tau)\) and \(f_2(\tau)\) using the initial conditions \((\Psi_1(0) \quad \Psi_2(0))\) as

\[
\begin{pmatrix}
\Psi_1(\tau) \\
\Psi_2(\tau)
\end{pmatrix} =
\begin{pmatrix}
f_0 \\
f^*_0
\end{pmatrix}
\begin{pmatrix}
a_{11}F_1 + b_1F_2 \\
a_{21}F_1 + b_2F_2
\end{pmatrix}
\begin{pmatrix}
\Psi_1(0) \\
\Psi_2(0)
\end{pmatrix},
\]

where

\[
F_{1,2} = \frac{i\partial_\tau f_{1,2} + \frac{\Delta}{\omega} f_{1,2}d\tau}{\frac{h}{\omega}}, a_1 = \frac{f_2(0)}{d}, a_2 = \frac{F_2}{d}|_{\tau=0},
\]

\[
b_1 = -\frac{f_1(0)}{d}, b_2 = \frac{F_1}{d}|_{\tau=0}, \frac{h}{\omega}d = -i(f_1\partial_\tau f_2 - f_2\partial_\tau f_1)|_{\tau=0}.
\]

Assuming that the wave function \((\Psi_1(0) \quad \Psi_2(0))\) is equal to \((1 \quad 0)\) at the initial time, the solution for the wave function (17) at time \(\tau\) is given by

\[
\begin{pmatrix}
\Psi_1(\tau) \\
\Psi_2(\tau)
\end{pmatrix} =
\begin{pmatrix}
f \\
f^*
\end{pmatrix}
\begin{pmatrix}
a_{11}F_1 + b_1F_2 \\
a_{21}F_1 + b_2F_2
\end{pmatrix}.
\]

4
The probability of a transition requiring a spin flip over time $\tau$ is

$$P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta, k) = |a_1 f_1 + b_1 f_2|^2. \quad (20)$$

Thus, the formula describing the transition probability could be expressed through functions $f_1(\tau), f_2(\tau)$ using the formulae in (18) and (20) as

$$P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta, k) = \frac{h^2}{\omega^2} \left| \frac{f_1(\tau) f_2(0) - f_2(\tau) f_1(0)}{(f_1(\tau) \partial_\tau f_2(\tau) - f_2(\tau) \partial_\tau f_1(\tau))|_{\tau=0}} \right|^2. \quad (21)$$

The Rabi result [1] provided by Eq. (14) at $k = 0$ stipulates that $f_1(\tau) = \cos \frac{\Omega R}{\omega} \tau$, $f_2(\tau) = \sin \frac{\Omega R}{\omega} \tau$, and the transition probability is

$$P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta = 0, k = 0) = \frac{h^2}{\Omega^2 R} \sin^2 \frac{\Omega R}{\omega} \tau. \quad (22)$$

Eq.(14) is simplified at $0 \leq k \leq 1$ in case of a sharp fundamental resonance with $\Delta = 0$:

$$\partial_\tau \varphi_2(\tau) + \frac{h^2}{\omega^2} \varphi_2(\tau) = 0. \quad (23)$$

Therefore, $f_1(\tau, \Delta = 0, k) = \cos \frac{\hbar}{\omega} \tau$, $f_2(\tau, \Delta = 0, k) = \sin \frac{\hbar}{\omega} \tau$ and Eq. (19) is solved explicitly

$$\begin{pmatrix} \psi_1(\tau) \\ \psi_2(\tau) \end{pmatrix} = \begin{pmatrix} f \cos \frac{\hbar}{\omega} \tau \\ -i f^* \sin \frac{\hbar}{\omega} \tau \end{pmatrix}. \quad (24)$$

Obviously, the transition probability is independent of the $k$ modulus and given by

$$P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta = 0, 0 \leq k \leq 1) = \sin^2 \frac{\hbar}{\omega} \tau. \quad (25)$$

The fundamental resonance is stable at any value of the $k$ modulus with respect to consistent variations of the longitudinal and traversal magnetic fields. In other words, a distortion in the traversal field is fully compensated by a corresponding distortion in the longitudinal field.

