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Quantum hysteresis loops in microscopic system: The loop area as a dynamical parameter

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Abstract. The area enclosed by hysteresis loops in a periodically forced bistable microscopic system at zero-temperature is examined by using the time dependent Hellmann–Feynman theorem and the Fourier grid Hamiltonian recipe for solving time-dependent Schrödinger equation. Effects of non-zero temperatures are explored with reference to a symmetric double well potential. The barrier crossing or, relaxation rates are shown to correlate systematically with the area of the loop. The possible use of hysteresis loop area in designing field parameters for optimal control is suggested.

Keywords. Quantum hysteresis; stochastic resonance; quantum dynamics; Fourier grid methods; stochastically perturbed systems.

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1. Introduction

The thermodynamic response of an interacting many particle system placed in an oscillating external field will oscillate with appropriate change in the form. Any delay in relaxation will however, cause the response to lag behind, creating a thermodynamic response-field loop of non-vanishing area. The phenomenon has been called dynamic hysteresis [1,2]. When the time period of oscillation of the driving field is much less than the relaxation time of the thermodynamic system, the hysteresis loop loses its symmetry about its origin. The dynamically broken symmetry may then lead to the appearance of a new thermodynamic phase. One then says that a dynamic phase transition has taken place due to the presence of two competing time scales, namely the relaxation time of the system and the time period of the external field.

An associated problem concerns the stochastic resonances in bistable systems that are periodically driven in the presence of stochastic noise. If the weak periodic modulation is in resonance with the Kramer's frequency of the thermodynamic system it may ultimately succeed in setting off periodic phase changes in the entire macroscopic system [3–5].

Can a microscopic system at zero temperature reveal similar response in appropriate cases? In what follows we explore this possibility with a wave function based descrip-

tion. That means we make use of pure state dynamical description of our quantum system. Let the quantum system be described by a one dimensional bi-stable potential [$V(x)$], the most well known example of which is the symmetric double well potential. The system is assumed to be initially in the ground state (Ψ_L) localized in the left well when the periodic field is switched on. Ψ_L is not an eigenstate of the symmetric double well potential as it is not a parity eigenstate. It is a symmetry-broken state formed by the superposition of the lowest even and odd parity eigenstates. We may anticipate therefore that Ψ_L $\left[\psi_L = \frac{1}{\sqrt{2}}(\psi_0^+ + \psi_0^-)\right]$ will slowly evolve into the parity eigenstate $(\psi_0^{\pm})$ by tunneling, even in the absence of any external field. The switched on external time varying field couples to the system and delivers energy to it. As time elapses, the higher states begin to be populated and the system crosses over to the other well (the state $\Psi_R = \frac{1}{\sqrt{2}}(\psi_0^+ - \psi_0^-)$) by barrier crossing and tunneling. As the driving field of a fixed frequency sweeps through one period, the population in the excited states may not relax at the same rate, causing a relaxation delay. If the system response is measured by $\langle x(t)\rangle$, it may not retrace its path as one cycle is completed, creating an $\langle x(t)\rangle$-field loop with non-vanishing area. We call them hysteresis loops of our microscopic system. The area itself would measure the amount of energy dissipated per cycle of the driving field and can be an important parameter in understanding some features of the dynamics of driven bi-stable quantum systems. We note here that the dissipated energy over a cycle of the periodic field is distributed among the *higher energy levels* which act as an '*internal bath*'. There is no external bath. As more and more energy is dumped into the higher energy levels, de-excitation sets in, affecting the dissipation of the wave packet. After many cycles therefore, the initially localized wave packet would disperse and the loops would disappear. If the intensity or the frequency of the light is high, the loop may get distorted even during one cycle.

