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LETTER TO THE EDITOR

Macroscopic quantum coherence and tunnelling in a double well potential

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Abstract. The quantum tunnelling and coherence of a particle moving in a biased or unbiased double well potential and subject to ohmic dissipation is considered. The complete time dependence of the reduced density matrix is determined for the case where the dimensionless friction constant $\alpha \ll 1$.

There has recently been a great deal of interest in the effects of dissipation upon the dynamics of a quantum mechanical particle moving in a double well potential. This is on account of its relation to macroscopic quantum phenomena which are expected to be exhibited by the magnetic flux trapped within a SQUID (Caldeira and Leggett 1983a).

In the case where the double well is symmetric (and hence unbiased) the associated phenomena are referred to as quantum coherence. These have been studied in thermodynamic (i.e. imaginary time) formulations (Chakravarty 1982, Bray and Moore 1982) and in real time (Zwerger 1983a, b, Chakravarty and Leggett 1984).

In the case where there is a small bias away from a symmetric double well potential, the decay from the upper well into the lower is referred to as quantum tunnelling. This has been studied in imaginary time (Weiss *et al* 1985) and in both real and imaginary time (Fisher and Dorsey 1985) for the case of large damping ($\alpha > 1$).

Related work on this subject is on the nature of the heat bath (Chang and Chakravarty 1985) and photoinduced tunnelling (Chakravarty and Kivelson 1983).

The approach adopted in this work is distinct from previous approaches in that we consider the equation of motion that the reduced density matrix obeys. This is particularly advantageous in the physically interesting weak damping regime ($\alpha \ll 1$) which previous approaches can reach only with difficulty. In this regime our approach can determine essentially all of the dymamics of the system (for both zero and finite temperatures) from the solution of a simple differential equation. Additionally the effects of non-zero bias are easily treated in this formalism and hence tunnelling and coherence may be considered simultaneously.

Following most of the previous authors, we shall work in the two lowest-level subspace of the particle and model the dissipation by linear coupling to harmonic oscillators. We thus have a spin boson Hamiltonian

$$H = -\frac{\hbar\Delta}{2}\sigma_x + \frac{\hbar\varepsilon}{2}\sigma_z + \sum_\alpha \left(\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha\omega_\alpha^2 x_\alpha^2}{2} + \frac{q_0}{2}\sigma_z\lambda_\alpha x_\alpha\right) \tag{1}$$

in which $(q_0/2)\sigma_z$ represents the coordinate of the particle and Δ corresponds to a tunnel matrix element between the two minima.

All information on the environment necessary for a reduced description of the spin is contained in the spectral density (Caldeira and Leggett 1981)

$$J(\omega) \equiv \frac{\pi}{2} \sum_\alpha \frac{\lambda_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha). \tag{2}$$

The object we shall study in this Letter is the reduced density matrix. This is obtained by integrating out the environmental oscillators (Feynman and Vernon 1963) assuming the full density matrix factorised at time $t = 0$, corresponding to the environment in equilibrium at temperature T. In a basis in which σ_z is diagonal we find a reduced density matrix at a time t (compare Caldeira and Leggett 1983b):

$$\rho(\sigma, \sigma_2; t) = \sum_{\sigma_3\sigma_4 = \pm 1} J(\sigma_1\sigma_2 t | \sigma_3\sigma_4 0)\rho(\sigma_3\sigma_4 0). \tag{3}$$

The propagator J of equation (3) can be written as a double path integral over spin variables:

$$J(\sigma_1\sigma_2 t | \sigma_3\sigma_4 0) = \int_{\sigma_3 0}^{\sigma_1 t} \mathrm{d}[\sigma] \int_{\sigma_4 0}^{\sigma_2 t} \mathrm{d}[\nu] A[\sigma]A^*[\nu]F[\sigma, \nu] \tag{4}$$

in which $\sigma(u)$ and $\nu(u)$ are spin 'trajectories' taking the values ± 1. $\sigma(u)$ goes from σ_3 at time 0 and reaches σ_1 at time t etc.

