Lectures on theory of dissipative tunneling

Mark Dykman & Leonid Pryadko

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Chapter I Problem of escape

Lecture 1

Classical Brownian motion and escape problem.

Investigation of transport phenomena is a very important area of physics. Many quantities that are measured in experiment are immediately related to transport—whether this is conductivity, which is determined by electron transport in a conductor, or light absorption spectrum, etc. In a naive picture of transport there is something that moves and "carries" what is transported. For example, an electron is diffusing through a conductor and carries electric charge.It is implied in this picture that

- (i) a "carrier" is a good (quasi)particle, its lifetime is large compared to \hbar/E where E is its characteristic energy, and
- (ii) the scattering events ("collisions") happen occasionally: the duration of a collision $t_{\rm col} \ll \Gamma^{-1}$ where Γ scattering rate; therefore collisions occur successively in time and do not interfere.

Obviously, (i) and (ii) are interrelated with each other.

The physical problems are: What are "carriers" and "scatterers" in a particular system and how do the carriers move? For example, is it a nearly free motion with occasional scattering as described above, or incoherent jumps between localized states, with the duration of a jump small compared to the intervals between the jumps—again, a very *similar* picture, in a sense? Where and when does this picture apply? What happens if it does not—what are the most substantial corrections

to the kinetic-equation approximation? How can we calculate transport coefficients?

In the first part of the course we will be dealing with the transport of a particle which moves in a "regular" potential and is coupled to a thermal bath, and we will start with the simplest problem: how does a particle escape from a metastable state? We know that the escape is thermally activated for high temperatures and is due to quantum tunnelling for T = 0. But how does the transition from one regime to another occur?



Fig. 1.2.

Apart from the obvious difference between classical and quantum approaches the two



Fig. 1.1.

concepts of the escape are different in one more respect: thermal activation implies that there is a bath which, on one hand, provides relaxation towards the stable state, and, on the other hand, provides the particle with the energy sufficient to escape. In the quantum picture coupling to a bath is often ignored. But to get a complete picture we have to take it into account (and we apparently have to do that if we want to describe experiment).



Fig. 1.3.

The role of coupling to a bath is even more apparent if one thinks about resonant tunnelling. What is the correct language when we describe the states of a dust particle on a desk if there is a periodic array of the desks? Is the particle "smeared" over the desks, which is hard to believe? Why not? If we have zero temperature-will the particle be smeared

coherently, or could it be that the tunnelling matrix element between equivalent states is equal to zero?

The work on the classical theory of transport phenomena goes back to Einstein. Nearly 90 years ago he analyzed diffusion of particles in liquid and gave the theory of Brownian motion. Although this theory is studied at high school I shall remind it a little bit and use it in the analysis of the classical theory of escape; as we shall see that there is still something to think over.

1.1 Qualitative picture of escape from a metastable state

The problem of escape of a thermal equilibrium Brownian particle was considered by Kramers more than 50 years ago, and this work has a very special status: not enough classical to be noncited, but yet quite well-known to have more than 100 citations a year. The problem is immediately related to many physical systems, there is a huge number of experiments, including very recent ones, although initially it was formulated in chemistry as the problem of a chemical reaction rate. Let us first analyze it qualitatively.



Fig. 1.4.

If we have a particle which experiences friction and is moving in a potential it will go down to the potential minimum over the characteristic relaxation time $t_{\rm rel}$. This motion is simple: it is described by mechanical equations of motion, and we have a simple trajectory. On having arrived to the vicinity of the stable state the particle will perform small fluctuations about this state.

There will also occasionally occur large fluctuations, and one of these fluctuations will give rise to the escape. Obviously, if a system arrives to a given point away from the potential minimum as a result of a fluctuation it moves along a random path, this path is not described by simple mechanical equations of motion, and each path will be different from the others. However, the probability densities for the motion along different paths will be quite different (exponentially different, as we will see), and most likely all the paths will lie within a "narrow tube" around the most probable *optimal path*. The concept of the optimal path is the basic concept in the theory of large fluctuations—both of the classical fluctuations that we will be considering now and of quantum fluctuations that will be considered later. In a way, optimal paths of large fluctuations are complimentary to the classical dynamical trajectories in the absence of fluctuations.

1.2 Path-integral formulation of the theory of Brownian motion

To formulate the problem of the optimal path of a Brownian particle we shall go back to the initial Einstein's idea that a particle experiences collisions with the molecules of the surrounding liquid. Assume that a particle does not have a macroscopic velocity, let us evaluate the force f(t) acting on it (one component of the force). The collisions occur very frequently, at the instants $t_{col}^{(i)}$, with the momentum transfer p_i , therefore on the *coarse*grained time scale

$$f(t) = \frac{1}{\Delta t} \sum_{t < t_{\rm col}^{(i)} < t + \Delta t} p_i$$

We assume that there are *many* very weak collisions over Δt , each of them changing the position and the velocity of the particle only slightly.

Now we perform ensemble averaging (we have many Brownian particles), and, since all p_i are random and independent from each other, we get:

$$\langle f(t) \rangle = 0, \ \langle f^2(t) \rangle = \frac{2D}{\Delta t}, \ D = \frac{1}{2}\nu \langle p_i^2 \rangle$$
 (1.1)

where ν is the average frequency of the collisions. Obviously, the values of f(t) at the instants of time differing by more than Δt are uncorrelated. One more important thing to notice is that there is a simple interrelationship between the higher-order moments of f(t):

$$\langle f^{2n+1}(t) \rangle = 0, \ \langle f^{2n}(t) \rangle = \frac{(2n+1)!}{2^n n!} \left(\langle f^2(t) \rangle \right)^n$$
(1.2)

(notice the similarity with the proof of the Wick's theorem! We use very substantially that the number of collisions within Δt is large.) Eqs. (1.1), (1.2) tell that the probability distribution of f(t) is Gaussian on the discretized time scale,

$$p[f(t_1), f(t_2), \ldots] = \text{Const} \times \exp\left(-\frac{\Delta t}{4D}\sum_k f^2(t_k)\right), \ t_k - t_{k-1} = \Delta t$$

Now we take the limit $\Delta t \to 0$, and we get

$$\langle f(t) \rangle = 0, \ \langle f(t)f(t') \rangle = 2D\,\delta(t-t')$$
 (1.3)

Instead of the probability distribution of the discrete variables $f(t_k)$, now we will have a *probability density functional* that determines the probabilities of the various realizations of the *function* of a continuous variable t:

$$\mathcal{P}[f(t)] = \exp\left(-\frac{1}{4D}\int dt f^2(t)\right) \tag{1.4}$$

Averaging over various realizations of the force f(t) comes to the path integral over $\mathcal{D}f(t)$ with the weight $\mathcal{P}[f(t)]$. A very natural way to introduce path integrals! Notice that Eq. (1.3) follows from Eq. (1.4) immediately. A random process with the probability density functional (1.4) is called white Gaussian noise ("white" because its power spectrum is independent of frequency).

We are interested not in the evolution of the force but in the dynamics of the Brownian particle. This dynamics is described by the equation first suggested (in a more simple situation) by Langevin in 1908 and called Langevin equation:

$$\ddot{q} + 2\Gamma\dot{q} + U'(q) = f(t) \tag{1.5}$$

In writing Eq. (1.5) we have assumed simple viscous friction, 2Γ is the friction coefficient, and we have set the mass of the particle equal to 1. Of course, the form of the "regular" force that provides the dissipation and the form of the correlators of the random force f(t)are interrelated. Qualitatively, both forces result from coupling to the bath, and it is clear that when there is no memory, *i.e.*, the values of the random force in the successive instants of time are uncorrelated, the friction should be determined by the instantaneous value of the velocity as well. This can be also seen from the "microscopic" model of the force created by multiple collisions if one accounts for the velocity of a Brownian particle. More generally, the instantaneous form of the viscous friction assumed in Eq. (1.5), as well as its magnitude (1.7) found below, follow directly from the correlator (1.3) because of the fluctuation-dissipation theorem.

Here, we shall relate the characteristic noise intensity D and the friction coefficient Γ in a very simple way. Let us consider a motion in the absence of the potential, *i.e.* "free" Brownian motion, described by the equation

$$\dot{p} + 2\Gamma p = f(t), \quad p = \dot{q}. \tag{1.6}$$

The solution of this equation

$$p(t) = p_0 e^{-2\Gamma t} + \int_0^t e^{-2\Gamma(t-t')} f(t') dt'$$

and its averages obtained with Eq. (1.3)

$$\langle p(t) \rangle = p_0 e^{-2\Gamma t}, \qquad \langle p^2(t) \rangle = p_0^2 e^{-4\Gamma t} + \frac{D}{2\Gamma} \left(1 - e^{-4\Gamma t} \right)$$

imply that the initial momentum p(0) gets "forgotten", and for $t \gg \Gamma^{-1}$

$$\langle p(t) \rangle = 0, \quad \langle p^2(t) \rangle = D/2\Gamma$$

(see Prob. 1.2 at p. 17 for an alternative derivation). In thermal equilibrium the average squared momentum $\langle p^2 \rangle = T$, and we obtain

$$D = 2\Gamma T, \tag{1.7}$$

which is also the result of the fluctuation-dissipation theorem as applied to the present case.

From the formal point of view Eq. (1.5) is a *stochastic differential equation*: the righthand side of it is a random function (sometimes in mathematics the term "SDE" is used in a bit narrower sense). The solution is also a random function—as one would expect it to be. The probability density functional (1.4) gives not only the probability densities of various realizations of the time-dependent force, but also the probability densities of various paths taken by the system (this idea goes back to Feynman). It makes it simple to explain the idea of the optimal path in the case of the small noise intensity D.

1.3 Variational functional for the optimal path.

It is obvious that for small D the system mostly fluctuates in a narrow vicinity of its stable state. If the system arrives to a point away from this state, it has to have been driven by a *finite* force f(t) that overcame the potential force U'(q) and the friction. The probabilities of all appropriate realizations of f(t) are exponentially small, as seen from Eq. (1.4), and also they are exponentially different for various realizations. The most probable realization is the one which gives the minimum to the functional in the exponent provided the system arrives to a given point. Alternatively, one can say that the most probable (optimal) path is the one that minimizes the functional

$$\mathcal{R}[q,\dot{q}] = \int dt \left(\ddot{q} + 2\Gamma\dot{q} + U'(q)\right)^2.$$
(1.8)

The minimum should be taken with respect to the paths that arrive to a given point $(q, p \equiv \dot{q})$ at a given instant of time t. In stationary conditions this instant does not differ from any other instant of time. Therefore we can consider only the paths that start from the stable state $q_{\rm st}$ at $t \to -\infty$, so that the complete set of boundary conditions becomes

$$q(t) = q, \ p(t) = p, \ q(-\infty) = q_{\rm st}, \ p(-\infty) = 0.$$
 (1.9)

The above formulation of the theory of large classical fluctuations is sometimes called the instanton formulation. We shall see later why this term is appropriate, to some extent, and what is the difference with the "orthodoxal" instanton formulation. Using the boundary conditions (1.9), one can show (see Prob. 1.1 at p. 17) that the correct variational equation of motion for the paths that provide a minimum to the functional (1.8) is

$$\ddot{q} - 2\Gamma\dot{q} + U'(q) = 0,$$
 (1.10)

and the corresponding minimal value of the functional

$$R(q,p) = \min \mathcal{R} = 8\Gamma\left(\frac{1}{2}p^2 + U(q) - U(q_{\rm st})\right). \tag{1.11}$$

The probability density to arrive to a given point (q, p) is given by $\exp(-R(q, p)/4D)$, up to a prefactor—the expression looks familiar if you allow for Eq. (1.7)! But notice that we have not only recovered the known result, but also have found the *way* along which the system moves to a given remote point.

Of course, the real value of this formulation is determined by the fact that it makes it possible to analyze fluctuations in systems away from thermal equilibrium. Beware: there are pitfalls! It's not at all that simple to find the optimal paths in this case—there is no this special time-reversal symmetry inherent to the problem we have been considering. And, of course, the probability density is not given by the Gibbs distribution.

1.4 The Fokker-Planck equation

A different approach to the description of the random motion of the Brownian particle (1.5) is based on the equation for its transition probability density. It is seen from Eq. (1.4) that the probability of realization of the force f(t) within a given time interval (t_1, t_2) is *independent* of the values f(t) has had away from this interval. Therefore if we know the values of q, p at $t = t_1$ we can find the probability density distribution $w(q, p; t_2)$ for $t_2 \ge t_1$, and this distribution will be *independent* of the values of q(t), p(t) for $t < t_1$. This property is called Markovian, and random processes that have it are called Markov processes (I will not be strictly rigorous from the mathematical point of view, sorry). Markov processes play crucial role both in classical and in quantum theory of transport phenomena: we shall see that quantum/classical kinetic equations hold when the corresponding processes are Markovian. The important feature (noticed by Einstein) is that they should be Markovian on the *coarsened* time scale, *i.e.*, for "slow" time. And all averaging we have done so far and we will be doing in the future should be performed prior to the coarsening: the order of the transitions is important (there is a well-known Ito vs. Stratonovich controversy on this issue).

We shall consider the equation for the transition probability density $w(q, p; t|q_0, p_0; t_0)$, *i.e.* the probability density for a particle placed at q_0, p_0 at the initial instant t_0 to be at q, pat the instant t: this quantity describes everything we need. Define

$$w(q, p; t) = \langle \delta(q - q(t)) \,\delta(p - p(t)) \rangle, \tag{1.12}$$

where q(t), p(t) are given by Eq. (1.5) and the condition $\dot{q}(t) = p(t)$. Then

$$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial q}(pw) - \frac{\partial}{\partial p}\left\langle \left[-2\Gamma p - U'(q) + f(t)\right] \,\delta(q - q(t))\,\delta(p - p(t))\right\rangle \tag{1.13}$$

It is straightforward to average the first two terms in the angular braket. To perform averaging in the last term we notice that

$$p(t) = p(t - \delta t) + \int_{t - \delta t}^{t} dt [-2\Gamma p - U'(q) + f(t)]$$
(1.14)

If we assume δt here is small, expand the last delta-function in Eq. (1.13) in the integral from $t - \delta t$ to t and allow for Eq. (1.3), we will arrive at

$$\frac{\partial w}{\partial t} = -\frac{\partial pw}{\partial q} - \frac{\partial \left[-2\Gamma p - U'(q)\right]w}{\partial p} + D\frac{\partial^2 w}{\partial p^2}$$
(1.15)

The last equation (and equations of a similar sort) are usually called Fokker-Planck equation. For the first time such equation was written by Einstein in the so-called overdamped case (when one can neglect inertia and drop the term \ddot{q} in Eq. (1.5); see Prob. 1.3 at p. 17). The form (1.15) was suggested by Klein and Kramers. Notice that Eq. (1.15) is in a way a continuity equation (it is also sometimes called Boltzmann equation, or vice versa, Boltzmann equation is called Fokker-Planck equation): if we think of w as a density of a system in the phase space, then the "current density" along the q-axis is equal to pw, and that along the p-axis is equal to $(-2\Gamma p - U')w - D\partial w/\partial p$; the last term is the diffusion current.