We propose in what follows, how one can easily calculate the loop area and examine possible uses of it. The question of simulating the dynamics in a non-zero temperature situation is also explored. We should mention here that quantum hysteresis has been an active area of contemporary research. For example, the dynamical phases in quantum hysteresis has been carefully analysed by Rao *et al* [6] and Dhar *et al* [7] recently. Dynamical hysteresis and stochastic resonance in quantum 2-level systems have been discussed in detail by Pareek *et al* [8].

2. The method

Let a particle of mass m, move in a symmetric double well potential $V(x)$. The Hamiltonian of the system is then given by

$$H_0 = \frac{P_x^2}{2m} + V_0(x). \tag{1}$$

When an external periodic field (ϵ_x) where

$$\epsilon_x = \epsilon_x^0 \sin\omega t$$

is switched on, the perturbed time-dependent Hamiltonian is given by

$$H(x,t) = H_0 + \epsilon_x^0 ex \sin\omega t = H_0 + V'(x,t). \tag{2}$$

The evolution of the perturbed system is governed by Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(x,t)\rangle = [H_0 + V'(x,t)]|\Psi(x,t)\rangle. \tag{3}$$

The quasi-energy of the system at any instant of time is given by $\langle E(t)\rangle$ where

$$\langle E(t)\rangle = \langle H(t)\rangle. \tag{4}$$

Since we represent the system by a well defined Hamiltonian and describe the relevant state by a wave function, we are in the regime of pure state quantum dynamics. We may invoke therefore the time-dependent Hellmann–Feynman theorem [9,10] for pure states to calculate time dependence of the quasi-energy $\langle E(t)\rangle$, to have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle E(t)\rangle &= \left\langle \frac{\mathrm{d}}{\mathrm{d}t}H(t)\right\rangle \\ &= \left\langle \frac{\mathrm{d}}{\mathrm{d}t}(H_0 + \epsilon_x^0 ex\sin\omega t)\right\rangle \\ &= \epsilon_x^0 e\omega\langle x(t)\rangle\cos\omega t.\end{aligned} \tag{5}$$

Integrating over one cycle of the applied field, we have

$$\int_0^\tau \mathrm{d}\langle E(t)\rangle = \epsilon_x^0 e\omega\int_0^\tau \langle x(t)\rangle\cos\omega t\mathrm{d}t$$

i.e.

$$\Delta E(\tau) = \epsilon_x^0 e\omega\int_0^{\frac{2\pi}{\omega}}\langle x(t)\rangle\cos\omega t\mathrm{d}t. \tag{6}$$

In eq. (6), $\Delta E(t)$ is the energy dissipated during one cycle of the field. To calculate the integral on the right hand side, we need to know how $\langle x(t)\rangle$ varies over one cycle. The information can be obtained by solving eq. (3) for $|\Psi(x,t)\rangle$ by the time-dependent Fourier grid Hamiltonian method [11–14]. In this method we express $|\Psi(x,t)\rangle$ on an uniformly discretized coordinate grid as follows

$$|\Psi(x,t)\rangle \equiv \sum_{p=1}^{n} w_p(t)|x_p\rangle\Delta x,$$

where $\langle x_p|x_q\rangle\Delta x = \delta_{pq}$, $\omega_p(t) = \Psi(x_p,t)$. The use of the Dirac–Frenkel time-dependent variational principle then directly leads to the evolution equation for the grid point amplitudes:

$$\dot{w}_p(t) = \frac{1}{i\hbar}\left[\sum_{q=1}^{n}\langle x_p|H|x_q\rangle w_q(t)\right] \tag{7}$$

for $p = 1, 2, \ldots, n$.

