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EFFECTIVE MASS APPROXIMATION FOR TUNNELING STATES WITH DISSIPATION *

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ABSTRACT

The dissipative tunnelling in an asymmetric double-well potential is studied at low temperature. With effective mass approximation, the dissipation can be replaced by a temperature-dependent effective mass. The effective mass increases with decreasing temperature and becomes infinite at $T = 0$. The partition function of the system is derived, which has the same form as that of a non-dissipative tunneling system. Some possible applications in glasses and heavy fermion system are also discussed.

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A Simple model for a particle tunneling in a double-well potential has been used in many physical and chemical problems. In the past, it has been treated as an isolated system in which there is no interaction to its nearby environment. Recently, there has been great interest in the dissipative effect of the environment on the tunneling (Chakravarty 1982; Bray and Moore 1982, Chakravarty and Kivelson 1983; Chakravarty and Leggett 1984; Grabert and Weiss 1985; Fisher and Dorsey 1985). Most recent investigations concentrate on the influence of the dissipation on the mean tunneling rate. It has been shown (Chakravarty 1982; Bray and Moore 1982) that the mean tunneling rate depends on the parameter $\varphi_0 = 4x_0^2\eta/\pi\hbar$ ($\pm x_0$ are the locations of the potential minima, η is the Ohmic dissipative coefficient). For $\varphi_0 > 2$, the mean tunneling rate decreases as temperature decreases, and a spontaneous symmetry breaking takes place at $T=0$. However, there has been few discussions about the partition function of the dissipative tunneling system. Because of the infrared divergence (Chakravarty and Kivelson 1985), it is difficult to reduce the partition function to a simple form by which one can easily find the thermal dynamical properties of the dissipative tunneling system. Such a partition function is very important in understanding the anomalous thermal dynamical properties of glasses (Phillips 1981), A15 superconductors(Yu and Anderson 1984) and heavy fermion systems (Czycholl 1986).

It is well established that when a particle interacts with a field,it becomes "dressed" in the point of the view of quantum field theory. In this case, the interaction with the field is absorbed as an effective mass of the "dressed" particle and it looks like a free particle. One example is an electron moving in a polar crystal. Because of the interaction with ions, the distortion of the crystal lattice will move with the electron when it moves about. This electron together with its distorted environment forms a "dressed" particle called polaron. One can find the effective mass of polaron by the technique of path integration (Feynmann and Hibbs 1965). In analogy to polaron, we raise the following question: whether and how the dissipative influence on the tunneling can be replaced by an effective mass, and then how to reduce the partition function of the dissipative tunneling system to a simple form. We will answer the above question in this paper.

Let us consider a system in which a particle, with "bare" mass m_0, tunnels in an adiabatic double-well potential and interacts with its environment. Following Caldeira and Leggett (Caldeira and Leggett 1981),the dissipative interaction of the particle with its environment can be modeled by linear coupling to a set of harmonic oscillators. The Hamiltonian for the system is

$$H = \frac{1}{2}m_0\dot{x}^2 + V(x) + \frac{1}{2}\sum_k(\dot{Q}_k^2 + \omega_k Q_k^2) + x\sum_k C_k Q_k + x^2\sum_k \frac{C_k^2}{2\omega_k} . \tag{1}$$

where the asymmetric double-well potential is

$$V = \frac{1}{2}\alpha(x \pm x_0)^2 \pm \epsilon . \tag{2}$$

The final term in eq.(1) is the shift of the zero-point energy of the oscillators due to the coupling. Following Chakravarty and Kivelson (Chakravarty and Kivelson 1985), we get the partition function as

$$Z = \sum_{\{x\}} \mathcal{D}_x \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} ds\left[T_{eff}(x) + V(x)\right]\right\} , \tag{3}$$

where $\beta = 1/k\,T$. The effective kinetic energy is

$$T_{eff} = \frac{1}{2}m_0\dot{x}^2 + \frac{\eta}{4\pi}\int_0^{\beta\hbar} ds' \frac{(x(s) - x(s'))^2}{\{(\beta\hbar/\pi)\sin[\pi(s-s')/\beta\hbar]\}^2} , \tag{4}$$

with Ohmic dissipative coefficient

$$\eta = \frac{\pi}{2\omega}\sum_k \frac{C_k^2}{\omega_k}\delta(\omega_k - \omega) . \tag{5}$$

