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Interference and coherent tunnelling in dissipative quantum systems[1])

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Abstract. In this paper I briefly review some important results on quantum interference and coherent tunnelling in dissipative systems emphasizing their relevance to some fundamental questions in quantum mechanics.

1. Introduction

When we are studying the quantum dynamics of any physical system, the first thing we need to know is its Hamiltonian. Once we know it we can describe the time evolution of the physical state of this system by solving the corresponding Schrödinger equation. Most of the time the systems whose dynamics we wish to study are not isolated. When this happens we have basically two kinds of problems. The first kind deals with systems which are acted by external forces whose time evolution is known. In this case a Hamiltonian can still be found and one either solves the corresponding Schrödinger equation (whenever it is possible) or make use of the well-known methods of perturbation theory.

The second kind of problems involving non-isolated systems deals with those systems whose *classical dynamics* is properly described by an equation of motion which cannot be obtained by the application of Hamilton equations to any Hamiltonian. The paradigm of this second kind of problems is the Brownian Motion. As we all know the classical example of this motion is the study of the dynamics of a heavy particle in a viscous fluid (by *heavy,* I mean that this particle is more massive than the molecules of the host fluid), which is described by the so-called Langevin equation [1]

$$M\ddot{q} + \eta\dot{q} + V'(q) = f(t) \tag{1.1}$$

where M is the mass of the particle, η is a phenomenological damping constant, $V(q)$ is the external potential acting on the particle and $f(t)$ is a fluctuating force

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which obeys the relations

$$\langle f(t)\rangle = 0 \quad \text{and} \quad \langle f(t)f(t')\rangle = 2\eta kT\,\delta(t-t') \tag{1.2}$$

where k is the Boltzmann constant, T is the temperature of the fluid and $\langle\ \rangle$ stands for the ensemble average of identically prepared systems.

Like any other phenomenological equation (1.1) has a restricted range of validity. It is reasonable to use Langevin equations when;

- The mass, M, of the Brownian particle is such that $M \gg m$, where m is the mass of the molecules of the viscous fluid and
- we are interested in the long time behaviour of the system. By this I mean times long compared to the typical collision time of the particles components of the fluid.

What I am particularly interested in doing is to study the quantum mechanics of dissipative systems such as a Brownian particle. Although most of the examples I will present in this lecture deal only with this specific case, the technique to be employed below can be easily generalized to many other dissipative systems.

At this point, the first question the reader should be asking is whether the quantum limit of typical Brownian systems is necessary at all. In many cases where equation (1.1) can be applied the answer is obviously *no*. However there are very special kinds of systems for which it is indeed necessary to think about Quantum Brownian Motion. One example is a superconducting ring closed by a weak link [2] which is found in the literature as SQUIDS (superconducting quantum interference devices).

The flux trapped inside a SQUID ring obeys the following Langevin equation [3]

$$C\ddot{\phi} + \frac{1}{R_n}\dot{\phi} + \frac{dU}{d\phi} = I_f \tag{1.3}$$

where $\langle I_f\rangle = 0$, $\langle I_f(t)I_f(t')\rangle = (2kT/R_n)\,\delta(t-t')$,

$$U(\phi) = \frac{(\phi-\phi_x)^2}{2L} - I_c\phi_0\cos\frac{2\pi\phi}{\phi_0} \tag{1.4}$$

and the quantities introduced above are:

C–capacitance of the weak link
R_n–normal resistance of the link
I_c–critical current of the link
ϕ_0–$h/2e$ (flux quantum)
ϕ_x–flux due to the application of an external magnetic field perpendicular to the ring.