These equations can be numerically integrated, once $\{w_q(0)\}_{q=1,n}$ are supplied leading to the values of $\{w_q(t)\}_{p=1,n}$. $\langle\Psi(x,t)|x|\Psi(x,t)\rangle = \langle x(t)\rangle$ is then given by

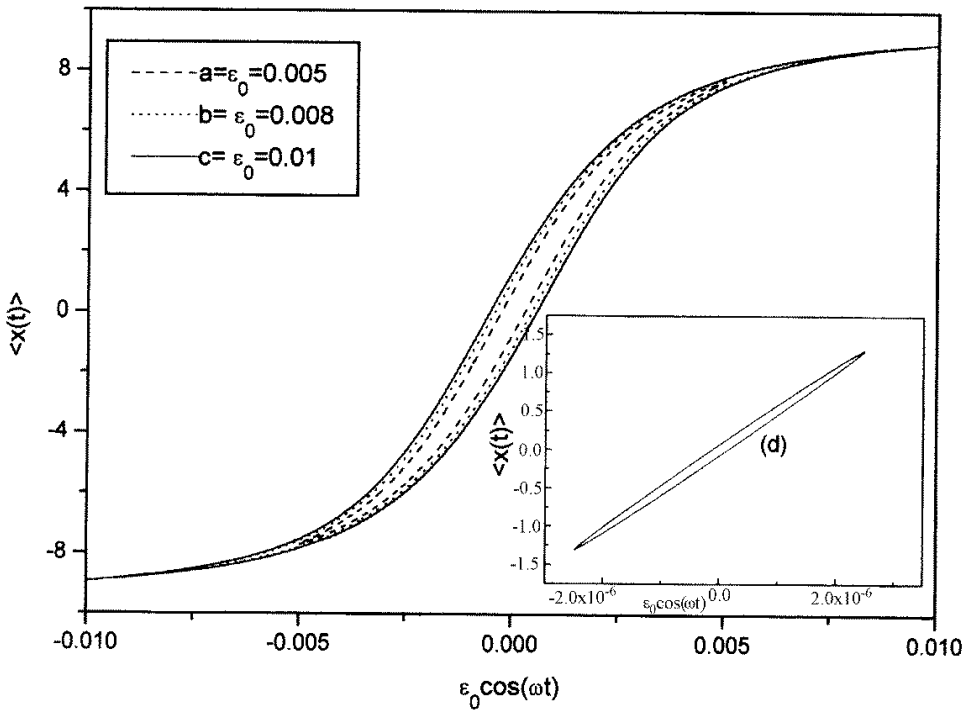

Figure 1(a–d). Hysteresis loop for different peak field intensities (ϵ_x^0) at zero temperature at a fixed frequency of the driving field ($\omega = 0.005$ a.u). Note the behaviour of the loop area as $\epsilon_x^0 \to 0$ (inset).

$$\langle x(t)\rangle = \sum_p |w_p(t)|^2 x_p$$

which is put back on the right hand side of eq. (6) and integration is carried out numerically. For the *zero temperature case*, $\Psi(x,t)$ is chosen as an eigenfunction of the unperturbed Hamiltonian (H_0) while for the non-zero temperature case the initial state [$\Psi(x,0)$] is chosen as a superposition of the eigenstates of H_0 with amplitudes (C_i) so chosen that $|C_i|^2$s reproduce the Boltzmann distribution of population among different eigenstates of H_0 (see ref. [15]) at the given temperature, the phases of the superposition being chosen randomly. This way, we hope to simulate a wave function based description at a non-zero temperature.

3. Results and discussion

3.1 *Quantum hysteresis loop and their areas* ($T = 0$ *case*)

The symmetric double well potential $V(x)$ used has the form $V(x) \equiv ax^4 - bx^2$ with $a = 0.01, b = 0.02$, all in atomic units. With these parameter values, the potential supports

