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Effects of nuclear spins on the coherent evolution of a phase qubit

Geordie Rose and Anatoly Yu Smirnov

D-Wave Systems Inc., 320-1985 West Broadway, Vancouver, Canada BC V6J 4Y3

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Abstract
The role of nuclear spins in decoherence and dephasing of a solid-state phase qubit is investigated. Both effects of static spin environment and spin polarization fluctuations in time are considered on the basis of non-Markovian Langevin–Bloch equations. We find conditions when coupling of a phase qubit to a bath of nuclear spins does not impair coherent evolution of the qubit.

1. Introduction

An analysis of decoherence and dephasing in quantum systems interacting with an environment has attracted great attention in recent years. This problem is of particular importance for a physical implementation of quantum computers, and, especially, for solid-state designs of qubits [1–6]. Such designs can be produced by means of well developed lithographic methods and offer advantages of scalability and flexibility. A disadvantage of solid-state qubits lies in the fact that their operating states are highly coupled to environment degrees of freedom. To get around this obstacle several models of phase qubits were proposed [3–6]. These qubits utilizing a superconducting phase as a dynamical variable with two macroscopically distinguishable values are effectively decoupled from charge degrees of freedom. In the general case the characteristic property of the phase qubit is the presence of a small magnetic flux which has two opposite directions in the different states of the qubit. An interaction of the magnetic field created by the flux with a bath of nuclear spins will be an important mechanism resulting in destroying a quantum superposition of the qubit's states and in statistical dispersion of characteristics of different qubits. In this work we develop a mathematical model describing the contribution of nuclear spins to decoherence and inhomogeneous broadening of phase qubits and determine conditions when nuclear spins have only a slight effect on the operation of the qubit. The problem of the spin-bath-mediated decoherence in phase qubits has been previously discussed in [8–10]. In papers [8, 9] particular attention has been given to the case of the static spin environment when the nuclear or paramagnetic spins have been subjected to the action of many magnetic fields, including the magnetic field from the qubit together with an external magnetic field and dipolar fields from other spins. By means of the instanton technique Prokof'ev and Stamp [9] have obtained, in particular, some estimations for the dephasing rates of the phase qubit in the static spin environment. It should be noted that the simple model considered in our paper allows us not only to get the same estimations but also to describe in detail a time evolution of the qubit's variables, and, especially, to determine the spectrum of all possible frequencies of quantum beats in the ensemble of qubits. This is a must for a correct analysis of logical operations in the ensemble of qubits. We suppose here that the magnetic field created by the qubit dominates over other magnetic fields acting on the nuclear spins. This assumption would hold for the qubit's design based on small grain-boundary junctions between d-wave superconductors [4, 5, 7, 11].

Besides the static case, in this paper we consider a contribution of spin–lattice relaxation to the decoherence rate of the phase qubit. This phenomenon, which is completely ignored in the above-mentioned paper [9], leads to true decoherence [12] as distinct from dephasing caused by the static spins. A qualitative estimation of effects of time-dependent spin fluctuations on the superconducting persistent current qubit has been performed in [10]. In [10] nuclear spins are supposed to be in the state of thermal equilibrium despite the fact that the qubit's magnetic field oscillates with a high frequency determined by splitting of the two lowest-energy states. Under such conditions an application of the fluctuation–dissipation theorem for the calculation of the qubit's decoherence rate as done in [10] casts some doubt. A longitudinal relaxation of nuclear spins takes long enough time T_1; however, many nuclear spins will contribute to the qubit's decoherence, so that the total decoherence rate of the qubit will be proportional not only to the damping rate of a single nuclear spin T_1^{-1} but also to the number of spins in the qubit's area. It follows herefrom that the mechanism of the qubit's decoherence due to spin–lattice relaxation is competitive with other mechanisms and, at least, cannot be rejected without more circumstantial consideration.

This paper is organized as follows. The next section is devoted to the formulation of the problem. In section 3 we analyse inhomogeneous broadening in the ensemble of qubits caused by a static spin environment. Decoherence rates of the qubit interacting with a spin polarization fluctuating in time are calculated in section 4.

2. Model

As mentioned above, there is a spontaneous flux ($\Phi \sim 10^{-2}$–$10^{-3}\Phi_0$) concentrated in the central part of the phase qubit and having opposite directions in two degenerate equilibrium states $\pm\varphi_0$ [3–6]. This flux creates the corresponding magnetic field $\boldsymbol{B}_0(\boldsymbol{r})$, which also has two directions: along and opposite to the z-axis, $\pm B_0(\boldsymbol{r})$ at different values of the qubit's phase. The existence of a two-well potential for the phase difference in the asymmetric grain-boundary Josephson junctions in d-wave cuprates directly follows from the experimental results obtained in [7]. A doubly degenerate ground state of such a junction is split into the symmetric and antisymmetric states with Δ being the energy difference between them. The qubit's two-level system is conveniently described by the Pauli matrices τ_x, τ_y, τ_z, so the tunnelling Hamiltonian is given by the expression $H_0 = (\Delta/2)\tau_z$. The eigenvalues ± 1 of the matrix τ_x correspond to the positioning of the qubit in the right-hand potential well (φ_0) or in the left-hand well ($-\varphi_0$), whereas the eigenvalues of the matrix τ_z correspond to the energy levels $\pm(\Delta/2)$ of the antibonding (antisymmetric) and bonding (symmetric) states. The magnetic field produced by the qubit can be also represented as a matrix: $\hat{B}_0 = \tau_x B_0(\boldsymbol{r})$ with $\int B(\boldsymbol{r})\,\mathrm{d}S = \Phi$.

