Quantum Measurement of a Single Spin using Magnetic Resonance Force Microscopy

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Single-spin detection is one of the important challenges facing the development of several new technologies, e.g. single-spin transistors and solid-state quantum computation. Magnetic resonance force microscopy with a cyclic adiabatic inversion, which utilizes a cantilever oscillations driven by a single spin, is a promising technique to solve this problem. We have studied the quantum dynamics of a single spin interacting with a quasiclassical cantilever. It was found that in a similar fashion to the Stern-Gerlach interferometer the quantum dynamics generates a quantum superposition of two quasiclassical trajectories of the cantilever which are related to the two spin projections on the direction of the effective magnetic field in the rotating reference frame. Our results show that quantum jumps will not prevent a single-spin measurement if the coupling between the cantilever vibrations and the spin is small in comparison with the amplitude of the radio-frequency external field.
Modern solid-state technologies are approaching the level at which manipulating a single electron, atom, electron or nuclear spin becomes extremely important. The future successful development of these technologies depends significantly on development of single-particle measurement methods. While a single electron charge can be detected using a single-electron transistor, methods for detection of a single electron (or nuclear) spin in solids are still not available. However, many proposals for solid-state nano-devices require a single-electron (or nucleus) spin measurement. There are a few proposals for a solid-state single-spin measurement based on the swap operation of a spin state to a charge state \([1]\), scanning tunneling microscopy \([2]\), or magnetic resonant force microscopy (MRFM) \([3,4]\).

In this paper, we consider a MRFM single-spin measurement. One of the most promising MRFM techniques is based on the cyclic adiabatic inversion (CAI) of electron or nuclear spins \([5]\). In this technique, the frequency of the spin inversion is in the resonance with the frequency of the mechanical vibrations of the ultrathin cantilever, which allows one to amplify the extremely weak force of a spin on the cantilever. The CIA MRFM method was successfully implemented as an alternative to the electron and nuclear magnetic resonance for macroscopic ensembles of spins \([5,6]\). It has already achieved a sensitivity, which is equivalent to detection of approximately 200 polarized electron spins \([7]\).

It is clear that the resonant amplification of the cantilever vibrations by a single spin cannot be considered as a classical process. Indeed, the driving force acting on the cantilever is quantized, since it is proportional to the spin projection. As a result, quantum jumps could appear in the cantilever motion, which might prevent the resonant amplification of the cantilever oscillations. In fact, the problem of quantum jumps is a very general one. It always arises in a continuous observation of a single quantum particle. Despite extensive study \([8]\), the quantum jumps in a mechanical motion of classical detectors and their effect on a measurement of a quantum system have not been investigated. The analysis of these quantum effects and their influence on a single-spin detection in CAI MRFM are the main subjects of this paper.

We consider the cantilever-spin system shown in Fig. 1. A single spin \(S = 1/2\) is
placed on the cantilever tip. The tip can oscillate only in the $z$-direction. The ferromagnetic particle, whose magnetic moment points in the positive $z$-direction, produces a non-uniform magnetic field which acts on the spin. The uniform magnetic field, $\vec{B}_0$, oriented in the positive $z$-direction, determines the ground state of the spin. The rotating radio frequency (rf) magnetic field, $\vec{B}_1$, induces transitions between the ground state and the excited state of the spin. The origin is chosen to be the equilibrium position of the cantilever tip with no ferromagnetic particle. The rf magnetic field can be written as $B_x = B_1 \cos[\omega t + \varphi(t)]$, $B_y = -B_1 \sin[\omega t + \varphi(t)]$, where $\varphi(t)$ is a periodic change in phase with the frequency of the cantilever, required for a CAI of the spin. A non-uniform magnetic field produces a force on the spin which depends on the spin direction. If the spin direction is changed with a frequency which equals to the cantilever resonant frequency, the amplitude of the cantilever vibrations increases so that it can be detected by optical methods.

