Noise Effect on Resonant Tunneling in the Nanoscale Molecular Magnet (Fe_8)

Masamichi Nishino, Keiji Saito, and Seiji Miyashita

Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo Bunkyo-ku, Tokyo 113-0033, Japan

Abstract

We study the effect of noise on the resonant tunneling for a realistic model of Fe_8. We discuss both the static and dynamical effect of noise on the estimation of tunnel splitting by the use of the Landau-Zener-Stückelberg (LZS) formula.

Key words: Fe_8; resonant tunneling; tunnel splitting; noise

1. Introduction

Since nanoscale molecular magnets (Mn_{12}, Fe_8, etc.) were reported to exhibit unprecedented features, much effort has been exerted to the quantum tunneling of magnetization. The tunneling dynamics has been studied from the viewpoint of the nonadiabatic transition [1–3]. The transition probability in the two level system is given by the Landau-Zener-Stückelberg (LZS) formula [4]. This formula is useful to pure quantum dynamics. However, in real systems fluctuation and dissipation affect the process of quantum dynamics. At low enough temperatures, effects of the ubiquitous hyperfine field within the molecule and the dipole field of other molecules become significant for the relaxation process. Therefore, we have to take notice of estimating the tunnel splitting by the use of LZS formula. We have already studied the effect of noise in the case $S = 1/2$ and clarified that the effect of noise cannot be negligible and the estimated gap deviates from the true tunnel splitting [5]. Here we study the noise effect of a realistic model with $S = 10$ for Fe_8 [6–8]. It is found that the estimated gap coincides with the true gap in the fast sweeping regime, while the effect of noise cannot be negligible in the slow sweeping regime.

2. Estimation of the tunnel splitting

We consider the following Hamiltonian which is adopted for the molecular magnet of Fe_8.

$$\hat{H}(t) = -D(S^z)^2 + E((S^x)^2 - (S^y)^2) + C((S^+)^4 + (S^-)^4) - \tilde{h}(t)S^z + \hat{H}^{\rm noise}(t), \tag{1}$$

where we set $D = 0.292$(K), $E = 0.046$(K), and $C = -2.9 \times 10^{-5}$(K) [6]. The field ($\tilde{h}(t)$) in the z-direction is swept linearly with time. We calculate the tunneling probability under the influence of the noise. We adopt $\hat{H}^{\rm noise}(t) = h_\alpha(t)S^\alpha$, where α denotes a direction of x, y, or z. Here $h(t)$ is a random gaussian noise and has an exponential-decaying autocorrelation. We define B as the amplitude of the noise [5]. Using the LZS formula, the tunneling probability p between the magnetizations m and m' in the sweeping field is given as a function of the energy gap $\Delta E_{m,m'}$ and the sweeping velocity $c(=\frac{dH_z}{dt})$: $p = 1 - \exp(\frac{-\pi(\Delta E_{m,m'})^2}{2\hbar|m-m'|c})$. In the experiments, p was estimated for given c and the tunnel splitting was estimated as a function of the velocity making use this formula. Here we estimate the effect of noise on estimation of the tunnel splitting by evaluating the following quantity.

[1] Corresponding author. E-mail: nishino@spin.t.u-tokyo.ac.jp

$$\Delta \equiv \frac{\Delta E_{\rm eff}}{\Delta E_{m,m'}},\ \Delta E_{\rm eff} \equiv \sqrt{-\frac{2\hbar|m-m'|c\ln(1-p)}{\pi}}. \quad (2)$$

$\Delta E_{m,m'}$ is the true energy gap and $\Delta E_{\rm eff}$ is the estimated energy gap from the obtained values of c and p. We can evaluate the effect of noise by estimating how much Δ deviates from 1.

3. Results and Discussion

In the beginning, we focus on the regime of the fast sweeping because the estimated gap shows no velocity dependence in the experiments [7,8]. In this regime, the noise could be considered to be static [5]. The tunnel splitting $\Delta E_{-10,10}$ is estimated numerically as 0.452×10^{-7} (K) for the system (1).