1.5 Kramers' solution of the escape problem

Independently of the way it was initially prepared, a system in a confining potential should eventually reach the thermal equilibrium, characterized by the familiar Gibbs distribution

$$w_{\rm st}(q, p) = Z^{-1} \exp\left(-\frac{E(q, p)}{T}\right),$$

$$E(q, p) = \frac{p^2}{2} + U(q),$$

$$Z = \int dq \, dp \, \exp(-E(q, p)/T),$$
(1.16)

One can easily see that this indeed is a stationary solution of Eq. (1.15), provided the fluctuation-dissipation theorem is satisfied, *i.e.* $T \equiv D/2\Gamma$. However, this solution is apparently inapplicable to the case of a potential well from which the system can escape to infinity. The solution for this case was suggested by Kramers.

The basic idea is that if the noise intensity is small enough, $T \ll \Delta U$, there is a strong hierarchy of times. A system placed initially inside the potential well will thermalize over the time $\sim \Gamma^{-1}$, and far inside the well the form of the distribution will be close to Eq. (1.16) (with Z being a certain constant). This distribution will be gradually decreasing in intensity because of the flux away from the well. The characteristic time over which it will change is determined by the escape probability $W \propto \exp(-\Delta U/T) \ll \Gamma$. Therefore within the time interval

$$\Gamma^{-1} \ll t \ll W^{-1}$$



Fig. 1.5.

both the intrawell distribution and the flux

$$j = \int dp \, p \, w(q, p; t) \tag{1.17}$$

are stationary (obviously, the solution (1.16) gives j = 0). The flux should be small, and far inside the well it can be neglected. However, it may become substantial near the barrier

top (q = 0) where the distribution (1.16) is exponentially small. We need to find another stationary solution of Eq. (1.15) other than Eq. (1.16), which describes such a flow near the barrier top, asymptotically approaches the equilibrium solution in the well, and at the same time disappears outside the barrier. We can simplify these requirements by factorising the desired time-independent solution of Eq. (1.15) into a product

$$w_1(p,q) = C(p,q) e^{-E(p,q)/T}$$

where C(p,q) is another unknown function which tends to a constant value as we move into the well and to zero outside the well. The function C satisfies the following equation

$$p \frac{\partial C}{\partial q} + (2\Gamma p - U'(q)) \frac{\partial C}{\partial p} - D \frac{\partial^2 C}{\partial p^2} = 0, \qquad (1.18)$$

which is still too hard to solve in general (but for the overdamped case, see Prob. 1.3 at p. 3). However, if the special case of the barrier parabolic near the top, $U(q) \approx U(0) - \frac{1}{2}\Omega^2 q^2$, there exists a solution that depends on the linear combination $\xi = q - \lambda p$ of the coordinate q and the momentum p, $C(p,q) = f(\xi)$, where λ is so far an unknown constant which must be chosen to render Eq. (1.18) an ordinary differential equation. After this substitution Eq. (1.18) becomes

$$[(1 - 2\Gamma\lambda)p - \Omega^2\lambda q]f' - D\lambda^2 f'' = 0, \qquad (1.19)$$

where the expression in square brackets must depend only on the combination $\xi = q - \lambda p$. Therefore $1 - 2\lambda\Gamma = \Omega^2\lambda^2$, which gives $\lambda_{\pm}\Omega^2 = -\Gamma \pm (\Gamma^2 + \Omega^2)^{1/2}$, and the solution of the reduced FPE can be written as

$$f_{\pm}(\xi) = \text{Const}_1 \int \exp{-\frac{\Omega^2 \xi^2}{2\lambda_{\pm} D}} d\xi + \text{Const}_2.$$

Only the function f_+ with positive value $\lambda \equiv \lambda_+$ can satisfy the boundary condition at infinity, and the solution of the original Fokker-Planck equation (1.15) can be finally written as

$$w_1(q,p) = \operatorname{Const} \exp\left(-\frac{p^2 - \Omega^2 q^2}{2T}\right) \int_{q-\lambda p}^{\infty} d\xi \, \exp\left(-\frac{\Omega^2 \xi^2}{4\lambda \Gamma T}\right).$$
(1.20)

This solution satisfies the physical boundary conditions that the distribution should vanish for $q \to \infty$ and that it should take on the form (1.16) for q approaching the interior of the well, *i.e.* in the range $\lambda p - q \gg \sqrt{\lambda \Gamma T}/\Omega$. By evaluating the flux (1.17) (*e.g.*, for q = 0—it does not depend on q near the barrier top), one arrives at the expression for the escape probability:

$$W = \frac{1}{2\pi} [\lambda \,\omega_0 \,\Omega] \exp\left(-\Delta U/T\right), \qquad \text{where} \quad \omega_0^2 = U''(q_{\text{st}}). \tag{1.21}$$

Eq. (1.21) gives both the exponent and the prefactor of the escape probability of the classical Brownian particle, in the broad range of parameters. The situation, however, becomes much more complicated when quantum effects come into play!

¹Clearly, the existence of such substitution is related to the fact that the variational equation (1.10) of motion for the escaping trajectory becomes linear in quadratic potential; the same values of λ can be obtained by looking for the solutions in the form $q(t) = \exp t/\lambda$.

1.A Dissipation by phonons

We discussed some implications of the "real" Brownian motion of a particle due to multiple collitions with other particles that constitute the thermal bath. Because the particle experiences so many collisions during any reasonably short time interval, the resulting force is delta-correlated at the coarsened time scale, while the friction has a simple form without any memory, or retardation effects. The derived equations of dissipative dynamics are very general and apply to many systems. In part to illustrate the generality of these equations, and in part to introduce an easy to quantize implementation of the Brownian dynamics, we will consider two "truly" microscopic models of Brownian motion. Both correspond to the linear coupling of a system to a "bosonic bath", with the Hamiltonian of the form

$$H = H_0 + H_b + H_i, \qquad (1.22)$$
$$H_0 = \frac{1}{2}p^2 + U(q), \quad H_b = \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right), \quad H_i = \sum_{\mu} \left(f_{\mu} q \, q_{\mu} + \frac{1}{2}(f_{\mu}/\omega_{\mu})^2 q^2\right),$$

where q, p are the coordinate and momentum of the system, whereas q_{μ} , p_{μ} are the coordinates and momenta of the eigenmodes of the bath. Notice that the coordinate-dependent terms in H_b and H_i can be written as $(1/2) \sum_{\mu} \left[(f_{\mu}/\omega_{\mu}) q + \omega_{\mu}q_{\mu} \right]^2$ which makes the structure of the expression better understandable; one may also say that the last term in H_i allows for (a part of) the polaron effect of the renormalization of the spectrum of a particle.

The equations of motion corresponding to the Hamiltonian (1.22) are of the form

$$\ddot{q} + U'(q) = -\sum_{\mu} f_{\mu} q_{\mu} - \sum_{\mu} (f_{\mu}/\omega_{\mu})^2 q, \qquad (1.23)$$

$$\ddot{q}_{\mu} + \omega_{\mu}^2 q_{\mu} = -f_{\mu} q.$$
 (1.24)

Let us assume that we know the initial (t=0) conditions q(0), p(0), $q_{\mu}(0) \equiv A_{\mu} \cos \phi_{\mu}$, $p_{\mu}(0) \equiv -A_{\mu}\omega_{\mu} \sin \phi_{\mu}$ for both the system and the thermal bath, where A_{μ}, ϕ_{μ} are the amplitudes and the initial phases of the vibrations of the bath. Then, for a given trajectory q(t) of the system, we can find the motion of the bath by solving the linear equations (1.24), and plug the solutions

$$q_{\mu}(t) = A_{\mu} \cos(\omega_{\mu} t + \phi_{\mu}) - \frac{f_{\mu}}{\omega_{\mu}} \int_{0}^{t} \sin \omega_{\mu}(t - \tau) q(\tau) d\tau$$

back into Eq. (1.23). As a result, we obtain the independent equation of motion for the system which self-consistently accounts for the dynamical response of the bath,

$$\ddot{q}(t) + U'(q) = L[q(t)] + f(t), \qquad f(t) = -\sum_{\mu} f_{\mu} A_{\mu} \cos(\omega_{\mu} t + \phi_{\mu})$$
(1.25)

$$L[q(t)] = \frac{2}{\pi} \int_0^\infty d\omega F(\omega) \int_0^t d\tau \sin(\omega\tau) q(t-\tau) - q(t) \frac{2}{\pi} \int \frac{d\omega}{\omega} F(\omega). \quad (1.26)$$

Here the function

$$F(\omega) = \frac{\pi}{2} \sum_{\mu} (f_{\mu}^2 / \omega_{\mu}) \,\delta(\omega - \omega_{\mu}) \tag{1.27}$$

has the meaning of the density of states of the bath weighted with the coupling constants. Obviously, the frequency integration interval should be wide enough to include the frequencies ω_{μ} of all oscillators included in the bath Hamiltonian H_b .

Apparently, Eq. (1.25) does not have a form of the equation of motion for Brownian particle: we have a *retarded* self-action mediated by the bath, and, generally, the force f(t)is not δ -correlated. Therefore, we need to figure out whether this equation *can* describe the "unretarded" Brownian motion in principle, with the appropriate choice for the coupling function $F(\omega)$, and also whether this choice can be justified physically, at least for some systems. Eventually, we shall answer both questions positively. Here, we shall answer the first question by considering the special form (1.28) of the coupling function $F(\omega)$. As we shall see later, this choice, the so called "Ohmic dissipation" case, is physically reasonable for describing the system coupled to a *fermionic* bath. In the next section, we shall show that the non-retarded Langevin equation also arises naturally for a harmonic (or weakly anharmonic) oscillator, with nearly parabolic potential U(q).

Let us consider Eq. (1.25) in the special case of "Ohmic dissipation", with the function $F(\omega)$ of the form

$$F(\omega) = 2\Gamma\,\omega\exp(-\epsilon\,\omega),\tag{1.28}$$

where ϵ is a cutoff parameter, which defines the fast time in the system, similar to the duration of a collision with a molecule for a Brownian particle. Now the frequency integration in Eq. (1.25) can be done explicitly, with the result

$$\frac{2}{\pi} \int_0^\infty F(\omega) \sin(\omega\tau) \, d\omega = -\frac{1}{\pi} \frac{d}{d\tau} \frac{4\Gamma\epsilon}{\epsilon^2 + \tau^2}, \quad \frac{2}{\pi} \int_0^\infty \frac{d\omega}{\omega} F(\omega) = \frac{4\Gamma}{\pi\epsilon}.$$

After performing the integration by parts in the first term of Eq. (1.25),

$$L[q(t)] = -\frac{4\Gamma q(t)}{\pi\epsilon} - \frac{4\Gamma}{\pi\epsilon} \left. \frac{q(t-\tau)\epsilon}{\tau^2 + \epsilon^2} \right|_0^t - \frac{4\Gamma}{\pi\epsilon} \int_0^t \frac{d\tau \dot{q}(t-\tau)\epsilon}{\tau^2 + \epsilon^2},$$

in the limit $\epsilon \ll t$, and assuming q(t) varies slowly on the time scale ϵ , we finally obtain

$$L[q] = -2\Gamma \dot{q}(t) \tag{1.29}$$

(to be consistent, we have to put sign t as a coefficient in the last equation; in what follows we assume t > 0). So, we do arrive at the right form of the friction force!

To analyze the form of the random force f(t) in Eq. (1.25), we assume that at the instant t = 0 the amplitudes A_{μ} and the phases ϕ_{μ} were random and corresponded to thermal equilibrium of the bath, *i.e.*, we assume that the phases ϕ_{μ} are uniformly distributed over the interval $[0, 2\pi]$ and

$$\langle A_{\mu}^2 \rangle = 2T/\omega_{\mu}^2$$

Because each of the coupling constants f_{μ} is very small, for the specific form (1.28) of the coupling function $F(\omega)$ one can show that the force f(t) is a Gaussian random process, and

$$\langle f(t) \rangle = 0, \qquad \langle f(t)f(t') \rangle = T \sum_{\mu} (f_{\mu}^2/\omega_{\mu}^2) \cos[\omega_{\mu}(t-t')] \to 4\Gamma T \delta(t-t').$$
(1.30)

Certainly, this result is not very surprising: it was expected from the fluctuation-dissipation theorem and the fact that the friction term (1.29) is unretarded.

Eq. (1.25) with the friction term L[q] given by Eq. (1.29) and the Gaussian δ -correlated random force (1.30) is exactly the Langevin equation for Brownian motion we had before. We have, therefore, managed to show that Brownian motion can, at least in principle, arise because of the coupling to the bath of harmonic oscillators.

1.B Kinetics of a harmonic oscillator coupled to a bath

The equations of motion of a classical system coupled to a bath may also be effectively unretarded in the case of a quite general form of the coupling function $F(\omega)$ (unlike the special form (1.28)), provided the dynamical system itself has a "fast" time, while the coupling is weak. In this case the effect of the bath must accumulate over many periods of nearly-coherent motion of the system. As we shall see, this results in the absence of the retardation on the coarsened (slow) time scale, even though the "real" dynamics of the system is retarded (non-Markovian).



Fig. 1.6.