For a tunneling path consisting of 2n flips (see Fig.1), we can write

$$\int_0^{\beta\hbar} T_{eff}\, ds = \frac{4nx_0}{\tau} m_{eff} . \tag{6}$$

The effective mass is

$$m_{eff} = m_0 + \frac{\eta\tau}{\pi}A , \tag{7}$$

with

$$A = \frac{3}{2} - \frac{1}{n}\sum_{i>j}\ln\left(\frac{S_i - S_j}{\tau}\right) . \tag{8}$$

for "rare" flips, namely

$$S_i - S_j >> \tau \quad (i, j = 1, 2, \cdots, 2n) . \tag{9}$$

In the sense of the effective mass, the cutoff is given by the reciprocal of the zero-point vibrational frequency of the "dressed" particle, instead of the "bare" particle, in the potential minimum:

$$\tau = m_{eff}^{1/2}\alpha^{-1/2} . \tag{10}$$

m_{eff} must be solved self-consistently by eqs.(7),(8) and (10). At the lowest-order approximation, $\ln\tau$ can be replaced by $\ln\tau_0$, where τ_0 is determined by the "bare" particle. Then we have

$$m_{eff} = m_0 + \frac{\eta^2A^2}{2\pi^2\alpha} + \frac{\eta A}{2\pi\alpha^{1/2}}\left[\frac{\eta^2A^2}{\pi^2\alpha} + 4m_0\right]^{1/2} . \tag{11}$$

A is a complex function of n and it depends on the arrangement of "imagine time" $\{S_i\}$. S_i is in the range $0 \leqslant S_i \leqslant \beta\hbar$, then without the loss of generality, we may assume

$$S_i - S_j = \beta\hbar f(i,j) . \tag{12}$$

Therefore we have

$$A = \frac{3}{2} + \ln\frac{T_0}{T} - \frac{1}{n}\sum_{i>j}(-1)^{i-j}\ln f(i,j) . \tag{13}$$

where $T_0 = \hbar\omega_0/k_B$, ω_0 is the zero-point vibrational frequency of the "bare" particle. Eq.(13) shows that the effective mass of the "dressed" particle depends on two factors: temperature and the tunneling path. The path-dependence of a tunneling particle, in the presence of phonons at zero temperature, was first investigated by Sethna with an instanton path approach (Sethna 1981). From "rare" flips condition (9) and eq.(12), we have

$$\frac{\beta\hbar}{\tau} >> \frac{1}{f(i,j)} > \prod_{2n\geqslant i>m}\left[f(i,m)^{(-1)^{i-m}}/f(i,m+1)^{(-1)^{i-m}}\right] , \tag{14}$$

where m is an arbitrary odd number satisfied $0 < m < 2n$. In deriving eq.(14), we have used the factor that $f(i,j) < f(i+1,j)$ and $f(i,j) > f(i,j+1)$. It is easy to find from eq.(14) that

$$\ln\frac{\beta\hbar}{\tau} \cong \ln\frac{T_0}{T} >> \frac{1}{n}\sum_{i>j}(-1)^{i-j}\ln f(i,j) . \tag{15}$$

This result tell us that temperature has dominant influence on the effective mass, under the "rare" flips condition. At low temperature ($T \to 0$), we have

$$A \cong \ln\left(\frac{T_0}{T}\right), \tag{16}$$

$$m_{eff} \cong \frac{\eta^2}{\alpha\pi^2} \ln^2\left(\frac{T_0}{T}\right). \tag{17}$$

Such temperature-dependent effective mass gives the effective tunneling splitting as

$$\begin{aligned}\Delta_{eff} &= \hbar\alpha^{1/2} m_{eff}^{-1/2} \exp\left[-\frac{2x_0^2}{\hbar}(m_{eff}\alpha)^{1/2}\right] \\ &\cong \frac{\alpha\hbar\pi}{\eta\ln(T_0/T)} (T/T_0)^{2x_0^2\eta/\pi\hbar}.\end{aligned} \tag{18}$$