Knowing the wave function in (24) makes it possible to find the polarization vector $\vec{P}$ defined by

$$P_i = (\Psi(t) \sigma_i \Psi(t)) \quad (i = x, y, z). \quad (26)$$

A simple calculation produces

$$\vec{P} = (\text{sn}\gamma_m H_0 t \sin \gamma_m h_0 t, -\text{cn}\gamma_m H_0 t \sin \gamma_m h_0 t, \cos \gamma_m h_0 t). \quad (27)$$
The polarization vector satisfies the Bloch equation

\[ \partial_t \vec{P} = \gamma_m [\vec{H}, \vec{P}], \quad \gamma_m = \frac{g\mu_0}{\hbar}. \tag{28} \]

### 3 Reduction to Heun equation

A general case where both the detuning (9) and the modulus of the elliptical functions are different from zero requires changing the variable in Eq. (14) and taking advantage of the doubly periodicity of the elliptical functions.

It is known that

\[ \text{sn}(\tau' + iK') = \frac{1}{k\text{sn}\tau}, \quad \text{cn}(\tau' + iK') = -i \frac{d\text{n}\tau'}{k\text{sn}\tau'}, \quad 0 < k < 1, \tag{29} \]

where the full elliptical integral of the first kind \( K' \) is

\[ K' = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1 - k'^2 \sin^2 \varphi}} d\varphi, \quad k^2 + k'^2 = 1. \tag{30} \]

Let us switch to a half-variable in functions \( \text{sn}\tau', \text{dn}\tau' \) using

\[ \text{sn}\tau' = \frac{2\text{sn}\frac{\tau'}{2} \text{cn}\frac{\tau'}{2} \text{dn}\frac{\tau'}{2}}{1 - k^2 \text{sn}^4\frac{\tau'}{2}}, \quad \text{dn}\tau' = \frac{d\text{n}\frac{\tau'}{2} - k^2 \text{sn}^2\frac{\tau'}{2} \text{cn}^2\frac{\tau'}{2}}{1 - k^2 \text{sn}^4\frac{\tau'}{2}} \tag{31} \]

and introducing a new independent variable

\[ z = \text{sn}^2\frac{\tau'}{2} = \frac{k^{-\frac{1}{2}} (1 + k) \text{sn}\frac{\tau}{2} - i \text{cn}\frac{\tau}{2} \text{dn}\frac{\tau}{2}}{1 + k \text{sn}^2\frac{\tau}{2}}, \tag{32} \]

we arrive at the algebraic form of an equation for function \( \varphi_2(\tau) \equiv y(z) \) after simple transformations:

\[ \partial_{zz} y + \left( \frac{A_1}{z} + \frac{A_2}{z - 1} + \frac{A_3}{z - k^2} \right) \partial_z y + \left( \frac{B_1}{z^2} + \frac{B_2}{(z - 1)^2} + \frac{B_3}{(z - k^2)^2} + \frac{C_1}{z} + \frac{C_2}{z - 1} + \frac{C_3}{z - k^2} \right) y = 0, \tag{33} \]
where

\[ A_1 = A_2 = A_3 = \frac{1}{2}, \quad B_1 = B_2 = a - b, \quad B_3 = -(a + b), \]

\[ a = \frac{\Delta}{4\omega}, \quad b = \frac{\Delta^2}{4\omega^2}. \]  

(34)

\[ C_1 = 2(a - b) - 2bk^2 + \frac{\Omega_R^2}{\omega^2}, \]

(35)

\[ C_2 = -2(a - b) - (a + b) + \frac{1}{k^2 - 1}[a(k^2 - 1) - b(k^2 + 1) + \frac{\Omega_R^2}{\omega^2}], \]

(36)

\[ C_3 = k^2(a + b) - \frac{1}{k^2 - 1}[a(k^2 - 1) - b(k^2 + 1) + \frac{\Omega_R^2}{\omega^2}]. \]

(37)

The values of \( C_1, \ C_2, \ C_3 \) are linked through

\[ C_1 + C_2 + C_3 = 0. \]  

(38)

The functional form of the coefficients in Eq. (33) under the condition in (38) is necessary and sufficient to classify this equation as Fuchs’ [7].