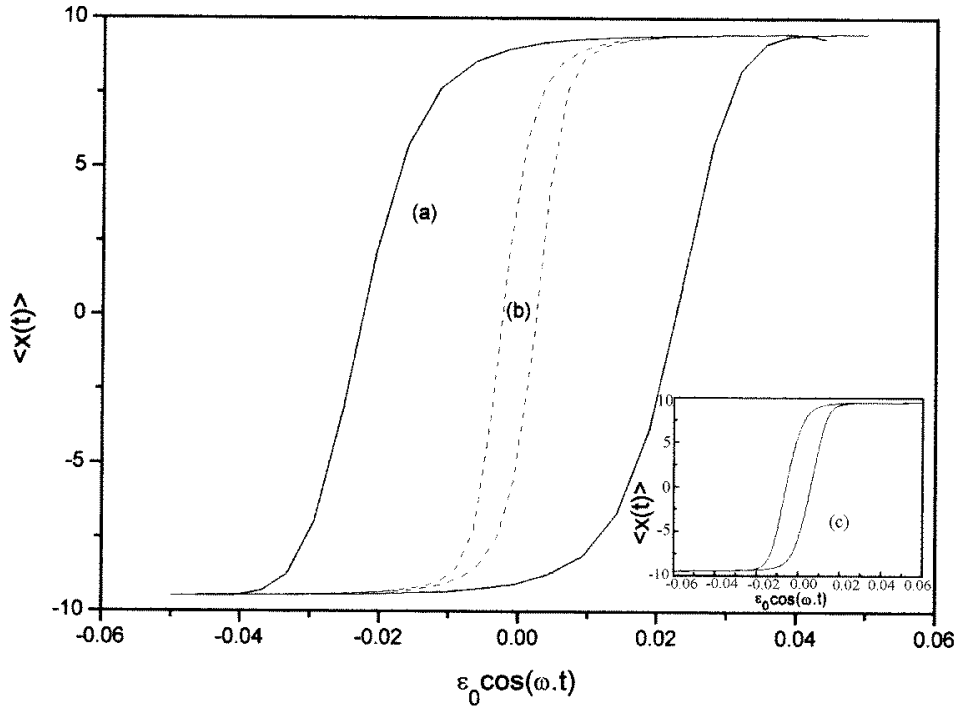

Figure 2(a–c). Hysteresis loop for different frequencies (ω) of the driving field at zero temperature when intensity ($\epsilon_x^0 = 0.05$ a.u) is fixed. Inset is the loop as $\omega \to 0$.

4 states under the barrier. From eq. (6), it follows that if $\langle x(t)\rangle$ is plotted against $\mathcal{F}_t = \epsilon_x^0 \cos\omega t$, the area enclosed by $\langle x(t)\rangle - \mathcal{F}_t$ loop when multiplied by ωe will give the value of $\Delta E(t)$. It is obvious that $\Delta E(t) \to 0$ as $\epsilon_x^0 \to 0$. Figures 1a–d demonstrates how the loop area shrinks as $\epsilon_x^0 \to 0$ in the $T = 0$ case. The magnitude of energy dissipation in one cycle can also be modulated by changing the amplitude of the external field. At higher field strengths, $\langle x(t)\rangle$ lags appreciably behind the field, thereby creating larger hysteresis loops. The reverse happens as ϵ_x^0 decreases. Figures 2a–c, on the other hand, display the response of the quantum hysteresis loop as $\omega \to 0$. In either case the area does not vanish linearly either as a function of ω or ϵ_0. When we monitor the calculated area of the hysteresis loop as a function of ω, it shows a clear maximum at $\omega(=\omega_0)$ that nearly corresponds to the $0 \to 1$ transition frequency or the tunneling splitting (figure 3b). The barrier crossing rate computed under similar condition is also seen to pass through a maximum (figure 3a) at the same frequency ω_0. The frequency at which hysteresis is maximal therefore appears to be dominantly shaped by tunneling at $T = 0^\circ$ K. The barrier crossing rate has been calculated by monitoring the rate of the growth of probability of the system within the perimeters of the right well (P_R) and then calculating the time-derivative of $\ln P_R$ [16]. Figure 4a displays how the computed barrier crossing rate constant at $T = 0^\circ$ K varies with changes in the intensity of the external periodic field (for a given $\omega = 0.005$). There is increase, followed by saturation. The computed hysteresis loop area behaves similarly

