We consider a simple version of a cyclic adiabatic inversion (CAI) technique in magnetic resonance force microscopy (MRFM). We study the problem: What component of the spin is measured in the CAI MRFM? We show that the non-destructive detection of the cantilever vibrations provides a measurement of the spin component along the effective magnetic field. This result is based on numerical simulations of the Hamiltonian dynamics (the Schrödinger equation) and the numerical solution of the master equation.

**I. INTRODUCTION**

Magnetic resonance force microscopy (MRFM) is approaching its ultimate goal: a single spin detection [1–3]. The most promising approach to single spin detection is, probably, cyclic adiabatic inversion (CAI) [1]. In this approach, the magnetic moment of the sample changes its direction adiabatically following the effective magnetic field. The CAI of the spin may act as an “external force” driving the resonant vibrations of the cantilever or it may affect the frequency of the cantilever vibrations driven by another source (e.g. the modern “OSCAR” technique [3]).

The fundamental question which arises in MRFM single-spin measurement is the following: What component of the spin is measured by this technique? Indeed, in a simple geometry the cantilever tip oscillating along the z-axis interacts with the z-component of the spin and, consequently, is expected to measure the spin z-component. From the other side, adiabatic inversion assumes that the approximate integral of motion is the spin component along the effective magnetic field which rotates in the x−z plane. Thus, one might expect that the cantilever measures the spin component along the effective magnetic field in the rotating reference frame.

In this work we consider the macroscopic cantilever as itself the measuring device interacting with an environment. We assume that the influence of an additional (e.g. optical) device which detects the cantilever vibrations is small. This corresponds to the current MRFM technique. In Section II we discuss the quantum dynamics of the quasi-classical cantilever which describes a generation of the Schrödinger cat state associated with two possible projections of the spin. In Section III we include an interaction of the cantilever with an environment inherent to any measurement processes. The latter leads to the decoherence of the two possible trajectories of the cantilever due to interaction with the environment.

**II. HAMILTONIAN DYNAMICS**

We considering the simple setup shown in Fig. 1.

The ferromagnetic particle with a magnetic moment \( \vec{m} \) is mounted on the cantilever tip. The permanent magnetic field, \( \vec{B}_0 \), points in the positive z-direction. A rotating rf field in the x−y plane, \( \vec{B}_1 \sim \exp[i(\tau - \varphi(t))] \), is resonant with the spin precession around the z-axis.

The frequency modulation of \( \vec{B}_1 \) causes the CAI of the spin. Under resonant conditions, when the period of the cantilever vibrations matches the period of the CAI, the amplitude of the cantilever vibrations is expected to increase providing the detection of the spin.

The quantum Hamiltonian of the system in the rotating frame (in terms of dimensionless parameters) can be written as

\[
\mathcal{H} = (\vec{g}^2 + \vec{z}^2)/2 + \varphi(\tau)S_z - \epsilon S_x - 2\eta z S_z. \tag{1}
\]

Here

\[
p_x = p_x/p_q, \quad z = Z/Z_q, \tag{2}
\]

\( \vec{S} \) is the electron spin operator, \( \epsilon = \gamma B_1/\omega_c, \quad \dot{\varphi} = d\varphi/d\tau, \quad \eta = gF/2F_q, \quad p_x \) and \( Z \) are the operators of the effective momentum and coordinate of the cantilever tip; \( \gamma = g\mu_B/\hbar \) is the spin gyromagnetic ratio (absolute value); \( \omega_c \) is the cantilever frequency; \( F \) is the magnetic force between the ferromagnetic particle and the cantilever tip is at the origin (\( z = 0 \)). The origin is chosen at the equilibrium position of the cantilever with no spin; \( \tau = \omega_c t \) is a dimensionless time. The units of the coordinate, momentum, and force are given by

\[
Z_q = (h\omega_c/k_c)^{1/2}, \quad p_q = \hbar/Z_q, \quad F_q = k_c Z_q, \tag{3}
\]

where \( k_c \) is the cantilever spring constant. Note, that we treat an electron spin of a paramagnetic atom whose direction is opposite to the direction of the atomic magnetic
moment. We assume in (1) that the transverse magnetic field points in the negative $x$-direction of the rotating frame.

