Rabi oscillations and quantum beats in a qubit in distorted magnetic field

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In a two-level system the time-periodic modulation of the magnetic field stabilizing the magnetic resonance position has been investigated. It was shown that the fundamental resonance is stable with respect to consistent variation of the longitudinal and transverse magnetic fields. The time-dependency of the Rabi oscillations and quantum beats of the spin flip probability was numerically researched in different parameter regimes taking into account dissipation and decoherence in the Lindblad form. The present study may be useful in the analysis of interference experiments and for manipulation of quantum bits.

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1. Introduction

Now world science centers dealt with a problem of a construction of quantum computers in which the algorithms of calculations based on the coherent mechanism of quantum processes are used. The idea of a quantum computer will consist in the construction of computer on the basis of quantum bits, instead of classical elementary cells.

The laws of quantum mechanics determining the behavior of quantum bits, provide huge advantages in the speed of calculations of a quantum computer in the comparison with a classical computer. In an NMR computer the manipulation of quantum bits (nuclear spins) is extremely important.

In the standard implementation of the magnetic resonance a constant magnetic field is perpendicular to linearly polarized, variable in time t monochromatic magnetic field. The shift of resonance frequency (the Bloch–Ziegert shift) appears [1]. The goal of the paper consists in the proposal and research of such magnetic field configuration, at which one the position of a main resonance is determined only by the Larmor frequency at arbitrary parameters of a system. This can be reached by generalizing the Rabi model [2]. Rabi studied the temporal dynamics of the particle with dipole magnetic moment and spin 1/2 in a constant magnetic field H_0 , directed along the z axis, and an alternating magnetic field perpendicular to it, rotating uniformly with a frequency $\omega/2\pi$: $H_x = h_0 \cos \omega t$, $H_y = h_0 \sin \omega t$, h_0 is the transverse field amplitude.

There are several methods for modulating magnetic fields while studying the phenomenon of magnetic resonance, depending on the goal of research (see [3] and references therein). In Refs. 4–6, without taking dissipation into account, it is investigated the temporal evolution of particle with dipole magnetic moment and spin 1/2 in a distorted magnetic field

$$\mathbf{H}(t) = (h_0 \operatorname{cn}(\omega t, k), h_0 \operatorname{sn}(\omega t, k), H_0 \operatorname{dn}(\omega t, k)), \quad (1)$$

where one cn, sn, dn are the Jacobi elliptic functions [7]. Such a modulation of the field upon variation of the modulus *k* of elliptic functions from zero to unity describes a class of field shapes from trigonometric $[cn(\omega t, 0) = cos \omega t, sn(\omega t, 0) = sin \omega t, dn(\omega t, 0) = 1]$ [2] to $[cn(\omega t, 1) = 1/ch \omega t, sn(\omega t, 1) = th \omega t, dn(\omega t, 1) = 1/ch \omega t]$ pulsed exponential [7]. The elliptic functions cn $(\omega t, k)$, $sn(\omega t, k)$ have a real period of $4K / \omega$, while dn $(\omega t, k)$ has a real period half as long. Here *K* is the complete elliptic integral of the first kind [7]. In other words, though the field is periodic with total real period of $4K / \omega$, it is seen that the frequency of amplitude modulation of the longitudinal field is twice that of the amplitude modulation of the transverse field. Such a field is called harmonized. In the paper [5] it was predicted that the position of the magnetic resonance would be stabilized in the field (1). In the work [6] the influence of a dissipation and decoherence on a stabilization has been studied. In the present work we study the transition of the Rabi oscillations into beats depending on the initial conditions and parameters describing the variable magnetic field (1).

2. Model

The dynamics of a spin 1/2 particle (qubit) with magnetic moment in an ac magnetic field $\mathbf{H}(t)$ will be described in the formalism of the density matrix ρ with a dissipative environment taken into account with the help of the Liouville–von Neumann–Lindblad (LvNL) equation [8] (we set $\hbar = 1$)

$$i\partial_{\tau}\rho = [\hat{H},\rho] - \frac{i}{2\omega} \sum_{i=1}^{3} (L_i^+ L_i \rho + \rho L_i^+ L_i - 2L_i^+ \rho L_i)$$
 (2)

with the Hermitian Hamiltonian

$$\hat{H} = \begin{pmatrix} \frac{\omega_0}{2\omega} \operatorname{dn}(\tau, k) & \frac{\omega_1}{2\omega} (\operatorname{cn}(\tau, k) - i \operatorname{sn}(\tau, k)) \\ \frac{\omega_1}{2\omega} (\operatorname{cn}(\tau, k) + i \operatorname{sn}(\tau, k)) & -\frac{\omega_0}{2\omega} \operatorname{dn}(\tau, k) \end{pmatrix}$$
(3)

in which dimensionless independent variable $\tau = \omega t$, $\omega_0 = g\mu_0 H_0$ is the Larmor frequency, $\omega_1 = g\mu_0 h_0$ is the amplitude of transverse field in terms of angular frequency, g is the factor Lande, μ_0 is the Bohr magneton. The operators L_i are chosen in the form $L_i = \sigma_i \sqrt{\Gamma_i/2}$ [9], where the Γ_i are phenomenological constants, which take into account the decoherence and dissipation in the system, and the σ are the Pauli matrixes.