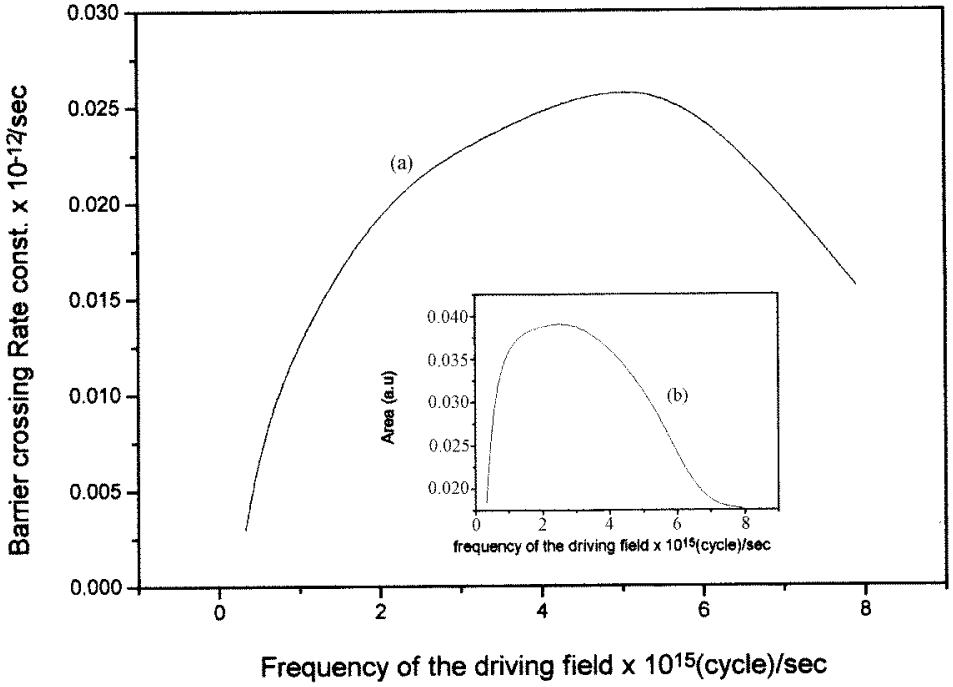

Figure 3. (**a**) Barrier crossing rate constant at zero temperature against the frequency (ω) of the driving field. (**b**) Inset is the corresponding plot for the area of loop against ω.

as shown in figure 4b (inset). The present exploration of dynamic hysteresis in microscopic systems or quantum hysteresis can be extended to non-zero temperatures.

3.2 *Quantum hysteresis at $T > 0$*

For T>0, when more than one level are populated, the shape of the hysteresis loop becomes quite different (figure 5a). Apparently, it breaks into a number of smaller loops. The total enclosed area, however responds to different perturbations quite systematically. As ω increases the loop disappears (figure 5b), and there is a sharp transition in $\langle x(t)\rangle$. Apparently, the state localized in the left well makes a sharp transition to the right well, when the frequency of the driving field exceeds a critical value.

The initial state which has been chosen to be consistent with Boltzmann population of different levels at the given temperature is strongly localized in the left well. As the periodic field is switched on, the population relaxes. We have followed the relaxation (figure 5c) by monitoring $\langle x(t)\rangle$ as a function of time and computing d/d($t\langle x(t)\rangle$) numerically. That leads to the average relaxation rate constant which is plotted against temperature. The hysteresis loop area has also been computed and plotted against T. The computed area and