Consider a harmonic oscillator coupled to a bath, described by the Hamiltonian (1.22) with the potential

$$U(q) = \frac{1}{2}\omega_0^2 q^2.$$
(1.31)

In the absence of the bath, the harmonic motion of this oscillator will have a well-defined amplitude and phase. The weak coupling to the thermal bath would create a slow modulation of the harmonic motion. In order to describe this modulation, let us perform the canonical transformation to the "rotating" frame,

$$q(t) = (2\omega_0)^{-1/2} \left[u(t)e^{-i\omega_0 t} + u^*(t)e^{i\omega_0 t} \right], \qquad (1.32)$$

$$p(t) \equiv \dot{q}(t) = -i(\omega_0/2)^{1/2} \left[u(t)e^{-i\omega_0 t} - u^*(t)e^{i\omega_0 t} \right].$$
(1.33)

The introduced complex amplitudes u(t), $u^*(t)$ are not independent; in order for Eq. (1.33) to be consistent, these coordinates must be related by the expression

$$\dot{u}(t)e^{-i\omega_0 t} + \dot{u}^*(t)e^{i\omega_0 t} = 0.$$
(1.34)

Because of this constraint, the acceleration term in the equation of motion (1.25) is expressed in terms of *first* derivatives only, and the result combined with Eq. (1.34) can be trivially reduced to the following set of two first-order differential equations for u(t), $u^*(t)$:

$$\dot{u}(t) = i(2\omega_0)^{-1/2} e^{i\omega_0 t} \left[L[q] + f(t) \right], \quad \dot{u}^*(t) = -i(2\omega_0)^{-1/2} e^{-i\omega_0 t} \left[L[q] + f(t) \right]$$
(1.35)

If the coupling to the bath is weak enough, these amplitudes will remain nearly a constant for the time $\sim \omega_0^{-1}$. Therefore, (the validity of this approximation will be checked later) we can replace $q(t-\tau)$ in the integral operator L[q] in Eq. (1.35) by the first term of expansion

$$q(t-\tau) = (2\omega_0)^{-1/2} e^{-i\omega_0(t-\tau)} \left(u(t) + \sum_{n=1}^{\infty} (-\tau)^n \frac{d^n}{dt^n} u(t) \right) + \text{c.c.},$$
(1.36)

and obtain,

$$i(2\omega_0)^{-1/2} e^{i\omega_0 t} L[q(t)] \approx \frac{iu(t)}{\pi\omega_0} \int d\omega F(\omega) \left[\int_0^t \sin(\omega\tau) e^{i\omega_0\tau} d\tau - \frac{1}{\omega} \right]$$
$$= \frac{iu(t)}{\pi\omega_0} \int d\omega F(\omega) \left[\frac{1 - e^{i(\omega+\omega_0)t}}{2(\omega+\omega_0)} + \frac{1 - e^{i(\omega_0-\omega)t}}{2(\omega-\omega_0)} - \frac{1}{\omega} \right]$$

Assuming the function $F(\omega)$ is smooth in a vicinity of the point $\omega = \omega_0$, we can use the following *asymptotic* expressions to evaluate the integral over ω :

$$\frac{\sin[(\omega - \omega_0)t]}{\omega - \omega_0} \to \pi \delta(\omega - \omega_0), \quad \frac{1 - \cos[(\omega \pm \omega_0)t]}{\omega \pm \omega_0} \to \text{v.p.} \ (\omega \pm \omega_0)^{-1},$$

where v.p. means that the principal value of the corresponding integral over ω should be taken). Then, keeping only the first term in the expansion of $q(t - \tau)$, and ignoring the non-resonant terms depending on the sum of the frequencies, we get the equation describing the slow dynamics of the system

$$\dot{u}(t) = -\Gamma u(t) - iP u(t) + i(2\omega_0)^{-1/2} e^{i\omega_0 t} f(t), \qquad (1.37)$$

where

$$\Gamma = F(\omega_0)/2\omega_0, \quad P = \frac{\omega_0}{\pi} \text{ v.p.} \int d\omega F(\omega) \left[\omega(\omega_0^2 - \omega^2)\right]^{-1}.$$
 (1.38)

Eq. (1.37) implies that the function u(t) varies very slowly, over the characteristic time

$$\Gamma^{-1}, |P|^{-1} \gg \omega_0^{-1}.$$

Using this inequality, we can check the self-consistency of our approximation, *i.e.* that the higher-order terms $\sim \tau^n d^n u/dt^n$ omitted in L[q] are small. The contribution due to these terms can be estimated by replacing τ^n under the integral by the *n*-th derivative over ω_0 , with the result $[d^n\Gamma/d^n\omega_0] d^n u/dt^n$, $[d^n P/d^n\omega_0] d^n u/dt^n$, which, indeed, is negligible for smooth enough responce function $F(\omega)$.

It can be shown (see Prob. 1.9 at p. 18) that on the time scale coarsened over the interval of the order of ω_0^{-1} (and over the characteristic width ω_c of the function $F(\omega)$) the forces $f(t) \cos(\omega_0 t)$ and $f(t) \sin(\omega_0 t)$ are asymptotically independent and δ -correlated. The final form of the equations for the slowly varying complex amplitudes of the oscillator is of the form:

$$\dot{u} = -\Gamma u - iP u + \tilde{f}(t), \quad \dot{u}^* = -\Gamma u^* + iP u^* + \tilde{f}^*(t)$$

$$\langle \tilde{f}(t) \rangle = 0, \quad \langle \tilde{f}(t)\tilde{f}(t') \rangle = 0, \quad \langle \tilde{f}(t)\tilde{f}^*(t') \rangle = [2\Gamma T/\omega_0] \,\delta(t - t').$$

$$(1.39)$$

Once again, the δ -function here is defined for the coarsened (slow) time; it should be understood that it has a peak of the width $\sim \max[\omega_0^{-1}, \omega_c^{-1}]$.

Problems

▶ **Problem 1.1** (page 83)

Find the optimal path for a fluctuating Brownian particle that minimizes the functional



$$\begin{split} \mathcal{R} &= \int \, dt (\ddot{q} + 2\Gamma \dot{q} + U'(q))^2 \\ q(t) &= q, \ \ \dot{q}(t) = p, \ \ q(-\infty) = q_{\rm st}, \ \ \dot{q}(-\infty) = 0, \end{split}$$

where q_{st} is the position of the minimum of the potential U(q) (in fact, the solution here means a second-order differential equation for q(t)). Find the corresponding value of the functional as a function of q, p. Explain why the equation for the optimal path takes the particular form you will have found: think about minimal work that a thermal bath has to do to bring the system to a particular

state.

▶ **Problem 1.2** (page 85)

Rederive the expression (1.7) in the presence of an arbitrary potential U(q). You may find it helpful to prove the formula $\langle p(t)f(t)\rangle = D$ first.

▶ **Problem 1.3** (page 85)

Brownian motion of an overdamped particle is described by the Langevin equation

$$\dot{Q} + U'(Q) = f(t), \quad \langle f(t) \rangle = 0, \quad \langle f(t)f(t') \rangle = 2D\delta(t - t')$$

The corresponding Fokker-Planck equation (FPE) is of the form

$$\frac{\partial w}{\partial t} = \frac{\partial [U'(Q)w]}{\partial Q} + D \frac{\partial^2 w}{\partial Q^2}$$

where $w \equiv w(Q, t)$ is the probability density. This FPE can be transformed to a Schrödingerlike equation for the function

$$\phi(Q,t) = e^{U(Q)/2D} w(Q,t).$$

The lowest eigenvalue of the corresponding equation is identically zero (why?), and the corresponding eigenfunction is $C \exp(-U(Q)/2D)$.

Find the lowest nonzero eigenvalue and the corresponding eigenfunction for the double-well potential U(Q) as shown in Fig. 1.8 in the limit of small D. Notice that the potential in the Schrödinger-like equation will have three wells in this case; be careful if you decide to apply the





known results of quantum mechanics for level splitting in the two-well potential.

▶ **Problem 1.4** (page 86)

Find the optimal fluctuational path for the overdamped Brownian motion.

▶ **Problem 1.5** (page 87)

When deriving the optimal path functional (1.8) from Eqs. (1.5), (1.7), we changed the pathintegration variables from f(t) to q(t), but ignored the corresponding Jacobian. Explain why this was an adequate approximation. Find the path integral description of an *overdamped* particle in the external potential U(q) in terms of the particle's coordinate q(t).

▶ **Problem 1.6** (page 88)

In the course of escape from a potential well a Brownian particle goes back and forth over the top of the barrier. Find the ratio of the ingoing and outgoing flows.

▶ **Problem 1.7** (page 88)

Consider the quantum problem of decay and find the lifetime of a metastable state in the potential well shown at page 11. Assume that the wave function is semiclassical both outside and well inside the barrier U(q), and that the potential is parabolic near its minimum.

▶ **Problem 1.8** (page 90)

For a classical system coupled to a bath of harmonic oscillators described by an arbitrary coupling function $F(\omega)$, derive the relationship between the correlator of the random force $\langle f(t) f(t') \rangle$ and the retarded dissipation rate $\kappa(t)$, defined by the equation

$$L[q(t)] = -2 \int_{-\infty}^{t} \kappa(t - t') \,\dot{q}(t') \,dt'.$$

▶ **Problem 1.9** (page 91)

Derive quantum Langevin equation for a harmonic oscillator linearly coupled to a phonon bath. Use the operators

$$a = (\omega_0/2)^{1/2}q + i(2\omega_0)^{-1/2}p, \quad a^+ = (\omega_0/2)^{1/2}q - i(2\omega_0)^{-1/2}p.$$

Assume the coupling to be weak. Evaluate, on the coarsened time scale, the evolution of the average values $\langle a^n(t) (a^+)^m(t) \rangle$.

▶ **Problem 1.10** (page 92)

Find the power spectrum of voltage fluctuations on a resistor R (for comparatively low frequencies, in particular for $\hbar\omega \ll T$). Consider a resistor in a circuit that consists of a capacitor C, a solenoid with an inductance L, and the resistor itself, held at temperature T, and use standard expressions for the energies stored in a capacitor and in a solenoid.

Lecture 2

Quantum escape problem.

2.1 The Crossover from Classical to Quantum Escape.

Classical formulation of the problem of escape from a metastable state is based substantially on the fact that relaxation is sufficiently fast—much faster than the escape rate. Otherwise, there would be no such thing as the rate of escape from a metastable state, and the outgoing current would depend on the initial preparation of the system.

Quite differently, the "standard" quantum formulation is based on the notion of the escape from a given quantum state. In quasiclassical approximation a particle escapes from the level n with the probability

$$W(E_n) = \frac{\omega(E_n)}{2\pi} \exp\left(-2S\left(E_n\right)\right), \quad (2.1)$$



where the tunneling action

$$S(E) = \int_{q_1}^{q_2} dq \, \left[2m(U(q) - E)\right]^{1/2}, \qquad (2.2)$$

 $q_{1,2}$ are the turning points, and we set the Planck constant $\hbar = 1$. The preexponential factor tells how often the particle "hits" the potential wall, and S is the "action" for the motion under the barrier.

If the system is coupled to a bath then, strictly speaking, its energy spectrum becomes continuous, and the Gibbs distribution over the energy levels is formed. We shall ignore the continuity of the spectrum for a moment and consider only the consequences of the equilibrium thermal energy distribution. At finite temperatures the system occupies not only the lowest energy level, but also the excited ones, and it may have energies higher than the barrier height, too. Therefore, there always exists a possibility of a purely activation escape over the barrier. If this is not the dominating mechanism, however, we may write the total escape rate as the sum of the tunneling rates for different levels weighted with the populations of the levels,

$$W = Z^{-1} \sum_{n} W(E_n) \exp(-E_n/T), \quad Z = \text{Tr} \exp(-H/T),$$
 (2.3)

where H is the Hamiltonian of the system. If the temperature is high enough (but not too high), the energy levels from which the system is most likely to escape may be (and often are) close to each other. Then, using the fact that in quasiclassics $\Delta E_n = E_{n+1} - E_n \approx \omega(E)$, the sum in Eq. (2.3) may be replaced by the integral

$$W = Z^{-1} \int \frac{dE}{\omega(E)} W(E) \exp(-E/T) = Z^{-1} \int dE \exp(-2S(E) - E/T).$$
(2.4)

As usual in the problem of escape, the integrand is such a rapidly changing function of energy that only a close vicinity of its maximum will dominate the value of the whole expression. This means that we can evaluate the integral over E by the method of steepest descent,

$$W \approx Z^{-1} \left[4\pi \left(\partial^2 S / \partial E^2 \right) \right]^{-1/2} \exp(-R), \qquad (2.5)$$

where both the prefactor and the exponent

$$R = 2S(E) + \frac{E}{T}, \qquad 2\frac{\partial S}{\partial E} = -\frac{1}{T}, \qquad (2.6)$$

The derived equation for this "optimal"

energy has a very simple meaning if we no-

tice that the action S(E) corresponds to that for a classical motion in the inverted

potential -U(q). It is known from classical mechanics that the period of the motion is equal to $\tau_p = 2|\partial S/\partial E|$, *i.e.*, the transitions occur, most likely, from the energy

levels for which the period of the oscilla-

tions in the inverted potential is equal to

Ε

the reciprocal temperature.

must be calculated at the same energy, given by the second expression above.



Fig. 2.2. The energy derivative of the tunneling action (2.2) is proportional to the period of oscillations in the "inverted" potential.

For a generic form of the inverted potential, the period of oscillations is limited from below, and Eq. (2.6) does not have a solution for arbitrarily large temperatures T. Often the energy dependence of the period of oscillations in the inverted potential $\tau_p(E)$ is monotonic, as illustrated in Fig. 2.3, and in this case the smallest period is determined by the curvature



of the potential near the top of the barrier, and, consequently, the solution of Eq. (2.6) will disappear at temperatures larger than

$$T_0 = \Omega/2\pi. \tag{2.7}$$

Thus defined characteristic temperature T_0 is the crossover temperature: the escape rate is determined by the quantum tunnelling on one side of T_0 , whereas on the other side of T_0

escape is thermally activated (note, however, that there are important quantum corrections to the prefactor, for not too high temperatures).

