Microstrip Resonator as a Measuring Device for a Single Molecule Magnet

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Abstract — A single molecule magnet (SMM) could be used as a qubit in quantum information processing. In this work, we suggested a method for the measurement of the SMM state with a microstrip resonator. In our method the frequency of the electron spin resonance adiabatically approaches to the fundamental frequency of the microstrip resonator. The shift of the resonator frequency is maximal near the crossing point. This shift depends on the initial state of the SMM and can be used for the measurement of the initial state. We have used the classical approach for description of the SMM dynamics and the interaction between the microstrip and SMM. We have obtained an analytical expression for the resonator maximum frequency shift and performed numerical analysis in the vicinity of the crossing point.

1. INTRODUCTION

In quantum information processing, single molecule magnets (SMM) can be used as qubits [2]. Measurement of the qubit state is fundamental to a successful quantum computer. A microstrip resonator recently became an important tool in quantum information processing [3]. In this paper, we suggest using a microstrip resonator as a method to measure the SMM spin state. We consider the adiabatic spin dynamics assuming that, the SMM magnetic moment remains parallel or antiparallel to the effective magnetic field. In this work, we use the classical equations of motion for the SMM magnetic moment. The microstrip was described in an equivalent circuit model. Only the rotating component of the transversal field on the SMM was taken into consideration and the anisotropy field was ignored.

2. SMM-MICROSTRIP SYSTEM

A diagram of a microstrip resonator is shown in Fig. 1. The microstrip resonator can be represented by an LC circuit. In terms of the physical shape of the microstrip resonator, the parameters, $C$ and $L$, can be approximated as:

$$C = \frac{\varepsilon wl}{d}, \quad L = \frac{\mu_0ld}{w}$$

(1)

where $\varepsilon$ is the permittivity of the dielectric substrate, $\mu_0$ is the permeability of free space, $w$ and $l$ are the width and the length of the microstrip, and $d$ is the distance between the microstrip and the metallic plate as shown in Fig. 1 [1].

We consider a SMM that is experiencing a permanent external magnetic field together with a transversal magnetic field created by a microstrip. The dynamics of the SMM is governed by the following equation

$$\ddot{m} = -\gamma (m \times (B_1 \cos(\omega t)\hat{x} + B_1 \sin(\omega t)\hat{y} + B_{ext} \hat{z}))$$

(2)

where $\vec{m} = m_x \hat{x} + m_y \hat{y} + m_z \hat{z}$ is the magnetic moment of SMM, $\gamma$ is the absolute value of the electronic gyromagnetic ratio, $B_1$ is the magnitude of the transversal rotating magnetic field of frequency $\omega$ caused by the microstrip resonator and $B_{ext}$ is the magnitude of the external permanent magnetic field, which points in the positive $z$-direction. (Only the resonant rotating component of the transversal field is taken into consideration.) Letting $m_+ = m_x + im_y = \pm m_o e^{i\omega t}$, where $m_o$ is the magnitude of the transversal magnetic moment, we describe the two stationary solutions in the rotating system of coordinates, where

$$m_o = \frac{\gamma B_1 m}{\sqrt{(\gamma B_1)^2 + (\gamma B_{ext} - \omega)^2}}.$$  

(3)

The magnitude of the magnetic moment is $m = \sqrt{m_o^2 + m_+^2}$. The two stationary solutions describe the magnetic moment, parallel or antiparallel to the effective field in the rotating system.
Figure 1: Microstrip resonator and magnetic moment, $\vec{m}$, of the SMM at an instant when the magnetic moment of the SMM points in the positive $x$-direction. $l$ and $w$ are the length and the width of the microstrip, $s$ is the distance between the substrate and the SMM.

3. EQUATION FOR RESONATOR FREQUENCY

We assume that the oscillating component of the magnetic moment, $m_x$, generates an $emf$ in the equivalent circuit of the microstrip resonator

$$emf = -\frac{d\Phi}{dt} = -k' \frac{dm_x}{dt}$$  \hspace{1cm} (4)

where $k'$ is a parameter determined by the geometry of the microstrip. Applying Kirchhoff’s rules to an LC circuit with the $emf$ from Eq. (4) and taking its time derivative, we get

$$-\frac{I}{C} - L\ddot{I} - k\dot{m}_x = 0$$  \hspace{1cm} (5)

In order to find the eigenfrequency of the resonator affected by the SMM, we put

$$I = I_o e^{i\omega t}, \hspace{0.5cm} m_x = \kappa m_o e^{i\omega t}$$  \hspace{1cm} (6)

The parameter, $\kappa = \pm 1$, respectively describes the magnetic moment parallel or antiparallel to the effective field in the rotating system. In the zeroth approximation putting $k' = 0$ we obtain the resonator frequency, $\omega = \omega_o = \frac{1}{\sqrt{LC}}$.