In the reference frame rotating with the frequency of the transversal magnetic field, $\omega + d\varphi/dt$, the Hamiltonian of the “cantilever-spin” system is,

$$
\mathcal{H} = \frac{P_z^2}{2m_c^*} + \frac{m_c^* \omega_c^2 Z^2}{2} - \hbar \left( \omega_L - \omega - \frac{d\varphi}{dt} \right) S_z - \hbar \omega_1 S_x - g \mu \frac{\partial B_z}{\partial Z} Z S_z.
$$

In Eq. (1), $Z$ is the coordinate of the oscillator which describes the dynamics of the quasi-classical cantilever tip; $P_z$ is its momentum, $m_c^*$ and $\omega_c$ are the effective mass and the frequency of the cantilever (the mass of the cantilever is: $m_c = 4m_c^*$); $S_z$ and $S_x$ are the $z$- and the $x$-components of the spin; $\omega_L = \gamma B_z$ (at $z=0$) is its Larmor frequency; $\omega_1 = \gamma B_1$ is the Rabi (or nutation) frequency; $\gamma = g \mu / \hbar$ is the gyromagnetic ratio of the spin; $g$ and $\mu$ are the g-factor and the nuclear magneton. (We consider for definiteness a nuclear spin, but the results can be applied also to an electron spin.)

We assume that $\omega = \omega_L$, which means that the average frequency of the rf field, $\omega$, is equal to the Larmor frequency of the spin in the permanent magnetic field. Using the dimensionless variables: $\tau = \omega_c t$ and $z = Z \sqrt{m_c^* \omega_c / \hbar}$ the spin-cantilever dynamics is described in the rotating frame, by the following Heisenberg operator equation,

$$
d^2 z/d\tau^2 + z = 2\eta S_z, \quad d\vec{S}/d\tau = [\vec{S} \times \vec{B}_{eff}],
$$

(2)
where \( \vec{B}_{\text{eff}} = (\epsilon, 0, -d\phi/d\tau + 2\eta z) \) is the dimensionless effective magnetic field, \( \epsilon = \omega_1/\omega_c \) and \( \eta = g\mu(\partial B_z/\partial Z)/(2\sqrt{m^*\omega_3^2\hbar}) \). Thus, our model includes two dimensionless parameters, \( \epsilon \) and \( \eta \). The first one is the dimensionless amplitude of the rf field, and the second one describes the interaction of a single spin with a cantilever mechanical vibrations due to a non-uniform magnetic field produced by the ferromagnetic particle. Note that the term \( d\phi/d\tau \) in \( \vec{B}_{\text{eff}} \) is caused by the phase modulation of the transversal magnetic field. The other part of the z-component of the effective magnetic field, \( 2\eta z \), describes a nonlinear effect – a back reaction of the cantilever vibrations on the spin.

If the adiabatic conditions (\( |d^2\phi/d\tau^2| \ll \epsilon^2 \)) are satisfied and the nonlinear effects are small in comparison to the effects of the rf field, the average spin is “captured” by the effective magnetic field. More precisely, it precesses around the effective magnetic field in such a way that the angle between the directions of the average spin and the effective magnetic field approximately remains constant. In CAI MRFM, the value of \( d\phi/d\tau \) changes periodically with the period of the cantilever (\( 2\pi \) in our dimensionless variables). As a result, the effective magnetic field and the average spin change their directions with the same period. This leads to a resonant excitation of the cantilever vibrations.

To test our model, we considered the classical limit of the macroscopic number of spins and the classical cantilever. Replacing the operators \( S_x \) and \( S_z \) in Eq. (2) by the sums of operators over all spins in the sample and neglecting the quantum correlation effects, we obtain the classical equations of motion for the total average spin and for the cantilever. We solved these classical equations numerically for the parameters corresponding to the experiment with protons in ammonium nitrate [5]. To estimate the amplitude of stationary vibrations of the cantilever within the Hamiltonian approach, we consider the time, \( \tau = Q_c \), where \( Q_c \) is the quality factor of the cantilever. We obtained for the amplitude of stationary vibrations of the cantilever \( Z_{\text{max}} \approx 15 \text{ nm} \), which is close to the experimental value in [5], \( Z_{\text{max}} \approx 16 \text{ nm} \).

Since a cantilever can be considered as a quasi-classical measuring device, one might
expect smooth increase of the cantilever amplitude also in a measurement of a single spin. However, a single spin z-component can accept only two values, \( s_z = \pm 1/2 \). Therefore, smooth resonant vibrations of the quasi-classical cantilever driven by the continuous oscillations of \( s_z \) seem to violate the principles of quantum mechanics. From this point of view, one should face quantum jumps rather than smooth oscillations of the cantilever. Such jumps could prevent the increase of the amplitude of the cantilever vibrations and a single-spin detection. To resolve this problem we consider the quantum dynamics of the single spin-quasiclassical cantilever system. The dimensionless Schrödinger equation can be written in the form,

\[
\frac{i}{\hbar} \frac{\partial \Psi(z, s_z, \tau)}{\partial \tau} = \mathcal{H}' \Psi(z, s_z, \tau), \quad \Psi(z, s_z, \tau) = \begin{pmatrix} \Psi_1(z, \tau) \\ \Psi_2(z, \tau) \end{pmatrix},
\]

where \( \Psi(z, s_z, \tau) \) is a dimensionless spinor, \( \mathcal{H}' = \mathcal{H}/\hbar \omega_c \) is the dimensionless Hamiltonian. The functions \( \Psi_{1,2}(z, \tau) \) are the complex amplitudes to find a spin in the state \( |s_z = \pm 1/2 \rangle \) and a cantilever at the point \( z \) at time \( \tau \).