The equation of motion (1.4) is obviously analogous to the one of a particle of coordinate ϕ subject to a potential $U(\phi)$. Changing the external field to which the SQUID ring is subject, one can distort the shape of $U(\phi)$ (see Fig. 1) and,

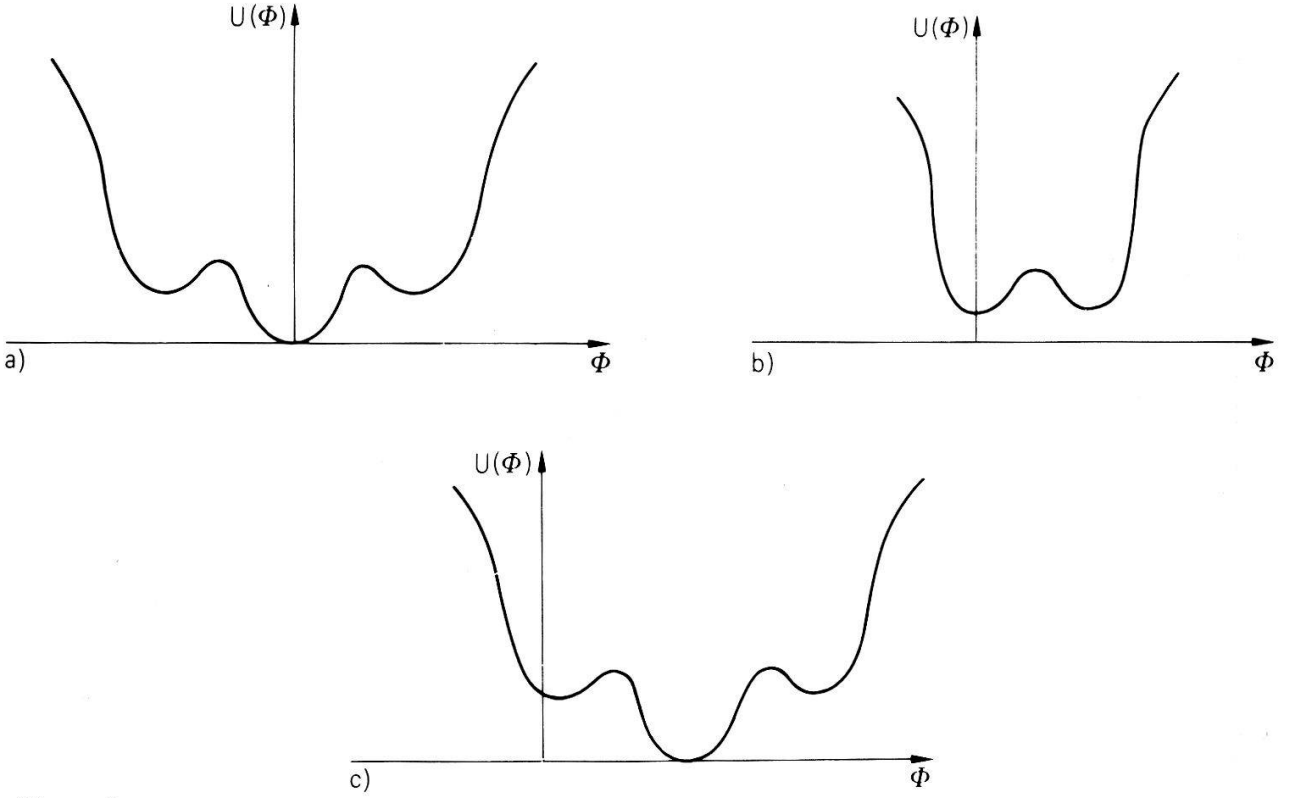

Figure 1

The potential $U(\phi)$ for: a) $\phi_x = 0$, b) $\phi_x = \frac{\phi_0}{2}$, c) $\phi_x = \phi_0$

consequently, vary the stability conditions of the system. The typical frequency, ω, of oscillation at one of the possible metastable equilibrium positions of $U(\phi)$ is of the order of $2\ (I_c/C\phi_0)^{1/2}$ which can be quite high depending on the capacitance and critical current of the link. For example, if $I_c \sim 10^{-5}$ A and $C \sim 10^{-12}$ F one has $\hbar\omega/k \sim 1°$ K and quantum effects would be observable at easily attainable temperatures. It should be emphasized here that the values I have just mentioned for I_c and C are quite reasonable within the new technology of building weak links and junctions in general (see, for example, Ref. 4).