With respect to actual “reading” devices we consider a realistic scenario for the MRFM technique which involves non-destructive measurements of the amplitude, frequency, and phase of the cantilever vibrations, for example by using a fiber-optic interferometer operating in the infrared region. We assume that the optical detection of cantilever vibrations does not influence significantly the cantilever-spin dynamics. (In practice, this means that the disturbance caused by the optical radiation is smaller than the thermal noise of the cantilever.)

In this section we do not consider the interaction with the environment which provides the measurement itself. (See also [4].) Thus, we use the Schrödinger equation,

$$i \dot{\Psi} = \mathcal{H} \Psi,$$  

(4)

for computer simulations of the cantilever-spin dynamics. In the $z - S_z$-representation, the wave function, $\Psi$, is a spinor. It contains two components, $\Psi(z, 1/2, \tau)$ and $\Psi(z, -1/2, \tau)$, which correspond to the two possible values of $S_z$. Using the expansion over the eigenfunctions, $u_n$, of the oscillator Hamiltonian, $(p_z^2 + z^2)/2$, we write these two components of the cantilever-spin wave function in the form,

$$\Psi(z, 1/2, \tau) = \sum_{n=0}^{\infty} A_n(\tau) u_n, \quad \Psi(z, -1/2, \tau) = \sum_{n=0}^{\infty} B_n(\tau) u_n,$$  

(5)

and derive equations for the amplitudes, $A_n$ and $B_n$,

$$i A_n = (n+1/2 + \dot{\phi}/2) A_n - (\eta/\sqrt{2})(\sqrt{n} A_{n-1} + \sqrt{n+1} A_{n+1}) - (\epsilon/2) B_n,$$  

(6)

$$i B_n = (n-1/2 + \dot{\phi}/2) B_n + (\eta/\sqrt{2})(\sqrt{n} B_{n-1} + \sqrt{n+1} B_{n+1}) - (\epsilon/2) A_n.$$  

(7)

The initial conditions describe the quasi-classical state of the cantilever tip and a spin which points in the positive $z$-direction,

$$A_n(0) = (\alpha^n / \sqrt{n!}) \exp(-|\alpha|^2/2), \quad B_n(0) = 0,$$  

(8)

$$\alpha = |\langle z(0) \rangle + i \langle p_z(0) \rangle| / \sqrt{2}.$$  

In our computer simulations we used the following parameter values,

$$\eta = 0.3, \quad \epsilon = 400, \quad \dot{\phi} = -6000 + 300 \tau \text{ if } \tau \leq 20,$$  

and

$$\dot{\phi} = 1000 \sin(\tau - 20) \text{ if } \tau > 20.$$  

The main results of our simulations are the following. The wave function of the cantilever-spin system, which is initially a product of the cantilever and spin parts, quickly becomes entangled. The probability distribution to find the cantilever at the point $z$ at time $\tau$,

$$P(z, \tau) = |\Psi(z, 1/2, \tau)|^2 + |\Psi(z, -1/2, \tau)|^2,$$  

(9)

splits into two peaks, “big” and “small” peaks. (See Fig. 2.) When the peaks are separated, the wave function of the cantilever-spin system can be represented as a sum of two spinors,

$$\Psi(z, s, \tau) = \Psi^{(1)}(z, s, \tau) + \Psi^{(2)}(z, s, \tau),$$  

(10)

where the upper indices “1” and “2” refer to the big and the small peaks, correspondingly. It was found with the accuracy to 1% that both spinor wave functions, $\Psi^{(k)}(z, s, \tau) \quad (k = 1, 2)$, can be represented as a product of the cantilever and spin functions,

$$\Psi^{(k)}(z, s, \tau) = R^{(k)}(z, \tau) \chi^{(k)}(s, \tau),$$  

(11)

where $\chi^{(1)}(s, \tau)$ describes the spin which points in the direction of the external effective field, $(\epsilon, 0, -\dot{\phi}(\tau))$, and $\chi^{(2)}(s, \tau)$ describes the spin which points in the opposite direction. The ratio of the probabilities for the big and the small peak is determined by the initial angle between the external effective magnetic field and the spin,

$$\int |R^{(2)}(z, \tau)|^2 dz \int |R^{(1)}(z, \tau)|^2 dz = \tan^2(\Theta/2),$$  