The variable $\sigma(u)$ changes sign ('spin flips') at times $\{t_n\}$ and

$$\int \mathrm{d}[\sigma] = \sum_n \int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} \ldots \int_0^{t_2} \mathrm{d}t_1. \tag{5}$$

The sum is over all flips consistent with the boundary conditions. $A[\sigma]$ is the probability amplitude for a given trajectory $\sigma(u)$ in the forward time direction and in the absence of the environment. Following and slightly generalising Chakravarty and Leggett (1984), we have

$$A[\sigma] = \left(\frac{\mathrm{i}\Delta}{2}\right)^n \exp\left(\frac{-\mathrm{i}\varepsilon}{2} \int_0^t \mathrm{d}u\, \sigma(u)\right). \tag{6}$$

The index n is the number of flips in $\sigma(u)$.

The forward and backward trajectories in the path integral of equation (4) are coupled by the influence functional $F[\sigma, \nu]$ (Feynman and Vernon 1963). This takes the form (see e.g. Caldeira and Leggett 1983b; with $q(u) \rightarrow (q_0/2)\sigma(u)$)

$$\begin{aligned} F[\sigma, \nu] = \exp&\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{q_0}{2}\right)^2\right] \int_0^t \mathrm{d}u \int_0^u \mathrm{d}v [\sigma(u) - \nu(u)][\sigma(v) + \nu(v)] Q_1'(u - v) \\ &\times \exp\left[-\frac{1}{\hbar}\left(\frac{q_0}{2}\right)^2\right] \int_0^t \mathrm{d}u \int_0^u \mathrm{d}v [\sigma(u) - \nu(u)]\,[\sigma(v) - \nu(v)] Q_2(u - v) \end{aligned} \tag{7}$$

with

$$Q_1'(u) \equiv \frac{\partial}{\partial u} Q_1(u), \qquad Q_1(u) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{J(\omega)}{\omega} \cos \omega u \tag{8}$$

$$Q_2(u) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} J(\omega) \coth\left(\frac{\omega\tau}{2}\right) \cos \omega u \tag{9}$$

and

$$\tau \equiv \hbar / k_\mathrm{B} T. \tag{10}$$

We shall now use a similar procedure to that of Chang and Waxman (1985) and derive the equation of motion that the propagator J obeys.

First we consider the factor $\int_{\sigma 30}^{\sigma 1 t} \mathrm{d}[\sigma] A[\sigma]$ in equation (4). We write

$$\int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} = \int_0^{t-\delta} \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} + \delta \int_0^{t-\delta} \mathrm{d}t_{n-1} + \mathrm{O}(\delta^2) \tag{11}$$

and

$$\int_0^t \mathrm{d}u\, \sigma(u) = \int_0^{t-\delta} \mathrm{d}u\, \sigma(u) + \delta\sigma_1 + \mathrm{O}(\delta^2). \tag{12}$$

Hence we can write

$$\int_{\sigma 30}^{\sigma_1 t} \mathrm{d}[\sigma] A[\sigma] = \left(1 - \frac{\mathrm{i}\varepsilon\delta\sigma_1}{2}\right) \int_{\sigma 30}^{\sigma_1, t-\delta} \mathrm{d}[\sigma] A[\sigma]$$
$$+ \delta\left(\frac{\mathrm{i}\Delta}{2}\right) \int_{\sigma 30}^{-\sigma_1, t-\delta} \mathrm{d}[\sigma] A[\sigma] + \mathrm{O}(\delta^2). \tag{13}$$

Note that the second term of this equation has an end point now of $-\sigma_1$ (not σ_1) since equation (11) results in this term having one fewer integration and hence one flip less. A similar result holds for the backward time trajectory $\nu(u)$.

In order to find an analogous expansion for the influence functional of equation (7) we use the result for a general function of u and v; $f(u, v)$:

$$\int_0^t \mathrm{d}u \int_0^u \mathrm{d}v\, f(u, v) = \int_0^{t-\delta} \mathrm{d}u \int_0^u \mathrm{d}v\, f(u, v) + \delta \int_0^{t-\delta} \mathrm{d}v\, f(t-\delta, v) + \mathrm{O}(\delta^2). \tag{14}$$