Next, we obtain the frequency of the resonator-SMM system in the first approximation. The transversal oscillating magnetic field at the SMM location is assumed to to be $B_x = kI$, where $k$ depends on the geometry of the microstrip. We take into consideration, only the resonant rotating component of the transversal field with the magnitude $B_1 = \frac{1}{2}kI_o$. From Eq. (5) and taking into consideration Eq. (3), one obtains

$$I_o \left( -\frac{1}{C} + L\omega^2 + \frac{\kappa^2 k'^2 m_o^2}{\sqrt{\gamma^2 k^2 T_o^2 + 4(\gamma B_{ext} - \omega)^2}} \right) = 0$$  \hspace{1cm} (7)

Letting $A = \gamma k' m_o L$, $D = \gamma k I_o$, $r = \gamma B_{ext}/\omega_o$, and $x = \omega/\omega_o$, one gets

$$-1 + x^2 + \frac{\kappa A x^2}{\sqrt{D^2 + 4\omega_o^2(r - x)^2}} = 0$$  \hspace{1cm} (8)

We will use the following parameters for estimation: $\gamma = 1.761 \times 10^{11} \text{ s}^{-1} T^{-1}$, $s = 252 \text{ nm}$ (we assume the distance between the SMM and the microstrip is 2 nm, and the thickness of the microstrip is 250 nm), $w = 0.4 \text{ mm}$, $m = 1.85 \times 10^{-22} \text{ JT}^{-1}$ (this corresponds to SMM, Mn$_{12}$-Acetate, with $m = 20 \mu_B$, i.e., $S = 10$), $l = 1.5 \text{ mm}$, and $d = 5 \text{ mm}$, $\epsilon = 13\epsilon_o$. With these parameters, we have $k = 1.57 \times 10^{-3} \text{ TA}^{-1}$, $k' = 3.02 \times 10^3 \text{ Hm}^{-2}$, $L = 23.6 \text{ nH}$, $C = 13.8 \text{ fF}$, $\omega_o/2\pi = 8.82 \text{ GHz}$, $D/T_o = 2.77 \times 10^8 \text{ s}^{-1} \text{ A}^{-1}$, and $A = 6.57 \times 10^{-3} \text{ s}^{-1}$. 
Figure 2: The dependence of the relative frequency shift on \( \frac{\gamma B_{\text{ext}} - \omega}{\omega_o} \) for \( I_o = 1 \mu \text{A} \). (a) \( \kappa = 1 \) and (b) \( \kappa = -1 \).

Figure 3: Relative frequency shift for different current amplitudes and \( \kappa = -1 \). All other parameters are the same as in Fig. 2. The function, \( \omega = \gamma B_{\text{ext}} \), is represented by the dashed line.

At the crossing point, \( x = 1 \), the relative frequency shift, \( |\epsilon| \), is maximum when \( D \to 0 \) i.e., when the current approaches zero

\[
|\epsilon(I_o \to 0)| = \frac{1}{2} \sqrt{\frac{A}{\omega_o}} = \frac{1}{2} \sqrt{\frac{\gamma k k' m}{L\omega_o}}
\]  

With our parameters, the maximum relative frequency shift at the crossing point is approximately \( 1.72 \times 10^{-7} \).

The classical description of the microstrip is valid if the microstrip energy is much greater than its energy quantum: \( \frac{1}{2} L I_o^2 \gg \hbar \omega_o \). Taking \( \frac{1}{2} L I_o^2 / 2 = 10 \hbar \omega_o \), we obtain the lower bound for the current amplitude: \( I_o \geq I'_o = \sqrt{20 \hbar \omega_o / L} \). For our parameters, we have \( I'_o = 7.04 \times 10^{-8} \text{ A} \). For current amplitude, \( I'_o \), the relative frequency shift is approximately the same as for \( I_o \to 0 \).
4. HYSTERESIS BEHAVIOR OF THE MICROSTRIP FREQUENCY

With our parameters and current amplitude \( I_o = 1 \mu A \), we numerically solved Eq. (8). The relative frequency shift of the resonator as a function of the ratio \( \gamma B_{ext} - \omega_0 \) is shown in Fig. 2. When \( \kappa = 1 \), Eq. (8) has three real positive solutions in the region, \(-1.18 \times 10^{-5} \leq r - 1 \leq -3.45 \times 10^{-7}\), and one real positive solution outside this region. When \( \kappa = -1 \), Eq. (8) has three positive real solutions in the region, \(3.45 \times 10^{-7} \leq r - 1 \leq 1.18 \times 10^{-5}\), and one real positive solution outside the region. One can see that the maximum resonator frequency shift is not at the crossing point. The maximum relative frequency shift, \(|\epsilon|_{\text{max}}\), for our parameters is approximately \(1.18 \times 10^{-6}\) for \( \kappa = \pm 1 \). For the minimum value of the “classical current amplitude”, \( I_o = I'_o \), we have approximately \(1.69 \times 10^{-4}\). This value is the maximum frequency shift one can expect to observe.

We numerically determined that the hysteresis behavior disappears with current, \( I_o \), approximately greater than \(10^{-4} A\). Fig. 3 shows the relative frequency shift for different current amplitudes.