Nuclear spins in the area of the qubit are subjected to the action of this magnetic field, and their energy operator appears as follows [10]:

$$H_s = -\tau_x \sum_i g\mu_{Ni} B(r_i)(\sigma_i)_z \qquad (1)$$

where μ_{Ni} is the nuclear magneton, $(\sigma_i)_z$ is the z-projection of the Pauli matrix describing the

ith nuclear spin and $B(r_i)$ is the magnetic field induced by the qubit at the point r_i, where the ith nuclear spin is located. Here we take a sum over all nuclear spins placed in the qubit's area. The effect of any external magnetic field on the nuclear spins is supposed to be small compared with the action of the qubit's magnetic field.

To consider an internal dynamics and fluctuations in the system of nuclear spins we suppose that the ith nuclear spin is coupled to the dissipative environment with variables $\{Q_x(t), Q_y(t), Q_z(t)\}_i$. This coupling has the form

$$H_N = -\sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{Q}_i. \tag{2}$$

For example, a heat bath of acoustic phonons is described by the variable [13]

$$\boldsymbol{Q}_i = V^{-1/2}\boldsymbol{G}\sum_q \sqrt{\frac{\hbar|\boldsymbol{q}|}{\rho c_s}}\mathrm{i}(b_q - b^+_{-q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i}.$$

Here b^+_q, b_q are creation–annihilation operators of acoustic phonons with wavevectors $\boldsymbol{q}$ and the sound velocity c_s; $\boldsymbol{G}$ is a constant of spin–phonon coupling; ρ and V are the density and the volume of the crystal, respectively.

The total Hamiltonian of our system will look like

$$H = \frac{\Delta}{2}\tau_z - P\tau_x - \sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{Q}_i + H_B. \tag{3}$$

Here

$$P = \sum_i \frac{\Delta_i}{2}(\sigma_i)_z \tag{4}$$

is the operator of Zeeman energy of nuclear spins in the fixed qubit's magnetic field, $\Delta_i = 2g\mu_{Ni}B(r_i)$ is the Zeeman frequency of the ith nucleus and H_B is the Hamiltonian of the free heat bath. In the case of acoustic phonons the Hamiltonian H_B will look like

$$H_B = \sum_q \hbar c_s|\boldsymbol{q}|(b^+_q b_q + 1/2).$$

We suppose that the free heat bath (without the interaction with the spins) is in thermal equilibrium with a temperature T.

It follows from the Hamiltonian (3) that the time evolution of the qubit's quasispin described by the matrices τ_x, τ_y, τ_z is governed by the equations

$$\begin{aligned}\dot{\tau}_x &= -\Delta\tau_y \\ \dot{\tau}_y &= \Delta\tau_x + 2\tau_z P \\ \dot{\tau}_z &= -2\tau_y P.\end{aligned} \tag{5}$$

Direct and indirect interactions between different nuclear spins are neglected in this model. In view of the a great number of nuclear spins in the qubit's area the influence of these spins on the qubit's dephasing can be quite considerable. Fortunately, the main part of the spin polarization, P_0, is almost static and determined by the initial spin configuration of the given qubit. This part differs in different qubits, as well as in the same qubit but taken at the time of the next logical operation. These fluctuations result in statistical dispersion of properties of qubits followed by the impact on the entanglement of qubits. In the next section we shall analyse a contribution of the static spin polarization without resorting to the perturbation theory. Besides the static part the spin polarization will include a small part fluctuating in time. This part $\tilde{P}(t) = P(t) - P_0$ is supposed to be here due to the spin–lattice interaction and results in destroying the quantum coherence of each individual qubit.

3. Inhomogeneous broadening

In this section we consider effects of the *static* spin environment ($P = P_0$) on the time evolution of the qubit's ensemble without taking into account the component fluctuating in time. The interaction between the qubit degrees of freedom and the static nuclear spins is not supposed to be weak. Each of the qubits has a specific distribution of nuclear spins. We have to average the qubit's operators over all configurations of nuclear spins to obtain information about the time evolution of the qubit's ensemble, for example, information about frequencies of quantum beats (tunnelling oscillations) of different qubits. Our goal is to find conditions when the frequency dispersion of the qubit's ensemble due to the interaction with nuclear spins will not influence the performance of logical operations, especially the entanglement of different qubits.

In this case the time evolution of the qubit's operators is described by equations (5) with the time-independent spin polarization $P = P_0$. A direct solution of the system (5) of differential equations (with $P = P_0$) gives us the formula

$$\tau_x(t) = \left[1 - \frac{\Delta^2}{\Omega^2}(1 - \cos\Omega t)\right]\tau_x(0) - \Delta\frac{\sin\Omega t}{\Omega}\tau_y(0) - \frac{2\Delta P_0}{\Omega^2}(1 - \cos\Omega t)\tau_z(0) \tag{6}$$

that represents oscillations of qubit variables with a frequency $\Omega^2 = \Delta^2 + 4P_0^2$ in a specific spin environment characterized by the parameter P_0. However, this parameter is changed when we proceed to the next qubit. To study a variety of possible evolutions we have to average expression (6) over an ensemble of all spin configurations. In the general case, it can be done by means of Fourier transforms, when the dependence on P_0 is transferred from the frequency $\Omega^2 = \Delta^2 + 4P_0^2$ to the exponent $e^{i\xi P_0}$, for example,

$$\left\langle\frac{\sin\Omega t}{\Omega}\right\rangle = \left\langle\int d\xi\, e^{i\xi P_0}F(\xi)\right\rangle \tag{7}$$

with

$$F(\xi) = \frac{1}{2\pi}\int_0^\infty dx\,\cos(\xi x)\frac{\sin 2t\sqrt{(\Delta/2)^2 + x^2}}{\sqrt{(\Delta/2)^2 + x^2}}. \tag{8}$$