If one now neglects the influence of damping and quantizes this system in the canonical way, one is faced with the possibility of studying a rich variety of quantum effects just by changing the external field. One can study the quantum behaviour of the SQUID in the classically accessible region (Fig. 1a) or coherent tunnelling (Fig. 1b) or still decay by quantum tunnelling (Fig. 1c). There are, however, two important questions about these considerations:

(1) What is the meaning of this secondary quantization about which I have been talking?
(2) How can one reconcile damped equations of motion with the process of quantization?

The answer for the first one is not that hard for the SQUID ring. As we know, $\phi = \oint \vec{A} \cdot d\vec{l}$ and, therefore, I have been talking about quantization of the electromagnetic field generated by this superconducting circuit in some indirect

way. The second question is somewhat harder and is partially the goal of next section.

Now that I hope to have convinced the reader about the need to study the quantum regime of a Brownian particle I shall mention that in this lecture I will only present some interesting results about interference of wave packets of Brownian particles and coherent tunnelling in a bistable potential (Fig. 1b). Other applications of the same formalism to be used below can be found in [5] or [6].

Before I go into the formalism of the problem I would like to emphasize the importance of our future results when applied to the specific case of a SQUID ring. Once one looks at the electronic states corresponding to the metastable (or stable) values of ϕ in Fig. 1, realizes that they are finite current states involving a macroscopic number of electrons (Cooper pairs). Therefore if one talks about something as coherent tunnelling (Fig. 1b) between two fluxoid states it is the same as talking about a superposition of two states involving a macroscopic number of particles

$$\psi = \psi_R(x_1 \cdots x_N) \pm \psi_L(x_1 \cdots x_N) \tag{1.5}$$

where $\psi_R(\psi_L)$ is the condensate wavefunction of electrons moving with finite current (zero current). Since these are macroscopic quantum states this question is basically the same as the one inspired by the Schrödinger's Cat. Therefore a more careful study of this problem is very important in discussions on the foundations of quantum mechanics.

2. The basic approach

Many people have tried to answer the second question above by very different methods. However, all these attempts fall into two main categories; [5]

- new schemes of quantization for non-isolated systems, or
- dynamics of subsystems (system of interest-plus-reservoir approach).

In this work I shall concentrate on the second possibility. The reason for this choice is simply because I know of no dissipative system in nature which is not coupled to an external reservoir.

Once one has made this choice there are still two possibilities;

- start with a first principle Hamiltonian of the system-plus-reservoir and solve a possibly complicated problem, or
- start with a simple Hamiltonian of the system-plus-reservoir and impose some conditions on the model in such a way that the appropriate classical limit is recovered.

Since in the great majority of cases one does not know enough about the reservoir to which the Brownian variable (the system of interest) is coupled, the

second possibility seems again to be the most attractive one and the specific model I shall employ is defined in what follows.

Let us suppose that the Hamiltonian of the complete system is given by

$$H = H_s + H_{\text{int}} + H_R + \text{C.T.} \tag{2.1}$$

where

$$H_s = \frac{p^2}{2M} + V(q); \qquad H_{\text{int}} = \sum_k C_k q_k q; \qquad H_R = \sum_k \frac{p_k^2}{2m_k} + \tfrac{1}{2} m_k \omega_k^2 q_k^2$$

and C.T. is a counter term [5, 6]; C.T. $= \sum_k (C_k^2/2m_k\omega_k^2)q^2$. Let us also introduce a spectral function $J(\omega)$ defined as

$$J(\omega) \equiv \sum_k \frac{\pi C_k^2}{2m_k\omega_k}\,\delta(\omega - \omega_k) = \begin{cases} \eta\omega & \text{if} \quad \omega < \Omega \\ 0 & \text{if} \quad \omega > \Omega \end{cases} \tag{2.2}$$

where Ω is a very high frequency.