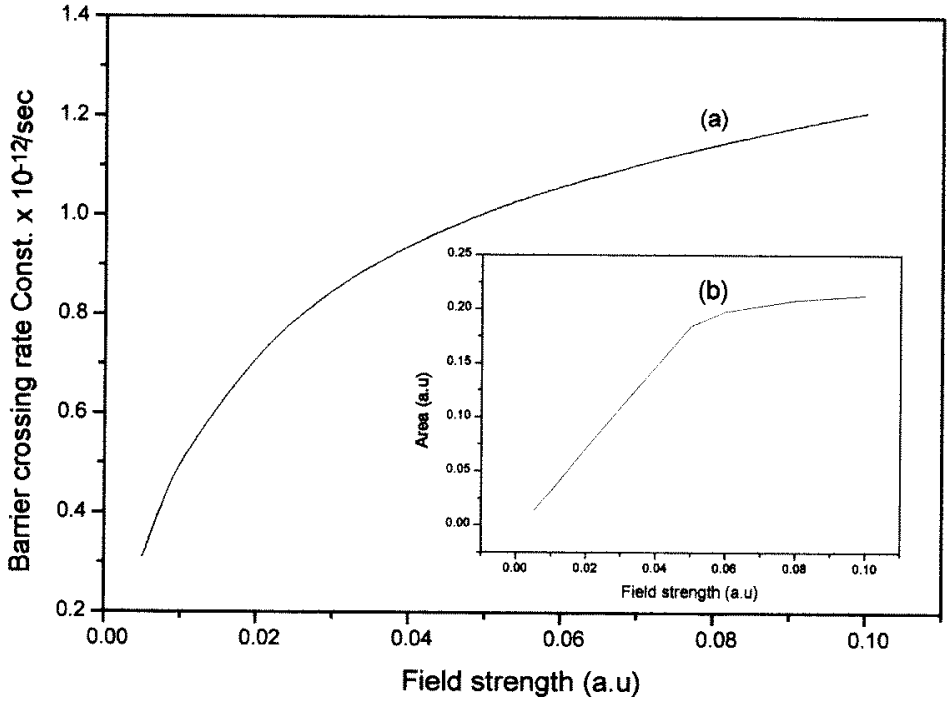

Figure 4. (**a**) Barrier crossing rate constant at zero temperature against the intensity of the driving field. (**b**) Inset is the corresponding plot for loop area against the intensity.

the rate constant are seen to grow almost exponentially with temperature. The relaxation thus appears to be dominated by over-barrier process at $T > 0$.

The loop area at a particular temperature also shows a resonance-like behaviour as a function of the frequency of the driving field (figure 5d). The *maximum* corresponds to a frequency $\omega = \omega'$ which is somewhat *red shifted* with respect to the resonance frequency (ω_0) in the zero temperature case. The computed barrier crossing rate constant at this temperature shows an identical type of ω-dependence (figure 5e). That ω' for which the rate is maximal is different from ω_0 for which maximum crossing rate was observed at $T = 0$, suggests that the barrier crossing at $T > 0$ is not dominated by coherent tunneling. Thus, an enhancement of the reaction rate at non-zero temperatures seems possible to achieve by tuning the frequency of the external field to the near resonance frequency. However, the new resonance frequencies may be quite different from the tunneling frequencies at zero temperature. For an optimal control, the new frequencies need to be determined. It is in this context that hysteresis loop area can be an useful quantity for designing the optimal field parameters. When the potential is made to fluctuate, quantum analogue of stochastic resonance may set in [17]. We are exploring this aspect at present. The results already available indicate the possibility of stochastic resonance affecting barrier crossing rates. We hope to return to the problem in the near future [17].