We apply this result to the two integrals in the exponent of the influence functional and expand the exponential to $\mathrm{O}(\delta)$. Combining the result obtained by this procedure with equation (13) and its counterpart for $\nu(u)$, we are able to expand the right-hand side of equation (4) up to $\mathrm{O}(\delta)$. Dividing the resulting equation by δ and taking the limit $\delta \to 0$, we obtain the equation of motion that the propagator obeys:

$$\mathrm{i}\hbar \frac{\partial}{\partial t} J(\sigma_1\sigma_2 t | \sigma_3\sigma_4 0) = -\frac{\hbar\Delta}{2} [J(-\sigma_1\sigma_2 t | \sigma_3\sigma_4 0) - J(\sigma_1 - \sigma_2 t | \sigma_3\sigma_4 0)]$$
$$+ \frac{\hbar\varepsilon}{2}(\sigma_1 - \sigma_2) J(\sigma_1\sigma_2 t | \sigma_3\sigma_4 0)$$
$$+ \left(\frac{q_0}{2}\right)^2 (\sigma_1 - \sigma_2) \int_0^t \mathrm{d}v\, Q_1'(t-v) \langle \sigma(v) + \nu(v) \rangle$$
$$- \mathrm{i}\left(\frac{q_0}{2}\right)^2 (\sigma_1 - \sigma_2) \int_0^t \mathrm{d}v\, Q_2(t-v) \langle \sigma(v) - \nu(v) \rangle. \tag{15}$$

In equation (15) we have introduced the notation

$$\langle \sigma(v) \pm \nu(v) \rangle = \int_{\sigma 30}^{\sigma_1 t} \mathrm{d}[\sigma] \int_{\sigma 40}^{\sigma_2 t} \mathrm{d}[\nu][\sigma(v) \pm \nu(v)]A[\sigma]A^*[\nu]F[\sigma, \nu]. \tag{16}$$

Equation (15) may profitably be compared with the corresponding equation for a coordinate degree of freedom (Chang and Waxman 1985). Equation (15) is a general result for a spin boson system of the type considered. We shall specialise to the case of ohmic dissipation (Caldeira and Leggett 1983a). In this case we take

$$J(\omega) = \eta\omega \exp(-\omega/\omega_c) \tag{17}$$

where ω_c is a frequency large compared with Δ. It is an excellent approximation to take $Q_1(u)$ to be a delta function:

$$Q_1(u) = \frac{n}{\pi} \frac{\omega_c^{-1}}{\omega_c^{-2} + u^2} \simeq \eta\delta(u). \tag{18}$$

The dimensionless friction constant which determines the coupling of the environment to the spin is

$$\alpha \equiv \eta q_0^2/2\pi\hbar. \tag{19}$$

For the physically interesting case of weak damping ($\alpha \ll 1$) we make the approximation of replacing $\langle \sigma(v) - \nu(v) \rangle$ of equation (15) by its undamped ($\alpha = 0$) value, $\langle \sigma(v) - \nu(v) \rangle_0$. It is straightforward to evaluate this quantity since

$$\langle \sigma(v) \rangle_0 = \langle \sigma_1 | \exp(-\mathrm{i}H_0 t/\hbar)\sigma_z(v)|\sigma_3\rangle\langle\sigma_2|\exp(-\mathrm{i}H_0 t/\hbar)|\sigma_4\rangle^* \tag{20}$$

$$\sigma_z(v) = \exp(\mathrm{i}H_0 v/\hbar)\sigma_z \exp(-\mathrm{i}H_0 v/\hbar) \tag{21}$$

and H_0 is the Hamiltonian of the spin alone. We find

$$\begin{aligned}\langle \sigma(v) - \nu(v) \rangle_0 = {} & f_1(t-v)[J(-\sigma_1\sigma_2 t|\sigma_3\sigma_4 0) - J(\sigma_1 - \sigma_2 t|\sigma_3\sigma_4 0)] \\ & - \mathrm{i}f_2(t-v)[\sigma_1 J(-\sigma_1\sigma_2 t|\sigma_3\sigma_4 0) + \sigma_2 J(\sigma_1 - \sigma_2 t|\sigma_3\sigma_4 0] \\ & + f_3(t-v)(\sigma_1 - \sigma_2)J(\sigma_1\sigma_2 t|\sigma_3\sigma_4 0)\end{aligned} \tag{22}$$

in which

$$f_1(s) = n_x n_z(1 - \cos(bs)) \tag{23}$$

$$f_2(s) = -n_x \sin(bs) \tag{24}$$

$$f_3(s) = n_z^2 + (1 - n_z^2)\cos(bs) \tag{25}$$

$$\boldsymbol{n} = \boldsymbol{b}/b \qquad \boldsymbol{b} = (-\Delta, 0, \varepsilon) \qquad b = |\boldsymbol{b}|. \tag{26}$$

Use of equation (22) in equation (15) results in a non-trivial simplification since we now have a differential equation for the propagator. Using equation (3), we can 'fold in' an initial density matrix and hence we obtain an equation of motion for the reduced density matrix.