The reason behind this choice is very simple; in the classical limit it reproduces equations (1.1) and (1.2). The Hamilton equations of the system read

$$M\ddot{q} + V'(q) = \sum_k C_k q_k - \sum_k \frac{C_k^2}{m_k\omega_k^2} q \tag{2.3}$$

$$m_k\ddot{q}_k + m_k\omega_k^2 q_k = C_k q \tag{2.4}$$

Taking the Laplace transform of (2.4) and substituting in (2.3) one has

$$\begin{aligned} M\ddot{q} + V'(q) = {} & \frac{1}{2\pi i}\int_{\varepsilon-i\infty}^{\varepsilon+i\infty} \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{s^2+\omega_k^2} + \frac{s q_k(0)}{s^2+\omega_k^2} \right\} e^{st}\, ds \\ & - \frac{d}{dt}\left\{ \sum_k \frac{C_k^2}{m_k\omega_k^2} \frac{1}{2\pi i} \int_{\varepsilon-i\infty}^{\varepsilon+i\infty} \frac{s\tilde{q}(s)}{s^2+\omega_k^2} e^{st}\, ds \right\} \end{aligned} \tag{2.5}$$

Using the convolution theorem and the spectral function (2.2) the second term in the RHS of (2.5) can be approximated by $\eta\dot{q}$ while the first term (call it $f(t)$) obeys the relations (1.2) once we impose that

$$\langle \dot{q}_k(0) \rangle = \langle q_k(0) \rangle = \langle \dot{q}_k(0) q_{k'}(0) \rangle = 0;$$

$$\langle \dot{q}_k(0) \dot{q}_{k'}(0) \rangle = \frac{kT}{m_k}\,\delta_{kk'}$$

and

$$\langle q_k(0) q_{k'}(0) \rangle = \frac{kT}{m_k\omega_k^2}\,\delta_{kk'} \tag{2.6}$$

where the last two expressions follow directly from the equipartition theorem.

In general one is interested in studying average values of operators of the system only, or,

$$\langle \hat{0}(p, q) \rangle = \text{tr}_{RS}[\rho\hat{0}] \tag{2.7}$$

where ρ is the density operator of the system-plus-reservoir. Therefore, since $\hat{0}$ does not depend on reservoir operators, one has

$$\langle \hat{0} \rangle = \mathrm{tr}_S [(\mathrm{tr}_R \rho)\hat{0}] = \mathrm{tr}_S [\tilde{\rho}\hat{0}] \tag{2.8}$$

where $\tilde{\rho} \equiv \mathrm{tr}_R \rho$ is the reduced density operator of the system. This is the quantity in which I shall be interested from now on. In particular, I shall work with the Feynman path integral [7] representation of $\tilde{\rho}$ because in many cases of interest these integrals are either exactly soluble or very well approximated by the saddle point method. On top of this, I shall be avoiding the use of $N+1$ dimensional wave functions.

In order to study the dynamics of the Brownian particle we need to find its reduced density operator at any time t. In the coordinate representation we can write it as

$$\tilde{\rho}(x, y, t) = \int dR_1\, dR_2 \cdots dR_N \, \langle x\vec{R}|\, \rho(t)\, |y\vec{R}\rangle \tag{2.9}$$

where $\vec{R}$ is a general configuration of the environmental oscillators and

$$\rho(t) = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar} \tag{2.10}$$

is the density operator of the total system. Following the same procedure as in [5, 7] one gets

$$\tilde{\rho}(x, y, t) = \int\int dx'\, dy' J(x, y, t; x', y', 0)\tilde{\rho}(x', y', 0) \tag{2.11}$$

where

$$J(x, y, t; x', y', 0) = \int_{x'}^{x} \int_{y'}^{y} Dx(\tau)Dy(\tau) \exp \frac{i}{\hbar} S_0[x(\tau)] \times \exp -\frac{i}{\hbar} S_0[y(\tau)] * F[x(\tau), y(\tau)] \tag{2.12}$$

with $S_0[z(\tau)]$ being the action correspondent to H_s in (2.1) and

$$F[x(\tau), y(\tau)] = \exp -\frac{i}{\hbar}\frac{\eta}{2}\int_0^t d\tau(\dot{x}(\tau) + \dot{y}(\tau))(x(\tau) - y(\tau)) \times \exp -\frac{\eta}{\pi\hbar}\int_0^\infty d\omega\, \omega \coth\frac{\hbar\omega}{2kT}\int_0^t d\tau \int_0^\tau d\sigma * [x(\tau) - y(\tau)] \cos\omega(\tau - \sigma)[x(\sigma) - y(\sigma)] \tag{2.13}$$