Eq. (33) may be simplified through substituting the dependent variable \[ y(z) = w(z)v(z), \quad w(z) = z^p(z - 1)^q(z - \frac{1}{k^2})^r, \]

(39)

where \( p, q, r \) are both solutions to the indicial equations and characteristic exponents in the vicinity of the following points

\[ z = \alpha_1 = 0, \quad z = \alpha_2 = 1, \quad z = \alpha_3 = \frac{1}{k^2} \]

(40)

The solutions may be found from the indicial equations:

\[ p(p - 1) + \frac{1}{2}p + B_1 = 0 \Rightarrow p = \frac{1}{4} \pm \frac{\Delta}{2\omega} - \frac{1}{4}, \]

(41)

\[ q(q - 1) + \frac{1}{2}q + B_2 = 0 \Rightarrow q = \frac{1}{4} \pm \frac{\Delta}{2\omega} - \frac{1}{4}, \]

(42)

\[ r(r - 1) + \frac{1}{2}r + B_3 = 0 \Rightarrow r = \frac{1}{4} \pm \frac{\Delta}{2\omega} + \frac{1}{4}. \]

(43)
The characteristic exponents in the vicinity of $z = \infty$ are determined from the indicial equation \[7\]

\[
\rho^\infty (\rho^\infty - 1) + (2 - \sum_{k=1}^{3} A_k) \rho^\infty + \sum_{k=1}^{3} (B_k + \alpha_k C_k) = 0,
\]

which takes the following form using (34-37), (40)

\[
\rho^\infty (\rho^\infty - 1) + \frac{1}{2} \rho^\infty + B_3 = 0 \Rightarrow \rho^\infty = \frac{1}{4} \pm \frac{\Delta}{2\omega} + \frac{1}{4}.
\]  

Thus, we obtain the Heun equation with real parameters \[8\] for function $v(z)$ in the Klein-Bôcher-Ince form \[9\,\[10\]

\[
\partial_{zz} v + \left( \frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\epsilon}{z-k^2} \right) \partial_z v + \frac{\alpha \beta z - q_a}{z(z-1)(z-k^2)} v = 0,
\]

where

\[
\gamma = 2p + \frac{1}{2}, \quad \delta = 2q + \frac{1}{2}, \quad \epsilon = 2r + \frac{1}{2}, \quad \alpha = \rho_+^\infty + p + q + r, \quad \beta = \rho_-^\infty + p + q + r.
\]

The accessory parameter $q_a$ is given by

\[
q_a = \gamma r + \frac{1}{2} p - \frac{C_1 - \gamma q - \frac{1}{2} p}{k^2}.
\]

It is easy to verify that the Fuchs’ condition is satisfied:

\[
\gamma + \delta + \epsilon = \alpha + \beta + 1.
\]

The Riemann symbol that characterizes the form of the solutions to Heun equation (46) is given by

\[
P = \begin{pmatrix}
0 & 1 & \frac{1}{k^2} & \infty
\hline
0 & 0 & 0 & \alpha & z; & q_a
\hline
\gamma - 1 & 1 - \delta & 1 - \epsilon & \beta
\end{pmatrix}.
\]