(12)

where $\Theta$ is the initial direction of the external effective magnetic field $(\tan \Theta = -\epsilon / \dot{\phi}(0) = 1/15)$. If the initial conditions describe a spin which points, for example, in the positive $x$-direction $(A_n(0) = B_n(0))$, our simulations reveal two peaks with approximately equal amplitudes. Thus, the Hamiltonian dynamics clearly indicates that the quasi-classical cantilever will measure the spin component along the effective magnetic field. Certainly,
in the frames of the Hamiltonian approach we cannot
describe the measurement itself: the coherence between
the two cantilever peaks does not disappear. In other
words, the Schrödinger equation describes the macro-
scopic Schrödinger cat state of the cantilever without ef-
facts of decoherence.

III. MASTER EQUATION

In the previous section, we have presented indications
that the cantilever “measures” the spin component along
the direction of the effective magnetic field. In this sec-
tion we describe the measurement process. During the
measurement process the coherence between two can-
tilever trajectories disappears. It means that the reduced
density-matrix of the cantilever-spin system becomes a
statistical mixture representing two possible trajectories
of the system. The main question we are going to answer
is the following: Does the cantilever, which interacts with
the environment, measure the spin component along the
effective magnetic field?

To answer this question, we studied the dynamics of the
cantilever-spin system using the master equation. Our
purpose is not just to simulate the expected exper-
iment but rather to present a qualitative verification of
the conclusion obtained in the previous section. That is
why we consider the simplest “ohmic” model of the envi-
ronment in the high-temperature approximation [5]. In
this approximation the environment is described as an
ensemble of harmonic oscillators. The number of oscilla-
tors per unit frequency is proportional to the frequency
in the region below the chosen “cutoff” frequency, Ω, and
\(k_B T \gg h\Omega\). The master equation for the density matrix,
\(ρ\), in the high-temperature approximation, is

\[
\frac{∂ρ_{ss'}(z,z',τ)}{∂τ} = \left[ i \left( \frac{∂^2}{∂z^2} - \frac{∂^2}{∂z'^2} \right) - \frac{β}{2}(z - z')^2 \right] ρ_{ss'}(z,z',τ) + \left[ 2iη(z's' - zs) + i\dot{ϕ}(s' - s) \right] ρ_{ss'}(z,z',τ) - \frac{ε}{2} \left[ ρ_{ss'}(z,z',τ) - ρ_{ss'}(z',z,τ) \right].
\]

Here \(s, s' = ±1/2\), \(s = -s\), \(s' = -s'\), \(D = k_B T/h\omega_c\),
\(β = 1/Q\), where \(Q\) is the quality factor of the cantilever.
Again, we use the expansion over the eigenfunctions, \(u_n\),
\[
ρ_{ss'}(z,z',τ) = \sum_{n,m} A_{n,m}^{s,s'}(τ) u_n(z) u_m^*(z').
\]

Next, we solve numerically the system of equations for
the amplitudes, \(A_{n,m}^{s,s'}(τ)\),

\[
A_{n,m}^{s,s'}(τ) = \left( \begin{array}{c} i\dot{ϕ}(s' - s) + β/2 - (n + m + 1)Dβ - i(n - m) \end{array} A_{n,m}^{s,s'}(τ) - \frac{ε}{2} \left[ A_{n,m}^{s,s'}(τ) - A_{m,n}^{s,s'}(τ) \right].
\]

Below we describe the results of our computer sim-
ulations for the values of parameters in (8). First,
setting \(β = D = 0\) we obtain the density matrix,
\(ρ_{ss'}(z,z',τ)\), which exactly corresponds to the wave func-
tion, \(Ψ(z, s, τ)\), derived from the Schrödinger equation.

