Dissipation in Quantum Systems

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1 Introduction - Motivation

In the last century, the English R.Brown observed that small particles immersed in a viscous fluid exhibit an extremely irregular motion. If no external force is applied to the particle, its average velocity is zero, $\langle \vec{v} \rangle = 0$ and its variance $\langle v^2 \rangle$ is finite. The averages are taken over an ensemble of systems identically prepared. This phenomenon is since then known as "Brownian Motion".

The theoretical treatment is given through the Langevin equation

$$\begin{aligned} M\ddot{q} + \eta\dot{q} + V'(q) &= f(t) \qquad (1) \\ \langle f(t) \rangle &= 0 \qquad \langle f(t)f(t') \rangle = 2\eta k_B T \delta(t-t') \end{aligned}$$

Here, M is the mass of the particle, η is the dissipation constant, $V(q)$ is an external potential and $f(t)$ is a fluctuating force. This phenomenological equation offers a good description only if:
- the mass M of the Brownian particle is much larger than the mass m of the molecules composing the viscous fluid, $M \gg m$.
- we are interested in the behavior of the particle at times t much larger than the average time τ between molecular collisions.

Although we have used a classical example to introduce the idea of Brownian motion, other examples are available. For instance, the dynamics of the magnetic flux in the interior of an RLC circuit obeys the equation

$$\begin{aligned} C\ddot{\phi} + \frac{RC}{L}\dot{\phi} + \frac{\phi}{L} &= I_f(t) \\ \langle I_f(t) \rangle &= 0 \qquad \langle I_f(t)\, I_f(t') \rangle = \frac{2RCk_BT}{L}\delta(t-t') \end{aligned}$$

Most of the systems exhibit a purely classical motion. The typical frequency $1/\sqrt{LC}$ of the circuit is such that $\hbar/\sqrt{LC} \ll k_B T$, even at low temperatures. The quantum effects are negligible when $\hbar\omega_0/k_B \equiv T_0 \ll 1K$,
where ${\omega_0}^2 \equiv \frac{V''(q_0)}{M}$ with $V'(q_0) = 0$ and $V''(q_0) > 0$.

However, some superconducting micro-circuits have been recently created with $T_0 \lesssim 1K$. In this case, quantum effects should be observed. The paradigm of these systems is the so called SQUID - Superconducting QUantum Interference Device, which is a superconducting ring closed by a weak contact. The magnetic flux in the interior of the ring is described by a Langevin equation under the action of a "potential" $U(\phi)$. This potential can be controlled by an external magnetic field, and can assume different forms, which are appropriate for the observation of different quantum effects.

Later in this script, there will be a brief introduction about SQUID's. Although this system exhibits quantum effects, we should notice that:
1 The dynamical values are macroscopic, i.e., they originate from effects

involving a macroscopically large number of particles. Hence, which is the physical meaning of this "macroscopic quantization"? In the particular case of the SQUID, we know that $\phi = \oint \vec{A} \cdot d\vec{l}$ along the superconducting ring. Hence, here we are actually quantizing the electromagnetic field subject to the boundary conditions imposed by the physics of superconducting materials and weak contacts. In other cases the interpretation is not so obvious. Here, we will assume that the quantization is possible "a priori".

2 The second problem concerns the quantization of non-isolated systems. Equation (1) exhibits a dissipative term of the form $\eta\dot{q}$ and a fluctuating force $f(t)$. We know that there is no Hamiltonian, so that the Hamilton equations reproduce (1). Hence, we cannot apply the canonical quantization rules to this system. The question is: how to reconcile the usual quantization procedure with dissipative equations of motion?

Finally, if we can answer the last question, which will be the influence of the dissipative and fluctuating terms in the quantum effects mentioned above? Is it possible to have a description only in terms of phenomenological constants, for instance, η?

We will try to find a quantum system which reproduces the Langevin equation in the classical limit. In order to solve the problem of the system being non-isolated, we will couple the system of interest to a reservoir, and then we quantize the composite system in the usual way. Finally, we eliminate the reservoir variables and study the effective dynamics of the system of interest. This method was originally proposed by Senitzki for studying the relaxation of the normal modes of the EM-field in a cavity.

The composite system is described by the Hamiltonian

$$H \;=\; H_R \,+\, H_I \,+ H_S$$

R : reservoir , I : interaction , S : system of interest

Hence, we can compute the density operator of the composite system through

$$\hat{\rho}(t) \;=\; e^{-\frac{iHt}{\hbar}}\,\hat{\rho}(0)\,e^{\frac{iHt}{\hbar}}$$

As we are interested only in operators referring to the system S, $\hat{O} = \hat{O}(p,q)$, we have

$$\langle \hat{O}(p,q) \rangle \;=\; tr_{RS}\{\hat{\rho}(t)\,\hat{O}\} \;=\; tr_S\{[tr_R\,\hat{\rho}(t)]\,\hat{O}\} \;=\; tr_S\{\tilde{\rho}(t)\,\hat{O}\}$$

where tr_R and tr_S represent the partial trace with respect to R and S, and

$$\tilde{\rho}(t) \;\equiv\; tr_R\,\hat{\rho}(t)$$

is the reduced density operator of the system of interest. Then, we have to choose H_R and H_I so that $\tilde{\rho}(t)$ will reproduce in the classical limit the result

expected from the classical theory of Brownian Motion. But before proceeding further with the dissipative theory, let us first study two specific phenomena that will be fundamentally important for us in these lectures.

2 Superconductivity as a "Macroscopic Quantum State"

A superconductor is a charged superfluid. Therefore, a wave function ψ is associated with a macroscopic number of electrons which are "condensate" in the same quantum state. The "particles" with mass m^* and charge e^* can be described as a whole by a macroscopic wave function

$$\psi = \sqrt{n_s} e^{i\varphi}, \tag{2}$$

where φ is a phase common to all the particles, and n_s is their density in the macrostate. The electric current density in the presence of a vector potential $\mathbf{A}$ is then given by

$$\mathbf{J} = \frac{e^*\hbar}{2m^*i}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] - \frac{e^{*2}\mathbf{A}}{m^*c}\psi^*\psi \tag{3}$$

Using then Eq. (2) into Eq. (3), we obtain that

$$\mathbf{J} = \frac{n_s e^*}{m^*}\left(\hbar\nabla\varphi - \frac{e^*}{c}\mathbf{A}\right) \tag{4}$$

2.1 Flux quantization

Recalling that the current $\mathbf{J} = n_s e^* \mathbf{v}$ we have that $\hbar\nabla\varphi = m^*\mathbf{v} + e^*\mathbf{A}/c$. Now, integrating this equation along a path Γ from position 1 to 2 one has

$$\int_1^2 \left(m^*\mathbf{v} + \frac{e^*}{c}\mathbf{A}\right)\cdot d\mathbf{r} = \hbar(\varphi_2 - \varphi_1) \tag{5}$$

because it is an integral of a gradient field. On the other hand, as φ is the phase of a wave function which must be single valued, the integral along a closed loop ($1 = 2$ above) must yield

$$\oint \left(m^*\mathbf{v} + \frac{e^*}{c}\mathbf{A}\right)\cdot d\mathbf{r} = \frac{e^*}{c}\oint \left(\Lambda\mathbf{J} + \mathbf{A}\right)\cdot d\mathbf{r} = 2\pi n\hbar \tag{6}$$

where n is an integer and $\Lambda = m^*c/e^{*2}n_s$. Therefore, with $e^* = 2e$ we find

$$\oint \left(\Lambda\mathbf{J} + \mathbf{A}\right)\cdot d\mathbf{r} = \frac{2\pi n\hbar c}{2\,e} \equiv n\phi_0 \tag{7}$$

where $\phi_0 = hc/2e \approx 2.09 \times 10^{-7}$gauss cm^2. For a simply connected superconductor where $\mathbf{A}$ and $\mathbf{J}$ are continuous functions the integral (7) is zero. However,

in a multiply connected region (a thick ring for example), this is no longer true. If we integrate (5) along a closed path Γ deep into the ring where there is no current, it yields

$$\oint \mathbf{A} \cdot d\mathbf{r} = \int \mathbf{B} \cdot d\mathbf{s} = n\phi_0 \tag{8}$$

where $d\mathbf{s}$ is an element of area on any surface bounded by Γ and we have used $\mathbf{B} = \nabla \times \mathbf{A}$ and the Stoke's theorem. From the above equation we see that the magnetic flux through a superconducting ring is quantized in units of ϕ_0.

2.2 The Josephson effect

Suppose that we have two pieces of superconductors separated by a non-superconducting material of thickness d. We call them 1 and 2. If d is very large the two superconductors do not feel each other's presence and the dynamics of their condensates should obey two decoupled Schrödinger equations

$$\begin{aligned} i\hbar\dot{\psi_1} &= E_1\psi_1 \\ i\hbar\dot{\psi_2} &= E_2\psi_2. \end{aligned} \tag{9}$$

Now if d is such that there is a substantial overlap between the two condensate wave functions it is reasonable to assume that we now have

$$\begin{aligned} i\hbar\dot{\psi_1} &= E_1\psi_1 + \Delta\psi_2 \\ i\hbar\dot{\psi_2} &= E_2\psi_2 + \Delta^*\psi_1. \end{aligned} \tag{10}$$

This arrangement is known in the literature as a *Josephson junction*.

