Single-spin measurements for quantum computation using magnetic resonance force microscopy

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Abstract

The quantum theory of a single-spin measurement using a magnetic resonance force microscopy is presented. We use an oscillating cantilever-driven adiabatic reversals technique. The frequency shift of the cantilever vibrations is estimated. We show that the frequency shift causes the formation of the Schrödinger cat state for the cantilever. The interaction between the cantilever and the environment quickly destroys the coherence between the two cantilever trajectories. It is shown that using partial adiabatic reversals one can obtain a significant increase in the frequency shift. We discuss the possibility of sub-magneton spin density detection in molecules using magnetic resonance force microscopy.

Keywords: Magnetic resonance force microscopy, magnetic resonance, cantilever, quantum measurement, Schrödinger cat state, decoherence, single spin measurement.

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I. INTRODUCTION

The oscillating cantilever-driven adiabatic reversals (OSCAR) technique first proposed in [1] is currently the most promising way for a single-spin detection using magnetic resonance force microscopy (MFMR). We consider the setup first implemented in [2]. In this setup the cantilever axis is perpendicular to the surface of the sample. The cantilever tip (CT) with an attached ferromagnetic particle oscillates along the x-axis, which is parallel to the surface of the sample. The external permanent magnetic field, $\vec{B}_{ext}$, is perpendicular to the surface of the sample in the positive z-direction. A single spin, placed near the surface of the sample, experiences both the external field $\vec{B}_{ext}$ and the dipole field $\vec{B}_d$ produced by the ferromagnetic particle.

Suppose that at time $t = 0$ the CT is in its right end position, and one applies a rotating *rf* field in the transverse x-y plane with frequency $\gamma(B_{ext}+B_{d0})$, where γ is the magnitude of the electronic gyromagnetic ratio and B_{d0} is the dipole field B_{dz} for the equilibrium CT position $X_c = 0$. At t=0 the dipole field B_{dz} is greater than B_{d0}. One quarter of the CT period later we have $B_{dz} = B_{d0}$, and the resonance frequency of the spin matches the *rf* field frequency. Then the dipole field B_{dz} becomes smaller than B_{d0}, and so on. The effective magnetic field in the rotating frame has the components, $\vec{B}_{eff} = (B_1, 0, B_{dz} - B_{d0})$. This field experiences periodic reversals with the frequency of the CT vibrations. If the adiabatic conditions are satisfied, the spin experiences adiabatic reversals following the effective magnetic field. The magnetic force produced by the spin on the ferromagnetic particle attached to the CT is $-g\mu_B|\partial B_z/\partial x|S_z$. Here we consider only the x-component of the magnetic force caused by the adiabatic reversals of the z-component of the spin. g is the electron g-factor and $\partial B_z/\partial x$ is the magnetic field gradient at the location of the spin. When the CT coordinate X_c is positive, then S_z is negative, and the magnetic force on the CT points in the positive x-direction. When $X_c < 0$, then the magnetic force points in the negative x-direction. Thus, the magnetic force is opposite to the effective spring force and causes a decrease of the CT vibrational frequency. The change of the CT vibrational frequency is the OSCAR signal, which must be detected. If the *rf* field is turned on when the CT is at the left end position, then the spin points in the direction of the effective magnetic field, and the CT vibrational frequency increases.

II. HAMILTONIAN OF THE CT-SPIN SYSTEM AND QUANTITATIVE ANALYSIS OF ITS DYNAMICS

We use the following dimensionless parameters: $x_c = X_c/X_0$, $p_c = P_c/P_0$, $\epsilon = \gamma B_1/\omega_c$, and $\eta = \gamma/2(\hbar/k_c\omega_c)^{1/2}|\partial B_z/\partial x|$, where X_c and P_c are the coordinate and the momentum of the CT, k_c and ω_c are the effective spring constant and the angular frequency of the CT. X_0 and P_0 are the "quantum units" of the coordinate and the momentum: $X_0 = \hbar\omega_c/k_c$, $P_0 = \hbar/X_0$. In these units the Hamiltonian of the CT-spin system can be written as $\mathcal{H} = (x_c^2 + p_c^2)/2 + \epsilon S_x + 2\eta x_c S_z$. Here the first term describes the unperturbed CT energy, the second term describes the interaction between the spin and the *rf* field, and the last term describes the CT-spin interaction. This Hamiltonian is written in the rotating system of coordinates, the rotating magnetic field points in the positive x-direction.

Neglecting oscillations with twice the CT frequency, we can estimate the magnetic force on CT as $-2\eta S_z = \pm\eta^2 x/\sqrt{2\eta^2 x_m^2 + \epsilon^2}$, where x_m is the CT amplitude. The corresponding frequency shift is $\Delta\omega_c/\omega_c = \mp\eta^2/\sqrt{2\eta^2 x_m^2 + \epsilon^2}$. From the experimental data [2] we have for the CT amplitude $x_m = 1.2 \times 10^5$ and $|\Delta\omega_c/\omega_c| = 4.7 \times 10^{-7}$.

The condition for adiabatic motion in terms of dimensionless parameters is $2\eta x_m << \epsilon^2$. To provide full reversals of the effective field one requires $\epsilon << 2\eta x_m$. It follows from this that one could increase the frequency shift by reducing the amplitude of the CT vibrations x_m and the *rf* field ϵ. Taking $\epsilon \approx 2\eta x_m$ we still satisfy the adiabatic condition but violate the condition of full reversals. Thus, one could increase the frequency shift by sacrificing the total reversal of the spin.

We simulate the Schrödinger dynamics using the dimensionless Schrödinger equation $i\partial\Psi/\partial\tau = \mathcal{H}\Psi$, $\tau = \omega_c t$. The initial conditions describe the quasiclassical state of the CT and the spin pointing in the positive z-direction. The results of our simulations are similar to those described in our previous publications [3–5]. The probability distribution for the CT gradually splits into two peaks. The first peak corresponds to the average spin pointing in the direction of the effective magnetic field for the first trajectory, the second peak describes the spin pointing in the direction of the effective field for the second trajectory. The Fourier spectrum of the CT motion clearly indicates two possible frequencies of the CT vibrations.

This phenomenon can be considered as the manifestation of the Stern-Gerlach effect in the OSCAR technique. The Hamiltonian dynamics describes a Schrödinger cat state of the CT. Two CT trajectories develop simultaneously in the process of quantum evolution. To simulate the decoherence caused by the interaction of the CT with the environment we used the simplest master equation: an ohmic model in the high-temperature approximation [6]. The results of these simulations are similar to those obtained in [4, 5]. The Schrödinger cat state transforms into a statistical mixture of two possible CT trajectories.

Finally, we would like to discuss the possibility of sub-magneton detection of the single electron spin density. To analyze this possibility we have chosen the beta carotene cation radical, which plays an important role in the active sites of proteins. In this molecule a single spin is delocalized along a chain of double bonds. To obtain the spatial distribution of the spin density we have used spin-restricted Kohn-Sham method with B3LYP exchange–correlation functional in Dunning's double zeta basis set. We assume that the molecule is placed in the x-z plane near the surface of the sample with its axis parallel to the x-axis. Suppose that we "divide" the molecule into three equal parts of length 1.05 nm. Our computations show that the integrated spin densities in these fragments are, correspondingly, 26%,48.4%, and 25.6%. If the CT amplitude were about 1 nm the OSCAR technique would detect the sub-magneton local spin density in this molecule.

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