We denote by ρ the 2×2 matrix with elements $\rho(\sigma_1\sigma_2; t)$. The polarisation vector $\boldsymbol{a}$ defined by

$$\rho = \tfrac{1}{2}(1 + \boldsymbol{a} \cdot \boldsymbol{\sigma}) \tag{27}$$

satisfies a differential equation of motion obtained from that of the density matrix. We find the simple result

$$\frac{\partial \boldsymbol{a}}{\partial t} = \boldsymbol{b} \times \boldsymbol{a} + \chi \hat{e}_x - \hat{e}_z \times (\boldsymbol{\psi}(t) \times \boldsymbol{a}) \tag{28}$$

in which†

$$\chi \equiv \left(\frac{4}{\hbar}\right)\left(\frac{\eta}{2}\right)\left(\frac{q_0}{2}\right)^2 f_2'(0) \tag{29}$$

and

$$\boldsymbol{\psi}(t) = (\psi_1(t), \psi_2(t), \psi_3(t)) \tag{30}$$

with

$$\psi_j(t) \equiv -\frac{4}{\hbar}\left(\frac{q_0}{2}\right)^2 \int_0^t \mathrm{d}v\, f_j(v) Q_2(v) \qquad (j = 1, 2, 3) \tag{31}$$

and $\hat{e}_x$, $\hat{e}_z$ are unit vectors along the X, Z axes respectively.

Equation (28) is the central result of this work. We emphasise that it holds for weak damping, $\alpha \ll 1$.

Let us make some comments on equation (28). Firstly for times large compared with τ the functions $\psi_j(t)$ become essentially independent of time‡. Here we shall ignore this transient behaviour and concentrate on longer-time properties. Secondly the equation exhibits irreversibility (damped oscillatory solutions in general) such that the solutions obtained by taking the limit $t \to \infty$ are, for $\alpha \to 0$, thermal equilibrium results.

To make the connection with the work on coherence we consider equation (28) for the asymmetry parameter $\varepsilon = 0$. We find for $a_z(t)$ the damped equation of motion

$$\ddot{a}_z + \Delta^2(1 - \psi_2/\Delta) a_z = \psi_3 \dot{a}_z. \tag{32}$$

This corresponds to the particle tunnelling at renormalised frequency

$$\Delta_r = \Delta(1 - \psi_2/\Delta)^{1/2} \simeq \Delta \exp(-\psi_2/2\Delta). \tag{33}$$

We find

$$\begin{aligned} \psi_2 &= -2\alpha\Delta \ln(c_1 \hbar\Delta/\hbar\omega_c) \qquad && (k_B T \ll \hbar\Delta) \\ &= -2\alpha\Delta \ln(c_2 k_B T/\hbar\omega_c) \qquad && (k_B T \gg \hbar\Delta) \end{aligned} \tag{34}$$

with c_1 and c_2 constants of order unity which are dependent on the precise way the spectral density cuts off at high frequencies. The inverse damping time $-\psi_3$ can be written down in closed form

$$-\psi_3 = \pi\alpha\Delta \coth(\hbar\Delta/2k_B T) \tag{35}$$

and for small α we obtain the temperature-dependent Q factor of the damped oscillations

$$Q \simeq (1/\pi\alpha) \tanh(\hbar\Delta/2k_B T). \tag{36}$$

† Strictly χ is independent of time t only if $\omega_c t \gg 1$.

‡ The dependence of ψ on time t may, for very low temperatures, result in significant deviations from damped oscillatory behaviour. I thank A J Leggett for informing me of his and his co-workers' results, which alerted me to this. I also thank him for bringing to my attention the related work of Harris and Silbey (1983).

The zero-temperature results of equations (32), (34), (35) and (36) closely correspond to results found by Chakravarty and Leggett (1984) in the small-α limit.

For the case of tunnelling, we shall simply state the result we find, namely that for small α we have essentially exponential decay into the thermal equilibrium configuration at a rate (to lowest order in α) given by

$$\Gamma = \frac{\pi\alpha\Delta^2}{\varepsilon}\coth\left(\frac{\hbar\varepsilon}{2k_B T}\right) \qquad (\varepsilon \gg \Delta). \tag{37}$$

There obviously exist a rich set of phenomena associated with the central result of this work, equation (28). We plan to discuss some of these in the near future.

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