Let us for simplicity choose $\Delta \in \Re$ and $\mathbf{A} = 0$. Then writing $\psi = \sqrt{n_s}e^{i\varphi}$ for each wave function in (10) we can easily get

$$-\hbar\dot{\varphi}_1 = \Delta\sqrt{\frac{n_2}{n_1}}\cos(\varphi_2 - \varphi_1) + E_1, \tag{11}$$

a similar equation for φ_2 (where one should exchange $1 \leftrightarrow 2$) and also

$$\dot{n}_1 = \frac{2\Delta}{\hbar}\sqrt{n_1 n_2}\sin(\varphi_2 - \varphi_1) = -\dot{n}_2. \tag{12}$$

As $\dot{n}_2$ gives us the current through the junction we can write

$$j = j_0 \sin\bar{\varphi} \tag{13}$$

$$\dot{\bar{\varphi}} = \frac{2eV}{\hbar} \tag{14}$$

where we assumed $n_1 \approx n_2$, $\sqrt{n_1 n_2} = n_s$ and

$$\bar{\varphi} \equiv \varphi_1 - \varphi_2, \quad j_0 \equiv \frac{2n_s\Delta}{\hbar} \quad \text{and} \quad \frac{E_2 - E_1}{\hbar} = \frac{2eV}{\hbar}. \tag{15}$$

What (13,14) tell us is that the difference between the phases of the wave functions on each superconductor can adjust itself to allow for the transport of a constant current, without any measurable voltage, up to a critical value j_0. Beyond this value, a voltage will develop between the two sides of the junction. This is the celebrated *Josephson effect*.

These two particular effects will be very important for us in discussing the devices we will be treating in these lectures.

2.3 Superconducting quantum interference devices (SQUIDs)

Our first device consists of a superconducting ring closed by a Josephson junction (see Fig.(1)). We shall be particularly interested in the so-called *weak links* (metallic junctions or point contacts).

Let us suppose that our SQUID ring is subject to an external field perpendicular to its plane and we wish to study the dynamics of the total magnetic flux comprised by the ring. If we had an ordinary ring we have just seen that the total flux would be quantized in units of ϕ_0. However, in this new example this quantization rule will be slightly modified.

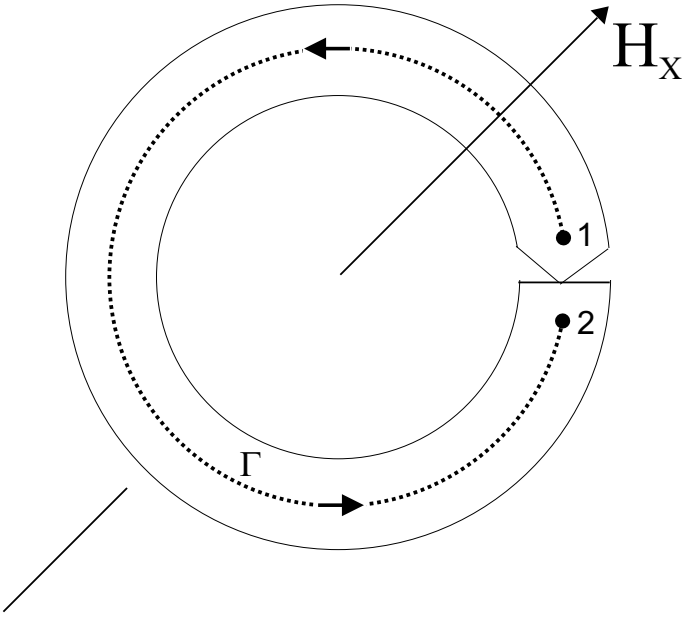

Figure 1: SQUID ring

This modification comes about because if the two points 1 and 2 in (5) are located right on the two terminals of the junction (see Fig. 1) it must be more

carefully analyzed. Let us rewrite it as

$$\int_1^2 \mathbf{J}\cdot d\mathbf{r} = \frac{n_s e^* \hbar}{m^*}\int_1^2 \nabla\varphi\cdot d\mathbf{r} - \frac{n_s e^* \hbar}{m^*}\frac{2\pi}{\phi_0}\int_1^2 \mathbf{A}\cdot d\mathbf{r}. \tag{16}$$

The term on the lhs of (16) still vanishes if Γ is a path deep into the superconducting ring. The last integral on the rhs, due to the continuity of $\mathbf{A}$, can be approximated by the integral along a closed loop which results in the flux ϕ through the ring. The only term that deserves more attention is the remaining one which we split as

$$\int_\Gamma \nabla\varphi\cdot d\mathbf{r} = \oint \nabla\varphi\cdot d\mathbf{r} - \int_2^1 \nabla\varphi\cdot d\mathbf{r} \tag{17}$$

to conclude that, since φ is a phase we have

$$\int_\Gamma \nabla\varphi\cdot d\mathbf{r} = 2\pi n - \bar{\varphi} \tag{18}$$

where $\bar{\varphi} \equiv \varphi_1 - \varphi_2$. Consequently, we can write the new quantization relation in the SQUID as

$$\phi + \frac{\phi_0}{2\pi}\bar{\varphi} = n\phi_0. \tag{19}$$

It should be noticed that when $\bar{\varphi} = 0$ one recovers the usual flux quantization of an uniform ring.

Now let us analyze the behavior of the total magnetic flux inside the SQUID ring. As we know from elementary electrodynamics the total flux can be written as

$$\phi = \phi_x + Li \tag{20}$$

where ϕ_x is the flux due to the external field H_x perpendicular to the rings plane, L is the self-inductance of the ring and i its total current. The latter, in the so-called *resistively shunted junction* (RSJ) model [1], can be decomposed as

Josephson current : this is the current component due to the tunnelling of Cooper pairs through the link and is given by (13)

$$i_s = i_0 \sin\bar{\varphi} \tag{21}$$

Normal current : this originates from the two-fluid model and obeys Ohm's law

$$i_N = \frac{V}{R} \tag{22}$$

where V is the voltage across the junction and R the normal resistance of the material in its normal phase.

Polarization current : this last bit comes from the fact that there is a finite junction capacitance and it reads

$$i_c = C\dot{V} \tag{23}$$

where C is the above-mentioned capacitance.

Assuming that the total current is given by the sum of these 3 components one gets

$$i = i_0 \sin\bar{\varphi} + \frac{V}{R} + C\dot{V} \tag{24}$$

which inserted in (20) reads

$$\frac{\phi_x - \phi}{L} = i_0 \sin\frac{2\pi\phi}{\phi_0} + \frac{\dot{\phi}}{R} + C\ddot{\phi} \tag{25}$$

where we used that $V = -\dot{\phi}$. This is the equation of motion of a particle of "coordinate" ϕ in a potential (see Fig. 2)

$$U(\phi) = \frac{(\phi - \phi_x)^2}{2L} - \frac{\phi_0 i_0}{2\pi}\cos\frac{2\pi\phi}{\phi_0} \tag{26}$$

and (25) becomes

$$C\ddot{\phi} + \frac{\dot{\phi}}{R} + U'(\phi) = 0 \tag{27}$$

where, as usual, $U'(\phi) \equiv dU/d\phi$.

In reality one should add a white noise fluctuating current $I_f(t)$ to the rhs of (27) in order to properly account for the thermodynamical equilibrium properties of the system [2]. With this additional term (27) is nothing but the well-known classical *Langevin equation* for the *Brownian motion* [2].

In order to appreciate the diversity of the physical phenomena in (26), it is worth analyzing that potential in some detail.

The minima of $U(\phi)$ are the solutions, ϕ_m, of $U'(\phi) = 0$ subject to $U''(\phi_m) > 0$. This leads us to two distinct cases:
(i) $2\pi\frac{Li_0}{\phi_0} > 1 \Longrightarrow$ several minima;
(ii) $2\pi\frac{Li_0}{\phi_0} \leq 1 \Longrightarrow$ only one minimum.

In Figs. 2,3 and 4 we sketch the form of $U(\phi)$ for three distinct values of the external flux ϕ_x for the case (i) above.

Suppose that at $t = 0$ there is no external field and the superconducting current is zero. In this case the equilibrium value of the flux inside the SQUID is also zero (point P in Fig.(2)). As we slowly turn on the external field H_x, the potential $U(\phi)$ changes accordingly and the equilibrium value of ϕ adiabatically follows its potential well until it becomes an inflection point of $U(\phi)$. In this example we clearly see that the initial equilibrium position moving from $P \rightarrow P' \rightarrow P''$. It is worth noticing that the adiabatic approximation is valid only when dH_x/dt is much smaller than any typical frequency resulting from (27),

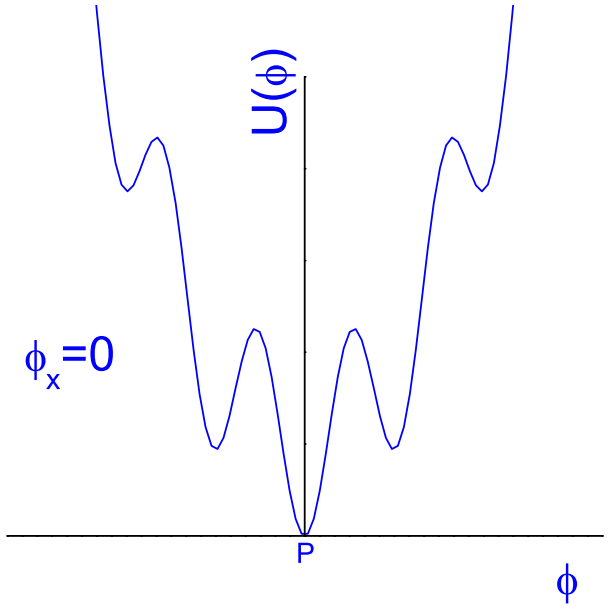

Figure 2: Potential energy for $\phi_x = 0$

namely, $[U''(\phi_m)/C]^{1/2}$ or $1/2RC$. In this way it is possible to see a broad region of values of H_x throughout which the initial flux changes from a stable to a bistable and, finally, a metastable configuration.

The realization that the dynamics of ϕ is really Brownian comes through the study of the decay of its metastable configuration by thermal fluctuations [3]. Here, as H_x increases, the value of ϕ that adiabatically evolves from $\phi = 0$ might jump to its neighboring minimum before H_x reaches H_x^*, the field at which the initial local minimum would become an inflection point of $U(\phi)$. The mechanism responsible for this transition is thermal activation over the potential barrier that keeps this configuration metastable. The probability of decaying from the metastable state in the SQUID ring nicely fits the results obtained by regarding ϕ as the coordinate of a Brownian particle.