The derived escape rate (2.5) fails near the crossover temperature T_0 since the steepest descent method does not apply here. More careful estimate above the transition, $T > T_0$ gives $R \approx \Delta U/T$ (where ΔU is the total barrier height), and for $T < T_0$, assuming the barrier nearly parabolic and the period $\tau_p(E)$ nearly linear in E near the barrier top,

$$R \approx \Delta U/T - \left| 2\tau_p' \right|^{-1} \left(T^{-1} - T_0^{-1} \right)^2.$$

Clearly, in this range of temperatures the quantum correction decreases the tunneling exponent R, and thus alleviates the escape, as one would naïvely expect.

Unfortunately, the argument works only in a rather narrow range of the relaxation rates. The dissipation must be not too small so that the quantized energy levels near the barrier top would not be depleted because of the escape, and not too large so that the energy levels remain well-defined and the quantum-mechanical expression for the tunneling rate is applicable.

2.2 Escape Probability and Partition Function

Strictly speaking, if a particle is capable of tunneling out of the potential well, it must have a continuous energy spectrum. The discrete energy levels associated with the original closed well are transformed into poles of the scattering amplitude analytically continued to complex values of energy. If the escape rate is small enough, these singularities are very close to the real axis, and they can be observed in various spectra as sharp absorption or emission peaks. If the properties of the system are dominated by such peaks, we can ignore the fact that the spectrum is continuous, and describe the system in terms of eigenstates of complex energy.

In order to benefit from such a description, we need to reformulate the escape problem as a non-Hermitian one. This can be done by imposing the boundary conditions of unidirectional flow far enough outside the well. Such conditions agree with our intuitive understanding of escape as the motion away to infinity with no chance of scattering back. Now, it is easy to relate the escape rate, or the rate of the reduction of the population of the state inside the well with the imaginary part of



Fig. 2.4. The integration in Eq. (2.8) is performed over the shaded region.

the corresponding energy. This relation can be obtained by multiplying the equations

$$H\psi = E\psi, \quad H\psi^* = E^*\psi^*,$$

where

$$H = -\frac{1}{2m}\nabla^2 + U(q),$$

by ψ^* and ψ , respectively, and integrating the difference over the interval including the well and, partly, the area outside the barrier, as illustrated in Fig. 2.4,

$$-2\operatorname{Im} E \int_{-\infty}^{q_0} |\psi|^2 \, dq = \frac{1}{2i\,m} \left(\psi^* \frac{\partial\psi}{\partial q} - \frac{\partial\psi^*}{\partial q} \,\psi \right). \tag{2.8}$$

Since the wave function is mostly concentrated inside the integration interval, the integral gives the population of the well, while the r.h.s. of the obtained expression is exactly the outgoing current j. Defining the escape rate as the ratio of the current to the population of the well,

$$W = j \left[\int dq \, |\psi|^2 \right]^{-1},$$

$$W(E_n) = -2 \operatorname{Im} E_n.$$
(2.9)

we obtain

For a multi-level many-dimensional system the expression for the overall probability of escape may be obtained by averaging the obtained equation over the states of the system. Assuming that the imaginary parts of the energies are small, we get

$$W = 2T \operatorname{Im} \sum_{n} Z^{-1} \exp(-E_n/T) = 2T \operatorname{Im} \ln Z = -2 \operatorname{Im} F.$$
 (2.10)

It is not surprising that the partition function and the free energy are complex, since we are analyzing the problem where a particle can escape to infinity. Another question is how good and how general the obtained expressions are. First, we assumed that Im E is small for all energies, which is certainly not true for the states close or above the barrier top, and one would expect that Eq. (2.10) should be modified when such energies become substantial. For not too small damping the modification becomes important in the range $T > T_0$ [T_0 defined by Eq. (2.7) is the crossover temperature], but it comes just to an extra prefactor. This prefactor can be found by accounts for the overbarrier reflection, which changes the expression for the escape probability (*cf.* the discussion above), and also for the modification of the expression for the partition function. The limit of very small dissipation rate, although mathematically rather involved, can be easily understood on the physical grounds: the tunneling rate is governed by the depletion of the area close, or even not very close to the barrier top and, respectively, by the difference between the real and the equilibrium Gibbs distributions used in Eq. (2.10).

Generally, the matter is delicate when the particle is coupled to a bath, since in this case we have an infinite number of degrees of freedom, and all time scales are present; the very fact that the particle is away from the well does not mean that it will not be drawn back as a result of relaxation of the bath. From a formal point of view, these problems arise because the current is determined by a two-particle Green's function, whereas the partition function is determined by the one-particle Green's function, and, in general, a two-particle Green's function is not expressed in terms of the one-particle one. Clearly, the approach does not apply to the case of nonequilibrium systems like optically bistable systems, or electrons in a Penning trap excited by a cyclotron radiation, or bistable chemical and biochemical systems with in- and outgoing flows, *etc*. However, in many cases of physical interest Eq. (2.10) (or its modification for $T > T_0$) does apply to systems coupled to a thermal bath, and enables us to answer a few important physical questions including the following:

- (i) Does the dissipation increase or decrease the tunnelling probability? What is the effect of small dissipation?
- (ii) How does escape occur in the case of a heavily damped (overdamped) motion?

In order to answer these questions, it is convenient to analyze Eq. (2.10) in the path integral representation.

2.3 Path Integral Formulation

The path integral formulation of quantum mechanics is based on the fact that the amplitude $K(q_f, t; q_i; t_0)$ of the transition from a point q_i occupied at the instant t_0 to the final point q_f over the time interval $t_f - t_i > 0$, is given by the path integral of the exponent of the classical action,

$$\psi(q_f, t_f) = \int dq_i \, K(q_f, t_f; q_i; t_0) \, \psi(q_i, t_0), \quad K(q_f, t_f; q_i; t_0) = \int \mathcal{D}q(t) \, \exp(iS[q(t)]),$$

where

$$S[q(t)] = \int_{t_0}^{t_f} dt \, L(\dot{q}, q),$$

and $L(\dot{q}, q)$ is the *classical* Lagrangian of the system, which we will assume to be timeindependent. For a particle with the mass m = 1 moving in a potential U(q),

$$L(\dot{q},q) = \frac{1}{2} \, \dot{q}^2 - U(q)$$

Alternatively, the Feynman's amplitude K can be expressed in terms of the complete set of the eigenvalues E_n and eigenfunctions $\psi_n(q)$ of the quantum-mechanical Hamiltonian of the system (for a particle mentioned above $H = \frac{1}{2}p^2 + U(q)$):

$$K(q_f, t_f; q_i; t_0) = \sum_n \psi_n^*(q_f) \,\psi_n(q_i) \,\exp\left[-iE_n(t_f - t_i)\right].$$
(2.11)

The generalization to a system with many degress of freedom is straightforward. Usually, the operator $K(q_f, t_f; q_i; t_i)$ is called a propagator, but this term is also used in other meanings; Feynman often called it just a kernel.

The representation (2.11) implies that the equilibrium partition function of the system can be written in terms of the kernel K as:

$$Z = \int dq \sum_{n} \psi_{n}^{*}(q)\psi_{n}(q) \exp(-\beta E_{n}) = \int dq K(q, -i\beta; q, 0), \qquad (2.12)$$

where $\beta \equiv T^{-1}$. Therefore, in order to find the partition function Z we have to evaluate the trace of the Feynman's propagator K for *imaginary* time interval $t = -i\beta$:

$$Z = \int_{q(0)=q(\beta)} \mathcal{D}q(\tau) \exp(-S_E[q(\tau)]), \quad S_E[q(\tau)] = \int_0^\beta d\tau \, L_E\left(\frac{dq}{d\tau}, q(\tau)\right), \tag{2.13}$$

where

$$L_E\left(\frac{dq}{d\tau},q(\tau)\right) = -L\left(i\frac{dq}{dt},q(it)\right).$$

The path integral in Eq. (2.13) is taken with respect to all periodic paths that come back to the initial point over the imaginary time $-i\beta$. The quantity S_E is often called the Euclidean action (in special relativity the metrics of the space-time becomes Euclidean when we switch to imaginary time). Correspondingly, the Lagrangian L_E is called Euclidean, too (mind the sign!). Generically, L_E is a functional of $q(\tau)$. For a particle with a unit mass moving in a potential U(q) the Euclidean Lagrangian has the simple form

$$L_E = \frac{1}{2} \left(\frac{dq}{d\tau}\right)^2 + U(q). \tag{2.14}$$

At low temperatures the imaginary time interval β is large, and the Euclidean action (in the units of \hbar !) is huge for the majority of the paths, and, quite similar to what we had in the classical problem, it is strongly different for different paths. Therefore the path integral may be evaluated by the method of steepest descent, *i.e.*, we have to find the extreme paths $\bar{q}(\tau)$ that satisfy the equation

$$\frac{\delta S_E[q]}{\delta q(\tau)} = 0. \tag{2.15}$$

Here $\delta/\delta q(\tau)$ means the functional derivative with respect to $q(\tau)$. In particular, for the Lagrangian (2.14) the variational equation takes a standard form of the Lagrangian equation of motion

$$-\frac{d}{d\tau}\frac{\partial L_E}{\partial (dq/d\tau)} + \frac{\partial L_E}{\partial q} = 0, \quad q(0) = q(\beta).$$
(2.15a)

For systems with a metastable state Eqs. (2.15) or (2.15a) have several solutions.



At very low temperatures the particle is mostly localized in the vicinity of the stable (or metastable) position $q_{\rm st}$, and the solution of Eq. (2.15) that provides the main contribution to the partition function Z is trivial,

$$\bar{q}(\tau) = q_{\rm st}, \quad \bar{S}_E = \beta U(q_{\rm st}).$$
 (2.16)

It is easy to see that for a particle with the Euclidean Lagrangian (2.14) in a potential with a single minimum this is the only solution of the variational equation Eq. (2.15). The value of the Euclidean action \bar{S}_E evaluated along

the saddle point path provides the exponent of the partition function. The corresponding prefactor, as usual in the saddle point approximation, can be found by performing the Gaussian integration over the fluctuations around the saddle-point solution $\bar{q}(\tau)$, after expanding the action $S_E[q(\tau)]$ to quadratic order in $\delta q(\tau) \equiv q(\tau) - \bar{q}(\tau)$. Formally, this expansion can be written as

$$S_E \approx \bar{S}_E + \frac{1}{2} \int \int d\tau \, d\tau' \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} \delta q(\tau) \, \delta q(\tau'), \qquad (2.17)$$

where the functional derivatives are evaluated at the path $q(\tau) = \bar{q}(\tau)$.

The Gaussian integration can be conveniently performed after expanding the variation

$$\delta q(\tau) = \sum_{n} c_n q_n(\tau) \tag{2.18}$$

over the solutions of the eigenvalue problem

$$\int_0^\beta d\tau' \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} q_n(\tau') = \lambda_n q_n(\tau), \quad q_n(\beta) = q_n(0).$$
(2.19)

The kernel of this equation is symmetric, and the functions $q_n(\tau)$ can be always chosen to form a complete orthonormal set,

$$\int_0^\beta d\tau \, q_n(\tau) q_m(\tau) = \delta_{nm}$$

and the action (2.17) becomes

$$S_E \approx \bar{S}_E + \frac{1}{2} \sum_n \lambda_n c_n^2, \quad q(\tau) = \bar{q}(\tau) + \sum_n c_n q_n(\tau).$$
 (2.20)

Now we can rewrite the integral over arbitrary paths $q(\tau)$ as an integral over the coefficients c_n of the expansion (2.18),

$$\int \mathcal{D}q(\tau) \longrightarrow N \prod_n \int dc_n / (2\pi)^{1/2}$$

where the overall constant N depends on the normalization; in the following the specific value of N will not be substantial.

Equation (2.20) implies that at low temperatures the main contribution to the partition function can be written as

$$Z_0 \approx N \left[\det \left(\delta^2 S_E / \delta q^2 \right) \right]^{-1/2} e^{-\beta U(q_{\rm st})} \equiv N e^{-\beta U(q_{\rm st})} \prod_n \lambda_n^{-1/2}.$$
(2.21)

This defines the determinant in terms of the eigenvalue problem (2.19). For the timeindependent extremal path (2.16) which minimises the Euclidean action for a particle in a potential well, the eigenvalue equations (2.19) can be written as

$$-\frac{d^2q_n}{d\tau^2} + U''(q_{\rm st}) q_n(\tau) = \lambda_n q_n(\tau), \quad q_n(\beta) = q_n(0),$$

while the corresponding determinant in Eq. (2.21) is sometimes denoted as

$$\det\left(\delta^2 S_E/\delta q^2\right) = \det\left[-(d^2/d\tau^2) + U''(q_{\rm st})\right]$$

The solution of the obtained eigenvalue problem is trivial, and the resulting eigenvalues are of the form

$$\lambda_n = U''(q_{\rm st}) + \frac{4n^2\pi^2}{\beta^2}, \quad n = 0, \pm 1, \dots$$

Our next step will be to find the contribution to the partition function Z from other extremal paths that exist in the case of a metastable potential.



2.4 Bounces

Fig. 2.6. The extremal trajectories visualized as the motion in the inverted potential.

These extremal paths, which can be obtained as a solution of the variational problem (2.15a), include one more time-independent solution $q(\tau) = q_{top}$, located at the top of the potential barrier, and a variety of time-dependent solutions that can be visualized as non-linear oscillations in the inverted potential -U(q). The timeindependent solution $q(\tau) = q_{top}$, which only explores the vicinity of the top of the potential barrier, is associated with activational transport. This solution, important at the temperatures close or above the crossover, $T \gtrsim T_0$, will be considered in Sec. 3.1. Here we are interested in calcu-

lating the escape rate at very small temperatures, $T \ll T_0$, which is dominated by a very special extremal trajectory called the bounce. It corresponds to the motion that starts very close to the top of the inverted potential -U(q) (*i.e.*, near the stable point $q_{\rm st}$) with nearly zero velocity, goes far away from $q_{\rm st}$ accross the well of the inverted potential -U(q), and then bounces back, with the total energy

$$E = \frac{1}{2} \left(\frac{dq}{d\tau}\right)^2 - U(q)$$

close to the potential energy $-U(q_{\rm st})$ in the stationary point.