After calculating the integral (8), we get for $F(\xi)$

$$F(\xi) = \frac{1}{4}J_0\left(\frac{\Delta}{2}\sqrt{4t^2 - \xi^2}\right)\theta(2t - |\xi|) \tag{9}$$

where $\theta(2t - |\xi|)$ is the Heaviside step function, and J_0 is the Bessel function. In formula (7) we average the function $\exp(i\xi P_0)$ or $\cos(\xi P_0)$ over the spin configurations:

$$\left\langle\frac{\sin\Omega t}{\Omega}\right\rangle = \frac{1}{2}\int_0^{2t} d\xi\,\langle\cos\xi P_0\rangle J_0\left(\frac{\Delta}{2}\sqrt{4t^2 - \xi^2}\right). \tag{10}$$

The characteristic functional of the spin ensemble can be represented as

$$\begin{aligned}\langle e^{i\xi P_0}\rangle &= \left\langle\exp\left(i\xi\sum_i\frac{\Delta_i}{2}(s_i)_z\right)\right\rangle \\ &= \left\langle\exp\left(i\frac{\Delta_1\xi}{2}(s_1)_z\right)\cdots\exp\left(i\frac{\Delta_{2N}\xi}{2}(s_{2N})_z\right)\right\rangle \\ &= \cos\left(\frac{\Delta_1\xi}{2}\right)\cdots\cos\left(\frac{\Delta_{2N}\xi}{2}\right) = \prod_{i=1}^{2N}\cos\left(\frac{\Delta_i\xi}{2}\right).\end{aligned} \tag{11}$$

Here $2N$ is the total number of nuclear spins in the qubit's volume. As a result, for the averaged function (10) we obtain

$$\left\langle \frac{\sin \Omega t}{\Omega} \right\rangle = \frac{1}{2} \int_0^{2t} \mathrm{d}\xi \, \cos\left(\frac{\Delta_1 \xi}{2}\right) \cdots \cos\left(\frac{\Delta_{2N} \xi}{2}\right) J_0\left(\frac{\Delta}{2}\sqrt{4t^2 - \xi^2}\right). \quad (12)$$

For the sake of simplicity we restrict ourselves to the case of the homogeneous magnetic field created by the flux: $B(r_1) = \cdots = B(r_{2N})$, and $\Delta_1 = \cdots = \Delta_{2N} = \Delta_0$. It should be mentioned that in the real case the dispersion in Δ_i can be of the order of its average value $\langle \Delta_i \rangle$. However, as it follows from equation (18) derived below, taking into account this dispersion will change an estimation for the dephasing rate $\Delta\omega$ by a factor of order four that is negligibly small compared with possible variation in the number of nuclear spins $2N \sim 10^7$–10^8. With the above-mentioned approximation we get

$$\prod_{i=1}^{2N} \cos\left(\frac{\Delta_i \xi}{2}\right) = \cos^{2N}\left(\frac{\Delta_0 \xi}{2}\right) = 2^{-2N} \sum_{k=0}^{2N} C_{2N}^k \cos[\Delta_0 (N-k)\xi] \quad (13)$$

with C_{2N}^k being the binomial coefficients. Calculating integrals gives us the simple formula

$$\left\langle \frac{\sin \Omega t}{\Omega} \right\rangle = 2^{-2N} \sum_{m=-N}^{m=N} C_{2N}^{N-m} \frac{\sin\left(t\sqrt{4\Delta_0^2 m^2 + \Delta^2}\right)}{\sqrt{4\Delta_0^2 m^2 + \Delta^2}}. \quad (14)$$

As a result, the time evolution of the qubit's variable averaged over nuclear spin configurations is given by the following expression:

$$\langle \tau_x(t) \rangle = 2^{-2N} \sum_{m=-N}^{m=N} C_{2N}^{N-m} \left[1 - \Delta^2 \frac{1 - \cos\left(t\sqrt{4\Delta_0^2 m^2 + \Delta^2}\right)}{4\Delta_0^2 m^2 + \Delta^2} \right] \tau_x(0)$$
$$- 2^{-2N} \sum_{m=-N}^{m=N} C_{2N}^{N-m} \Delta \frac{\sin\left(t\sqrt{4\Delta_0^2 m^2 + \Delta^2}\right)}{\sqrt{4\Delta_0^2 m^2 + \Delta^2}} \tau_y(0). \quad (15)$$

In the case of zero Zeeman frequency ($\Delta_0 = 0$) the phase differences of all identical qubits in our ensemble will oscillate with the same frequencies equal to tunnel splitting Δ. Otherwise, the frequencies of quantum beats of different qubits can take the spectrum of values $\omega_m = \sqrt{4\Delta_0^2 m^2 + \Delta^2}$ with $m = 0, 1, \ldots, N$, because each of these qubits has its own quasistatic distribution of nuclear spins (up or down), and, therefore, its own energy of interaction with these spins. Changing an orientation of a single nuclear spin, for example from up to down, will change the interaction energy between this spin and the qubit by the value of Δ_0. This fact results in the discrete character of the qubit's frequencies. During the time of one logical operation the frequency of the given qubit is equal to one of the frequencies ω_m. But in the time of performing the next operation separated from the first operation by the interval that is in excess of the spin–lattice relaxation time T_1 this qubit can be characterized by another frequency from the set $\{\omega_m\}$. The adjacent qubits can also have different frequencies that will affect entanglement processes. The dispersion of the qubit's freqiencies is described by the binomial coefficients