In the following we compare the above results with those of renormalization group method. With the straight tunneling path as before and also following Chakravarty and Kivelson, we get the partition function for the symmetric case ($\epsilon = 0$)

$$Z = \sum_{n=0}^{\infty} y_0^{2n} \int_0^{\beta\hbar} \frac{dS_{2n}}{\tau_0} \int_0^{S_{2n}-\tau_0} \frac{dS_{2n-1}}{\tau_0} \cdots \int_0^{S_2-\tau_0} \frac{dS_1}{\tau_0} \exp\left\{\varphi_0 \sum_{i>j} (-1)^{i-j} \ln\left(\frac{S_i-S_j}{\tau_0}\right)\right\}, \tag{19}$$

with

$$y_0 = \Delta_0\tau_0/\hbar, \qquad \varphi_0 = 4x_0^2\eta/\pi\hbar, \tag{20}$$

where Δ_0 is "bare" tunneling splitting. Following Anderson and Yural (Anderson and Yural 1971), we obtain the scaling relation as

$$\frac{dy}{d\ln\tau} = (1-\varphi/2)\,y, \tag{21}$$

$$\frac{d\varphi}{d\ln\tau} = -\varphi y^2. \tag{22}$$

The renomalization group flows can be divided into two regions, corresponding to two phases. $\varphi_0 = 2$ is the critical point. For $\varphi_0 > 2$, fugacity y decreases with increasing of τ ; while for $\varphi_0 < 2$, y increases with increasing of τ. When $\varphi_0 >> 2$ ($2x_0^2\eta/\pi\hbar >> 1$), eq.(21) gives (Bray and Moore 1982)

$$\Delta_{re} = \Delta_0 (T/T_0)^{2x_0^2\eta/\pi\hbar}, \tag{23}$$

which has the same asymptotic behavior as that given in eq.(18). It has been suggested that eq.(18) be valid only for $2x_0^2\eta/\pi\hbar = \varphi_0/2 > 1$. Such a restriction may be found by the "rare" flips condition in the present effective mass description. As mentioned before the interaction with the environment has been included in the effective mass of the "dressed" particle, therefore it oscillates with frequency $\Delta_{eff}/\hbar$ between the two wells ($\epsilon = 0$). The average number of flips may be estimated by

$$\bar{n} \sim \beta\hbar/(\hbar/\Delta_{eff}) = \Delta_{eff}/k_B T. \tag{24}$$

Substituting eq.(18) yields

$$\bar{n} \sim T^{\varphi_0/2-1}. \tag{25}$$

Then the "rare" flips condition requires $\varphi_0/2 - 1 > 0$ or $\varphi_0 > 2$.

Eqs.(7) and (8) indicate the $m_{eff} \to \infty$ and $\Delta_{eff} \to 0$ as $T \to 0$, i.e. a spontaneous symmetry breaking takes place ($\epsilon = 0$). Such a phenomenon may be understood physically in the following way. According to the definition of Ohmic dissipative coefficient, we have

$$\alpha = \varphi_0/2 = x_0^2 \sum_k \frac{C_k^2}{\omega_k} \delta(\omega_k - \omega)/\hbar\omega. \tag{26}$$

Keeping in mind that α is actually independent of ω, we therefore have the identity

$$\alpha = \frac{1}{\omega_0}\int_0^{\omega_0} \alpha\, d\omega = x_0^2 \sum_k \frac{C_k^2}{2\omega_k^2} \Big/ \frac{1}{2}\hbar\omega_0, \tag{27}$$

which clearly gives the physical meaning of α (or φ_0). $\hbar\omega_0/2$ is the zero-point vibrational energy of the tunneling particle. While $x_0^2\sum_k C_k^2/2\omega_k^2$ is the energy transferred from the tunneling particle to the environment at T = 0 according to eq.(1). For $\alpha > 1$ ($\varphi_0 > 2$), such energy is larger than the total energy of the tunneling particle. Hence, the spontaneous symmetry breaking, or self-trapping phenomenon having analogy to polaron problem, takes place. For $\alpha < 1$ ($\varphi_0 < 2$) however, only part of the total energy of the tunneling particle is transferred, and such a case does not take place.