To describe the cantilever as a sub-system close to the classical limit, we choose the initial wave function of the cantilever in the coherent state \( |\alpha \rangle \). Namely, it was taken in the form, \( \Psi_1(z, 0) = \sum_{n=0}^{\infty} A_n(0) |n\rangle, \quad \Psi_2(z, 0) = 0, \) and \( A_n(0) = (\alpha^n/n!) \exp(-|\alpha|^2/2) \), where \( |n\rangle \) is an eigenstate of the oscillator (cantilever) without spin. The initial average values of the coordinate and momentum are related to \( \alpha \) as \( \langle z \rangle = \frac{1}{\sqrt{2}} (\alpha^* + \alpha), \quad \langle p_z \rangle = \frac{i}{\sqrt{2}} (\alpha^* - \alpha) \). In order to correspond the classical limit, we took \( |\alpha|^2 \gg 1 \).

For numerical simulation of the single-spin-cantilever dynamics we used the value of the interaction parameter \( \eta = 0.3 \). Currently this value is not feasible in experiments with a nuclear spin, but can be achieved in experiments with a single electron spin. For instance, for the cantilever parameters from [9] and the magnetic field gradient reported in [7], we obtain for a single electron spin \( \eta = 0.8 \). The phase modulation of the rf field was taken in the form \( d\varphi/d\tau = -6000 + 300\tau, \) (if \( \tau \leq 20 \)), and \( d\varphi/d\tau = 1000 \sin(\tau - 20), \) (if \( \tau > 20 \)), and the rf field amplitude, \( \epsilon = 400 \). For these parameters the effective magnetic field, \( 2\eta z \), produced by the cantilever vibrations on the spin remains small with respect to the amplitude of the
rf field.

The numerical simulations of the quantum dynamics reveal the formation of the asymmetric quasi-periodic Schrödinger cat (SC) state for the cantilever. Fig. 2 shows the typical probability distributions, \( P(z, \tau) = |\Psi_1(z, \tau)|^2 + |\Psi_2(z, \tau)|^2 \), for nine instants of time. Near \( \tau = 40 \), the probability distribution, \( P(z, \tau) \), splits in two asymmetric peaks. After this the separation between these two peaks varies periodically in time. The ratio of the peak amplitudes is about 1000 for chosen parameters (the probabilities are shown in the logarithmic scale).

It is clear that the small peak does not significantly influence the average coordinate of the cantilever. Fig. 3 shows the average coordinate of the cantilever, \( \langle z(\tau) \rangle \), and the corresponding standard deviation, \( \Delta(\tau) = [\langle z^2 \rangle - \langle z \rangle^2]^{1/2} \). One can see fast increase of the average amplitude of the cantilever vibrations, while the standard deviation still remains small. This, in fact, is related to the initial conditions of the spin, which was taken in the direction of the \( z \)-axis. For instance, if the spin initially points in the \( x \)-axis (\( \Psi_1(z, 0) = \Psi_2(z, 0) \)), our calculations show two large peaks with similar amplitudes.

The two peaks in the cantilever probability distribution, shown in Fig. 2, indicate two possible trajectories of the cantilever. As a result of the consequent measurement of the cantilever position the system selects one of the two trajectories. The crucial problem is the following: Do the two peaks of the SC state of the cantilever correspond to the definite spin states? To answer this question we studied the structure of the wave function of the cantilever-spin system. First we have found that both functions, \( \Psi_1(z, \tau) \) and \( \Psi_2(z, \tau) \), contribute to each peak. Fig. 4 illustrates the probability distributions, \( |\Psi_1(z, \tau)|^2 \) (red) and \( |\Psi_2(z, \tau)|^2 \) (blue), for nine instants of time. One can see that these functions have maxima at the same values of \( z \). Next, we analyzed the structures of the functions, \( \Psi_1(z, \tau) \) and \( \Psi_2(z, \tau) \). When two peaks are clearly separated we can represent each of these functions as a sum of two terms, corresponding to the “big” and “small” peaks,