The observation of the above-mentioned phenomena was made at temperatures of about 4 K (for a Nb SQUID). However if the temperature is lowered below 1 K thermal fluctuations are not so intense to trigger this process. On the other hand, for the SQUID parameters such as $C \simeq 10^{-12}$ F, $L \simeq 5 \times 10^{-10}$ H and $i_0 \simeq 10^{-5}$ A, one has $T_0 \equiv \hbar\omega/k \simeq 1$ K, where ω is one of the natural frequencies of the SQUID. This means that for $T \leq 1$ K quantum effects are important and therefore one should ask about the possibility of observing the same

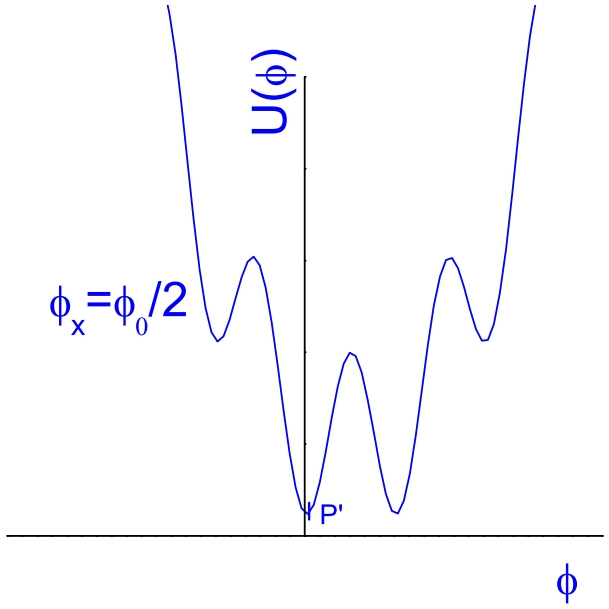

Figure 3: Potential energy for $\phi_x = \phi_0/2$

transition driven by another mechanism: for example, quantum tunnelling. In this case one should start by neglecting the dissipative term and proceeding with the canonical quantization applied to the Hamiltonian in terms of the flux variable which allows us to write a Schrödinger equation for the fictitious particle represented by the coordinate ϕ. From then onwards we can apply, for example, the standard WKB method to describe the tunnelling of the lowest energy state initially prepared about the metastable minimum of the potential (see Fig. (4)).

This procedure would not be useful only for studying the phenomenon of decay of a metastable configuration but one could also study the coherent tunnelling between two bistable configurations or the level structure within a stable potential well. In the former case we restrict ourselves to the two-dimensional Hilbert space spanned by the two lowest energy eigenstates of the potential of Fig. (3). Here, one can also apply approximation methods to describe the coherent tunnelling between the two bistable minima of that potential once the initial state is on one given side of the potential barrier.

We shall shortly address these issues and their interpretation in the next section.

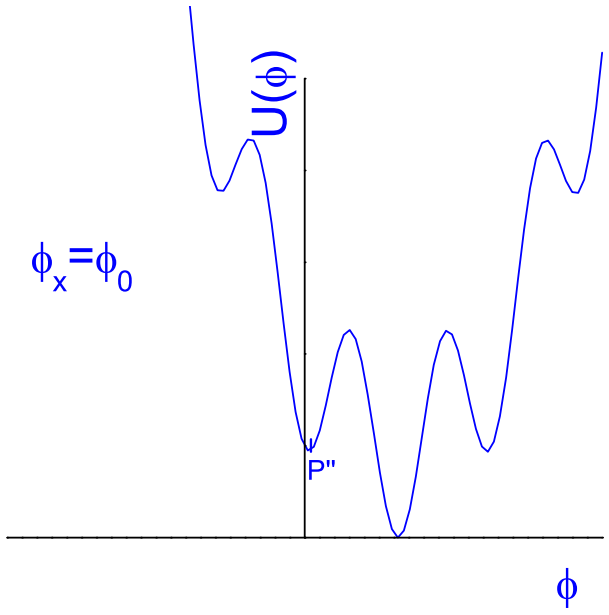

Figure 4: Potential energy for$\phi_x = \phi_0$

2.4 Current biased Josephson junctions (CBJJs)

Suppose we have now a weak link coupled to a current source which provides a constant current I_x to the system. In this case the variable of interest is the phase difference, $\bar{\varphi}$, across the weak link and here the RSJ model can be used as well.

We can easily get the dynamics of $\bar{\varphi}$ using (27) and the fact that the current biased junction is an extreme case of a huge SQUID such that $L \to \infty$, $\phi_x \to \infty$ but $\phi_x/L = I_x$, the current bias. Moreover, since the flux inside the ring ceases to make any sense for the junction with a current bias one must rewrite it in terms of the phase difference $\bar{\varphi}$ as (see (19))

$$\phi = -\frac{\phi_0}{2\pi}\,\bar{\varphi} \equiv \frac{\phi_0}{2\pi}\,\varphi \tag{28}$$

and (27) becomes

$$\frac{\phi_0}{2\pi}\,C\,\ddot{\varphi} + \frac{\phi_0}{2\pi R}\,\dot{\varphi} + U'(\varphi) = 0, \tag{29}$$

where

$$U(\varphi) = -I_x\,\frac{\phi_0}{2\pi}\,\varphi - E_J\,\cos\varphi, \tag{30}$$

where we have just defined *the Josephson coupling energy* as

$$E_J \equiv \frac{\phi_0 i_0}{2\pi}. \tag{31}$$

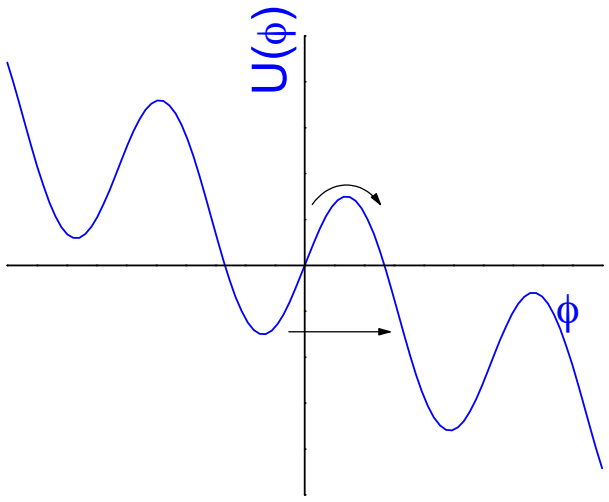

Figure 5: Washboard potential

When the external current is zero, there is no phase difference across the junction. As the external current is increased the phase across the junction adjusts itself so the current can cross the junction without the generation of any finite voltage. But, when $I_x \geq i_0$ (13,14) a finite voltage develops across the junction. In our mechanical analogy this means that the maxima and minima of the washboard potential coalesce at $I_x = i_0$ and beyond this value our particle runs downhill which means that φ varies with time. The current-voltage characteristic for a CBJJ is shown in Fig. (6)

However a finite voltage can be generated even before i_0 is reached because, once again, thermal fluctuations could drive our fictitious particle out of its equilibrium position by overcoming the potential barrier. Now, if the temperature is not high enough to create intense thermal fluctuations, one could also in this case enquire about the possibility of tunnelling induced voltage across the junction. This means that our fictitious particle of coordinate φ tunnels through the potential barrier provided by the washboard potential. Once again we must neglect the dissipative term in the equation of motion of φ in order to apply the canonical quantization procedure to this problem as well.

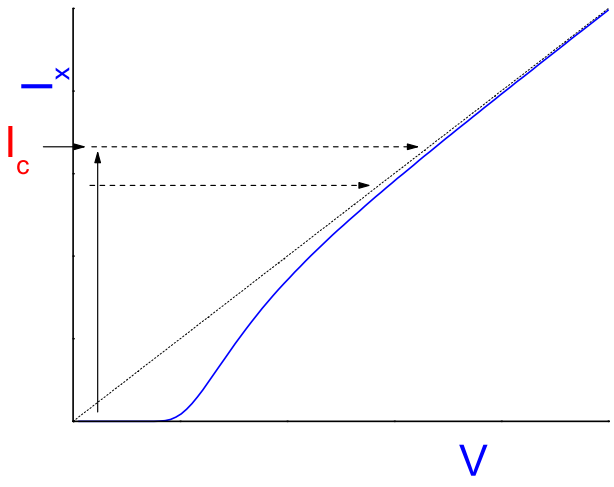

Figure 6: Voltage-current characteristic of a CBJJ

3 Dissipative quantum systems

As we have seen during our first lecture the equation of motion of the variable of interest of the superconducting devices we have introduced are all dissipative. This means that despite the quantum mechanical effects take place on the macroscopic level, this also happens to be the reason why the system cannot be treated as entirely isolated. It is very hard to isolate any of those devices, or to be more precise, the macroscopic variable of interest from its environment. Actually, it is not even true that they might be considered very weakly damped. As a general rule there is no restriction about the dissipative term and it can even be controlled by the experimentalist in such a way that they result in overdamped dynamics.

On the other hand it is known that there is no safe way to generalize the canonical quantization procedure in order to deal with dissipative systems on the quantum mechanical level [4]. The way out of this dilemma is to explicitly consider the fact that the dissipative system is always coupled to a given thermal environment. We know of no dissipative system in Nature which is not coupled to another system responsible for its losses. Therefore, before one tries to modify the canonical scheme of quantization we believe that it is more useful to apply the traditional methods to more realistic situations.

Conceptually the idea is very simple. However, in practice things are not as simple as they look. Once we have decided to explicitly consider the coupling

of the system of interest to the environment we must know what sort of system the latter is and how their mutual coupling takes place. This can be a very hard task.

Nevertheless, fundamentally different composite systems - system of interest-plus-environment - might have the former presenting Brownian dynamics in the classical limit. Although this appears to be an additional complication to our approach it actually gives us a chance to argue in favor of some simplifying hypothesis. For instance, we can assume that, regardless of their differences, they may share some common characteristics such as the behavior of their spectrum of excitations or the way they are acted by their Brownian particles.