We make the substitution $\rho = \alpha^{-1} r \alpha$ with the matrix

$$\alpha = \begin{pmatrix} f & 0 \\ 0 & f^* \end{pmatrix}, \text{ where the function } f \text{ is equal to}$$
$$f = \sqrt{\operatorname{cn} \tau - i \operatorname{sn} \tau}. \tag{4}$$

The equation for the transformed matrix r takes the form

$$i\partial_{\tau}r = \frac{\omega_1}{2\omega}[\sigma_x, r] + \frac{\delta_r}{2\omega}\mathrm{dn}\tau[\sigma_z, r] - \frac{i}{2\omega}\sum_{i=1}^3 (\alpha L_i^+ L_i \alpha^{-1} r + r\alpha L_i^+ L_i \alpha^{-1} - 2\alpha L_i \alpha^{-1} r\alpha L_i^+ \alpha^{-1})$$
(5)

in which detuning δ_r is equal to

$$\delta_r = \omega_0 - \omega. \tag{6}$$

As it is seen from Eq. (5) the detuning appears explicitly, i.e., the position of the principal resonance does not suffer a shift when the parameters of model are changed. In the case of a sharp resonance, when $\omega_0 = \omega$, in neglect of damping, the transition probability

$$P_{\frac{1}{2} \to -\frac{1}{2}}(\tau, \delta_r = 0) = \sin^2 \frac{\omega_1}{2\omega} \tau \tag{7}$$

does not contain modulus k, i.e., it is does not depend of the harmonized field deformation [4,5].

3. Decomplexification of LvNL equation

In the general case for an arbitrary detuning δ_r (6) we write the matrix *r* in the form of a decomposition in the complete set of Pauli matrices:

$$r = \frac{1}{2}(1 + \sigma \mathbf{R}), \quad r = r^{+}, \quad \text{Sp } r = 1,$$
 (8)

for all τ . We substitute the expression for r (8) in Eq. (5). As a result, we obtain the system of three first-order differential equations with periodic coefficients, with respect to unknown real functions R_x , R_y , R_z :

$$\partial_{\tau} R_{x} = -\frac{\delta_{r}}{\omega} \operatorname{dn} \tau R_{y} - \frac{\Gamma_{z}}{\omega} R_{x} - \frac{\Gamma_{x}}{\omega} (\operatorname{sn}^{2}(\tau, k) R_{x} - \operatorname{cn}(\tau, k) \operatorname{sn}(\tau, k) R_{y}) - \frac{\Gamma_{y}}{\omega} (\operatorname{cn}^{2}(\tau, k) R_{x} + \operatorname{cn}(\tau, k) \operatorname{sn}(\tau, k) R_{y}), \quad (9)$$

$$\partial_{\tau}R_{y} = \frac{\delta_{r}}{\omega} \operatorname{dn} \tau R_{x} - \frac{\omega_{1}}{\omega}R_{z} - \frac{\Gamma_{z}}{\omega}R_{y} - \frac{\Gamma_{x}}{\omega}(\operatorname{cn}^{2}(\tau,k)R_{y} - \operatorname{cn}(\tau,k)\operatorname{sn}(\tau,k)R_{x}) - \frac{\Gamma_{y}}{\omega}(\operatorname{cn}(\tau,k)\operatorname{sn}(\tau,k)R_{x} + \operatorname{sn}^{2}(\tau,k)R_{y}), (10)$$

$$\partial_{\tau} R_z = \frac{\omega_1}{\omega} R_y - \left(\frac{\Gamma_x}{\omega} + \frac{\Gamma_y}{\omega}\right) R_z.$$
 (11)

Now in terms R_x , R_y , R_z the density matrix ρ becomes

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + R_z & f^2 (R_x - iR_y) \\ f^{*2} (R_x + iR_y) & 1 - R_z \end{pmatrix}.$$
 (12)

The transition probability with spin flip is equal to the matrix element ρ_{22} that is

$$P_{\frac{1}{2}} \to -\frac{1}{2}(\tau, \delta_r, k) = \frac{1}{2}(1 - R_z).$$
(13)

Using expression (13) and set of Eqs. (9)–(11), it is easy to obtain a differential equation of the third order for the transition probability, which one we do not make out here. By the selection of decay constants $\Gamma_x = \Gamma_y = \Gamma_z = \Gamma$ the system (9)–(11) becomes

$$\partial_{\tau} R_x = -\frac{\delta_r}{\omega} \operatorname{dn} \tau R_y - \gamma R_x,$$
 (14)

$$\partial_{\tau} R_{y} = \frac{\delta_{r}}{\omega} \operatorname{dn} \tau R_{x} - \frac{\omega_{1}}{\omega} R_{z} - \gamma R_{y},$$
 (15)

$$\partial_{\tau}R_{z} = \frac{\omega_{1}}{\omega}R_{y} - \gamma R_{z},$$
 (16)

where $\gamma = 2\Gamma / \omega$.