It is easy to understand why the bounces play such a special role in the limit of large $\beta = T^{-1}$. First, the candidate solution must be a *periodic* solution, $q(0) = q(\beta)$, and therefore only the trajectories located in the barrier region, where the inverted potential provides a restoring force, may apply. This limits the allowed energies to the interval between the bottom of the well $-U(q_{st})$ and the top of the barrier $-U(q_{top})$, *i.e.*, the minimum of the inverted potential -U(q). Second, it is easy to see that in the considered limit the bounce has the smallest action out of all not-trivial



Fig. 2.7. A typical form of the bounce solution. A very important simplification comes from the fact that the displacement $q_{\text{bounce}} - q_{\text{st}}$ is *exponentially* small away from the peak, so that the functional form remains the same for all $T \ll T_0$.

trajectories. Indeed, the Euclidean action $S_E[q(\tau)]$ associated with a periodic solution $q(\tau)$ is equal to the action per one oscillation times the total number of the oscillations during the time interval β . This number is proportional to inverse temperature T^{-1} for the trajectories starting somewhere near the middle of the well of the inverted potential -U(q). As a result, the associated action will be extremely large for small T, which rules out the possibility that such solutions may be important.

2.4. BOUNCES

From the physical notion of the bounce as the trajectory in the inverted potential, it is clear that the particle spends most of the time (we are talking about the imaginary time!) near the local maximum $q_{\rm st}$ of the potential -U(q), then it performs a fast trip to the other side of the "well" over the time $\sim \Omega^{-1} \equiv |U''(q_{\rm top})|^{-1/2}$, and returns to the vicinity of the point $q_{\rm st}$. Clearly, the trajectory must lie entirely on one side of this point, *i.e.*, the function $\bar{q}(\tau) - q_{\rm st}$ has no nodes.

Analyzing the linearized equations of motion in the vicinity of the stationary point $q_{\rm st}$, it is easy to see that the particle approaches this point exponentially, with the characteristic time ω_0^{-1} determined by the frequency of oscillations near the bottom of the well, $\omega_0^2 = U''(q_{\rm st})$. Therefore, even though the solution $\bar{q}(\tau)$ depends on the total time interval β , for small enough temperatures, $2\pi T \ll \omega_0, \Omega$, the form of the bounce solution remains the same with exponential accuracy. The specific time interval when the fast motion actually occurs, in particular, the instant τ_0 when the system reaches the turning point at the opposite "potential wall", is arbitrary, and the extremal solution can be written in the form

$$\bar{q}(\tau) \equiv q_{\text{bounce}}(\tau - \tau_0) = Q(\tau - \tau_0) \tag{2.22}$$

with an arbitrary τ_0 . For our example of the particle moving in a static potential, the function $Q(\tau)$ is given by the solution of the equation

$$\frac{dQ}{d\tau} = \pm \left[2\left(U(Q) - U(q_{\rm st})\right)\right]^{1/2}$$

This equation is often easier to integrate in a closed form than finding the generic trajectories at arbitrary energy. For example, the generic motion in a quartic potential $U(q) = q^2/2 - q^4/4$ is described by elliptic functions. However, one can easily find that the bounce solution is $Q(\tau) = \pm \sqrt{2}/\cosh(\tau)$, where the plus (minus) sign corresponds to the tunneling under the left (right) wall. This local in time *soliton-like* structure of the bounce solution is very general and very important.

An immediate and quite remarkable consequence of the structure of the bounce solution (2.22) is that the function

$$q_1(\tau) = A_1^{-1} \frac{dQ(\tau - \tau_0)}{d\tau}, \quad A_1 = \left[\int_0^\beta d\tau \, \left(\frac{dQ(\tau)}{d\tau} \right)^2 \right]^{1/2}, \tag{2.23}$$

which has exactly one node, as follows from the fact that $Q(\tau) - q_{\rm st}$ has none, is the solution of the eigenvalue problem analogous to Eq. (2.19),

$$\int d\tau' \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} q_n(\tau') = \Lambda_n q_n(\tau), \quad q_n(\beta) = q_n(0), \quad (2.24)$$

with the eigenvalue $\Lambda_1 = 0$. Indeed, it is easy to see that

$$\int d\tau' \left. \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} \right|_{q(\tau) = Q(\tau - \tau_0)} \frac{dQ(\tau' - \tau_0)}{d\tau'} = -\frac{d}{d\tau_0} \left(\frac{\delta S_E}{\delta q(\tau)} \right|_{q(\tau) = Q(\tau - \tau_0)} \right) = 0,$$

where the last equality is a consequence of the fact that $Q(\tau - \tau_0)$ is the extremum of the action S_E . The presence of a zero eigenvalue signals that we are in trouble, and in fact we

have two problems. The first one is that the determinant that provides the prefactor and is equal to the square root of the product of the eigenvalues Λ_n of the problem (2.24) seems to vanish! Then the prefactor would diverge. To say it in other words, the action is "flat" in one of the "directions" in the functional space.

The most elegant way to deal with this problem is to use what is called a collective coordinate. We recall that the evaluation of the prefactor is based on reducing the path integral to that over the coefficients c_n of the expansion in the eigenfunctions $q_n(\tau)$,

$$q(\tau) = \bar{q}(\tau) + \sum_{n} c_n q_n(\tau), \quad \int \mathcal{D}q(\tau) \longrightarrow N \prod_n \int \frac{dc_n}{(2\pi)^{1/2}}$$
(2.25)

This reduction holds if the set of the functions $q_n(\tau)$ is complete and orthonormal, but the corresponding eigenvalues Λ_n may be arbitrary. The increment of the trajectory $\Delta q(\tau)$ related to the increment of c_1 is equal, as seen from the above expansion, to

$$\Delta q(\tau) = q_1(\tau) \,\Delta c_1$$

On the other hand, we have an "internal" degree of freedom related to the shift of the bounce $\bar{q}(\tau) = Q(\tau - \tau_0)$; by shifting the position of the bounce τ_0 we change $q(\tau)$, and this change may be accounted for as one of the variations of the trajectory $q(\tau)$ over which the path integration is performed,

$$\Delta q(\tau) = \frac{dQ(\tau - \tau_0)}{d\tau_0} \,\Delta \tau_0 = -A_1 \, q_1(\tau) \,\Delta \tau_0.$$

These equations provide the relationship between the increments Δc_1 and $\Delta \tau_0$, and the integral over c_1 can be evaluated explicitly

$$\int_{-\infty}^{\infty} \frac{dc_1}{(2\pi)^{1/2}} \longrightarrow \frac{A_1}{(2\pi)^{1/2}} \int_0^{\beta} d\tau_0 = \beta \frac{A_1}{(2\pi)^{1/2}},$$
(2.26)

where we used the fact that the action $S_E[q(\tau)]$ is invariant under the time shift $\tau \rightarrow \tau - \Delta \tau_0$, so that the integrand is actually independent of τ_0 . A more careful derivation of this important relationship is given in the Appendix 2.A.

Another issue related to the occurrence of the zero solution $\Lambda_1 = 0$ in the eigenvalue problem (2.24) is that this problem also has exactly one *negative* eigenvalue $\Lambda_0 < \Lambda_1 = 0$, as follows from the fact that the eigenfunction $q_1(\tau)$ has exactly one zero. This means that the bounce does *not* provide a minimum to the functional $S[q(\tau)]$ in the path integral, or, formally, the integral of $\exp\left(-\frac{1}{2}\Lambda_0 c_0^2\right)$ over dc_0 diverges. On the other hand, if we just wrote the result formally as $\propto (\Lambda_0)^{-1/2}$ we would have an imaginary number. But this is just what we were trying to get: we have been evaluating the *imaginary* part of the partition function Z, and now we see where this imaginary part comes from, formally.

The integral over c_0 in the case $\Lambda_0 < 0$ can be evaluated by analytic continuation. The arguments are subtle. We have to continue analytically the *shape* of the potential so that the latter changed from a stable to a metastable, and we have to follow the distortion of the contour of integration over c_0 . Eventually, instead of integration along the real axis of c_0 we have to arrive at the integration along the imaginary axis. In a way this is not that surprising

that we are doing this: as we know, path integrals in real time contain the integrals over the increment of the coordinate x with the integrands, for a free particle, of the form of $\exp(imx^2/2\hbar\Delta t)$, and these integrals are evaluated by the steepest descent method, too.

To gain an idea of what is going on let us consider an integral

$$J = \frac{1}{\sqrt{2\pi}} \int_0^\infty dz \, \exp(-az^2 - bz^3)$$

This integral converges for positive a, b. Let us now change $b \to b \exp(i\phi)$ and vary ϕ from zero to $-\pi$, so that b eventually changes its sign. We can keep the integral converging by shifting the contour of integration in complex plane, as illustrated with dashed line in Fig. 2.9. As usual



with analytic functions, it does not really matter what integration contour we take, as long as at $|z| \to \infty$ it ends up in the same shaded area. The imaginary part of the integral for $\phi = -\pi$ can be evaluated by the steepest descent method by integrating along the contour shown in Fig. 2.9 with solid line,

$$\operatorname{Im} J = \frac{1}{\sqrt{2\pi}} \operatorname{Im} \int_{2a/3|b|}^{K} dz \exp\left[-\frac{4a^{3}}{27b^{2}} + a\left(z - \frac{2a}{3|b|}\right)^{2}\right]$$
$$= \frac{1}{2\sqrt{2a}} \exp\left[-4a^{3}/27b^{2}\right],$$

where $|K| \to \infty$, $\arg K = \pi/3$, and we used the fact that the integration along the real axis does not contribute to the imaginary part of the integral. The obtained expression differs by a factor 1/2 from the result one would naïvely expect if the analytic continuation could be done simply by rotating the integration contour; this factor arises because we are integrating in one direction away from the real axis. If we changed from b to -b by rotating b in the upper halfplane, we would get Im J with the same absolute value but the opposite sign.

We can argue now that a similar thing must happen when we perform the integration over c_0 in the path integral, and in this case we will also get the factor 1/2. The existence of two signs of Im Z can be also understood from physical arguments: they



Fig. 2.9. The shaded areas indicate the regions where z^3 is negative.

correspond to two possible choices of the unidirectional flow far from the well when defining the non-Hermitian problem of escape; both signs can be obtained by analytic continuation from the original stable potential.

Now that we learned to perform the Gaussian integration when the second variation of

the action has zero and negative eigenvalues, we can write

Im
$$Z = \frac{1}{2} \beta \frac{A_1}{(2\pi)^{1/2}} N \left| \det' \left(\delta^2 S_E / \delta q^2 \right)_{\text{bounce}} \right|^{-1/2} \exp(-S_E[q_{\text{bounce}}]),$$
 (2.27)

where

$$\det' \left(\delta^2 S_E / \delta q^2 \right)_{\text{bounce}} \equiv \prod_{n \neq 1} \Lambda_n,$$

and the index "bounce" means that the corresponding quantities are evaluated for the bounce solution $\bar{q}(\tau) = q_{\text{bounce}}(\tau)$ of the variational problem (2.15) or (2.15a) (the eigenvalues Λ_n are evaluated for the eigenvalue problem that refers to that same solution), and the prime means that zero eigenvalue should be omitted when the determinant is evaluated.

Although we calculated only the imaginary part of the contribution of the bounce to the partition function, it is clear that the real part of the partition function at small temperatures is dominated by the vicinity of the (meta) stable point $q_{\rm st}$. Therefore, the correction to the real part will be relatively unimportant, and, using the fact that the normalization factor N is the same for integration around all extremal solutions, we can write the final expression for the escape rate $W = 2T \text{Im} \ln Z$ in the form

$$W = C \exp(-S_E[q_{\text{bounce}}]), \qquad C = \frac{A_1}{(2\pi)^{1/2}} \left[\frac{\det (\delta^2 S_E / \delta q^2)_{q=q_{\text{st}}}}{|\det' (\delta^2 S_E / \delta q^2)_{\text{bounce}}|} \right]^{1/2}$$
(2.28)

This expression provides a basis for the analysis of the escape rate in the case of a system coupled to a thermal bath.

2.A Appendix. Collective mode integration.

We shall discuss an alternative way to integrate over the zero-eigenvalue mode in Eq. (2.25). The integral in Gaussian approximation diverges because, even though the main contribution to the path integral is due to the paths that are close to the bounce solution $Q(\tau - \tau_0)$, the position of the bounce τ_0 is arbitrary in the interval $(0, \beta)$, and the associated variation can be large. To eliminate this zero-eigenvalue mode we need to choose the bounce solution with an "optimal" position for every variational trajectory $q(\tau)$. This can be done by looking for a value of τ_0 such that $q(\tau)$ is best approximated by $Q(\tau - \tau_0)$ "on the average", *i.e.* that the integral

$$M(\tau_0; q) \equiv \int_0^\beta d\tau \, [q(\tau) - Q(\tau - \tau_0)]^2 \tag{2.29}$$

reaches a minimum, which implies

$$f(\tau_0; q) \equiv \partial M(\tau_0; q) / \partial \tau_0 = -2 \int_0^\beta \dot{Q}(\tau - \tau_0) q(\tau) = 0.$$
 (2.30)

Clearly, $\tau_0 \equiv \tau_0[q(\tau)]$ defined by this equation is a *functional* of $q(\tau)$.