In what follows we will not attempt to justify the use of one specific model. We will choose a simple one which under certain conditions reproduces Brownian motion in the classical regime. Thus, the justification for the choice of the model will be provided *a posteriori*. However, it is worth mentioning that the employment of detailed microscopic models for some environments may show different quantum mechanical behaviors which turn out be very important in some cases.

3.1 The Model

Let us suppose our composite system can be described by the Lagrangian

$$L = L_S + L_I + L_R + L_{CT}, \tag{32}$$

where

$$L_S = \frac{1}{2} M \dot{q}^2 - V(q), \tag{33}$$

$$L_I = -\sum_k C_k \, q_k \, q, \tag{34}$$

$$L_R = \sum_k \frac{1}{2} m_k \dot{q}_k^2 - \sum_k \frac{1}{2} m_k \, \omega_k^2 \, q_k^2, \tag{35}$$

$$L_{CT} = -\sum_k \frac{1}{2} \frac{C_k^2}{m_k \, \omega_k^2} \, q^2, \tag{36}$$

are respectively the Lagrangian of the system of interest, interaction, reservoir, and counter-term (see below). The reservoir consists of a set of non-interacting harmonic oscillators of coordinates q_k, masses m_k and natural frequencies ω_k. Each one of them is coupled to the system of interest, which we will loosely call the system from now on, by a coupling constant C_k. A fairly general justification of this model was made in [5].

Initially we shall study the classical equations of motion resulting from (32). Writing the Euler-Lagrange equations of the composite system one has

$$M\ddot{q} = -V'(q) - \sum_k C_k\, q_k - \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\, q, \tag{37}$$

$$m_k\,\ddot{q}_k = -m_k\,\omega_k^2\, q_k - C_k\, q. \tag{38}$$

Taking the Laplace transform of (38) one gets

$$\tilde{q}_k(s) = \frac{\dot{q}_k(0)}{s^2+\omega_k^2} + \frac{s\,q_k(0)}{s^2+\omega_k^2} - \frac{C_k\,\tilde{q}(s)}{m_k\,(s^2+\omega_k^2)}, \tag{39}$$

which after the inverse transformation can be taken to (37) yielding

$$\begin{aligned} M\ddot{q} + V'(q) + \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\, q \;\; &= \;\; \frac{-1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty} \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{s^2+\omega_k^2} + \frac{s\,q_k(0)}{s^2+\omega_k^2} \right\} e^{s\,t}\, ds + \\ &+ \sum_k \frac{C_k^2}{m_k}\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty} \frac{\tilde{q}(s)}{s^2+\omega_k^2}\, e^{s\,t}\, ds. \end{aligned} \tag{40}$$

Thus using the identity

$$\frac{1}{s^2+\omega_k^2} = \frac{1}{\omega_k^2}\left\{1 - \frac{s^2}{s^2+\omega_k^2}\right\}, \tag{41}$$

we can show that the last term on the rhs of (40) generates a term that exactly cancels the last one on the lhs and the resulting equation is

$$\begin{aligned} & M\ddot{q} + V'(q) + \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty} \frac{s^2\,\tilde{q}(s)}{s^2+\omega_k^2}\, e^{s\,t}\, ds \\ = \;\; & \frac{-1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty} \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{s^2+\omega_k^2} + \frac{s\,q_k(0)}{s^2+\omega_k^2} \right\} e^{s\,t}\, ds. \end{aligned} \tag{42}$$

Then we see that the inclusion of L_{CT} in (32) was solely to cancel one extra harmonic contribution that would come from the coupling to the environmental oscillators.

The last term on the lhs of (42) can be rewritten as

$$\frac{d}{dt}\left\{ \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty} \frac{s\,\tilde{q}(s)}{s^2+\omega_k^2}\, e^{s\,t}\, ds \right\} \tag{43}$$

which with the help of the convolution theorem reads

$$\frac{d}{dt}\left\{ \sum_k \frac{C_k^2}{m_k\,\omega_k^2} \int_0^t \cos\left[\omega_k\,(t-t')\right]\, q(t')\, dt' \right\}. \tag{44}$$

In order to replace $\sum_k \longrightarrow \int d\omega$ let us introduce the spectral function $J(\omega)$ as

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{C_k^2}{m_k\,\omega_k}\,\delta\left(\omega - \omega_k\right), \tag{45}$$

which allows us to write

$$\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\cos\left[\omega_k\,\left(t-t'\right)\right] = \frac{2}{\pi}\int_0^\infty d\omega\,\frac{J(\omega)}{\omega}\cos\left[\omega\,\left(t-t'\right)\right]. \tag{46}$$

The function $J(\omega)$ is nothing but the imaginary part of the Fourier transform of the retarded dynamical susceptibility of the bath of oscillators, namely,

$$J(\omega) = \mathrm{Im}\mathcal{F}\left\{-i\,\theta\left(t-t'\right)\left\langle\left[\sum_k C_k\,q_k(t)\,,\,\sum_{k'} C_{k'}\,q_{k'}(t')\right]\right\rangle\right\}. \tag{47}$$

Now, assuming that

$$J(\omega) = \{\,\eta\,\omega \qquad \mathrm{if}\omega < \Omega, 0 \qquad \mathrm{if}\omega > \Omega, \tag{48}$$

where Ω is a high frequency cutoff that fixes the frequency (or time) scale of the problem, we can rewrite (46) as

$$\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\cos\left[\omega_k\,\left(t-t'\right)\right] = \frac{2}{\pi}\int_0^\Omega \eta\,\cos\left[\omega\,\left(t-t'\right)\right] = 2\,\eta\,\delta\left(t-t'\right), \tag{49}$$

where we took $\Omega \longrightarrow \infty$. This result allows us to rewrite Eq. (44) as

$$\frac{d}{dt}\int_0^t 2\,\eta\,\delta\left(t-t'\right)q(t')dt' = \eta\,\dot{q}. \tag{50}$$

Finally, the rhs of (42) can be interpreted as a force $f(t)$ depending on the initial conditions imposed on the oscillators of the bath. Suppose the environment is in thermodynamical equilibrium independently of the position of the external particle. Thus, using the equipartition theorem we have in the classical limit

$$\begin{aligned}
&\langle q_k(0)\rangle = \langle \dot{q}_k(0)\rangle = \langle \dot{q}_k(0)\,q_k(0)\rangle = 0,\\
&\langle \dot{q}_k(0)\,\dot{q}_{k'}(0)\rangle = \frac{k\,T}{m_k}\,\delta_{kk'},\\
&\langle q_k(0)\,q_{k'}(0)\rangle = \frac{k\,T}{m_k\,\omega_k^2}\,\delta_{kk'}.
\end{aligned} \tag{51}$$

Using these relations it can be shown that

$$\begin{aligned}
&\langle f(t)\rangle = 0 \qquad \text{and}\\
&\langle f(t)\,f(t')\rangle = 2\,\eta\,k\,T\,\delta\left(t-t'\right).
\end{aligned} \tag{52}$$

If we now insert (50) in (42) we finally have

$$M\,\ddot{q} + \eta\,\dot{q} + V'(q) = f(t), \tag{53}$$

where $f(t)$ satisfies (52). This is the well-known Langevin equation for the classical Brownian motion.

Along the deduction of (53) we have omitted some minor but crucial details which have to do with the specific choice of the initial state of the environment we have chosen. For instance, (50) is not strictly correct but a thorough analysis of this problem can be found in [6].

As a last remark we would like to mention that another completely equivalent way to write our model (32) is to replace the interaction Lagrangian (34) by

$$\tilde{L}_I = -\sum_k \tilde{C}_k\, q\, \dot{q}_k, \tag{54}$$

and omit L_{CT}. In this way we can define the canonical momenta p_k as

$$p_k = \frac{\partial L}{\partial \dot{q}_k} = m_k\,\dot{q}_k - \tilde{C}_k\, q, \tag{55}$$

and write

$$\tilde{H} = p\,\dot{q} + p_k\,\dot{q}_k - L = \frac{p^2}{2\,M} + V(q) + \sum_k \left\{ \frac{1}{2\,m_k}\Big(p_k + \tilde{C}_k\, q\Big)^2 + \frac{1}{2} m_k\,\omega_k^2\, q_k^2 \right\}, \tag{56}$$

Now, performing a canonical transformation $p \to p$, $q \to q$, $p \to m_k\,\omega_k\,q_k$, and $q_k \to p_k/m_k\,\omega_k$ and defining $C_k \equiv \tilde{C}_k\,\omega_k$ we have

$$H = \frac{p^2}{2M} + V(q) + \sum_k C_k q_k q + \sum_k \left\{ \frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 q_k^2 \right\} + \sum_k \frac{C_k^2}{2m_k\omega_k^2} q^2, \tag{57}$$

which has (32) as its corresponding Lagrangian. Therefore, the electromagnetic Lagragian with $\tilde{L}_I$ replacing L_I in (32) and no counter-term is completely equivalent to (32) itself. It is worth noticing that the spectral density $J(\omega)$ must be modified when expressed as a function of $\widetilde{C}_k$.

Now that we know a treatable model that generates the classical Brownian motion for the variable of interest ($q(t)$ in the present case) we can study the quantum mechanics of the composite system and extract from it only the part referring to the system of interest.

3.2 The Dynamical Reduced Density Operator

It is well-known from quantum mechanics that we can get all the information about a given subsystem S when we perform the partial trace of the total density operator $\hat{\rho}(t)$ with respect to those variables to which that subsystem is coupled. In what follows we shall briefly resume the essence of the method and then apply it to our specific model (32).