Finally, I wish to mention something about the problem of the initial condition in (2.6a). In general, one chooses $\rho(0) = \rho_R(0)\rho_S(0)$ [5, 7] where $\rho_R(0)$ refers only to the reservoir and $\rho_S(0)$ only to the system (obviously, $\tilde{\rho}(0) = \rho_S(0)$). Although this choice gives us almost all the expected results, some transients appear with a bizarre dependence on the cutoff frequency Ω. In order to overcome this problem one can choose a different initial condition as

$\rho(0) = \rho_{RS}(0)\rho_S(0)$ where $\rho_{RS}(0)$ is the density operator of the reservoir in the presence of the Brownian particle and $\rho_S(0) = \tilde{\rho}(0)$ is the result of a measurement on that particle only [8]. When this happens there is a slight modification in the influence functional, F, but it still retains its quadratic form. The great advantage of this new initial condition is the fact that all transients are now independent of Ω.

3. Applications

The study of (2.12) for simple potentials has been carried out in Ref. 5. In this lecture I will be interested in presenting the results of this double functional integral in the following examples.

3.1. *Quantum interference* [9]

Here, I wish to study the motion of a Brownian particle subject to a harmonic potential, $V(q) = \frac{1}{2}M\omega_0^2 q^2$, when its initial state is given by

$$\tilde{\rho}(x', y', 0) = \psi(x')\psi^*(y') \tag{3.1}$$

where

$$\psi(x) = \psi_1(x) + \psi_2(x) = N\left[\exp -\frac{x^2}{4\sigma^2} + \exp -\frac{(x - x_0)^2}{4\sigma^2}\right] \tag{3.2}$$

N being a normalization constant. Therefore, we initially have a superposition of two localized packets in a harmonic well.

When there is no damping ($\eta = 0$) everyone knows that

$$\rho(x, t) = \rho_1(xt) + \rho_2(xt) + 2\sqrt{\rho_1(xt)\rho_2(xt)}\cos\varphi(x, t) \tag{3.3}$$

where I have defined $\rho(x, t) \equiv \rho(x, x, t)$. This means that the total probability density is the sum of probability densities corresponding to the first and second packets and an interference term. If one now makes η finite (3.3) changes to

$$\rho(x, t) = \rho_1(x, t) + \rho_2(x, t) + 2\sqrt{\rho_1(x, t)\rho_2(x, t)}\cos\varphi(x, t)\exp -\Gamma t \tag{3.4}$$

where Γ can be analysed as below for very different conditions.

– High temperatures ($kT \gg \hbar\omega_0$)

$$\Gamma = \begin{cases} \dfrac{2NkT}{\hbar\omega_0}\gamma \quad \text{if} \quad \omega_0 \gg \gamma \quad \text{and} \quad \hbar\omega_0^2/2kT\gamma \gg 1 & \text{(3.5a)} \\ \left(\dfrac{4}{3}\dfrac{NkT\gamma}{\hbar\omega_0^2}\right)^{1/3}\omega_0 \quad \text{if} \quad \omega_0 \gg \gamma \quad \text{and} \quad \hbar\omega_0^2/2kT\gamma \ll 1 & \text{(3.5b)} \\ \dfrac{2NkT}{\hbar\omega_0}\dfrac{\omega_0^2}{2\gamma} \quad \text{if} \quad \omega_0 \ll \gamma & \text{(3.5c)} \end{cases}$$

– Low temperature ($kT \ll \hbar\omega_0$)

$$\Gamma = \begin{cases} N\gamma & \text{if} \quad \gamma \ll \omega_0 \qquad (3.6a) \\ \dfrac{N\omega_0^2}{2\gamma} & \text{if} \quad \gamma \gg \omega_0 \qquad (3.6b) \end{cases}$$

The quantity N is a measure of the mean number of energy quanta present in the system at $t = 0$; $N \equiv x_0^2/2\sigma^2$. Therefore, one can say that if the two initial wave packets are well separated ($N \gg 1$) $\Gamma^{-1} \ll \gamma^{-1}$. In other words, the interference fringes are destroyed much faster than the relaxation time of the system (γ^{-1}).