We estimate numerically the dependence of the gap on static noise h_x and h_y, and approximate them by an algebraic function $f(h) = \Delta E_{-10,10} + \alpha h^2$, where $\alpha = -1.356\times10^{-6}$ (K/T^2) for h_x and $\alpha = 2.056\times10^{-6}$ (K/T^2) for h_y. The error bar of α is within 10^{-11}. The values of the gap ΔE in the presence of h_y and the fitting function $f(h_y)$ are shown in Fig. 1. We find that $0.997 \leq \Delta_x \leq 1$ and $1 \leq \Delta_y \leq 1.005$ [9] when $B{=}\sqrt{\langle h_y\rangle^2} \leq 0.1\times10^{-1}$ (T), whose energy scale is 10^6 times as large as the tunnel splitting $\Delta E_{-10,10}$. This holds true from $c = 10^{-5}$ to $c = 10^0$ (T/s), where the experiments were performed. This indicates that the estimated gap is equal to the true gap. This is because the transition from $m = -10$ to $m' = 10$ is the 20th perturbation process and the term of h_xS^x or h_yS^y can give only little effect on the transition process.

Next we investigate the dynamical effect of the noise. It is difficult to simulate time-dependent Schrödinger equation for the system (1) with realistic parameters. However the flowing parameter set is enough to investigate the dynamical effect of 20th perturbation: $D = 0.1$, $E = 0.07$, and $C = 0$. The tunnel splitting ($\Delta E_{-10,10}$) is 0.00113 and we set $B = \Delta E_{-10,10}/40$. We show the sweeping rate dependence of Δ_x in Fig. 2, where $\hbar = 1$. γ is the damping factor of the noise. Here the arrow of Fig. 2 shows the regime of sweeping rate corresponding to that of the experiment. It is found that the fluctuation of noise has an influence on the tunneling process and the estimated gap decreases in the slow sweeping region even if B is not so large. This tendency reproduces the experimental results qualitatively.

The system $S = 1/2$ is sensitive to the effect of noise and the estimated gap should be corrected by $O(\frac{B^2}{\Delta E^2})$ for the fast sweeping regime. On the other hand, the effect of noise can be ignored in the estimation of the tunnel splitting in the case $S = 10$. It is mainly due to the 20-th perturbation. However the fluctuation of noise gives an influence to the tunneling process in the slow sweeping regime regardless of the amplitude of noise. As a result, reduction of the estimated gap is observed in that regime, which reproduces the corresponding experimental data qualitatively.

In the experimental results, isotopically substituted Fe_8s show the different estimated values [7,8]. This difference cannot be explained within our modeling. A treatment from a more microscopic viewpoint may be necessary.

References

[1] S. Miyashita, J. Phys. Soc. Jpn. **64**, 3207 (1995); J. Phys. Soc. Jpn. **65**, 2734 (1996).

[2] S. Miyashita, K. Saito, and H. De Raedt, Phys. Rev. Lett. **80**, 1525 (1998)

[3] M. Nishino, H. Onishi, K. Yamaguchi, and S. Miyashita, Phys. Rev. B **62**, 9463 (2000).

[4] L. Landau, Phys. Z. Sowjetunion **2**, 46 (1932); C. Zener, Proc. R. Soc. London, Ser. A **137**, 696 (1932); E. C. G. Stückelberg, Helv. Phys. Acta **5**, 369 (1932).

[5] M. Nishino, K. Saito, and S. Miyashita, Phys. Rev. B **65**, 014403 (2002).

[6] W. Wernsdorfer and R. Sessoli, Science, **284** 133 (1999).

[7] W. Wernsdorfer, R. Sessoli, A. Caneschi, D. Gatteschi, and A. Cornia, EuroPhys. Lett. **50**, 552 (2000); J.Phys. Soc. Jpn. 69 (2000) Suppl.A.pp. 375, Frontiers in Magnetism.

[8] Wernsdorfer, cond-mat/0101104, to be published in Advanced in Chemical Physics, and references therein.

[9] M. Nishino, K. Saito, and S. Miyashita, Prog. Theo. Phys. in press.

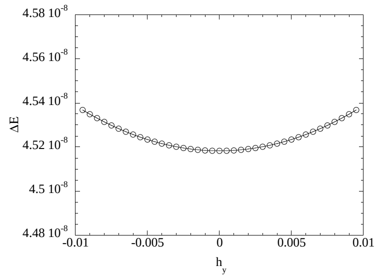

Fig. 1. $\Delta E(h_y)$ ($\circ$) and $f(h_y)$ (Solid line)

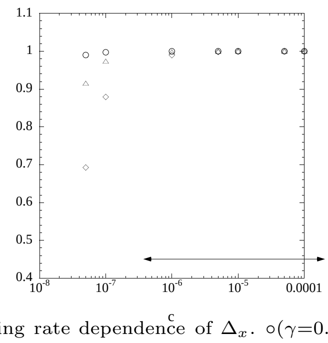

Fig. 2. Sweeping rate dependence of Δ_x. $\circ$(γ=0.01), $\triangle$(0.1). 1.0($\diamond$).