\[
\Psi_{1,2}(z, \tau) = \Psi_{1,2}^b(z, \tau) + \Psi_{1,2}^s(z, \tau).
\]
We have found that with accuracy up to 1% the ratio, \( \Psi_1(z, \tau)/\Psi_2(z, \tau) = -\Psi_2(z, \tau)/\Psi_1(z, \tau) = \kappa(\tau) \), where the \( \kappa(\tau) \) is a real function independent of \( z \). As a result, the total wave function can be represented in the form,

\[
\Psi(z, s_z, \tau) = \Psi^b(z, \tau)\chi^b(s_z, \tau) + \Psi^s(z, \tau)\chi^s(s_z, \tau),
\]

where \( \chi^b(s_z, \tau) \) and \( \chi^s(s_z, \tau) \) are spin wave functions, which are orthogonal to each other. Eq. (5) shows that each peak in the probability distribution of the cantilever coordinate corresponds to a definite spin wave function. We found that the average spin corresponding to the big peak \( \langle \chi^b | \vec{S} | \chi^b \rangle \) points in the direction of the vector \((\epsilon, 0, -d\varphi/d\tau)\), whereas \( \langle \chi^s | \vec{S} | \chi^s \rangle \) points in the opposite direction. Note that up to a small term, \( 2\eta z \), the vector \((\epsilon, 0, -d\varphi/d\tau)\) is the effective magnetic field acting on the spin (see Eq. (2)). The ratio of the integrated probabilities (\( \int P(z, \tau)dz \)) for the small and big peaks (\( \sim 10^{-3} \) in Fig. 2) can be easily estimated as \( \tan^2(\Theta/2) \), where \( \Theta \) is the initial angle between the effective field, \((\epsilon, 0, -d\varphi/d\tau)\), and the spin direction. Therefore by measuring the cantilever vibrations, one finds the spin in a definite state along or opposite to the effective magnetic field. Our numerical simulations show that starting with such a new initial condition, i.e. when the average spin points along or opposite to the effective field, the probability distribution \( P(z, \tau) \) shows again two peaks, as in Fig. 2, but the ratio of the integrated probabilities of these peaks is much less (\( \sim 10^{-6} \)). Thus for chosen parameters, the quantum jumps generated by a single spin measurement cannot prevent the amplification of the cantilever vibration amplitude, and thus the detection of a single spin.

So far, the described picture reminds the classical Stern-Gerlach effect in which the cantilever measures the spin component along the effective magnetic field. An appearance of the second peak, even if the average spin points initially in the direction of the effective magnetic field, provides a difference with the Stern-Gerlach effect. The origin of this peak is a small deviations from the adiabatic motion of the spin even at large amplitude of the effective field, and the back reaction of the cantilever vibrations on the spin. The next important question is the following: Is it possible to use CAI MRFM to measure the state of
a single spin? We studied numerically the phase of the cantilever vibrations when the initial spin points along or opposite the direction of the effective magnetic field. Our computer simulations show that the phases of the cantilever vibrations for these two initial conditions are significantly different. When the amplitude of the cantilever vibrations increases, the phase difference for two initial conditions approaches \( \pi \). Thus, the classical phase of the cantilever vibrations indicates the state of the spin relatively to the effective magnetic field. If the spin is initially in the superposition of these two states, it will acquire one of these states in the process of measurement.

In practical applications it would be very desirable to use CAI MRFM for measurement of the initial \( z \)-component of the spin. For this purpose one should provide the initial direction of the effective magnetic field to be a \( z \)-direction. Then, the initial \( z \)-component of the spin will coincide with its component relatively to the effective magnetic field. In our computer simulations presented in Figs. 2-4 we have assumed instantaneous increase of the amplitude of the \( rf \) field, at \( \tau = 0 \). It causes the initial angle between the directions of the spin and the effective magnetic field, \( \Theta \approx \epsilon / |d\varphi/d\tau| \approx 0.07 \). To eliminate this initial angle we simulated the quantum spin-cantilever dynamics for adiabatic increase of the \( rf \) field amplitude: \( \epsilon = 20\tau \) for \( \tau \leq 20 \), and \( \epsilon = 400 \) for \( \tau > 20 \). Dependence for \( d\varphi/d\tau \) was taken the same as in Figs. 2-4. The results of these simulations are qualitatively similar to those presented in Figs. 2-4, but the integrated probability of the small peak was reduced to its residual value \( \sim 10^{-6} \). Neglecting this small probability one can provide the measurement of the initial \( z \)-component of the spin.