This result can be understood in a very simple way. Let us work at $T = 0$ for simplicity and assume a very weak coupling between the particle and its environment. Initially the state of the composite system is given by

$$|\Phi\rangle = (|\psi_0\rangle + |\psi_1\rangle) \otimes |0\rangle \qquad (3.7)$$

where $|\psi_0\rangle$ is the ground state of the oscillator and $|\psi_1\rangle$ that packet with a finite displacement (see (3.2)). $|0\rangle$ is the ground state of the environment. Suppose we know that it takes $\tau = \gamma^{-1}$ for $|\psi_1\rangle$ the relax to the ground state of the system. Now, since $\langle\psi_1| H |\psi_1\rangle \sim N\hbar\omega_0$ let us investigate what is the new state of the composite system once $|\psi_1\rangle$ has lost one quantum of energy to the environment. Due to the coupling we have in (2.1) it must be given by

$$|\tilde{\Phi}\rangle \approx |\psi_0\rangle \otimes |0\rangle + |\tilde{\psi}_1\rangle \otimes |1\rangle \qquad (3.8)$$

where $|1\rangle$ is an excited state of the environment with energy $\hbar\omega_0$. Because $|0\rangle$ and $|1\rangle$ are orthogonal the reduced density operator becomes

$$\mathrm{tr}_R\, |\tilde{\phi}\rangle\langle\tilde{\phi}| \approx |\psi_0\rangle\langle\psi_0| + |\tilde{\psi}_1\rangle\langle\tilde{\psi}_1| \qquad (3.9)$$

which is obviously a mixture. On the other hand it takes about $\tau_d \approx \tau/N$ for $|\psi_1\rangle$ to lose $\hbar\omega_0$ to the environment in agreement with (3.6).

3.2 *Coherent tunnelling* [10]

The second application I wish to mention is the Brownian motion of a particle in the bistable potential

$$V(q) = -\tfrac{1}{2}M\omega_0^2 q^2 + \frac{\lambda}{4} q^4. \qquad (3.10)$$

In this example let us consider temperatures such that only the lowest two energy states of $V(q)$ can be populated. Then we are basically interested in a two state system coupled to the bath of oscillators and H_s and H_{int} in (2.1) can be replaced by

$$H_s = -\frac{\hbar}{2}\Delta_0\sigma_x \quad \text{and} \quad H_{\mathrm{int}} = \frac{q_0}{2}\sigma_z \sum_k C_k q_k \qquad (3.11)$$

where σ_i are Pauli matrices and q_0 the distance between the two minima of $V(q)$.

The path integral (2.12) has to be solved for hopping like paths and its solution is undoubtedly a formidable mathematical problem [10]. Computing $P(t) \equiv \langle \sigma_z(t) \rangle$ and expressing the results in terms of the dimensionless damping constant

$$\alpha \equiv \eta q_0^2 / 2\pi\hbar \tag{3.12}$$

and the renormalized splitting

$$\Delta_r = \begin{cases} \Delta_0 (\Delta_0/\Omega)^{\alpha/1-\alpha} & \alpha < 1 \\ 0 & \alpha > 1 \end{cases} \tag{3.13}$$

one can show that [10]

(a) If $\alpha > 1$ and $T = 0 \Rightarrow$ localization

(b) If $\alpha > 1$ and $T \neq 0$ or $\alpha < 1$ and $\alpha T \gtrsim \Delta_r$ $\Rightarrow P(t) = \exp -\frac{t}{\tau}$

where

$$\tau^{-1} = \frac{h\Delta_r^2}{kT} \frac{\sqrt{\pi}}{2} \frac{\Gamma(\alpha)}{\Gamma(\alpha + \frac{1}{2})} \left(\frac{\pi k T}{h \Delta_r} \right)^{2\alpha} \tag{3.14}$$