$$C_{2N}^{N-m} = \frac{(2N)!}{(N-m)!(N+m)!}$$

times 2^{-2N}. At large N and $m \ll N$ this function is approximated by the Gaussian distribution:

$$2^{-2N} C_{2N}^{N-m} \simeq \exp(-m^2/N)$$

so that the probable values of m are in the range from zero to $\sqrt{N}$. The maximum frequency of quantum beats is of order $\sqrt{4\Delta_0^2 N + \Delta^2}$. In the practically interesting case of weak coupling between nuclear spins and the qubit we obtain for the inhomogeneous broadening of the qubit's line

$$(\Delta\omega)_{\text{weak}} = 2N\frac{\Delta_0^2}{\Delta} \tag{16}$$

whereas for strong coupling we have

$$(\Delta\omega)_{\text{strong}} = \frac{\Delta^2}{\Delta_0\sqrt{2N}}. \tag{17}$$

In the framework of the instanon technique Prokof'ev and Stamp [9] have considered a more general model of the qubit's dephasing due to static nuclear spins, but at the final stage they have obtained the same estimations as those in equations (16), (17). This points to the ability of our simple mathematical model to describe properly the above-mentioned mechanism of the qubit's dephasing. It should be emphasized that besides estimations our model gives the mathematical expression for the time evolution of the qubit's variable $\langle\tau_x(t)\rangle$ (15), that is of great importance for an analysis of logical operations in the ensemble of qubits.

The static nuclear spin environment does not affect the time evolution of the qubit and, therefore, the performance of logical operations, if the number of nuclear spins, $2N$, interacting with the qubit is less than the ratio of tunnel splitting to Zeemann splitting squared:

$$2N < \frac{\Delta^2}{2\Delta_0^2}. \tag{18}$$

For the sake of estimation we consider the qubit's model with the linear size of the central area $l \simeq 10^{-5}$ cm. This size seems to be too small for designs considered in [3, 6], but it is very reasonable for qubits based on Josephson junctions between d-wave superconductors [4, 5, 7, 11]. As shown in [11] for this design the magnetic field produced by circulating spontaneous currents can be localized in the area with one side of about $10\xi_0$ (ξ_0 is the coherence length, $\xi_0 \sim 10^{-6}$ cm) and another side of about the width of the junction ($\sim$0.2 μm). Such small junctions are necessary also to eliminate experimentally defects and other irregularities [7]. Even with both sides of order 0.2 μm and with the magnetic flux created by the qubit of order $\Phi \simeq 10^{-2}\Phi_0$, $\Phi_0 = hc/2e$ we obtain that the qubit's magnetic field can reach the value 10 G, comparable to the dipole fields between the nuclear spins. Different components of $YBa_2Cu_3O_7$ have magnetic moments in the range from $-0.238(^{89}Y)$ to $3.075(^{65}Cu)$ nuclear magnetons. Because of this, for the Zeeman frequency of one nucleus in the qubit's magnetic field we get the estimation $\Delta_i \simeq 10^4$–$10^5(1/s)$, so $\Delta_i/\Delta \simeq 10^{-3}$–$10^{-4} \ll 1$, if $\Delta \simeq 10^8(1/s)$. As follows from equation (18), the number of nuclear spins coupled to the qubit should be less than 10^6–10^7 if we want to get rid of effects of the above-mentioned inhomogeneous broadening on the qubit's evolution. The magnetic field of the qubit cannot penetrate into the superconductors at depth in excess of the penetration length λ. Only nuclear spins located inside of the volume with third dimension smaller than the penetration length will be subjected to the action of the qubit's magnetic field. For a $YBa_2Cu_3O_7$ sample with cell sizes of order (3, 3, 11) Å there are almost $2N \sim 10^8$ nuclear spins in the qubit if the penetration length $\lambda \sim 10^{-5}$ cm. This number of nuclear spins is close enough to the above-mentioned requirements. With small decrease of the number of spins (or decrease of the ratio Δ_0^2/Δ^2) the statistical dispersion of frequencies of different qubits will be of little importance and the operation of the qubit under discussion will not be distorted by this mechanism of inhomogeneous broadening.

4. Decoherence of phase qubit in the spin bath

Now we analyse an effect of a nuclear spin polarization fluctuating in time on decoherence processes in the superconducting qubit. In this part we assume that the concentration of nuclear spins is sufficiently small, so that condition (18) is fulfilled and we can neglect any effect of static spin polarization on the evolution of the qubit: $P_0 = 0$, so that fluctuations of the spin polarizations are completely due to coupling of nuclear spins to the heat bath, for example to phonons. Now a contribution of the fluctuating component to the total Hamiltonian (3) of the system is supposed to be small compared with the tunnelling term $(\Delta/2)\tau_z$. Here we consider also weak coupling of nuclear spins to a dissipative environment, for example, to a phonon heat bath, as a source of fluctuations of nuclear spin polarization. This coupling results in the energy dissipation and thermalization of the spin system. In the weak-damping approximation when the energy of the interaction between spins and the heat bath is much less than the Zeeman frequency Δ_i we can find a dissipative evolution of nuclear spin operators σ_{zi} in the flipping magnetic field $\tau_x B_z(r_i)$ created by the qubit and calculate a correlation function

$$\langle[\tilde{P}(t), \tilde{P}(t')]_\pm\rangle = \langle\tilde{P}(t)\tilde{P}(t') \pm \tilde{P}(t')\tilde{P}(t)\rangle$$

with the polarization $\tilde{P}(t)$ being determined by equation (4):

$$\tilde{P}(t) = \sum_i \frac{\Delta_i}{2}[(\sigma_i)_z - \langle(\sigma_i)_z\rangle].$$