Suppose we have a general system described by the Hamiltonian

$$H = H_0(q,p) + H_I(q,q_k) + H_R(q_k,p_k) + H_{CT}, \tag{58}$$

where H_0, H_I, H_R and H_{CT} are, as usual, the Hamiltonians of the system, interaction, reservoir and counter-term, respectively. If we introduce the general vector $\mathbf{R} = (R_1, ..., R_N)$, where R_k is the value assumed by q_k we can write the coordinate representation of the total $\hat{\rho}(t)$

$$\begin{aligned}\hat{\rho}(x,\mathbf{R},y,\mathbf{Q},t) &= \int\int\int\int dx'dy'd\mathbf{R}'d\mathbf{Q}'\, K(x,\mathbf{R},t;x',\mathbf{R}',0)\, K^*(y,\mathbf{Q},t;y',\mathbf{Q}',0)\, \times \\ &\times\hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0)\end{aligned} \tag{59}$$

where

$$K(x,\mathbf{R},t;x',\mathbf{R}',0) = \left\langle x,\mathbf{R}|e^{-i\,H\,t/\hbar}|x',\mathbf{R}'\right\rangle, \tag{60}$$

is the quantum mechanical propagator of the whole universe $S+R$ and

$$\hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0) = \langle x',\mathbf{R}'|\hat{\rho}(0)|y',\mathbf{Q}'\rangle \tag{61}$$

the coordinate representation of its initial state. Taking the trace with respect to the environmental variables means to make $\mathbf{R} = \mathbf{Q}$ and integrate over it. Then, assuming that (61) is separable

$$\hat{\rho}(x',\mathbf{R}',y',\mathbf{Q}',0) = \hat{\rho}(x',y',0)\,\hat{\rho}(\mathbf{R}',\mathbf{Q}',0), \tag{62}$$

one reaches

$$\tilde{\rho}(x,y,t) = \int\int dx'dy'\, J(x,y,t;x',y',0)\,\hat{\rho}(x',y',0), \tag{63}$$

where

$$\begin{aligned}J(x,y,t;x',y',0) &= \int\int\int d\mathbf{R}'d\mathbf{Q}'d\mathbf{R}\left\{K(x,\mathbf{R},t;x',\mathbf{R}',0)\, K^*(y,\mathbf{R},t;y',\mathbf{Q}',0)\, \times\right. \\ &\left.\times\,\tilde{\rho}(\mathbf{R}',\mathbf{Q}',0)\right\}.\end{aligned} \tag{64}$$

Here we should notice that if S and R are decoupled $K(x,\mathbf{R},t;x',\mathbf{R}',0) = K_0(x,t;x',0)\,K_R(\mathbf{R},t;\mathbf{R}',0)$, which inserted in (64) yields

$$J(x,y,t;x',y',0) = K_0(x,t;x',0)\,K_0^*(y,t;y',0), \tag{65}$$

where we used that $\mathrm{tr}_R\{\hat{\rho}_R(t)\} = 1$. Thus J acts as a super-propagator of the reduced density operator of the system.

From (63) and (64) we see that all that is needed is to evaluate the total propagator $K(x,\mathbf{R},t;x',\mathbf{R}',0)$ since $\hat{\rho}(0)$ is assumed to be known. However, as the reservoir consists of a set of N oscillators, it is quite laborious to go on with its evaluation through conventional approaches such as the explicit use of

the environmental wave functions. Our approach is instead to appeal to the Feynman representation of K in terms of functional integrals which will prove more powerful than many other ways to deal with the same problem.

It can be shown [7] that in the functional integral representation the total propagator reads

$$K(x,\mathbf{R},t;x',\mathbf{R}',0)=\int_{x'}^{x}\int_{\mathbf{R}'}^{\mathbf{R}}\mathcal{D}x(t')\,\mathcal{D}\mathbf{R}(t')\,\exp\left\{\frac{i}{\hbar}S[x(t'),\mathbf{R}(t')]\right\}, \qquad (66)$$

where

$$S[x(t'),\mathbf{R}(t')]=\int_0^t L(x(t'),\mathbf{R}(t'),\dot{x}(t'),\dot{\mathbf{R}}(t'))\,dt', \qquad (67)$$

is the action of the composite system $R+S$. Those integrals in (66) must be evaluated over all the geometric paths $x(t')$ and $\mathbf{R}(t')$ such that $x(0)=x'$, $x(t)=x$, $\mathbf{R}(0)=\mathbf{R}'$, and $\mathbf{R}(t)=\mathbf{R}$.

Inserting (66) in (64) one reaches

$$\begin{aligned}J(x,y,t;x',y',0) &= \int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\,\mathcal{D}y(t')\,\exp\left\{\frac{i}{\hbar}\widetilde{S_0}[x(t')]\right\}\exp\left\{-\frac{i}{\hbar}\widetilde{S_0}[y(t')]\right\}\times \\ &\quad\times\mathcal{F}[x(t'),y(t')], \qquad (68)\end{aligned}$$

where $\widetilde{S_0}$ is the action of the system of interest when isolated, S_0, plus the counter-term action, S_{CT}, and

$$\begin{aligned}\mathcal{F}[x(t'),y(t')] &= \int\int\int d\mathbf{R}'\,d\mathbf{Q}'\,d\mathbf{R}\,\rho_R(\mathbf{R}',\mathbf{Q}',0)\int_{\mathbf{R}'}^{\mathbf{R}}\int_{\mathbf{Q}'}^{\mathbf{R}}\mathcal{D}\mathbf{R}(t')\,\mathcal{D}\mathbf{R}(t')\,\times \\ &\quad\times\exp\left\{\frac{i}{\hbar}\Big[S_I[x(t'),\mathbf{R}(t')]-S_I[y(t'),\mathbf{Q}(t')]+S_R[\mathbf{R}(t')]-S_R[\mathbf{Q}(t')]\Big]\right\}, \qquad (69)\end{aligned}$$

is the so-called influence functional [7, 8]. This functional is the average of the product of two time evolutions over the initial state of the environment . One is the time evolution of the environment when acted by the system of interest and the other is its time reversed partner. One needs these two histories to describe the time evolution of the reduced density operator of the system.

It is clear that this approach can be applied to several systems but it is unlikely to be exactly soluble in many cases. That is where our model (32) comes into play. Since our bath is harmonic one can easily compute its propagator when acted by the coordinate of the particle of interest (forced harmonic oscillators) and perform the average in (69) by assuming that the environment is in thermal equilibrium at a given temperature T [7, 9].

Although the integrals in (69) are all Gaussians we are not going to write the intermediate steps of their evaluation explicitly.

In order to compute the influence functional (69) we shall make explicit use of the expression for the propagator of the k^{th} environmental oscillator when it is acted by an external force $C_k x(t)$ which reads [9, 7]

$$K_{RI}^{(k)}=\sqrt{\frac{m_k\omega_k}{2\pi i\hbar\sin\omega_k t}}\,\exp\frac{i}{\hbar}S_{cl}^{(k)} \qquad (70)$$

where

$$S_{cl}^{(k)} = \frac{m_k\omega_k}{2\sin\omega_k t}\Big[\Big(R_k^2+{R'_k}^2\Big)\cos\omega_k t - 2R_kR'_k + \frac{2C_kR_k}{m_k\omega_k}\int_0^t x(t')\sin\omega_k t'dt' + \frac{2C_kR'_k}{m_k\omega_k}\int_0^t x(t')\sin\omega_k(t-t')dt' - \frac{2C_k^2}{m_k^2\omega_k^2}\int_0^t dt'\int_0^{t'} dt'' x(t')x(t'')\sin\omega_k(t-t')\sin\omega_k t''\Big]. \tag{71}$$

This and its time reversed counter-part must be multiplied by one another for all k and averaged over the initial state of the environment. In our particular problem we will assume that the environment is initially in thermal equilibrium at temperature T and therefore its density operator can be written as

$$\rho_R(\mathbf{R'},\mathbf{Q'},0) = \prod_k \rho_R^{(k)}(R'_k,Q'_k,0) =$$

$$= \prod_k \frac{m_k\omega_k}{2\pi\hbar\sinh\big(\frac{\hbar\omega_k}{k_BT}\big)}\exp-\left\{\frac{m_k\omega_k}{2\hbar\sinh\big(\frac{\hbar\omega_k}{k_BT}\big)}\Big[\Big({R'_k}^2+{Q'_k}^2\Big)\cosh\Big(\frac{\hbar\omega_k}{k_BT}\Big)-2R'_kQ'_k\Big]\right\}. \tag{72}$$

Since all the integrals in (69) are Gaussians we can readily evaluate them. Substituting (72,71,70) in (69) and the resulting expression in (68) one gets

$$J(x,y,t;x',y',0) = \int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\mathcal{D}y(t')\exp\frac{i}{\hbar}\Big\{\widetilde{S_0}[x(t')]-\widetilde{S_0}[y(t')] - \int_0^t\int_0^\tau d\tau d\sigma[x(\tau)-y(\tau)]\alpha_I(\tau-\sigma)[x(\sigma)+y(\sigma)]\Big\}\times \times \exp-\frac{1}{\hbar}\int_0^t\int_0^\tau d\tau d\sigma[x(\tau)-y(\tau)]\alpha_R(\tau-\sigma)[x(\sigma)-y(\sigma)]\Big\} \tag{73}$$

where

$$\alpha_R(\tau-\sigma) = \sum_k \frac{C_k^2}{2m_k\omega_k}\coth\frac{\hbar\omega_k}{2k_BT}\cos\omega_k(\tau-\sigma) \tag{74}$$

and

$$\alpha_I(\tau-\sigma) = -\sum_k \frac{C_k^2}{2m_k\omega_k}\sin\omega_k(\tau-\sigma). \tag{75}$$

Now using (45,48) we can rewrite these expressions as

$$\alpha_R(\tau-\sigma) = \frac{1}{\pi}\int_0^\Omega d\omega\ \eta\omega\coth\frac{\hbar\omega}{2k_BT}\cos\omega(\tau-\sigma) \tag{76}$$

and

$$\alpha_I(\tau-\sigma) = -\frac{1}{\pi}\int_0^\Omega d\omega\ \eta\omega \sin\omega(\tau-\sigma) = \frac{\eta}{\pi}\frac{d}{d(\tau-\sigma)}\int_0^\Omega d\omega\ \eta\omega\cos\omega(\tau-\sigma). \tag{77}$$

In order to obtain the final expression for (68) we must insert (76,77) into (73) . These substitutions must be carefully done, in particular the one involving the expression (77) . We shall not go into the details of this analysis but only warn the reader that in handling the limit $\Omega \to \infty$ and the resulting delta functions one must always interpret the instant $t = 0$ as $t = 0^+$. The physical reason for this lies once again on the choice we have made for our initial state of the whole system (61) . We refer the reader to [10] for a clear discussion on this issue.