Now we shall use the trick similar to the gauge-fixing procedure in the field theory. Let us introduce

$$1 = \int_0^\beta \delta\left(\tau' - \tau_0\left[q(\tau)\right]\right) \, d\tau'$$

under the integral in the exact partition function (2.13),

$$Z = \int_0^\beta d\tau' \int \mathcal{D}q(\tau) \exp(-S_E[q(\tau)]) \,\delta(\tau' - \tau_0[q(\tau)]) \tag{2.13a}$$

Since the partition function includes the integration over all possible time-translated trajectories, the integrand does not actually depend on τ' , and the integration over this variable is trivial. After selecting an arbitrary value $\tau' = \tau_0$, we can simplify the argument of the δ -function using the stationarity condition (2.30) and the formula $\delta(f(x)) = \delta(x) |f'(x)|^{-1}$, with the result

$$\operatorname{Im} Z = \beta \operatorname{Im} \int \mathcal{D}q(\tau) \exp(-S_E[q(\tau)]) \,\delta(f(\tau_0;q)) \,\left|\partial f(\tau_0;q)/\partial \tau_0\right|.$$
(2.31)

The linear functionals in this expression are

$$f(\tau_0; q) \equiv -2 \int_0^\beta \dot{Q}(\tau - \tau_0) q(\tau) = -2A_1 c_1, \qquad (2.32)$$

$$\partial f(\tau_0; q) / \partial \tau_0 \equiv 2 \int_0^\beta \ddot{Q}(\tau - \tau_0) q(\tau) = -2A_1^2 + 2A_1 \sum_n c_n b_n, \qquad (2.33)$$

where we used the expansion $q(\tau) = Q(\tau - \tau_0) + \sum c_n q_n(\tau)$, and the coefficients

$$b_n \equiv \int_0^\beta \dot{q}_1 q_n d\tau, \quad b_1 = 0.$$

Now we expand the Euclidean action in the exponent with the help of Eq. (2.20) and, keeping in mind the arguments about the analytic continuation of the formally-divergent integral over c_0 , we obtain

$$\operatorname{Im} Z = \beta N \int \prod_{n} \frac{dc_{n}}{(2\pi)^{1/2}} \,\delta(c_{1}) \, \left| A_{1} - \sum_{n} c_{n} \, b_{n} \right| \, e^{-\bar{S}_{E}} \, \exp\left(-\frac{1}{2} \sum_{n} \lambda_{n} \, c_{n}^{2}\right), \tag{2.34}$$

which can be further transformed after rescaling $c_n \to c_n \sqrt{\lambda_n}$ and a rotation,

Im
$$Z = \beta N \zeta_1 \frac{A_1}{\sqrt{2\pi}} e^{-\bar{S}_E} \prod |\lambda_n|^{-1/2},$$
 (2.35)

where the additional correction term

$$\zeta_1 \equiv \int \frac{d\xi}{(2\pi)^{1/2}} e^{-\xi^2/2} |1 - \alpha\xi| = \operatorname{erf}\left(1/\sqrt{2}\,\alpha\right) + \alpha\,\sqrt{\frac{2}{\pi}}\,\exp\left(-1/2\,\alpha^2\right), \text{ and } A_1^2\alpha^2 = \sum_{n \neq 1} \frac{b_n^2}{\lambda_n}.$$

The original assumption that $q(\tau)$ is close to $Q(\tau - \tau_0)$ with suitably chosen τ_0 is equivalent to the statement that α is very small (practically, $\alpha \leq 0.5$ is enough); in this case the correction term $\zeta_1 = 1$ with *exponential* accuracy, the whole expression is analytic to a good approximation, and, therefore, we restore the prescription

$$\int_{-\infty}^{\infty} \frac{dc_1}{(2\pi)^{1/2}} \longrightarrow \beta \frac{A_1}{(2\pi)^{1/2}}.$$
 (2.26')

Otherwise, if α is not small, even though we have a formally exact expression for the correction factor ζ_1 , we must admit that the integrand in Eq. (2.34) is not really an analytic function of c_0 , and the procedure of analytic continuation described in Sec. 2.4 becomes at best questionable.

Problems

▶ **Problem 2.1** (page 93)

(Re)derive the equation of motion for a current-biased Josephson junction. Assume that two identical superconductors are separated by a thin layer through which electron pairs can tunnel. In a simplie model the spatial dependence of the pair operators $\psi_{l,r}$ in the left and right superconductors is ignored, and the Hamiltonian of the pairs is

$$H = t \left(\psi_l^{\dagger} \psi_r + \psi_r^{\dagger} \psi_l \right) - 2eV \left(\psi_l^{\dagger} \psi_l - \psi_r^{\dagger} \psi_r \right), \quad \left[\psi_i, \psi_j^{\dagger} \right] = \delta_{ij}, \quad i, j = l, r,$$

where V is the potential difference accross the contact. Seek the solution of the equations of motion in the form

$$\psi_{l,r} = n_{l,r}^{1/2} \exp(i\phi_{l,r})$$

with the pair densities $n_l \approx n_r$, and arrive at the Josephson equation for the time derivative of the phase difference $\theta \equiv \phi_l - \phi_r$ as a function of V. Then, assuming that a capacitor C and a resistor R are switched in parallel to the contact, and the total current through the circuit is I, find the equation of motion for θ .



Fig. 2.10.

▶ **Problem 2.2** (page 94)

Find the temperature dependence of the exponent R in the quasiclassical escape rate formula for the temperatures close to the transition temperature T_0 , if the period of oscillations in inverted potential $\tau_p(E)$ is a linear function of the energy E, measured off the top of the potential barrier. What will happen if this dependence is nonmonotonic, like shown in Fig. 2.10? The latter dependence arises, e.g., for the potential $-U(q) = \frac{1}{2}q^2 + \frac{1}{4}q^4 + Aq$ for $|A| > 8/7^{3/2}$.

▶ **Problem 2.3** (page 95)

Check the explicit form of the bounce solution and find the associated action for a particle moving in a metastable quartic potential,

$$U(q) = \frac{1}{2}q^2 - \frac{1}{4}q^4.$$
 (2.36)

▶ **Problem 2.4** (page 95)

The prefactor in the former case can be found explicitly in the limit $\beta \to \infty$: positive eigenvalues belong to a continuous spectrum and can be found along the lines described in L&L "Quantum Mechanics", pp.79 - 81. Notice that there is only scattering forward for the potential of the form of $-3/\cosh^2 x$ ($\hbar = m = 1$). Therefore the eigenvalues are expressed in terms of the phase for this scattering. Also, when evaluating the ratio of the determinants (of the products $\prod_n \lambda_n$) you have to use the fact that the main contribution to each of them comes from large n, and for large n the eigenvalues for the problem linearized with respect to the bounce solution are close to those for the problem linearized about the stable state. The ratio of the difference of the eigenvalues to the eigenvalues themselves is small, and the product can be replaced by the exponent of the sum (over n) of the latter ratios. The problem is fairly complicated but you may try to think about it.

▶ **Problem 2.5** (page 97)

Consider a particle coupled to a phonon bath, with the Hamiltonian

$$H = \frac{1}{2}p^2 + U(q) + \frac{1}{2}\sum_k \left(p_k^2 + \omega_k^2 q_k^2\right) + \sum_k \left(f_k q q_k + \frac{1}{2}(f_k/\omega_k)^2 q^2\right),$$

Find the lowest-order coupling- (dissipation)-induced correction to the *exponent* for the escape probability for low temperatures. Does the escape probability increase or decrease because of the dissipation?

Lecture 3

Activational escape

3.1 Overbarrier transitions

We saw that the small-temperature tunneling rate of a metastable system is governed by the so called bounce solution of the variational problem (2.15a). These equations can be interpreted as the equations of motion of a particle moving in the reverted potential, illustrated in Fig. 2.6, while the bounce solution at small temperatures is shown in Fig. 2.7. As the temperature is increased, the shape of the bounce solution gradually changes.

Because the period β of the imaginary time orbit becomes comparable with the period of oscillations in the inverted potential, the extremal path does not have to spend such an enormous time near the bottom $q_{\rm st}$ of the original potential well. Therefore, the amplitude of the oscillations in inverted potential gradually decreases, and finally at the crossover temperature $T_0 = \Omega_0/2\pi$ only the harmonic motion with vanishingly small amplitude is possible (see, however, Prob. 3.2 at p. 32 for an alternative scenario). Near the crossover temperature the non-trivial bounce solution becomes very close to the stationary solution $q(\tau) = q_{\rm top}$ localized at the top of the barrier; this implies that the non-linear (usually quartic) terms in the expansion of the potential near the top of the barrier must be taken into account, and the steepest descent method does not work.

However, at higher temperatures, $T \gg T_0$, where, as we saw from a simplified quasiclassical calculation, the escape is governed by the classical overbarrier transport, the imaginary part of the partition function is once again dominated by the vicinity of a single extremal trajectory,

$$\bar{q}(\tau) = q_{\rm top}.\tag{3.1}$$

For the special case of an isolated particle, the Eucledian action

$$S_E = \int_0^\beta d\tau \, \left[\frac{1}{2} \left(\frac{dq}{d\tau} \right)^2 + U(q) \right] \tag{3.2}$$

calcuated along this trajectory is

 $S_E[\bar{q}] = U(q_{\text{top}})/T.$
Correspondingly, the escape rate, which is generally proportional to $\exp(-S_E[\bar{q}] + S_E[q_{st}])$, has the exponent $S_E[q_{top}] - S_E[q_{st}] = \Delta U/T$ —a familiar result from the theory of activational transitions.

Two questions to answer are: does the solution (3.1) provide an *imaginary* part of the partition function, and, if so, which of the solutions, this one or the bounce, defines the escape rate? The answer to the second question is determined by the temperature: for T well below the crossover temperature T_0 the action for the bounce solution is less than that for the activation one, and it is the quantum tunnelling that determines the escape. On the other hand, for T well above T_0 the escape occurs via activation. To see how T_0 emerges in the present formulation we have to analyze the prefactor; from this analysis we shall also see that the prefactor generates the imaginary part Im Z for the partition function.

Before calculating the prefactor, we need to remember that in weakly-dissipative systems the quantum mechanical states near the barrier top do not really have an equilibrium population—these states are dynamically depopulated by the escape. To account for this effect consistently within the quantum mechanical description, one has to allow for quite a few factors that we mentioned when the crossover temperature was considered: overbarrier reflection, inapplicability of the steepest descent in the case of $T \approx T_0$, etc. It turns out, however, that these effects can be accounted for by a simple modification of the escape probability formula (2.10).

In the classical limit the modified expression can be derived by comparing the imaginary part of the free energy calculated by analytically continuation of the the classical partition function

$$Z = \int dp \, dq \, \exp\left(-\frac{p^2}{2 T} - \frac{V(q)}{T}\right),$$

with the classical (e.g. Kramers') escape rate. The corrected relationship has the form

$$W = 2T_0 \operatorname{Im} \ln Z = -2 \frac{T_0}{T} \operatorname{Im} F.$$
 (3.3)

It is obvious that this expression calculated at the crossover temperature, $T = T_0$, gives the same result as the quantum-mechanical expression (2.10) applicable at $T < T_0$, which implies that the crossover does not have to be particularly broad. This turns out to be indeed the case: I. Affleck has shown that the crossover region between these two expressions is actually very narrow, $(\delta T/T_0)^2 \sim 1/R$, where R is the exponent in the escape rate expression.

The equations for the eigenfunctions of the variational problem linearized in the vicinity of the extremal solution (3.1) for a particle moving in a static potential are

$$-\frac{d^2q_n}{d\tau^2} + U''(q_{\text{top}}) q_n = \Lambda_n q_n, \quad q_n(\tau + \beta) = q_n(\tau).$$

The corresponding eigenvalues are $\Lambda_n = (2\pi nT)^2 - \Omega^2$, where, as usual, $-\Omega^2 \equiv U''(q_{\text{top}})$. As before, the crossover temperature $T_0 = \Omega/2\pi$; we work in the domain $T > T_0$. Therefore, there *is* a negative eigenvalue among Λ_n , but only one, the eigenvalue with n = 0. The integration along the corresponding direction has to be done by analytic continuation; as in the case of the bounce solution we pick up only the "outgoing wave", and the imaginary part of the partition function acquires an additional factor 1/2. The final expression for the imaginary part of the logarithm of the partition function is of the form

Im
$$\ln Z = \frac{1}{2} \frac{\omega_0}{\Omega} \prod_{n=1} \frac{(2\pi nT)^2 + \omega_0^2}{(2\pi nT)^2 - \Omega^2} \exp\left(-\frac{\Delta U}{T}\right),$$
 (3.4)

where $\omega_0 = [U''(q_{st})]^{1/2}$ is the frequency of oscillations about the minimum of the potential. Combining Eqs. (3.3) and (3.4), we obtain the overbarrier escape rate

$$W = \frac{\omega_0}{2\pi} \prod_{n=1} \frac{(2\pi nT)^2 + \omega_0^2}{(2\pi nT)^2 - \Omega^2} \exp\left(-\frac{\Delta U}{T}\right).$$
 (3.4*a*)

In the classical limit $T \gg \hbar \omega_0$, $\hbar \Omega$, the infinite products in the numerator and the denominator of the prefactor cancel, and Eq. (3.4a) goes over into the Kramers' result (1.21) in the absence of dissipation ($\Gamma = 0$). For smaller temperatures Eq. (3.4a) gives quantum corrections to the Kramers' theory. The other interesting thing obvious from Eq. (3.4) is that the theory appears to "know" that it applies only for temperatures high enough: when Tapproaches the crossover temperature $T_0 = \Omega/2\pi$, the prefactor diverges. The formal reason for this behavior is the emergency of the bounce solution and the associated "soft" mode. We shall not go into details of the analysis of the range $T \approx T_0$.

3.2 Partition function for a particle linearly coupled to a phonon bath.

The above analysis was substantially based on the assumption that the system has enough time to come to thermal equilibrium before escape occurs. This requires a not too small relaxation time. And yet we did not specify what is the *relaxation* that brings the system to the equilibrium. Of course, one could imagine considering a multivariable system with a continuous energy spectrum (including the *intrawell* states in the neglect of the decay), but still there would remain some uncertainty about how dense should the continuous spectrum be, *etc.* Now we shall be more consistent, and consider the escape of a system coupled to a thermal bath.