Here brackets $\langle\cdots\rangle$ mean averaging over the state of the equilibrium heat bath. It should be noted that equations (5) descriptive of the qubit's evolution incorporate the total spin polarization $P = \tilde{P} + \langle P\rangle$. However, the mean part of the polarization $\langle P\rangle$ leads only to small corrections for the tunnelling frequency Δ, and, therefore, it can be dropped out. At the same time the fluctuating part of the spin polarization $\tilde{P}$ causes the destruction of the qubit's coherence for the time interval which is equal to the relaxation time of the averaged x-projection $\langle\tau_x\rangle$ of the qubit's quasispin. The evolution of matrices τ_x, τ_y, τ_z is governed by equations (5) where $P = \tilde{P}(t)$. The fluctuating part of spin operator $\tilde{P}(t)$ includes contributions from many different spins and can be described approximately by Gaussian statistics. With this property in mind the mean value of the product of the qubit's matrix and the spin polarization, say, $\langle\tau_z\tilde{P}\rangle$, can be expressed as [14–16]

$$\langle\tau_z\tilde{P}\rangle = \left\langle\tfrac{1}{2}[\tau_z(t), \tilde{P}(t)]_+\right\rangle = \int \mathrm{d}t_1\, \tilde{M}_P(t, t_1)\langle \mathrm{i}[\tilde{\tau}_z(t), \tilde{\tau}_x(t_1)]_-\rangle.$$

Here

$$M_P(t, t_1) = \left\langle\tfrac{1}{2}[\tilde{P}(t), \tilde{P}(t_1)]_+\right\rangle \tag{19}$$

is the correlation function of the spin bath in the presence of flipping magnetic field created by the qubit, $[A, B]_\pm = AB \pm BA$, $\tilde{M}_P(t, t_1) = M_P(t, t_1)\theta(t - t_1)$ with $\theta(t - t_1)$ being the Heaviside step function. Averaging equation (5) over fluctuations of the Gaussian spin variable $\tilde{P}(t)$, i.e. eventually over the heat bath fluctuations, gives the non-Markovian equations [14–16] for the mean qubit variables

$$\begin{aligned}
\langle\dot{\tau}_x\rangle &= -\Delta\langle\tau_y\rangle \\
\langle\dot{\tau}_y\rangle &= \Delta\langle\tau_x\rangle + 2\int \mathrm{d}t_1\, \tilde{M}_P(t, t_1)\langle \mathrm{i}[\tau_z(t), \tau_x(t_1)]_-\rangle \\
\dot{\tau}_z &= -2\int \mathrm{d}t_1\, \tilde{M}_P(t, t_1)\langle \mathrm{i}[\tau_y(t), \tau_x(t_1)]_-\rangle.
\end{aligned} \tag{20}$$

As mentioned above time-dependent fluctuations of spin polarizations are supposed to be weak. Because of this, to calculate the commutators in equations (20) we can use the equations

$$\ddot{\tau}_x + \Delta^2\tau_x = 0$$

for the free oscillations of the qubit's variables without any spin polarization. Then, the commutators are expressed in terms of the qubit's matrices, for example,

$$\mathrm{i}[\tau_z(t), \tau_x(t_1)] = -2\tau_y(t)\cos\Delta(t-t_1) + 2\tau_x(t)\sin\Delta(t-t_1).$$

Ignoring the frequency shift of the qubit due to spin fluctuations we obtain the simple equation

$$\langle\ddot{\tau}_x\rangle + 2\Gamma\langle\dot{\tau}_x\rangle + \Delta^2\langle\tau_x\rangle = 0 \tag{21}$$

describing the relaxation of the qubit's oscillations between two wells with the relaxation rate

$$\Gamma = S_P(\Delta) \tag{22}$$

where

$$S_P(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega\tau} M_P(\tau) \tag{23}$$

is the spectral density of spin fluctuations. The relaxation of the qubit matrix τ_x to the equilibrium value is described by the expression

$$\langle\tau_x(t)\rangle = \left[\langle\tau_x(0)\rangle\cos(\Delta t) - \langle\tau_y(0)\rangle\sin(\Delta t)\right]\mathrm{e}^{-\Gamma t}. \tag{24}$$

The coefficient Γ (22) represents also the rate of the qubit's decoherence in the spin environment. To find this decoherence rate we have to calculate the spectral function $S_P(\omega)$ (23) and the correlation function $M_P(t, t_1)$ (19). Fluctuations of different spins are supposed to be independent. In view of this fact together with equation (4) the correlator $M_P(t, t_1)$ is proportional to the sum of correlation functions of z-projections of nuclear spins:

$$M_P(t, t_1) = \left\langle \frac{1}{2}[\tilde{P}(t), \tilde{P}(t_1)]_+ \right\rangle = \sum_i \frac{\Delta_i^2}{4} \left\langle \frac{1}{2}[(\sigma_i)_z(t), (\sigma_i)_z(t_1)]_+ \right\rangle. \tag{25}$$

Note that only the z-projection of the nuclear spins is coupled to the qubit because the qubit's magnetic field is always directed parallel to the z-axis while its magnitude oscillates with time.