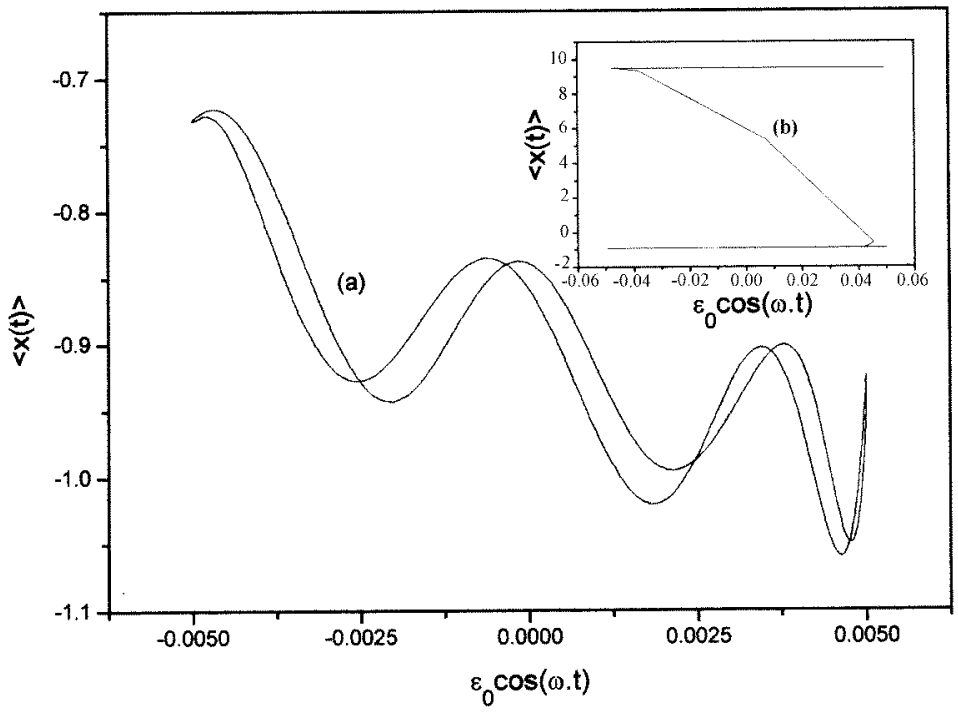

Figure 5a,b.

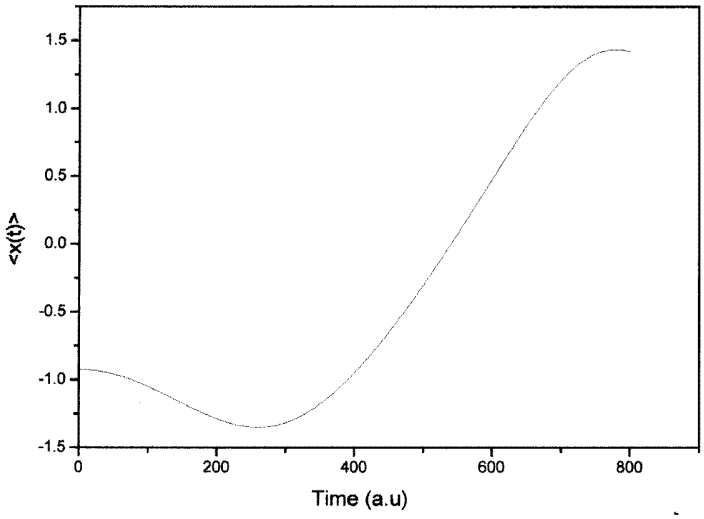

Figure 5c.