With the effective mass approximation, we can rewrite the partition function of system as

$$Z = \sum_{\{x\}} \int \mathcal{D}x \exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} ds\, H_{eff}(s)\right], \tag{28}$$

where the effective Hamiltonian is

$$H_{eff} = \frac{1}{2} m_{eff} \dot{x}^2 + V(x). \tag{29}$$

In other words, we have reduced the partition function of a dissipative tunneling problem into that of a nondissipative problem with the help of the effective mass approximation. At low temperature ($T \to 0$), eq.(28) becomes (Chakravarty and Kivelson 1985)

$$Z = 2\cosh[\beta(\epsilon^2 + \Delta_{eff}^2)^{1/2}]. \tag{30}$$

which is extremely simple compared with eq.(19) and can be easily studied. Eq.(30) maps to an effective two-level system (TLS).Because of the temperture-dependence of Δ_{eff}, we have a temperature-dependent TLS. These results may be helpful in understanding the anomalous thermal dynamical properties of glasses. It is believed that, in glasses there are low-energy elementary excitations: TLS, resulting from the atomic tunneling between an asymmetric double-well potentials (Phillips 1981).There are few discussions about the influence of the dissipation on the atomic tunneling states in glasses (Chen et al 1986, Chen et al 1987).By taking account of such an influence, we can subdivide the asymmetric double-well into two groups. The large one satisfies $x_0 > (\pi\hbar / 2\eta)^{1/2}$, corresponding to the temperature-dependent TLS, while the small one satisfies $x_0 < (\pi\hbar/2\eta)^{1/2}$, corresponding to the temperature-independent TLS. To explain the anomalous thermal dynamical properties of glasses, Varma et al have supposed that there are two kinds of TLS (Varma et al 1982): one is temperature-dependent and the other is not. The present results seems to provide a clearly physical base for their assumption. Recently, Fleurov and Trakhtenberg have found that the double- well potentials can be divided into two kinds: soft and rigid(Fleurov and Trakhtenberg 1986). Actually, these two kinds are very similar to the large and small groups mentioned above.Moreover,we have successfully explained the "excess T^3" anomaly in the specific heat and the "plateau" in

the thermal conductivity in glasses by introducing the temperature-dependent TLS (Chen and Wu 1986). The other possible application of the present theory is in the explanation of the anomalous thermal dynamical properties of heavy fermion systems. It is accepted that the f electrons with two nearly degenerate configurations may play an important role in these properties (Czycholl 1986). Because of the heavy effective mass ($10^2 \sim 10^3 m_e$) of f electrons found in these systems, we expect that the ordinary adiabatic approximation is no longer valid, and one must consider the dissipative influence of phonon environment. In this case,we predict that the effective mass of f electron will increase as temperature decreases. Such a behaviour has been observed in many experiments (Steward 1984).The detail investigation about this problem is beyond the scope of the present paper and will be given in a separate paper. Recently, Alexandrov et al have developed a bipolaron model for heavy fermion systems (Alexandrov et al 1986). Their model and the present model have the same physical foundation of a self-trapping nature resulting from the strong coupling of a particle with phonon environment.

In conclusion, we have studied the dissipative tunneling in an asymmetric double-well potential with the effective mass approximation. We found that at low temperature the dissipation can be replaced by a temperature-dependent effective mass. The calculated tunneling splitting is compared with that of the renormalization group theory. The present theory enables us to reduce the partition function of a dissipative tunneling problem to that of a nondissipative problem. We expect that some results may be helpful in understanding the anomalous thermal dynamical properties of glasses and heavy fermion systems.

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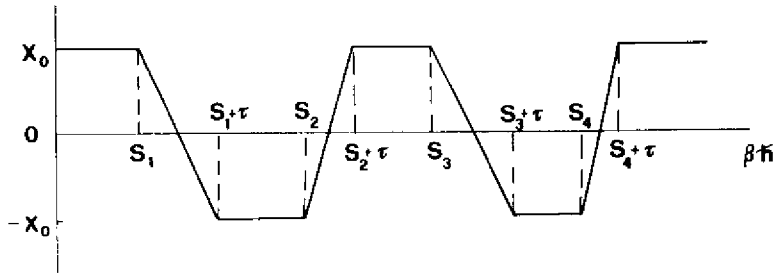

Fig.1 Tunneling path.