The calculation of the correlation function for the ith spin $\langle(1/2)[(\sigma_i)_z(t), (\sigma_i)_z(t_1)]_+\rangle$ in the presence of a flipping magnetic field and a heat bath is of interest by itself. This problem could be of importance for measuring the qubit's magnetic field by means of electronic spin resonance (ESR) in the free radical probe coated on the surface of the superconducting qubit. The flipping of the qubit's magnetic field will be reflected in the characteristics of the ESR signal. That is why this method can be used for detecting coherent and incoherent oscillations in the qubits.

To find the spectral function of the ith nuclear spin we start with the Hamiltonian

$$H_i = -\frac{\Delta_i}{2}\tau_x(\sigma_i)_z - (\sigma_i)_x Q_x - (\sigma_i)_y Q_y - (\sigma_i)_z Q_z. \tag{26}$$

The spin operators $(\sigma_i)_x$, $(\sigma_i)_y$, $(\sigma_i)_z$ obey the following equations:

$$\begin{aligned} \dot{\sigma_x} &= \Delta_i\tau_x\sigma_y - 2\sigma_z Q_y + 2\sigma_y Q_z \\ \dot{\sigma_y} &= -\Delta_i\tau_x\sigma_x + 2\sigma_z Q_x - 2\sigma_x Q_z \\ \dot{\sigma_z} &= -2\sigma_y Q_x + 2\sigma_x Q_y. \end{aligned} \tag{27}$$

Here we omit the index 'i' in spin operators. The heat bath operators $(Q_i)_\alpha$ are supposed to be independent for different spins ($i = 1, 2, \ldots, 2N$; $\alpha = x, y, z$), so that the response functions and the correlators of the free heat bath variables have the form

$$\langle\mathrm{i}[(Q_i)_\alpha^{(0)}(t), (Q_j)_\beta^{(0)}(t')]_-\rangle\theta(t-t') = \varphi(t, t')\delta_{ij}\delta_{\alpha\beta} \tag{28}$$

$$\langle(1/2)[(Q_i)_\alpha^{(0)}(t), (Q_j)_\beta^{(0)}(t')]_+\rangle = M(t, t')\delta_{ij}\delta_{\alpha\beta} \tag{29}$$

$\tilde{M}(t, t_1) = M(t, t_1)\theta(t - t_1)$, $\varphi(t, t') = \varphi(t - t')$, $M(t, t') = M(t - t')$. As mentioned above, the free heat bath, for example phonons without any interaction with spins, is in thermal equilibrium at temperature T. In this case the heat bath is characterized by the susceptibility

$$\chi(\omega) = \int \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega\tau}\varphi(\tau)$$

as well as the the spectral density of fluctuations

$$S(\omega) = \int \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega\tau} M(\tau)$$

which are related by the fluctuation–dissipation theorem

$$S(\omega) = \hbar\chi''(\omega)\coth(\hbar\omega/2T). \tag{30}$$

The imaginary part of the susceptibility, $\chi''(\omega)$, describes dissipative properties of the equilibrium heat bath.

Following the method developed in [14–16] we can derive from equations (27) the Langevin-like equations for the spin operators, especially, for the z-projection σ_z we are interested in. Due to the Gaussian statistics of unperturbed heat bath variables $Q_\alpha^{(0)}(t)(\alpha = x, y, z)$ the response of the heat bath to the action of the spin is linear in the spin matrices σ_α:

$$Q_\alpha(t) = Q_\alpha^{(0)}(t) + \int \mathrm{d}t_1\, \varphi(t - t_1)\sigma_\alpha(t_1). \tag{31}$$

After substituting these operators into equations (27) we have to eliminate the unperturbed heat bath variables $Q_\alpha^{(0)}(t)$ to obtain the equations only for spin variables. To do that the products $Q_\alpha^{(0)}(t)\sigma_\beta(t)(\beta = x, y, z)$ involved in the Heisenberg equations (27) are conveniently represented as

$$Q_\alpha^{(0)}(t)\sigma_\beta(t) = \{Q_\alpha^{(0)}(t), \sigma_\beta(t)\} + \int \mathrm{d}t_1\, \tilde{M}(t, t_1)\mathrm{i}[\sigma_\beta(t), \sigma_\alpha(t_1)]_-. \tag{32}$$

This formula can be considered as a definition of the brackets $\{\ldots\}$ having zero mean value:

$$\langle\{Q_\alpha^{(0)}(t), \sigma_\beta(t)\}\rangle = 0$$

because of the quantum Furutsu–Novikov theorem [14]. Introducing the fluctuation forces, for example,

$$\xi_z(t) = 2\{Q_y^{(0)}(t), \sigma_x(t)\} - 2\{Q_x^{(0)}(t), \sigma_y(t)\} \tag{33}$$

with zero mean values, $\langle\xi_z(t)\rangle = 0$, we obtain the Langevin-like equation for z-projection of the ith spin:

$$\dot{\sigma_z} = \xi_z - 2\int \mathrm{d}t_1\, \{\tilde{M}(t, t_1)\mathrm{i}[\sigma_y(t), \sigma_x(t_1)]_- + \varphi(t, t_1)(1/2)[\sigma_y(t), \sigma_x(t_1)]_+\}$$
$$+2\int \mathrm{d}t_1\, \{\tilde{M}(t, t_1)\mathrm{i}[\sigma_x(t), \sigma_y(t_1)]_- + \varphi(t, t_1)(1/2)[\sigma_x(t), \sigma_y(t_1)]_+\}. \tag{34}$$

The brackets $\{\ldots\}$ simplify also the problem of calculating correlation functions of the fluctuation forces. They merely imply that pairings of operators within the same brackets should be omitted in the process. As a result, the explicit expression for the fluctuation force ξ_z (33) together with the definition (32) allow us to get the following correlator:

$$\langle(1/2)[\xi_z(t), \xi_z(t')]_+\rangle = 2M(t, t')\langle[\sigma_x(t), \sigma_x(t')]_+ + [\sigma_y(t), \sigma_y(t')]_+\rangle. \tag{35}$$