Another point that deserves attention is that (77) carries an extra harmonic contribution which exactly cancels the counter-term action as expected.

Now that we hope to have settled these questions we must proceed and write

$$\begin{aligned} J(x,x',t;y,y',0) &= \int_{x'}^{x}\int_{y'}^{y}\mathcal{D}x(t')\mathcal{D}y(t')\times \\ &\times\exp\frac{i}{\hbar}\Big\{S_0[x(t')] - S_0[y(t')] - M\gamma\int_0^t (x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x})dt'\Big\}\times \\ &\times\exp -\frac{2M\gamma}{\pi\hbar}\int_0^\Omega d\omega\,\omega\,\coth\frac{\hbar\omega}{2k_BT}\int_0^t\int_0^\tau d\tau d\sigma[x(\tau)-y(\tau)]\cos\omega(\tau-\sigma)[x(\sigma)-y(\sigma)], \end{aligned} \tag{78}$$

where $\gamma \equiv \eta/2M$ is the relaxation constant of the system.

3.3 The Equilibrium Reduced Density Operator

Despite the fact that we have developed the expression for the real time evolution of $\widetilde{\rho}(x,y,t)$ there are several problems for which only the knowledge of the reduced density operator in equilibrium is necessary. It is also true that this operator can be obtained by taking the limit $t \to \infty$ of our previous time evolution but this task might be fairly difficult sometimes. However, there is a shortcut one can take by directly evaluating its functional integral representation in terms of the system variables only. The latter will prove very useful since it can be handled by some very suitable techniques.

The density operator for the composite system in equilibrium reads

$$\langle x\mathbf{R}|e^{-\beta H}|y\mathbf{Q}\rangle = \rho(x,\mathbf{R};y,\mathbf{Q},\beta) \tag{79}$$

where H is the hamiltonian of the complete system, $H = H_S + H_I + H_R + H_{CT}$, as in (57,58). This operator also admits a functional integral representation [7] that reads

$$\rho(x,\mathbf{R};y,\mathbf{Q},\beta) = \int_y^x\int_{\mathbf{Q}}^{\mathbf{R}}\mathcal{D}q(\tau)\mathcal{D}\mathbf{R}(\tau)\exp -\frac{1}{\hbar}S_E[q(\tau),\mathbf{R}(\tau)] \tag{80}$$

where

$$S_E[q(\tau),\mathbf{R}(\tau)] = \int_0^{\hbar\beta} d\tau \Big\{ \frac{1}{2}M\dot{q}^2 + V(q) + \sum_k \Big(C_k q R_k + \frac{1}{2}m_k \dot{R}_k^2 + \frac{1}{2}m_k\omega_k^2 R_k^2 \Big) \Big\} \tag{81}$$

is the so-called "Euclidean action" of the composite system. The reduced density operator of the particle is then

$$\begin{aligned} \tilde{\rho}(x,y,\beta) &\equiv \int d\mathbf{R}\, \rho(x,\mathbf{R};y,\mathbf{R},\beta) = \\ &= \int_y^x \mathcal{D}q(\tau) \int d\mathbf{R} \int_{\mathbf{R}}^{\mathbf{R}} \mathcal{D}\mathbf{R}(\tau) \exp -\frac{1}{\hbar} S_E[q(\tau),\mathbf{R}(\tau)] \end{aligned} \tag{82}$$

which also involves only Gaussian integrals over the environmental variables [5, 9]. Evaluating these integrals one reaches

$$\tilde{\rho}(x,y,\beta) = \tilde{\rho}_0(\beta) \int_y^x \mathcal{D}q(\tau)\, \exp -\frac{1}{\hbar}\widetilde{S}_E^{(0)}[q(\tau)]\, \exp \frac{\Lambda[q(\tau)]}{\hbar} \tag{83}$$

where

$$\tilde{\rho}_0(\beta) = \prod_k \frac{1}{2}\, \mathrm{cosech}\Big(\frac{\hbar\beta\omega_k}{2}\Big), \tag{84}$$

$$\widetilde{S}_E^{(0)}[q(\tau)] = S_E^{(0)}[q(\tau)] + S_{CT}[q(\tau)] = \int_0^{\hbar\beta} d\tau \Big\{ \frac{1}{2}M\dot{q}^2 + V(q) \Big\} + S_{CT}[q(\tau)], \tag{85}$$

and

$$\Lambda[q(\tau)] = \sum_k \frac{C_k^2}{4m_k\omega_k} \int_{-\infty}^{+\infty} d\tau' \int_0^{\hbar\beta} d\tau q(\tau) q(\tau') \exp -\omega_k |\tau - \tau'|. \tag{86}$$

Now, completing squares in the integrand of (86) one cancels the counter-term contribution for the Euclidean action and gets

$$\tilde{\rho}(x,y,\beta) = \tilde{\rho}_0(\beta) \int_y^x \mathcal{D}q(\tau)\, \exp -\frac{1}{\hbar} S_{eff}[q(\tau)] \tag{87}$$

where

$$S_{eff}[q(\tau)] = \int_0^{\hbar\beta} d\tau \Big\{ \frac{1}{2}M\dot{q}^2 + V(q) \Big\} + \frac{1}{2} \int_{-\infty}^{+\infty} d\tau' \int_0^{\hbar\beta} d\tau \alpha(\tau - \tau') \big\{ q(\tau) - q(\tau') \big\}^2 \tag{88}$$

and

$$\alpha(\tau - \tau') \equiv \sum_k \frac{C_k^2}{4m_k\omega_k} \exp -\omega_k |\tau - \tau'| = \frac{1}{2\pi} \int_0^{\infty} d\omega\, J(\omega) \exp -\omega_k |\tau - \tau'| \tag{89}$$

where, as usual, we have transformed the sum into an integral with the help of (45). For the specific case of interest, namely, ohmic dissipation, this becomes

$$\alpha(\tau - \tau') = \frac{1}{2\pi} \int_0^{\infty} d\omega\, \eta\omega \exp -\omega_k |\tau - \tau'| = \frac{\eta}{2\pi} \frac{1}{(\tau - \tau')^2} \tag{90}$$

3.4 Applications

Now let us apply the machinery we have just developed to some problems of interest.

3.4.1 Damped Harmonic Oscillator

This first application is the simplest one. We want to follow the time evolution of a harmonic oscillator coupled to our standard environment. We thus initially prepare a particle of mass M subject to a potential $V(q) = M\omega_0^2 q^2/2$ in a pure state given by the wave packet

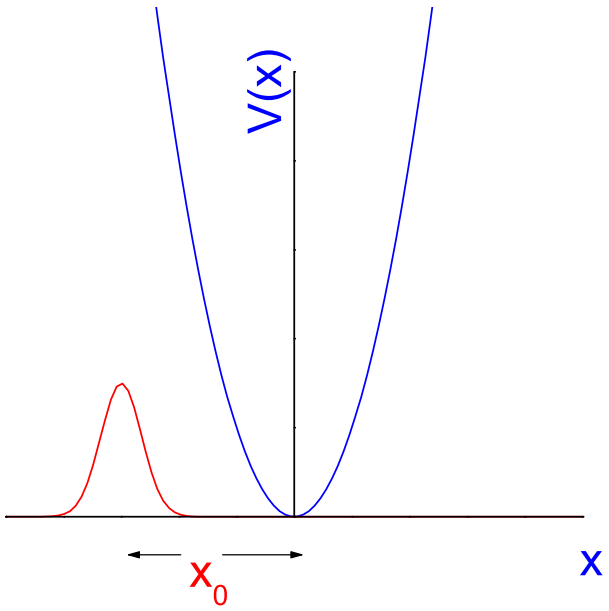

Figure 7: Gaussian wavepacket

$$\psi(x') = \frac{1}{(2\pi\sigma^2)^{1/4}} \exp \frac{ipx'}{h} \exp -\frac{x'^2}{4\sigma^2} \tag{91}$$

and allow it to interact with a the bath of oscillators which is in equilibrium at temperature T. Notice that this wavepacket corresponds to $x_0 = 0$ in fig.(7).

The first step of the calculation is to evaluate the specific form of the super-propagator $J(x,y,t;x',y',0)$ for the harmonic potential introduced above. Although the integrations might involve non-local kernels in time, they are all Gaussian and can be easily performed. We shall omit the details of their evaluation only to avoid encumbering the text with very long expressions. These can be found, for example, in [4].

Once this has been achieved we can perform the integration in (63), using the density operator built with (91), to finally get the reduced density operator of the damped harmonic oscillator at time t. Its diagonal element, which represents the probability density to find the particle at the position x, is given by

$$\tilde{\rho}(x,x,t) = \left(\frac{1}{2\pi\sigma^2(t)}\right)^{1/2} \exp -\frac{1}{2\sigma^2(t)}\left(x - x_0(t)\right)^2 \tag{92}$$

from which we can identify the time evolution of its center as $x_0(t)$. In the case of an underdamped oscillator ($\omega_0 > \gamma$), for example, it can be shown [4] that

$$x_0(t) = \frac{p}{M\omega}\sin\omega t\; e^{-\gamma t} \qquad \text{where} \qquad \omega = \sqrt{\omega_0^2 - \gamma^2} \tag{93}$$

which is exactly the classical trajectory of a harmonic particle with initial momentum p and position zero which are clearly the initial conditions obtained from (91).