We should also mention that the detection of a single electron spin in an atom can be used to determine the state of its nuclear spin \([10,11]\). Such a measurement is possible for an atom with a large hyperfine interaction in a high external magnetic field, because the electron spin frequency of the atom depends on the state of its nuclear spin.

In conclusion, we have analyzed the quantum effects in the single-spin measurement using cyclic adiabatic inversion (CAI) to drive cantilever vibrations in magnetic resonance force microscopy (MRFM). We investigated the quasi-classical cantilever interacting with a
single spin using Hamiltonian approach. We have shown that the spin-cantilever dynamics generates a Schrödinger-cat (SC) state for the cantilever. The two peaks of the probability distribution of the cantilever coordinate correspond approximately to the directions of the spin along or opposite to the direction of the effective magnetic field, in the rotating frame.

In this paper, we did not discuss the intriguing possibility of observing the SC state. This requires an estimate of the SC life time, which cannot be derived using our Hamiltonian which neglects the environment of the cantilever. Instead, we concentrated on a possibility of observing the resonant excitation of the cantilever vibrations, driving by a single spin. We demonstrated by a direct computation of the average cantilever position and its standard deviation as a function of time that the resonant amplification of the cantilever oscillations in indeed possible (for considered region of the system parameters), despite the quantum jumps of the single spin. In fact, the standard deviation of the cantilever coordinate becomes large only when the angle between the initial spin direction and the effective magnetic field approaching $\pi/2$. In this case the SC state appears with approximately equals peaks. However after an observation of the cantilever position the system appears in one of the peaks, and the following evolution of the cantilever coordinate shows again the resonant amplifications with a very small standard deviation.

We expect that taking into consideration the interaction with an environment will not change our conclusion. Such an interaction will cause the decoherence \[12\], which transforms the SC state into the statistical mixture. It is clear that this effect as well as the thermal vibrations of the cantilever (see, for example \[3,9\]), cannot prevent an observation of the driven oscillations of the cantilever if the corresponding rms amplitude exceeds the rms amplitude of the vibrational noise. Another effect of the interaction with the environment is the finite quality factor, $Q_c$, of the cantilever, which puts the limit on the increase of the cantilever vibrations. The stationary amplitude of the cantilever vibrations can be estimated in our Hamiltonian approach by putting $\tau = Q_c$.

Finally, we mention two other possible techniques for the cyclic spin inversion in MRFM. One of them is the standard Rabi technique. This assumes that in our notation $d\varphi/d\tau = 0,$
and $\epsilon = 1$, i.e. the Rabi frequency equals to the cantilever frequency. This technique seems to be simpler than the CAI MRFM. But the amplitude of the rf field, $\epsilon$, must be much greater than the effective field produced by the cantilever on the spin $2\eta z \ll \epsilon = 1$. In this case, the force acting on the cantilever is very small, and the amplification of the driven cantilever vibrations requires a long time, i.e. a large cantilever quality factor. Another technique assumes the application of short $\pi$-pulses which periodically change the direction of the spin in the time-interval, which is very short in comparison to the cantilever period $13$. If the time interval between successive pulses equals half of the cantilever period, this technique provides a resonant amplification of the cantilever vibrations. Testing this technique in MRFM experiments is a challenging problem.
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FIG. 1. The cantilever-spin system. $\vec{B}_0$ is the uniform permanent magnetic field; $\vec{B}_1$ is the rotating magnetic field; $\vec{M}$ is the magnetic moment of the ferromagnetic particle; $\vec{S}$ is a single spin.
FIG. 2. The probability distribution, $P(z)$, for the cantilever position. The values of parameters are: $\epsilon = 400$ and $\eta = 0.3$. The initial conditions are: $\langle z(0) \rangle = -20$, $\langle p_z(0) \rangle = 0$ (which correspond to $\alpha = -10\sqrt{2}$). The same parameters will be used in all figures below.
FIG. 3. Cantilever dynamics. (a) Average coordinate of the cantilever as a function of $\tau$ and (b) its standard deviation $\Delta(\tau) = \left[ \langle z^2(\tau) \rangle - \langle z(\tau) \rangle^2 \right]^{1/2}$.
FIG. 4. The probability distributions $P_i(z, \tau) = |\Psi_i(z, \tau)|^2$, $i = 1$ (red) and $i = 2$ (blue) for nine instants in time: $\tau_k = 92.08 + 0.8k$, $k = 0, 1, ..., 8$