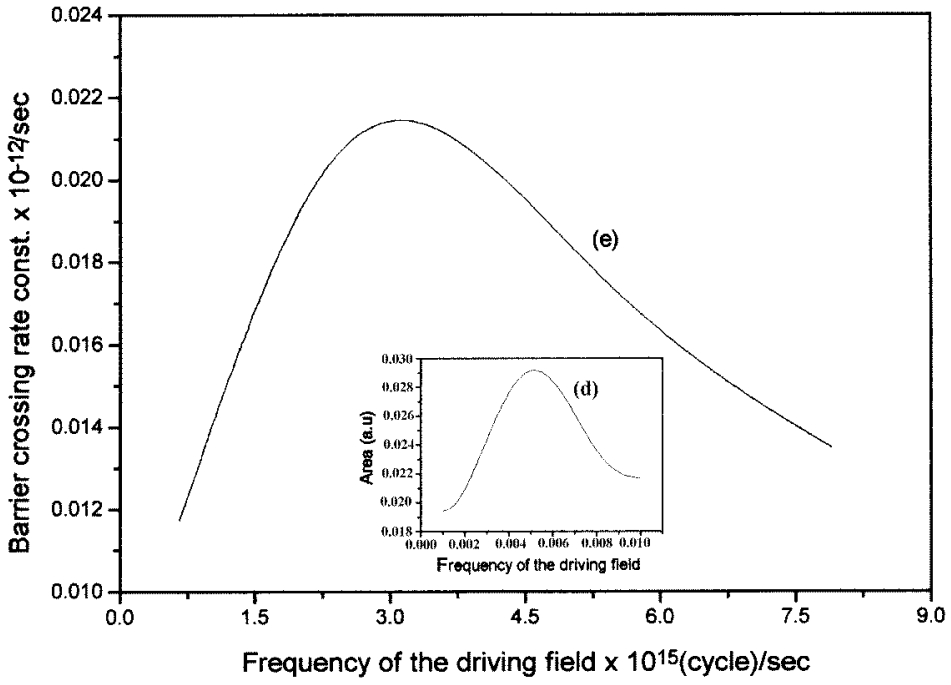

Figure 5. (**a**) Hysteresis loop at non-zero temperature ($T = 25^{\circ}$ K) at particular peak field intensity. (**b**) The phase transition-like behaviour when the frequency of the driving field is too high is shown (inset). (**c**) Relaxation profile of the system against time. (**d**) Inset is the loop area plotted against the driving frequency. (**e**) Barrier crossing rate constant at non-zero temperature against the frequency of the driving field.

4. Conclusion

The hysteresis and dynamic phase transition in a bistable *micro system* mirror their macroscopic analogues. The hysteresis loop area can be an useful quantity for identifying critical values of field parameters responsible for the onset of resonance-like response of the system, and thereby help in designing field parameters for optimal control.

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References

[1] J P Sethna, K A Dahmen, S Kantha, J A Krumhansl, B W Roberts and J D Shore, *Phys. Rev. Lett.* **70**, 3347 (1993)
[2] K A Dahmen and J P Sethna, *J. Phys.* **A30**, 5259 (1997)

[3] L Gammaitoni, P Hänggi, P Jung and F Marchesoni, *Rev. Mod. Phys.* **70**, 223 (1998)
[4] M Thorwart, P Reimann, P Jung and R F Fox, *Chem. Phys.* **235**, 61 (1998)
[5] S W Sides, P A Rikvold and M A Novotny, *Phys. Rev.* **E57**, 6512 (1998)
[6] M Rao, H R Krishnamurthy and R Pandit, *Phys. Rev.* **B42**, 856 (1990)
[7] D Dhar and P B Thomas, *J. Phys.* **A25**, 4967 (1992)
[8] N Kumar, T P Pareek and A M Jaynnavar, *Mod. Phys. Lett.* **B11**, 861 (1997)
[9] E F Hayes and R G Pass, *J. Chem. Phys.* **43**, 1831 (1965)
[10] S T Epstein and R E Johnson, *J. Chem. Phys.* **51**, 188 (1969)
[11] C C Marston and G G Balint Kurti, *J. Chem. Phys.* **91**, 3571 (1989)
[12] S Adhikari, P Dutta and S P Bhattacharyya, *Chem. Phys. Lett.* **199**, 574 (1992)
[13] S Adhikari and S P Bhattacharyya, *Phys. Lett.* **A172**, 155 (1992)
[14] N Balakrishnan, C Kalyanraman and N Sathyamurthy, *Phys. Rep.* **280**, 79 (1997)
[15] C K Mondal, P Chaudhury and S P Bhattacharyya, *Chem. Phys. Lett.* **311**, 400 (1999)
[16] P Sarkar and S P Bhattacharyya, *Phys. Lett.* **A238**, 141 (1998)
[17] C K Mondal and S P Bhattacharyya, (2000) in preparation