The width of the packet is clearly given by $\sigma^2(t)$ [4] which in the limit $t \to \infty$ reduces to

$$\sigma^2(\infty) = \frac{\hbar}{\pi}\int_0^\infty d\nu \coth\frac{\hbar\nu}{2kT}\left(\frac{1}{M}\frac{2\gamma\nu}{\left(\omega_0^2 - \nu^2\right)^2 + 4\gamma^2\nu^2}\right). \tag{94}$$

Recognizing the term inside the parenthesis in the integrand as the imaginary part of the susceptibility of a damped oscillator, $\chi''(\nu)$, we rewrite the above expression as

$$\sigma^2(\infty) = \frac{\hbar}{\pi}\int_0^\infty d\nu \coth\frac{\hbar\nu}{2kT}\chi''(\nu) \tag{95}$$

which is nothing but the celebrated *fluctuation - dissipation theorem*. Now, just for general information, one sees that the width of the probability density of the damped oscillator in equilibrium behaves as

$$\sigma^2(\infty) = \frac{\hbar}{2M\omega_0}f(\alpha) \qquad \left(\alpha \equiv \frac{\gamma}{\omega_0}\right) \tag{96}$$

where

$$f(\alpha) = \begin{cases} \frac{1}{\sqrt{1-\alpha^2}}\left(1 - \frac{2}{\pi}\tan^{-1}\frac{\alpha}{\sqrt{1-\alpha^2}}\right) & \text{if} \quad \alpha < 1 \\ \frac{1}{\sqrt{\alpha^2-1}}\frac{1}{\pi}\ln\left|\frac{\alpha+\sqrt{\alpha^2-1}}{\alpha-\sqrt{\alpha^2-1}}\right| & \text{if} \quad \alpha > 1 \end{cases} \tag{97}$$

This last expression shows us that the width of the packet always decreases with increasing dissipation which is a signature of a more efficient localization of a particle in a damped environment.

3.4.2 Decoherence

In this application we repeat exactly the same steps as before with the difference that now the initial state of the oscillator is given by (see Fig.(8))

$$\psi(x) = \psi_1(x) + \psi_2(x) = \tilde{\mathcal{N}}\left[\exp -\frac{x^2}{4\sigma^2} + \exp -\frac{(x+x_0)^2}{4\sigma^2}\right], \tag{98}$$

where $\tilde{\mathcal{N}}$ is a normalization constant. From this state one builds the initial

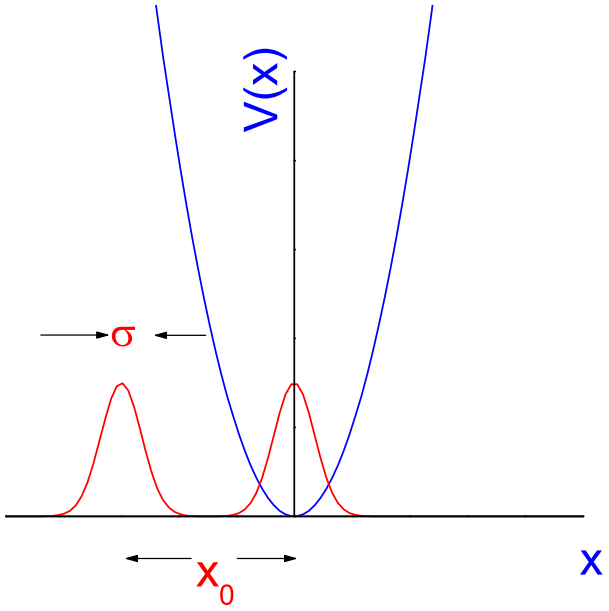

Figure 8: Delocalized initial state

density operator of the particle as

$$\rho(x', y', 0) = \rho_1(x', y', 0) + \rho_2(x', y', 0) + \rho_{int}(x', y', 0) \tag{99}$$

where $\rho_{int}(x', y', 0) = \psi_2(x')\psi_1^*(y') + \psi_1(x')\psi_2^*(y')$. The first (second) term on the rhs of (99) represents the wavepacket centered at the origin (position

$-x_0)$, whereas the last term represents the interference term between these two packets. When $x_0 \gg \sigma$ the latter term is negligible.

It is our intention to study the time evolution of $\widetilde{\rho}(x,x,t) \equiv \widetilde{\rho}(x,t)$ as before. As the time evolution is linear one has

$$\tilde{\rho}(x,t) = \tilde{\rho}_1(x,t) + \tilde{\rho}_2(x,t) + \tilde{\rho}_{int}(x,t) \tag{100}$$

where $\rho_1(x,t)$ and $\rho_2(x,t)$ are the probability densities corresponding to the time evolution of the initial wavepackets ψ_1 and ψ_2, respectively, and $\widetilde{\rho}_{int}(x,t)$ is obtained by

$$\tilde{\rho}_{int}(x,t) = \int dx'dy' J(x,x,t;x',y',0)\tilde{\rho}_{int}(x',y',0). \tag{101}$$

This integral can be readily evaluated and gives

$$\tilde{\rho}_{int}(x,t) = 2\sqrt{\tilde{\rho}_1(x,t)}\sqrt{\tilde{\rho}_2(x,t)}\cos\phi(x,t)\exp -f(t) \tag{102}$$

where $\phi(x,t)$ is a function that determines the interference pattern and $\exp -f(t)$ is an attenuation factor for the intensity of this pattern. It should be stressed that in an undamped system the interference pattern develops every time the two wave packets overlap. An interesting question is to compare the time scale for the destruction of the interference pattern with the relaxation time of the system (γ^{-1}). Once again we refer the reader to the details of this calculation elsewhere [11]. It can be shown that

$$\exp -f(t) \approx \exp -\Gamma t \tag{103}$$

where the general behavior of the so-called *decoherence rate* Γ is illustrated below,

$$\Gamma = \begin{cases} \text{high temperatures} & (\kappa \ll 1) \begin{cases} \frac{2NkT}{\hbar\omega_0}\gamma & \text{if } \gamma \ll \omega_0 \\ \frac{2NkT}{\hbar\omega_0}\frac{\omega_0^2}{2\gamma} & \text{if } \gamma \gg \omega_0 \end{cases} \\ \text{low temperatures} & (\kappa \gg 1) \begin{cases} N\gamma & \text{if } \gamma \ll \omega_0 \\ N\frac{\omega_0^2}{2\gamma} & \text{if } \gamma \gg \omega_0 \end{cases} \end{cases} \tag{104}$$

where $\kappa \equiv \hbar\omega_0/kT$ and $N \equiv x_0^2/4\sigma^2$ is a measure of the average number of quanta of energy initially present in the system and also the square distance between the two wavepackets in units of their width. So, for wavepackets initially prepared quite far apart from one another, the decoherence time is much shorter than the relaxation time of the system regardless of the strength of its damping term. This time scale is even shorter for high temperatures.

This result can be easily understood through the following analysis. Suppose that the initial state of the composite system can be approximated by

$$|\phi_1\rangle \approx \{|\psi_0\rangle + |\psi_z\rangle\} \otimes |0\rangle \tag{105}$$

where $|\psi_0\rangle + |\psi_z\rangle$ is the initial state of the system and $|0\rangle$ the ground state of the environment which we assume to be initially at zero temperature. Moreover, since $|\psi_z\rangle$ is displaced from the origin, the initial state of the system contains an average number N of quanta of energy.

After a time interval τ (the relaxation time of the system), the composite system will be in the state

$$|\phi_f\rangle = |\psi_0\rangle \otimes |N\rangle \tag{106}$$

where $|N\rangle$ is the state of the reservoir containing N quanta of energy $\hbar\omega_0$.

Now, let us investigate the state of the composite system once the oscillator has lost only one quantum of energy to the environment.

Since the emission of N quanta takes place in τ the emission of a single quantum is expected to happen within τ/N. On the other hand, once the interaction Hamiltonian of our model involves coordinate-coordinate coupling, the state of the composite system at this instant can be approximated by

$$|\phi_1\rangle \approx |\tilde{\psi}_z\rangle \otimes |1\rangle + |\tilde{\psi}_0\rangle \otimes |0\rangle \tag{107}$$

because states at different positions will correlate differently with the environment. Therefore, using the orthogonality between $|0\rangle$ and $|1\rangle$ we can compute the reduced density operator of the system as

$$\tilde{\rho} \equiv \mathrm{tr}_R |\phi_1\rangle\langle\phi_1| = |\tilde{\psi}_z\rangle\langle\tilde{\psi}_z| + |\tilde{\psi}_0\rangle\langle\tilde{\psi}_0| \tag{108}$$

which is a statistical mixture. So, since the off-diagonal terms have been washed out within such a short time scale the overlap of the wavepackets will present no interference pattern any more.

The finite temperature effect can also be accounted for with a very similar reasoning [11].

3.4.3 Dissipative Quantum Tunnelling

This is one of the examples where all that is needed can be extracted from the reduced density operator of the particle in equilibrium.

We are interested in studying the decay of a particle out of a metastable potential well. The potential we are going to employ in our exercise is given by (see Fig.(9))

$$V(q) = \frac{1}{2} M\omega_0^2 q^2 - \lambda q^3 \qquad (\lambda > 0). \tag{109}$$

As one usually does in the undamped case, a possible strategy here is to compute the imaginary part of the energy of the metastable state initially prepared as, for example, a Gaussian centered at the position $q = 0$. The difference is that we now have a composite system and, therefore, this imaginary part of

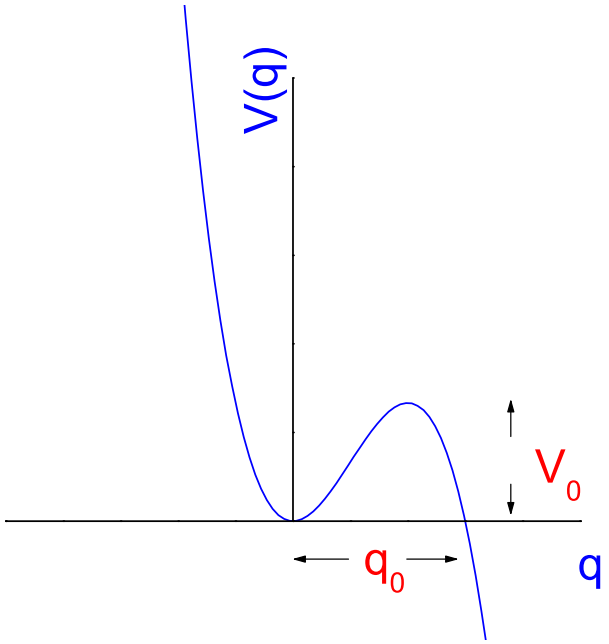

Figure 9: Metastable potential

the energy carries with it all the influence the environment might have in the tunnelling event of the particle.