In some special cases exact solutions of set (14)–(16) are presented in the work [6].

4. Numerical results

Let us consider behavior of transition probability depending on the pure initial conditions

$$R_x(0) = R_y(0) = 0, \quad R_z(0) = 1,$$
 (17)

$$R_x(0) = 1, \quad R_y(0) = 0, \quad R_z(0) = 0, \quad (18)$$

$$R_x(0) = R_y(0) = R_z(0) = 1/\sqrt{3}$$
, (19)

and the mixed initial condition

$$R_x(0) = R_y(0) = R_z(0) = 0.25 / \sqrt{3}$$
. (20)

The probability of a spin-flip transition is determined by the expression (13).

To perform the numerical simulation, we have chosen the parameters in units of $2\pi 100$ MHz: $\omega_0=1$ corresponds to the longitudinal field 2.3487 T for the proton resonance of a qubit. Without taking into account dissipative decoherence and at a resonance the formula (13) accepts an obvious form (7). When the detuning increases and k = 0, the frequency of oscillations increases, and the amplitude decreases, i.e., in the Rabi–Lindblad model damping oscillations are observed [6].

The spin-flip probabilities are presented at the initial condition (17) in Figs. 1 and 2. As it is seen from Fig. 1 the decoherence and dissipation reduce the amplitude of beats and their appreciable number. The period of beating and «the small period of oscillations» depend on initial conditions and the modulus k (Fig. 2). At frequency of an ac magnetic field ω much greater of the Larmor frequency ω_0 and the initial condition (17) the transition probability is closely to zero and equal 1/2 for the condition (18) (Fig. 3).

At all parameters and any initial conditions at the Rabi frequency $\Omega_R = \sqrt{\delta_r^2 + \omega_1^2} \approx \omega$ only damping oscillations



Fig. 1. Transition probabilities versus τ at $\Gamma = 0.005$ (top) and at $\Gamma = 0.001$ (bottom).

are observed. The evolution of initial condition (18) is more sensitive to the field deformation. Already for small k the beats arise (Fig. 4).

In Fig. 5 we present the dynamics of imaginary part of density matrix ρ_{12} (*y* component of the polarization vector) reduced by the factor 0.5 [6]. The real part ρ_{12}



Fig. 2. Beats for different modulus k.



Fig. 3. Rabi oscillations at big detuning. The top plot corresponds to initial condition (18), bottom (17).



Fig. 4. Transition probability at the initial condition (18).



Fig. 5. Imaginary part of density matrix ρ_{12} versus τ at the initial condition (18).



Fig. 6. Transition probabilities versus τ at the initial conditions: (19) (dot line), (20) (solid line).

(x component of the polarization vector) has the similar behavior.

In Fig. 6 we record the time evolution of transition probabilities for pure (19) (dot line) and mixed (20) (solid line) initial conditions. We see that the amplitude of oscillations for mixed conditions less then for pure conditions, but the period of beats do not changes.

We also record the time evolution of the entropy $S = -\text{Sp}(\rho \ln \rho) = -\lambda_1 \ln \lambda_1 - \lambda_2 \ln \lambda_2$, where λ_1, λ_2 are the eigenvalues of the density matrix ρ . The entropy increases monotonically from 0 to its asymptotic limit of ln 2. At resonance (solid line) the entropy keeps the mixing longer (Fig. 7).

The deformation of a field can be considered as the influence of an environment on the qubit dynamics [10].

It is necessary to note that at $\Gamma_x \neq \Gamma_y \neq \Gamma_z$ the beats are kept and the beat amplitudes change only insignificantly.



Fig. 7. Entropy versus τ at the initial condition (18).

Conclusion

Eventually the presence of dissipative decoherence levels the population of top and bottom levels. Depending on the field frequency, own frequency and a kind of initial conditions there are extremely a plenty of oscillations.

It would be desirable to do an experiment to check the theoretical predictions as to the stability of the magnetic resonance positions for different model parameters. Such an experiment would be an extension of the experimental situation in the circular polarized field. Since the parametric resonances in a harmonized magnetic field have a appreciable widths, it may be preferable to investigate magnetic resonance at parametric frequencies. This research reported here may find application in the analysis of interference experiments and for manipulation of qubits [11,12].

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