(c) If $\alpha = \frac{1}{2}$ at all $T \Rightarrow P(t) = \exp -\frac{t}{\tau}$

where

$$\tau^{-1} = \frac{\pi \Delta_0^2}{2\Omega} \tag{3.15}$$

(d) If $0 < \alpha < \frac{1}{2}$ $\quad \alpha T \lesssim \Delta_r$

$$\Rightarrow P(t) = \frac{1}{1-\alpha} \cos \left\{ \left[\cos \frac{\pi\alpha}{2(1-\alpha)} \right] \Delta_{\text{eff}} t \right\} \exp - \left\{ \left[\sin \left(\frac{\pi\alpha}{2(1-\alpha)} \right) \Delta_{\text{eff}} t \right] \right\}$$

+ incoherent relaxation

with

$$\Delta_{\text{eff}} = [\Gamma(1-2\alpha) \cos \pi\alpha]^{1/2(1-\alpha)} \Delta_r \tag{3.16}$$

(e) If $\frac{1}{2} < \alpha < 1$ $\quad T = 0$

$P(t) =$ incoherent relaxtion (probably)

These result are very important in the analysis of some fundamental quantum mechanical problems when they are applied to systems such as SQUID rings. However, before I start to touch these questions, I would like to say a few words about the localization phenomenon at $T = 0$ and $\alpha > 1$.

One can easily understand the localization by looking at the renormalized splitting Δ_r in (3.13). Because $\Delta_0/\Omega \ll 1$, Δ_r decreases as $\alpha \to 1$ and consequently there is a tendency for the renormalized energy splitting to vanish for $\alpha \geq 1$. Indeed this is really what happens because $\Delta_r = 0$ for $\alpha > 1$.

This result is obtained by noticing that the splitting in the composite system must be calculated by taking into account the fact that high frequency oscillators

should adjust adiabatically to the motion of the particle from one well to the other. Therefore the new splitting becomes

$$\Delta(\omega_l) = \Delta_0 \prod_{\alpha} \langle g_{\alpha+} \mid g_{\alpha-} \rangle \tag{3.17}$$

where $g_{\alpha+(-)}$ is the ground state of an oscillator with frequency ω_α ($\omega_\alpha > \omega_l > \Delta_0$) when the particle is on the right (left) well. Evaluating (3.17) one has

$$\Delta(\omega_l) = \Delta_0 \exp - \alpha \int_{\omega_l}^{\Omega} \frac{d\omega}{\omega} \tag{3.18}$$

Since $\Delta(\omega_l) < \Delta_0$ we may iterate this procedure using new oscillators in the range $\omega_l(\Delta_0) > \omega > \omega_l(\Delta) > \Delta$. The result converges to a finite Δ when $\alpha < 1$ while for $\alpha > 1$ Δ can be made vanishingly small (see (3.13)).

4. Conclusions

The two examples I treated in this lecture clearly show that the linear damping ($\eta\dot{q}$) tends to destroy quantum mechanical effects such as interference or coherent tunnelling. The main reason behind this is the nature of the coupling between the particle and its environment; being of the form qq_k we can think off the environment as trying to "observe" the coordinate of the particle. As a consequence the initially prepared pure state of that particle is reduced to a mixture within a very short time scale. How short clearly depends on how strong the coupling to the environment is.

In the particular example of the coherent tunnelling in a SQUID ring the "coordinate of the Brownian particle" actually is a collective variable which reflects the coherent motion of a macroscopic number of superconducting electrons. In this case the coupling to the environment only blocks one of the two macroscopically distinct states when $\alpha > 1$ (localization phenomenon mentioned above). For $\alpha < \frac{1}{2}$ one can still observe few coherent oscillations between these two states (see (3.16)) before it finally becomes a mixture. Therefore for sufficiently weakly damped SQUID's one should be able to observe few coherent superpositions of states involving a macroscopic number of particles (once again the Cat Paradox).

The latest statement clearly imposes some restrictions on our search for a measuring apparatus. If we decide to use a SQUID to measure the value of an observable with two eigenvalues (each one of them corresponding to the right or left value of the flux ϕ) we must prepare our device with parameters such that $\alpha > 1$. Notice that only with this restriction these conclusions are in agreement with the concept of the pointer basis [11].

If these predictions fail to be tested one should obviously need an alternative way to describe the physical phenomena at this level.

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