Let us start by writing the density operator of the composite system in equilibrium which reads

$$\rho_{eq}(x,\mathbf{R};y,\mathbf{Q},\beta)=\sum_n \psi_n(x,\mathbf{R})\psi_n^*(y,\mathbf{Q})\exp-\beta E_n. \tag{110}$$

The reduced density of the particle in equilibrium is then

$$\tilde{\rho}_{eq}(x,y,\beta)=\int d\mathbf{R}\rho_{eq}(x\mathbf{R};y\mathbf{R})=\int d\mathbf{R}\sum_n \psi_n(x,\mathbf{R})\psi_n^*(y,\mathbf{R})\exp-\beta E_n \tag{111}$$

or, using the functional integral representation,

$$\begin{aligned}\tilde{\rho}_{eq}(x,y,\beta)&=\int d\mathbf{R}\langle x\mathbf{R}|e^{-\beta H}|y\mathbf{R}\rangle\\ &=\int d\mathbf{R}\int_{y,\mathbf{R}}^{x,\mathbf{R}}\mathcal{D}q(\tau')\mathcal{D}\mathbf{R}(\tau')\exp-\frac{S_E}{\hbar}[q(\tau'),\mathbf{R}(\tau')]\end{aligned} \tag{112}$$

where H is the hamiltonian of the composite system and S_E its corresponding Euclidean action. The energy of the metastable state of the composite system

can be computed if we take the limit $\beta \to \infty$ in (111) when $x = y$. Defining $\tau \equiv \hbar\beta$ we have

$$\int d\mathbf{R}|\psi_0(0,\mathbf{R})|^2 e^{-\tau E_0/h} \approx \int d\mathbf{R} \int_{0,\mathbf{R}}^{0,\mathbf{R}} \mathcal{D}q(\tau')\mathcal{D}\mathbf{R}(\tau') \exp -\frac{S_E}{\hbar}[q(\tau'),\mathbf{R}(\tau')] \quad (113)$$

On the other hand the trace of the functional integral over $\mathbf{R}(\tau')$ in (113) has already been performed and the result is (87,88)

$$\tilde{\rho}(0,0,\beta) = \tilde{\rho}_0(\beta) \int_0^0 \mathcal{D}q(\tau') \exp -\frac{S_{eff}}{\hbar}[q(\tau')] \quad (114)$$

and

$$S_{eff}[q(\tau')] = \int_0^\tau \left\{ \frac{1}{2}M\dot{q}^2 + V(q) \right\} d\tau' + \frac{\eta}{4\pi} \int_{-\infty}^{\infty} d\tau'' \int_0^\tau d\tau' \frac{\{q(\tau') - q(\tau'')\}^2}{(\tau' - \tau'')^2} \quad (115)$$

Now we have to evaluate the path integral (114) in order to identify the imaginary part of the energy of the metastable state of the composite system through (113). We shall associate this quantity, which we denote by Γ from now onwards, to the effective decay rate of the metastable state of the system of interest influenced by the presence of the environment.

This computation is not simple. It involves the application of the saddle point method to the functional integral (114) once an appropriate analytic extension of the functional in that integrand has been performed. Those interested in the details of this calculation should find it in [5] for the case of zero temperature and [12] for the more general case. The main result at $T = 0$ is

$$\Gamma = A \exp -\frac{B}{\hbar} \quad (116)$$

where

$$B \equiv S_{eff}[q_c] = \int_{-\infty}^{\infty} \left\{ \frac{1}{2}M\dot{q}_c^2 + V(q_c) \right\} d\tau' + \frac{\eta}{4\pi} \int_{-\infty}^{\infty} d\tau' \int_{-\infty}^{\infty} d\tau'' \frac{\{q_c(\tau') - q_c(\tau'')\}^2}{(\tau' - \tau'')^2} \quad (117)$$

is the Euclidean action computed at a function of imaginary time $q_c(\tau)$. The latter is the so-called *bounce solution*, a non-trivial extremum (actually, a saddle point) of the imaginary time or Euclidean action [5].

The pre-factor A represents the fluctuations about this extremum solution and is proportional to the ratio of the determinants of two eigenvalue problems generated by the second functional derivative of the Euclidean action; one computed at a trivial solution and the other at the bounce. As stressed before this is a very subtle problem and the interested reader is urged to follow its details in [5] and [12].

Although both A and B increase with dissipation, the correction due to the modification of the action is the most important one since its contribution

comes through an exponential factor. This increase in the action is trivially seen because the term that depends on η is a positive definite integral. For weakly damped systems ($\omega_0 \gg \gamma$) this correction reads

$$\Delta B = \frac{45}{\pi^3}\,\zeta(3)\,\alpha B_0 = \frac{12}{\pi^3}\,\zeta(3)\,\eta\,\bar{q}^2 \tag{118}$$

where $\alpha \equiv \eta/2M$ and $\zeta(3) = \sum_{n=1}^{\infty} 1/n^3$. This result is obtained perturbatively over the undamped bounce solution $q_0(\tau)$ which has $\bar{q}$ as its maximum value. This is the coordinate of the exit point of the tunnelling particle in a semiclassical picture. In this case it basically coincides with the point where the cubic oscillator potential vanishes away from the origin.

In the case of strongly damped systems ($\gamma \gg \omega_0$) the bounce solution can also be found but it bears no resemblance to the undamped bounce. The total Euclidean action again increases and its final form is now

$$B = \frac{2\pi}{9}\,\eta\,\bar{q}^2 + O\left(\frac{\omega_0}{\gamma}\right) \tag{119}$$

where the new $\bar{q}$ is much larger than the one for the undamped solution. One could loosely say that as the particle tunnels and loses energy it will materialize on the other side of the barrier at a point further away from the exit point of the undamped case.

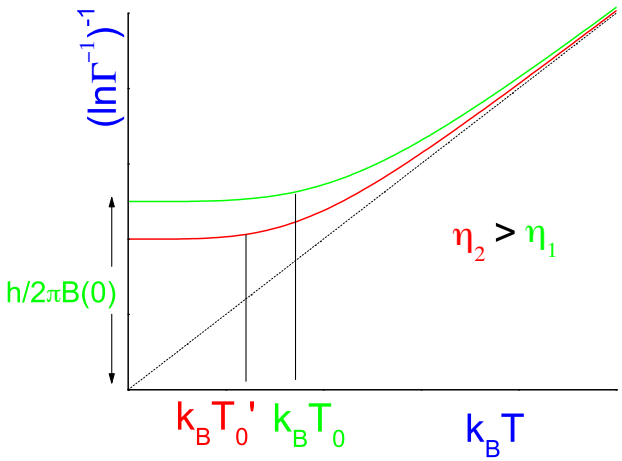

Figure 10: Escape rate as a function of the temperature

Although we shall not address the question of finite temperatures here we present the general behavior of $\Gamma(T)$ in fig.(10).

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Exercises -

1. Consider a system interacting with a reservoir, which is described by a Lagrangean

$$L = L_S + L_I + L_R$$

where

$$L_S = \tfrac{1}{2}M\dot{q}^2 - V_0(q)$$
$$L_I = -\textstyle\sum_k C_k q q_k$$
$$L_R = \textstyle\sum_k \left(\tfrac{1}{2}m_k\dot{q}_k^2 - \tfrac{1}{2}m_k\omega_k^2 q_k^2\right)$$

are respectively, the Lagrangean of the system (S), of interaction (I), and of the reservoir (R), which is formed by an ensemble of harmonic oscillators with coordinates q_k, mass m_k, and coupling constants C_k.
(a) Derive the equations of motion for q and q_k.
(b) Take the Laplace transform for the q_k equation and show that

$$\tilde{q}_k(s) = \frac{\dot{q}_k(0)}{s^2+\omega_k^2} + \frac{sq_k(0)}{s^2+\omega_k^2} + \frac{C_k\tilde{q}(s)}{m_k(s^2+\omega_k^2)}$$

Hint: Look, for instance, at the book of Arfken, Mathematical Methods for Physics, and find that $\mathcal{L}\{f^{(n)}(t)\} = s^n\mathcal{L}\{f(t)\} - s^{n-1}f(0) - s^{n-1}f'(0) - f^{(n-1)}(0)$.
2. Take now the inverse transform of $\tilde{q}_k(s)$ and substitute it into the equation of motion for q. Using the identity

$$\frac{1}{s^2+\omega_k^2} = \frac{1}{\omega_k^2}\left[1 - \frac{s^2}{s^2+\omega_k^2}\right],$$

derive Eq. (42) of the script.
3. Assuming an ohmic spectral function and using Eq. (49) of the script, show that the last term in the LHS of Eq. (42) becomes $\eta\dot{q}(t)$.
4. Use the equipartition theorem for an ohmic bath of harmonic oscillators to show that $< f(t) >= 0$ and $< f(t)f(t') >= 2\eta k_b T\delta(t-t')$.
5. Collect all the above results to show that the Caldeira-Leggett model reproduces the Langevin equation in the classical limit.
6. Show that the spectral function $J(\omega)$ defined in Eq. (45) of the script is nothing but the imaginary part of the Fourier transform of the (retarded) dynamical susceptibility of the oscillators bath in the classical limit,

$$J(\omega) = Im\mathcal{F}\left\{(i/\pi)\theta(t-t')\left\langle[c_k q_k(t), c_k q_k(t')]\right\rangle\right\}$$

7. The Caldeira-Leggett model describes the environment as a bath of harmonic oscillators. How good is this approximation, and when is it valid?