It should be emphasized that this result is not based on the fluctuation–dissipation theorem and will be valid in the case of strong non-equilibrium as well. However, here we resort to the approximation of weak coupling between the spin and the heat bath. With this approximation we are able to calculate the (anti-) commutators in equations (34), (35) by means of the equations describing the spin evolution in the time-varying qubit's magnetic field:

$$\begin{aligned}\sigma_x(t) &= \sigma_x(t_1)\cos\Lambda_i(t,t_1) + \sigma_y(t_1)\sin\Lambda_i(t,t_1)\\ \sigma_y(t) &= \sigma_y(t_1)\cos\Lambda_i(t,t_1) - \sigma_x(t_1)\sin\Lambda_i(t,t_1)\\ \sigma_z(t) &= \sigma_z(t_1)\end{aligned} \tag{36}$$

where

$$\Lambda_i(t,t_1) = \Delta_i \int_{t_1}^{t} \mathrm{d}t_2\, \tau_x(t_2). \tag{37}$$

The operators (36) obey equations (27) where all heat bath variables Q_α are omitted. Taking into consideration a free oscillation of the qubit operator $\tau_x(t)$ with the tunnelling frequency Δ we obtain for the function $\Lambda_i(t,t_1)$

$$\Lambda_i(t,t_1) = \frac{\Delta_i}{\Delta}\left[\tau_x(t)\sin\Delta(t-t_1) + \tau_y(t)(1-\cos\Delta(t-t_1))\right]. \tag{38}$$

With the properties of Pauli matrices we find also that

$$\cos\Lambda_i(t,t_1) = \cos\left(2\frac{\Delta_i}{\Delta}\sin\left[\frac{\Delta(t-t_1)}{2}\right]\right) \tag{39}$$

$$\begin{aligned}\sin\Lambda_i(t,t_1) &= 2\sin\left(2\frac{\Delta_i}{\Delta}\sin\left[\frac{\Delta(t-t_1)}{2}\right]\right)\\ &\quad\times\left(\tau_x(t)\cos\left[\frac{\Delta(t-t_1)}{2}\right] + \tau_y(t)\sin\left[\frac{\Delta(t-t_1)}{2}\right]\right).\end{aligned} \tag{40}$$

As a result, for z-projection of the ith spin operator we obtain the simple stochastic equation

$$\dot{\sigma}_z(t) + \int \mathrm{d}t_1\, \gamma_i(t,t_1)\sigma_z(t_1) = \xi_z(t) + v_i(t). \tag{41}$$

Here

$$\begin{aligned}\gamma_i(t,t_1) &= 8\tilde{M}(t,t_1)\cos\Lambda_i(t,t_1)\\ v_i(t) &= 4\int \mathrm{d}t_1\, \varphi(t,t_1)\sin\Lambda_i(t,t_1).\end{aligned} \tag{42}$$

The relaxation of the ith nuclear spin is determined by the real part $\gamma_i(\omega)$ of the Fourier transform of the function $\gamma_i(t,t_1)$:

$$\gamma_i(\omega) = 4\int_{-\infty}^{+\infty} \mathrm{d}\tau\, M(\tau)\cos(\omega\tau)\cos\left[2\frac{\Delta_i}{\Delta}\sin\left(\frac{\Delta\tau}{2}\right)\right]. \tag{43}$$

After a short calculation we derive the following formula for the function $\gamma_i(\omega)$:

$$\gamma_i(\omega) = 2\sum_m J_m\left(2\frac{\Delta_i}{\Delta}\right)\left[S\left(\omega - \frac{m\Delta}{2}\right) + S\left(\omega + \frac{m\Delta}{2}\right)\right]. \tag{44}$$

Here $J_m(z)$ is the Bessel function of mth order, and $S(\omega)$ is a spectral density of the heat bath fluctuations (30). It should be emphasized that it is formula (44) that gives a line width of the spin $1/2$ coupled to a heat bath in the presence of the flipping magnetic field created by the qubit. This line width can be measured in experiments on electronic or nuclear paramagnetic resonance.

It follows from equations (35), (36) that the Fourier transform of the correlation function of the fluctuation forces is also determined by the formula like equation (44):

$$\left\langle \tfrac{1}{2}[\xi_z^{(i)}(\omega), \xi_z^{(i)}]_+\right\rangle = 2\gamma_i(\omega). \tag{45}$$

As a result the spectral density of fluctuations of the ith nuclear spin

$$K_i(\omega) = \int \mathrm{d}t \left\langle \tfrac{1}{2}[(\sigma_i)_z(t), (\sigma_i)_z(0)]_+ \right\rangle \mathrm{e}^{\mathrm{i}\omega t}$$

is determined by the expression

$$K_i(\omega) = \frac{2\gamma_i(\omega)}{\omega^2 + \gamma_i^2(\omega)}$$

whereas the spectral density (23) has the simple form

$$S_P(\omega) = \frac{1}{2}\sum_i \Delta_i^2 \frac{\gamma_i(\omega)}{\omega^2 + \gamma_i^2(\omega)} \tag{46}$$

with the function $\gamma_i(\omega)$ given by equation (44).