Our numerical computations show that when the current amplitude decreases, the relative frequency shift \(|\epsilon|\) monotonically increases. We numerically infer that the extremum (maximum for \( \kappa = 1 \) and minimum for \( \kappa = -1 \)) value of \( x \) in Eq. (8), occurs when \( x = r \) i.e., \( \omega = \gamma B_{ext} \). With this substitution, we obtain the exact expression for the resonator frequency:

\[
x_{\text{ext}} = \sqrt{\frac{D}{D + \kappa A}} = \sqrt{\frac{L I_o}{L I_o + \kappa k'm}}
\]

Thus, the maximum frequency shift, \(|\epsilon|_{\text{max}}\), is given by the expression

\[
|\epsilon|_{\text{max}} = \sqrt{\frac{L I_o}{L I_o + \kappa k'm}} - 1
\]

For \( I_o = 1 \mu A \), the maximum frequency shift for a 20\( \mu B \) SMM is estimated as \(|\epsilon|_{\text{max}} \approx 1.18 \times 10^{-6}\) for \( \kappa = \pm 1 \).

Figure 4: Expected behavior of the resonator frequency for a decreasing magnetic field \( \kappa = \pm 1 \). The dashed line corresponds to \( \omega = \gamma B_{ext} \).

5. CONCLUSION

We have developed the theory of the SMM measurement with the microstrip resonator using a classical description of the microstrip resonator and the SMM spin dynamics. We derived an analytical expression for the maximum frequency shift of the resonator (Eq. (11)) and numerically determined the behavior of the relative frequency shift, \( \frac{\omega - \omega_0}{\omega_0} \), as a function of the ratio, \( \gamma B_{ext}/\omega_0 \). The hysteresis behavior of the resonator frequency was demonstrated. The maximum possible relative frequency shift for a 20\( \mu B \) SMM is estimated as \(|\epsilon|_{\text{max}} \approx 1.69 \times 10^{-4}\).

Next, we propose two methods to use the resonator frequency shift to find the spin state of the SMM. We consider only two initial states of the SMM, ones where the magnetic moment is parallel or anti-parallel to the external magnetic field. The two states can be distinguished using
the frequency shift of the microstrip resonator. Let the initial Larmor frequency, $\gamma B_{\text{ext}}$, be much greater than the frequency of the microstrip resonator, $\omega_0$. Then the Larmor frequency is slowly (adiabatically) lowered. The frequency shift, $\omega - \omega_0$, is negative if the magnetic moment was initially parallel to the external magnetic field. Otherwise, the frequency shift will be positive. Thus, using the sign of the resonator frequency shift one can distinguish these two states of the SMM: the ground state, $m_z = m$, and the upper state, $m_z = -m$. Note that the spin state can be measured non-destructively if we do not cross the point of frequency jump and adiabatically return to the initial value of the magnetic field $B_{\text{ext}}$.

Suppose that an experimental apparatus does not allow one to measure the sign of the frequency shift, $\omega - \omega_0$, but only its absolute value, $|\omega - \omega_0|$. In this case, the spin state of the SMM can still be determined. Assume that the external magnetic field adiabatically decreases from the values $\gamma B_{\text{ext}} \gg \omega_0$ to the value $B'$ in Fig. 4(a) and Fig. 4(b). The frequency jump is avoided so that the spin state can continue to change adiabatically. For current amplitude, $I_0 = 1 \mu\text{A}$, the relative frequency shift, $|\omega - \omega_0|/\omega_0$, is $7.13 \times 10^{-8}$ when $m_z = m$ and $4.15 \times 10^{-7}$ when $m_z = -m$. Thus, the relative frequency shift, $|\epsilon|$, at $B_{\text{ext}} = B'$ differs more than 5 times for the two initial states of the magnetic moment. Afterwards, the external magnetic field is increased back to its initial value. Therefore, a nondestructive measurement of the spin state of the SMM can be performed regardless of the sign of the frequency shift.

If the spin state of the SMM need not to be preserved, the magnetic field can be further decreased. If $m_z = m$, then the frequency shift, $|\omega - \omega_0|$ reaches its maximum value, $|\omega_a - \omega_o|$ in Fig. 4(a). This maximum value will be observed at $\gamma B_{\text{ext}} < \omega_0$. In the opposite case, $m_z = -m$, the maximum frequency shift for the decreasing field $B_{\text{ext}}$ is $|\omega_g - \omega_o|$ in Fig. 4(b). It will be observed at $\gamma B_{\text{ext}} > \omega_0$. Thus, decreasing the external magnetic field, $B_{\text{ext}}$, one can observe the frequency shift whose sign, absolute value and position are different for the two SMM spin states. Despite the fact that this method destructively measures the spin state of the SMM, the frequency shift, $|\epsilon|$, is permitted to reach its maximum possible value.

**ACKNOWLEDGMENT**

This work was supported by the NYU-Poly seed funds.

**REFERENCES**