The initial density matrix is represented as a product
of the cantilever and spin parts,

\[
ρ_{s,s'}(z,z',0) = Ψ(z,1/2,0)Ψ^*(z',1/2,0) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.
\]

The wave function, \(Ψ(z,1/2,0)\), describes the quasi-
classical state of the cantilever,

\[
Ψ(z,0) = \sum_{n=0}^{∞} A_n(0) u_n(z).
\]
The values $A_n(0)$ are given in (7). The initial values, $A_{n,m}^k(0)$, in (15) can be easily found from (16).

For $\tau > 0$, the density matrix describes the entangled state which cannot be represented as a product of the cantilever and spin parts. The initial peak of $\rho_{s,s'}(z, z', \tau)$ splits into two peaks which are centered along the diagonal $z = z'$, and two peaks centered at $z \neq z'$, off the diagonal. The density matrix can be represented approximately as a sum of four terms corresponding to four peaks,

$$
\rho_{s,s'}(z, z', \tau) = \rho^{(1)}_{s,s'} + \rho^{(2)}_{s,s'} + \rho^{(3)}_{s,s'} + \rho^{(4)}_{s,s'},
$$

where we omit variables, $z, z', \tau$. The matrices, $\rho^{(1)}$ and $\rho^{(2)}$, describe the “big” and “small” diagonal peaks; $\rho^{(3)}$ and $\rho^{(4)}$, describe the peaks centered at $z \neq z'$.

As an illustration, we show in Fig. 3 the quantity,

$$
|\rho_{1/2,1/2}(z, z', \tau) + \rho_{-1/2,-1/2}(z, z', \tau)|.
$$

We have found that with accuracy to 1% the density matrix, $\rho^{(1)}_{s,s'}(z, z', \tau)$, can be represented as a product of the coordinate and spin parts,

$$
\rho^{(1)}_{s,s'}(z, z', \tau) = \tilde{\chi}_{s,s'}^{(1)}(\tau) \chi_{s,s'}^{(1)}(\tau),
$$

where $\chi_{s,s'}^{(1)}(\tau)$ describes the spin which points in the direction of the external effective magnetic field ($\epsilon, 0, -\psi(\tau)$). A similar expression is valid for $\rho^{(2)}_{s,s'}(z, z', \tau)$. But in this case, $\chi_{s,s'}^{(2)}(\tau)$ describes a spin which points in the opposite direction.

First we note that in order to describe the measurement process (the decoherence), we have to consider an ensemble of quasi-classical cantilevers with the same initial conditions. At the same time, we are considering driven oscillations of the cantilever. So, the result of our simulations qualitatively does not depend on the initial conditions of the cantilever. Second, as we already mentioned, we are going to verify qualitatively the conclusion derived in the previous section rather than simulate the expected experiment. Thus, we choose the values of parameters which help us to save a computational time. Namely, we choose a relatively small (but still quasi-classical) values for the initial energy of the cantilever, and a relatively small value for the thermal parameter $D$ (without violating the high-temperature approximation which requires $D \gg 1$). The small initial energy of the cantilever allows us to reduce a number of basis functions, $u_n(z)$. A relatively small value of $D$ allows us to observe four well-separated peaks at relatively small values of time, $\tau$.

The initial uncertainty of the cantilever position is, $\delta z = 1/\sqrt{2}$. Due to thermal diffusion, the uncertainty of the cantilever position increases with time. Thus, we have two effects: i) the increase of the amplitude of the driven cantilever vibrations (similar to the Hamiltonian dynamics) and ii) the increase of the uncertainty of the cantilever position due to thermal diffusion. If the second effect dominates, the two positions of the diagonal peaks (i.e., peaks centered on the line $z = z'$) become indistinguishable. In this case, one cannot provide a spin measurement with two possible outcomes.