With the formulas (22), (46) we obtain the following expression for the decoherence rate (or the inverse decoherence time τ_d^{-1}) of the phase qubit

$$\Gamma = \frac{1}{\tau_\mathrm{d}} = \frac{1}{2}\sum_i \Delta_i^2 \frac{\gamma_i(\Delta)}{\Delta^2 + \gamma_i^2(\Delta)}. \tag{47}$$

In view of the fact that the relaxation rate of the ith nuclear spin, $\gamma_i(\Delta)$, or, in other words, an inverse longitudinal relaxation time $(1/T_1)_i$ of the ith spin, is much less than the qubit's frequency $\Delta : (1/T_1)_i = \gamma_i(\Delta) \ll \Delta$, we find that the qubit's decoherence rate is proportional to the sum of spin line widths γ_i due to spin coupling to a heat bath taken with the weights (Δ_i^2/Δ^2):

$$\frac{1}{\tau_\mathrm{d}} = \frac{1}{2}\sum_i \frac{\Delta_i^2}{\Delta^2}\gamma_i(\Delta) = \sum_i \frac{\Delta_i^2}{\Delta^2}\sum_m J_m\left(2\frac{\Delta_i}{\Delta}\right)\left[S\left(\Delta - \frac{m\Delta}{2}\right) + S\left(\Delta + \frac{m\Delta}{2}\right)\right]. \tag{48}$$

This formula takes into consideration oscillations of the qubit's magnetic field with the tunnelling frequency Δ. Usually Zeeman splitting Δ_i of the ith nuclear spin in the qubit's magnetic field as well as in the magnetic field created by other nuclear spins is much less than the frequency of quantum beats $\Delta : \Delta_i \ll \Delta$. Because of this, the term with $m = 0$ gives the major contribution to the sum in equation (48), and in this approximation the qubit's decoherence rate will look like

$$\frac{1}{\tau_\mathrm{d}} = 2\chi''(\Delta)\coth\left(\frac{\Delta}{2T}\right)\sum_i \frac{\Delta_i^2}{\Delta^2}. \tag{49}$$

Here $\chi''(\omega)$ is the imaginary part of the susceptibility of the heat bath with the temperature T. The interaction of nuclear spins with this heat bath, for example, with lattice vibrations, provides a mechanism of dissipation and thermalization in the spin system. If the heat bath temperature is in excess of the tunnel splitting, $T \gg \Delta$, the qubit's decoherence rate increases linearly with temperature:

$$\frac{1}{\tau_\mathrm{d}} = 4T\frac{\chi''(\Delta)}{\Delta}\sum_i \frac{\Delta_i^2}{\Delta^2}. \tag{50}$$

The nuclear spin–lattice relaxation time is usually measured at the field of order 10^4 G when the Zeeman frequency for one of our nuclei is $10^7(1/s)$. At this field and at the temperature $T \simeq 1$ K the spin–lattice relaxation rate is of order or less than $10(1/s)$ [17]. According to results by Morr and Wortis [18] the spin–lattice relaxation rate is approximately proportional to the applied magnetic field squared. Our decoherence time, τ_d (48)–(50), is determined by the spin–lattice relaxation rate $\gamma_i(\Delta)$ taken at the frequency Δ. For the qubit model mentioned at the end of section 3 we have $\Delta \simeq 10^8(1/s)$, that is more than the usual frequency $10^7(1/s)$ of relaxation time measurements by a factor of 10. So, the spin–lattice relaxation rate corresponding to our quantum beat frequency Δ will be estimated as $(1/T_1)_i = \gamma_i(\Delta) \sim 10^3(1/\text{s})$. For the same $YBa_2Cu_3O_7$ sample as in section 3 with $2N \sim 10^8$ nuclear spins the qubit's decoherence rate due to magnetic coupling to the nuclear spins is

$$\frac{1}{\tau_{\rm d}} \simeq 10^3(1/s).$$

This decoherence time is much more than the period of quantum beat oscillations, $\tau_{\rm d}\Delta \sim 10^5 \gg 1$, so that the necessary condition

$$\tau_{\rm tunnelling} < \tau_{\rm gate} < \tau_{\rm decoherence}$$

or

$$10^{-8}s < \tau_{\rm gate} < 10^{-3}s$$

holds if the nuclear spins are considered as the main decoherence mechanism. Nevertheless, as is evident from the foregoing, the mechanism of the qubit's decoherence related to the spin–lattice relaxation cannot be considered as improbable, especially as this mechanism causes true decoherence of a single qubit in distinction to dephasing occurring in the ensemble of qubits. It is necessary to emphasize that contributions of magnetic impurities and electrons in the normal conductor have to be taken into account as well for the correct estimation of the decoherence rate $\tau_{\rm d}^{-1}$.

5. Conclusions

We have considered a contribution of nuclear spins to the dephasing and decoherence of a phase qubit. An effect of the static spin environment has been analysed without resorting to perturbation theory. For this case we have found a condition (18) when dephasing or inhomogeneous broadening in an ensemble of qubits has no effect on the operation of a quantum computer. Decoherence rates (48)–(50) of the qubit weakly coupled to the heat bath of nuclear spins have been calculated as well; in so doing we have taken into account fluctuations of a spin polarization in time stemming from the interaction of nuclear spins with some basic dissipative environment, for example, with lattice vibrations. Interestingly, formulae for the relaxation rate $\gamma_i(\omega)$ (44) and for a spectral density $K_i(\omega)$ of fluctuations of an individual nuclear spin in the time-varying magnetic field of the qubit have been derived in the process. These formulae are also useful for understanding the electron spin resonance in the flipping magnetic field. For the realistic parameters of the phase qubit based on the YBCO crystal [4, 5, 11] we have estimated a decoherence time that meets the necessary condition for the successful operation of the qubit.

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