Let us start with the simplest case of linear coupling to a phonon bath. As we know, the Hamiltonian that describes the coupled system and the bath is

$$H = H_0 + H_b + H_i,$$

$$H_0 = \frac{1}{2}p^2 + U(q), \quad H_b = \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right), \quad H_i = \sum_{\mu} \left(f_{\mu} q q_{\mu} + \frac{1}{2}(f_{\mu}/\omega_{\mu})^2 q^2\right),$$

where q, p are the coordinate and momentum of the system, whereas q_{μ} , p_{μ} are the coordinates and momenta of the eigenmodes of the bath. We are interested in the dynamics of the system itself, and it would be nice to get rid of the dynamical variables of the bath (to "eliminate phonon variables"). Feynman found the way to do it, and indeed it is quite straightforward within the path-integral formalism (this is why we are using it; unfortunately, long is the way from the expression in the form of a path integral to something

"finite-dimensional", but sometimes we can get through it). As we know, we need just to evaluate the partition function which may be written as a path integral over all *periodic* multidimensional paths $q(0) = q(\beta)$, $q_{\mu}(0) = q_{\mu}(\beta)$ of the exponent of the Eucledian action of the system + bath $S_E^{(s+b)}$:

$$Z^{(s+b)} = \int \left(\prod_{\mu} \mathcal{D}q_{\mu}(\tau)\right) \int \mathcal{D}q(\tau) \exp\left(-S_E^{(s+b)}[q(\tau), \{q_{\mu}(\tau)\}]\right), \tag{3.5}$$

$$S_{E}^{(s+b)} = \int_{0}^{0} d\tau \left\{ \frac{1}{2} \left(\frac{dq}{d\tau} \right) + U(q) + \sum_{\mu} \left[\frac{1}{2} \left(\frac{dq_{\mu}}{d\tau} \right) + \frac{1}{2} \omega_{\mu}^{2} q_{\mu}^{2} + f_{\mu} q q_{\mu} + \frac{1}{2} \left(\frac{f_{\mu}}{\omega_{\mu}} \right) q^{2} \right] \right\}.$$

The action $S_E^{(s+b)}$ is quadratic in the variables q_{μ} , but there are not only quadratic, but also linear terms which describe the coupling to the system. This suggests that the integration over the bath variables q_{μ} can be done in the same way as one evaluates the integral of $\exp(-ax^2 - bx)$: one just changes variables $(x \to x - b/2a)$ to get rid of the linear term. To find the substitution one must find the extremum of the quadratic part by solving the equation $d(ax^2 + bx)/dx = 0$. We shall do the same, and write the extremum equation in terms of the functional derivative

$$\frac{\delta S_E^{(\rm s+b)}}{\delta q_\mu(\tau)} = 0 \quad \longrightarrow \quad -\frac{d^2 q_\mu}{d\tau^2} + \omega_\mu^2 q_\mu(\tau) + f_\mu q(\tau) = 0$$

The easiest way to solve these equations is to notice that both $q_{\mu}(\tau)$ and $q(\tau)$ are periodic, and therefore we may write the solution as

$$q_{\mu}(\tau) = q_{\mu}^{(0)}(\tau) - f_{\mu} \sum_{n} \left(\omega_{n}^{2} + \omega_{\mu}^{2}\right)^{-1} e^{-i\tau\omega_{n}} q_{M}(n), \quad q_{M}(n) \equiv \beta^{-1} \int_{0}^{\beta} d\tau \, q(\tau) e^{i\tau\omega_{n}}, \quad (3.6)$$

where $\omega_n \equiv 2\pi n/\beta$ are Matsubara frequencies. The term $q_{\mu}^{(0)}(\tau)$ is the solution of the equation of motion for the μ -th oscillator in the absence of the coupling to the system. Clearly, the path integral (3.5) can be understood just as a path integral over $q_{\mu}^{(0)}(\tau)$ —we just perform a linear shift of the functions $q_{\mu}(\tau)$.

We can now plug (3.6) into the expression for the action (3.5) and substantially simplify this expression by noticing that the action can be expanded in $q_{\mu}(\tau) - q_{\mu}^{(0)}(\tau)$ to the second order, and this expansion is *exact* (allow for the periodicity of the solution to notice that there are no boundary terms coming from the integration by parts). We can then transform the integral of the square of the first derivative into the integral of the product of the function by its second derivative, and we get, eventually:

$$S_{E}^{(s+b)} = S_{E}^{(eff)} + S_{E}^{(b)}, \quad S_{E}^{(b)} = \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{\mu} \left[\left(\frac{dq_{\mu}^{(0)}}{d\tau} \right)^{2} + \omega_{\mu}^{2} \left(q_{\mu}^{(0)} \right)^{2} \right]$$
$$S_{E}^{(eff)} \equiv S_{E}[q] = \int_{0}^{\beta} d\tau \left(\frac{1}{2} \left(\frac{dq}{d\tau} \right)^{2} + U(q) \right) + \frac{1}{2} \beta \sum_{n} \Phi_{n} q_{M}(n) q_{M}(-n). \quad (3.7)$$

The term $S_E^{(b)}$ corresponds, obviously, to the Euclidean action of the bath isolated from the system. The partition function of the system coupled to the bath is, therefore, factorized

into the product of the partition function of the *dissipating* system and the partition function of the bath uncoupled from it,

$$Z^{(s+b)} = Z Z^{(b)},$$

$$Z = \int_{q(0)=q(\beta)} \mathcal{D}q(\tau) \exp(-S_E[q]), \qquad Z^{(b)} = \prod_{\mu} \left[1 - \exp\left(-\beta\omega_{\mu}\right)\right]^{-1}.$$
(3.8)

The coefficients Φ_n in Eq. (3.7) are determined by the coupling of the system to the bath, and can be expressed in terms of the function $F(\omega)$ that gives the density of states of the bath weighted with the interaction:

$$\Phi_n = \frac{2}{\pi} \omega_n^2 \int d\omega \, \frac{\omega^{-1} F(\omega)}{\omega^2 + \omega_n^2}, \quad F(\omega) = \frac{\pi}{2} \sum_{\mu} \left(f_{\mu}^2 / \omega_{\mu} \right) \delta(\omega - \omega_{\mu}) \tag{3.9}$$

You may notice that these coefficients are simply proportional to the temperature Green's function

$$\mathcal{D}(\omega_n) = \int_0^\beta d\tau e^{i\tau\omega_n} \sum_{\mu,\mu'} \frac{f_\mu f_{\mu'}}{\omega_\mu \omega_{\mu'}} \left\langle q_\mu(\tau) q_{\mu'}(0) \right\rangle = \frac{2}{\pi} \int d\omega \frac{\omega^{-1} F(\omega)}{\omega^2 + \omega_n^2}$$

evaluated in the absence of the coupling.

We have thus performed what we wanted: all that remained from the coupling to a bath and from the infinite number of the dynamical variables of the bath in the partition function Z is just one extra term that depends on the cordinate of the system and is quadratic in this coordinate. At this point we can start investigating the various effects coming from the coupling, and these effects will depend, of course, on the form of the function $F(\omega)$. It is clear that to the zeroth order in the coupling we reproduce the partition function of the isolated system. The effects of weak coupling can be considered by perturbation theory.

3.3 Activational escape in the presence of dissipation

The distinctive feature of the action S_E given by Eq. (3.7), as compared with the action of an isolated particle, is that the effective Lagrangian is nonlocal in the imaginary time. This is particularly clear if we rewrite Eq. (3.7) in the form

$$S_E = \int_0^\beta d\tau \, \left(\frac{1}{2} \left(\frac{dq}{d\tau} \right)^2 + U(q) \right) + \frac{1}{2} \int_0^\beta \int_0^\beta d\tau \, d\tau' \, \kappa(\tau - \tau') q(\tau) q(\tau'), \tag{3.10}$$

where the non-local interaction strength

$$\kappa(\tau) \equiv \beta^{-1} \sum_{n} \Phi_n \, e^{-i\tau\omega_n}$$

This, certainly, agrees with the nonlocality we observed in our analysis of the classical particle coupled to a phonon bath: the real-time equation of motion was retarded.

Let us now analyze the trajectories that provide an extremum to the functional S_E . The Euler-Lagrange equation of motion is of the form

$$\frac{\delta S_E}{\delta q(\tau)} = 0, \quad \text{or} \quad -\frac{d^2 q}{d\tau^2} + U'(q) + \int_0^\beta \kappa(\tau - \tau')q(\tau') = 0.$$
(3.11)

From the explicit form of the expression for $\kappa(\tau)$ and for the coefficients Φ_n it follows that on average the retarded interaction vanishes,

$$\int_0^\beta\,d\tau\,\kappa(\tau)=0,$$

which agrees with our interpretation of this term as some sort of a non-local friction. Therefore Eq. (3.11) has a solution that corresponds to the particle resting at the minimum $q_{\rm st}$ of the potential U(q):

$$\bar{q} = q_{\rm st}; \qquad S_E[\bar{q}] = \beta U(q_{\rm st})$$

$$(3.12)$$

The eigenvalue problem (2.19)

$$-\frac{d^2q_n}{d\tau^2} + U''(\bar{q})q_n(\tau) + \int_0^\beta d\tau' \kappa(\tau - \tau')q_n(\tau') = \lambda_n q_n(\tau)$$
(3.13)

for the perturbations about the extremal solution can be easily solved for $\bar{q} = q_{st}$, with the result

$$\lambda_n = \omega_n^2 + U''(q_{\rm st}) + \Phi_n. \tag{3.14}$$

Clearly, all the eigenvalues (3.14) are positive. Notice, however, that the coupling to the bath changes the values of the eigenvalues even for the problem linearized about the stationary state.

For a metastable potential there is also a solution of the variational equation (3.11) that corresponds to the system staying at the top of the potential barrier, $\bar{q} = q_{\text{top}}$, with the action $S_E = \beta U(q_{\text{top}})$. The corresponding eigenvalues of the problem (3.13) are

$$\Lambda_n = \omega_n^2 - \Omega^2 + \Phi_n,$$

where, as usual, $-\Omega^2 = U''(q_{top})$ is the curvature of the potential at the top of the barrier. At high enough temperatures there is only one negative eigenvalue, $\Lambda_0 = U''(q_{top})$. The crossover temperature T_0 is defined as the temperature at which the smallest nonnegative eigenvalue of the problem (3.13) vanishes,

$$\omega_1^2 + \Phi_1 = |U''(q_{\text{top}})| \text{ for } T = T_0,$$

one can check that below this temperature there appears the non-trivial bounce solution for the non-local extremum equation (3.11).

It is straightforward now to reproduce the results for classical activation escape in the presence of dissipation. For $T > T_0$, we can just rewrite Eq. (3.4a) with the account taken of the dissipation-induced renormalization of the eigenvalues

$$W = \left(\frac{U''(q_{\rm st})}{|U''(q_{\rm top})|}\right)^{1/2} T_0 \prod_{n=1} \frac{\omega_n^2 + U''(q_{\rm st}) + \Phi_n}{\omega_n^2 - |U''(q_{\rm top})| + \Phi_n} \exp\left(-\frac{\Delta U}{T}\right).$$
(3.15)

In the case of Ohmic dissipation and in the limit $\hbar \to 0$ this expression safely goes over into the result obtained by Kramers.

Problems

▶ **Problem 3.1** (page 98)

By an explicit analytic continuation from positive values of λ , find the imaginary part of the *classical* partition function for a particle in a metastable potential

$$U(q) = \frac{q^2}{2} + \lambda \frac{q^4}{4}, \quad \lambda < 0$$

Compare your result with the Kramer's escape rate in the absence of dissipation ($\Gamma = 0$), and check Eq. (3.3) in this regime.

▶ **Problem 3.2** (page 99)

Show that for a particle linearly coupled to a phonon bath, with the Hamiltonian

$$H = \frac{1}{2}p^2 + U(q) + \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right) + \sum_{\mu} \left(f_{\mu}qq_{\mu} + \frac{1}{2}(f_{\mu}/\omega_{\mu})^2 q^2\right),$$

the term in the effective action that describes the nonlocal in time self-action of the particle can be written as

$$\delta S = \frac{1}{2} \int_{-\infty}^{\infty} d\tau' \int_{0}^{\beta} d\tau \, \alpha(\tau - \tau') \left[q(\tau) - q(\tau') \right]^{2},$$

where

$$\alpha(\tau - \tau') = \frac{1}{2\pi} \int d\omega F(\omega) \exp(-\omega|\tau|),$$

and we assume that $q(\tau) = q(\tau + \beta)$. The function $F(\omega)$ is the density of states of the bath weighted with coupling; its explicit form in terms of f_{μ}, ω_{μ} is given in Eq. (3.9). Notice the simple form of the function $\alpha(\tau)$ in the case of Ohmic coupling, $F(\omega) = 2\Gamma\omega \exp(-\epsilon\omega)$, $\epsilon \to +0$.

▶ **Problem 3.3** (page 100)

Find the bounce solution and evaluate action for an overdamped particle (Ohmic dissipation) in a cubic potential,

$$U(q) = 3U_0 \left(\frac{q}{q_0}\right)^2 \left(1 - \frac{2}{3}\frac{q}{q_0}\right).$$

"Overdamped" means that you can neglect the term with inertia, *i.e.*, the term $d^2q/d\tau^2$ in the equation of motion.

Hint: Seek the solution in the form $q(\tau) = \sum_{n} c_n \exp(i\omega_n \tau)$; the set of equations for c_n can be solved in the present case.

▶ **Problem 3.4** (page 102)

Evaluate the effective action for the coupling to a phonon bath of the form

$$H_i = \sum_{\mu} f_{\mu}(q) q_{\mu}.$$

Chapter II Resonant tunneling

Lecture 4

Instanton formulation

4.1 Ohmic dissipation

In the previous lecture we studied the quantum decay of a system in the presence of a dissipation caused by the coupling to a bath of harmonic oscillators (phonons). We traded the infinite number of phonon degrees of freedom for the retarded interaction, and arrived at the following effective Euclidean action

$$S_E = \int_0^\beta d\tau \, \left(\frac{1}{2} \left(\frac{dq}{d\tau}\right)^2 + U(q)\right) - \frac{1}{4} \int_0^\beta \int_0^\beta d\tau \, d\tau' \, \kappa(\tau - \tau') [q(\tau) - q(\tau')]^2, \tag{4.1}$$

where the retarded interaction

$$\kappa(\tau) = \beta^{-1} \sum_{n} \Phi_n e^{-i\tau\omega_n}, \quad \Phi_n = \omega_n^2 \frac{2}{\pi} \int d\omega \, \omega^{-1} [\omega^2 + \omega_n^2]^{-1} F(\omega)$$
(4.2)

can be expressed as the sum over the Matsubara frequences $\omega_n \equiv 2\pi nT$. The oscillator bath is described by the function $F(\omega)$, defined by Eq. (3.9) as the density of states of the bath weighted with the coupling. The effective action S_E written in the form (4.1) shows clearly that the nonlocal in time part of the action depends on how fast the function $q(\tau)$ varies in time. We emphasize that Eq. (4.1) formally holds even for $q(\tau)$ which are *not* necessarily periodic in τ : the derivation was based only on the periodicity of the *bath* variables with a period $\beta = T^{-1}$.