We have found that peaks centered on the diagonal retain the main properties described by the Hamiltonian dynamics. The density matrix, $\rho^{(k)}_{s,s'}(z, z', \tau)$, for $k = 1, 2$ can be approximately represented as a product of the cantilever and spin parts. The spin part of the matrix describes the spin which points in the direction of the external effective magnetic field ($k = 1$) or in the opposite direction ($k = 2$).

Next, we discuss the two peaks centered at $z \neq z'$. As an illustration, Figs. 4 and 5 show the contours of the quantities,

$$
|\rho_{1/2,1/2}(z, z', \tau) + \rho_{-1/2,-1/2}(z, z', \tau)|,
$$

and

$$
|\rho_{1/2,-1/2}(z, z', \tau) + \rho_{-1/2,1/2}(z, z', \tau)|,
$$

given in logarithmic scale. One can see the peaks centered at $z \neq z'$ as well as at $z = z'$. The peaks centered at $z \neq z'$ describe the coherence between the two cantilever positions. The amplitude of these peaks quickly decreases due to the decoherence. Thus, the master equation explicitly describes the process of measurement. The coherence between two cantilever trajectories (the macroscopic Schrödinger cat state) quickly disappears. As a result, the cantilever will “choose” one of two possible trajectories. Correspondingly, (depending on the cantilever trajectory) the spin will point in the direction of the effective magnetic field or in the opposite direction.

### IV. CONCLUSION

We have studied the quantum dynamics of the cantilever-spin system in a simple version of the cyclic adiabatic inversion (CAI) magnetic resonance force microscopy (MRFM). In this version, the spin experiences a CAI under the action of the external phase modulated rf magnetic field. If the frequency of CAI matches the cantilever frequency, the amplitude of the cantilever vibrations increases allowing single-spin detection. We have studied the problem: Which component of the spin is measured by the cantilever? We argue that one will measure the component of the spin along the direction of the effective magnetic field providing non-destructive detection of the cantilever vibrations. This result was first derived using computer simulations of the Hamiltonian dynamics (the Schrödinger equation). Then, it was confirmed by the numerical solution of the master equation. We have considered the case when the amplitude of the
driven cantilever vibrations was greater than the thermal noise. In this case, the phase of the driven vibrations depends on the spin component along the direction of the external effective magnetic field. Thus, detecting the phase of the cantilever vibrations one can measure the spin component along the effective magnetic field.  

We should mention that the direct relation between the cantilever trajectory and the direction of the spin has been verified for a transient process in the CAI MRFM. Our computer capabilities do not allow us to check this relation for the stationary cantilever vibrations at $\tau \gg Q$.  

Also, we completely ignored the direct interaction between the spin and the environment. We are now investigating this interaction.

FIG. 1. MRFM setup.

FIG. 2. The probability distribution, $P(z, \tau)$, for the cantilever position, in the logarithmic scale. 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 corresponds to $\alpha = -10\sqrt{2}$).

FIG. 3. Three-dimensional plot of log $|\rho_{1/2,1/2}(z, z', \tau) + \rho_{-1/2,-1/2}(z, z', \tau)|$, in the logarithmic scale. The values of parameters are: $\epsilon = 400$, $\eta = 0.3$, $\beta = D = 0$. The initial conditions are: $\langle z(0) \rangle = -4$, $\langle p_z(0) \rangle = 0$. The colors in Figs. 3-5 correspond to the following values for the logarithm of the density matrix: white (<-16), red (-16,-12), green (-12,-8), blue (-8,-4), yellow (>4).

FIG. 4. The contours for log $|\rho_{1/2,1/2}(z, z', \tau) + \rho_{-1/2,-1/2}(z, z', \tau)|$. The values of parameters are: $\epsilon = 400$, $\beta = 0.001$, and $D = 10$. The initial conditions are: $\langle z(0) \rangle = -4$, $\langle p_z(0) \rangle = 0$.

FIG. 5. The same as in Fig. 4, but for log $|\rho_{1/2,-1/2}(z, z', \tau) + \rho_{-1/2,1/2}(z, z', \tau)|$.

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