It is worth noting that the substitution in (39) could be done eight ways

\[
pqr \in \{ p_+ q_+ r_+, \, p_+ q_- r_+, \, p_+ q_+ r_-, \, p_+ q_- r_-, \, p_- q_+ r_+, \, p_- q_- r_+, \, p_- q_+ r_-, \, p_- q_- r_- \}.
\]
which sometimes allows to pick suitable characteristic exponents and accessory parameter for specific calculations. Thus, the linearly independent solutions to Eq. (14) are written as \( f_1 = wv_1, f_2 = wv_2 \), where \( v_1, v_2 \) belong to the fundamental system of solutions to the Heun equation (46). The probability of the transition with a spin flip is expressed through the solutions \( v_1, v_2 \) as:

\[
P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta, k) = \frac{\hbar^2}{\omega^2} \left| \frac{w(\tau)(v_1(\tau)v_2(0) - v_2(\tau)v_1(0))}{\left| w(\tau)(v_1(\tau)\partial_\tau v_2(\tau) - v_2(\tau)\partial_\tau v_1(\tau)) \right|_{\tau=0}} \right|^2. \tag{52}
\]

In practice, solutions to the Heun equation are obtained through a reduction of the parameter space for \( \gamma, \delta, \epsilon, \alpha, \beta, q \) taking into account that there are additional relationships between the parameters \([9]\) besides the condition in (49). An analysis of parametric resonances induced by a non-zero detuning and distortion of a magnetic field will be presented elsewhere.

4 Spin \( \geq \frac{1}{2} \)

Generalization for higher spin values is not difficult because the matrix in (17) is unitary due to the hermitian property of the Hamiltonian in Eq. (1):

\[
\begin{pmatrix}
  f(a_1F_1 + b_1F_2) & f(a_2F_1 + b_2F_2) \\
  f^*(a_1F_1 + b_1F_2) & f^*(a_2F_1 + b_2F_2)
\end{pmatrix} = D^\frac{1}{2}(\varphi, \theta, \psi),
\]

where \( D^\frac{1}{2}(\varphi, \theta, \psi) \) is a Wigner matrix. The Euler angles \( \varphi, \theta, \psi \) are determined from equations

\[
f(a_1F_1 + b_1F_2) = \cos \frac{\theta}{2} \exp \frac{i}{2} (\varphi + \psi), \tag{54}
\]

\[
f^*(a_1F_1 + b_1F_2) = i \sin \frac{\theta}{2} \exp -\frac{i}{2} (\varphi - \psi), \tag{55}
\]

\[
\sin^2 \frac{\theta}{2} = P_{\frac{1}{2} \rightarrow -\frac{1}{2}}(\tau, \Delta, k) \tag{56}
\]

and are independent of the magnitude of the angular momentum \( J [11] \). Therefore, the transition probability over time \( \tau \) from the state with a projection of angular momentum \( m \) into one with a projection \( m' \) for a particle
with a spin $J$ is given by

$$P_{m \rightarrow m'}(\tau, \Delta, k) = D_{mm'}^{(J)}(\varphi, \theta, \psi)^2 = [(J + m)!(J - m)!(J + m')!(J - m')!] \cos^{4J} \theta \frac{1}{2} \left[ \sum_{\nu} (-1)^{\nu} \frac{(\tan \frac{\theta}{2})^{2\nu - m + m'}}{\nu!(\nu - m + m')!(J + m - \nu)!(J - m' - \nu)!} \right]^2.$$  

(57)

The Wigner matrix in formula (57) is

$$D_{mm'}^{(J)}(\varphi, \theta, \psi) = i^{m' - m} e^{i(m\varphi + m'\psi)}[(J + m)!(J - m)!(J + m')!(J - m')!]^{\frac{1}{2}} \sum_{\nu} (-1)^{\nu} \frac{(\sin \frac{\theta}{2})^{2\nu - m + m'}(\cos \frac{\theta}{2})^{2J - 2\nu + m - m'}}{\nu!(\nu - m + m')!(J + m - \nu)!(J - m' - \nu)!}.$$  

(58)

and $m, m' = (-J, -J + 1, \ldots, J - 1, J)$.

## 5 Conclusion

The study presented in this work may be useful in analyzing the results of interference experiments [12], improving magnetic spectrometers, and the field of quantum computing.

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