In view of our former analysis and of the numerous experimental data on the tunnelling decay in Josephson junctions, it is interesting to analyze the effect of dissipation in the particular case when it is Ohmic, *i.e.* when

$$F(\omega) = 2\Gamma\omega \exp(-\epsilon\omega), \quad \Phi_n = 2\Gamma |\omega_n|.$$
(4.3)

Here, Γ is the friction coefficient (the dynamics of a system with the coupling (4.3) corresponds to the real time Brownian motion with the friction force $-2\Gamma \dot{q}$), and ϵ is the cutoff parameter which determines the fast time for a given system. For the Ohmic dissipation model (4.3), it is straightforward to evaluate the retarded interaction function,

$$\kappa(\tau) = -\frac{2\pi\Gamma\beta^{-2}}{\sin^2(\pi\tau/\beta)}.$$
(4.4)

On the whole, the nonlocal in time term in the Euclidean action (4.1) is positive, and we see that is does not have any divergences at $\tau = \tau'$ for smooth trajectories $q(\tau)$. The equation of motion for the path $\bar{q}(\tau)$ that provides an extremum to the action (4.1) is of the form

$$-\frac{d^2\bar{q}}{d\tau^2} + U'(\bar{q}) + \frac{2\pi\Gamma}{\beta^2} \mathcal{P} \int_0^\beta d\tau' \frac{\bar{q}(\tau) - \bar{q}(\tau')}{\sin^2(\pi(\tau - \tau')/\beta)} = 0,$$
(4.5)

where the symbol \mathcal{P} denotes that the principal value of the integral should be taken.

The major contribution to the action for the bounce-type solution $\bar{q}(\tau) = Q(\tau - \tau_0)$, where τ_0 is the position of the center of the bounce, comes from the range of comparatively small time increments $|\tau - \tau'|/\beta$. This contribution changes the asymptotics of the bounce solution from exponential to a power law. Indeed, in the time domain $\beta \gg |\tau - \tau_0| \gg [\omega_0]^{-1/2}$, where $\omega_0 \equiv [U''(q_{\rm st})]^{1/2}$ is the frequency of the vibrations about the minimum $q_{\rm st}$ of the potential well, the system is close to this minimum, $|q - q_{\rm st}| \ll |q_{\rm st} - q_{\rm top}|$, where $q_{\rm top}$ is the position of the top of the barrier, and the solution of Eq. (4.5) is asymptotically of the form

$$|\bar{q}(\tau) - q_{\rm st}| \sim \frac{\Gamma}{\omega_0^{3/2}} \frac{|q_{\rm top} - q_{\rm st}|}{(\tau - \tau_0)^2}$$

The interesting effects associated with the Ohmic dissipation are related to this long tail of the bounce solution. They may be dramatically strong for not very weak coupling in the situation of resonant tunnelling.

4.2 Instantons.

Fig. 4.1.

So far we have been considering only a single bounce solution, and this was good enough for the problem of decay of a metastable state. The situation is different if we are considering the **resonant tunnelling**: in this case the quantum tunneling lifts the degeneracy, and the partition function depends on the relative scale of the temperature and the tunnelling splitting (we assume both of them to be much smaller than the energies of intrawell vibrations):

$$Z = e^{-E_0/T} \left[e^{\Delta/2T} + e^{-\Delta/2T} \right],$$
 (4.6)

where E_0 is the energy of the intrawell state in the absence of the tunnelling, and Δ is the tunnelling splitting.

The partition function written in the form (4.6) suggests that the path integral can be used to evaluate the tunneling splitting—this is similar to the way we used the partition function to evaluate the escape rate from a metastable state. However, in the problem of the interwell tunnelling we do not expect the partition function Z to have an imaginary part, and we will not need to perform the analytic continuation of the path integral. This simplification, however, does not come free: the price is that we may no longer limit ourselves to the vicinity of a single extremal trajectory.

Let us start with a simple problem of the tunnelling of a particle in a symmetrical doublewell potential U(q) = U(-q), isolated from a bath: the conventional solution to this problem is given in L&L's *Quantum Mechanics*. The partition function Z is given by the path integral

$$Z = \int dq_0 \int_{q(0)=q_0}^{q(\beta)=q_0} \mathcal{D}q(\tau) \exp(-S_E[q]),$$

where we separated the integration over the end-point $q_0 = q(0) = q(\beta)$ of the periodic trajectory. As we shall see, this notation will be convenient for the analysis of multy-instanton solutions.

The action S_E corresponds to the motion of a particle in the inverted potential -U(q), and we count U(q) off from its value in the stable positions, $U(\pm q_{st}) = 0$. As in the escape problem, the main contribution to the partition function comes from the motion in the vicinity of the potential minima, *i.e.*, the maxima of the inverted potential -U. Clearly, there must be a separate contribution from the vicinity of the left maximum, $q = q_{\text{left}}$ and that from the vicinity of the right one, $q = q_{\text{right}} \equiv -q_{\text{left}}$. These contributions are equal by symmetry, and we can consider only one of them and then double the answer. The solution of the extremum equation

$$\frac{\delta S_E}{\delta q(\tau)} = 0, \tag{4.7}$$

localized in the vicinity of the point q_{left} , starting and ending at the point q_0 which is also close to q_{left} , can be written in the linear approximation

$$q(\tau) \approx q_{\text{left}} + (q_0 - q_{\text{left}}) \left[e^{-\omega_0 \tau} + e^{-\omega_0 (\beta - \tau)} \right], \quad S_E \approx \omega_0 (q_0 - q_{\text{left}})^2,$$
(4.8)

where $\omega_0 \equiv [U''(q_{\rm st})]^{1/2}$, and we assume that the temperature is small enough, $\omega_0 \beta \gg 1$.

As before, in order to find the preexponent, we need to diagonalize the second variation of the action S_E . Because the position of the particle at the ends of the integration interval is fixed, the corresponding eigenvalue problem is that with zero rather than periodic boundary conditions,

$$\int d\tau' \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} \tilde{q}_n(\tau') = \tilde{\lambda}_n \tilde{q}_n(\tau), \qquad \tilde{q}_n(0) = \tilde{q}_n(\beta) = 0.$$
(4.9)

The corresponding eigenvalues

$$\tilde{\lambda}_n = \omega_0^2 + n^2 \pi^2 T^2, \quad n = 1, 2, 3, \dots$$

are independent of q_0 , and the integral over q_0 can be immediately evaluated. The resulting expression for the partition function in the single-level approximation is known,

$$Z_0 = \int dq_0 \exp(-\omega_0 q_0^2) \,\tilde{M} \prod_{n=1}^{\infty} (\omega_0^2 + (n\pi/\beta)^2)^{-1/2} \approx \exp\left(-\frac{1}{2}\beta\omega_0\right), \qquad (4.10)$$

A less trivial contribution to the par-

tition function at small temperatures T

comes from the solution that starts near the left maximum of the inverted potential, goes to the other maximum, returns after spending some time there, and then possibly performs a few more excursions

of this sort, *i.e.*, this solution consists of the pairs of trajectories which are usually called a kink and an antikink. No-

tice that the action for a pair of kinks is not proportional to the total time inter-

val $\beta = T^{-1}$ as it would be for a solution

oscillating somewhere inside the well of

the inverted potential -U(q), with a pe-

where we intentionally ignored all excited levels in the well, in agreement with the approximation (which is convenient but not entirely necessary) we made in Eq. (4.8), and the assumed small temperature limit, $\omega\beta \gg 1$; the direct evaluation of the determinant is given in the Feynman's *Quantum Mechanics*... The factor \tilde{M} defines the normalization of the path integral, and, since we know the partition function Z_0 , its form can be derived from Eq. (4.10). Note also, that Eq. (4.10) accounts only for the states of the particle in the left well; it gives only a half of the partition function of the system in the absence of the tunnelling.



Fig. 4.2. A typical two-instanton solution. The "width" of each instanton is much smaller then the total time interval β .

riod ~ $|U''_{top}|^{-1/2}$. Such kinks are called instantons.

As an exercise, consider the fluctuations around a single instanton solution, as shown in Fig. 4.3. Clearly, this solution is *not* periodic in imaginary time and, therefore, the path integral

$$I_{\text{inst}} = \int_{q(0)=q_{\text{left}}}^{q(\beta)=q_{\text{right}}} \mathcal{D}q(\tau) \exp(-S_E[q]), \qquad (4.11)$$



taken over the paths that start at q_{left} for $\tau = 0$ and end at q_{right} after time β does not have a physical meaning of a partition function for some system. Nevertheless, this path integral will be important for the analysis of multi-instanton configuration. Within the steepest descent method we seek the solution $\tilde{q}(\tau)$ of the variational equation (4.7) with zero boundary conditions. Assuming that the total time interval greatly exceeds the characteristic reciprocal frequencies,

 $\beta \gg \omega_0^{-1}, |U_{\rm top}''|^{-1/2},$

Fig. 4.3. A typical extremal trajectory for the path integral (4.11).

the motion along the extremal trajec-

tory consists of a very slow exponential motion in a close vicinities of the maxima of the

inverted potential -U(q) (it takes nearly all the time β), and a "true" motion between these maxima that takes a time of the order of the reciprocal frequency of the intrawell vibrations. The extremal trajectory can be approximated as

$$\bar{q}(\tau) \approx Q_{\text{inst}}(\tau - \tau_0); \quad Q_{\text{inst}}(-\infty) = q_{\text{left}}, \quad Q_{\text{inst}}(\infty) = q_{\text{right}} \equiv -q_{\text{left}},$$
(4.12)

where the function $Q_{\text{inst}}(\tau - \tau_0)$ is an instanton (the term is used for the function $\bar{q}(\tau)$ as well). This solution has the shape of a kink centered at τ_0 , with a width $\sim |U''_{\text{top}}|^{-1/2}$, and it corresponds to the motion in the inverted potential with zero total energy,

$$\frac{dQ_{\text{inst}}}{d\tau} = \left[2U(Q_{\text{inst}})\right]^{1/2}, \quad S_{\text{inst}} = S_E[Q_{\text{inst}}] = \int_{q_{\text{left}}}^{q_{\text{right}}} dq \left[2U(q)\right]^{1/2}.$$
(4.13)

In a simple-minded version of the steepest descent method the path integral (4.11) would be given by the expression

$$I_{\text{inst}} = \tilde{M} \prod_{n} \tilde{\Lambda}_{n}^{-1/2} \exp(-S_{\text{inst}})$$

where Λ_n are the eigenvalues of the linear problem

$$\int_0^\beta d\tau' \frac{\delta^2 S_E}{\delta q(\tau) \delta q(\tau')} \,\tilde{q}_n(\tau') = \tilde{\Lambda}_n \tilde{q}_n(\tau), \quad \tilde{q}_n(0) = \tilde{q}_n(\beta) = 0. \tag{4.9a}$$

However, just like in the case of the fluctuations around the bounce solution, not all eigenvalues $\tilde{\Lambda}_n$ are positive. Specifically, it is easy to see that the function

$$\tilde{q}_0(\tau) = A_0^{-1} \frac{dQ_{\text{inst}}(\tau - \tau_0)}{d\tau}, \quad A_0 = \left[\int d\tau \left(\frac{dQ_{\text{inst}}(\tau)}{d\tau} \right)^2 \right]^{1/2}$$
(4.14)

is a normalized solution of the eigenvalue problem (4.9a) with zero eigenvalue, $\tilde{\Lambda}_0 = 0$. The proof is precisely the same as in the case of a bounce solution—we plug the function (4.14) into Eq. (4.9a) and check that the integrand becomes a full ordinary derivative with respect to the position of the instanton τ_0 of the first functional derivative of the action S_E , evaluated at $Q_{\text{inst}}(\tau - \tau_0)$. This functional derivative vanishes because the instanton solution satisfies the extremum equation (4.7). The prescription for dealing with the zero eigenvalue is, again, the same as in the case of the bounces, and we get, eventually

$$I_{\rm inst} = C_{\rm inst}(\beta) \exp(-S_{\rm inst}); \quad C_{\rm inst}(\beta) = \tilde{M} \frac{A_0}{(2\pi)^{1/2}} \beta \prod_{n=1}^{\infty} \tilde{\Lambda}_n^{-1/2}$$
(4.15)

Unlike the eigenvalue problem (2.24) for the fluctuations in the vicinity of the bounce solution, the equation (4.9a) does not have negative eigenvalues. This follows from the fact that the zero-eigenvalue solution (4.14) does not have nodes, which means that it is the ground state of the instanton eigenvalue problem. Therefore, unlike the bounce which can be viewed as a saddle-type extremum, an instanton provides a *local minimum* to the action. This is, of course, in a perfect agreement with our expectation that the partition function for a two-well potential has no imaginary part.

4.3 Instanton gas.

When analyzing the escape problem, we argued that the vicinity of multi-bounce extremal trajectories give an exponentially small contribution to the imaginary part of the partition function, and that such trajectories can be safely ignored. For the problem of resonant tunneling, however, Eq. (4.6) is non-linear in the tunneling amplitude Δ , and in order to obtain the partition function in this form we need to evaluate the contributions to the partition function from the solutions with an arbitrary number of instanton pairs. This is easy to understand on physical grounds: the level degeneracy is, in some sence, a measure of quantum mechanical delocalization between the wells; classically this implies that the particle moves back and forth between the minima.

The extremal equation (4.7) with the boundary conditions $q(0) = q(\beta) = q_0 \approx q_{\text{left}}$ has solutions with an *arbitrary* number of the kink-antikink pairs at sufficiently small temperatures. The simplest is the solution with one pair of instantons,

$$\bar{q}(\tau) = (q_0 - q_{\text{left}}) \left[\exp\left(-\omega_0 \tau\right) + \exp\left(-\omega_0 \left(\beta - \tau\right)\right) \right] + \bar{q}_{\rightleftharpoons}(\tau),$$

where

$$\bar{q}_{\rightleftharpoons}(\tau) \approx Q_{\text{inst}}(\tau - \tau_1) - Q_{\text{inst}}(\tau - \tau_2), \quad S_E[\bar{q}_{\rightleftharpoons}] = 2S_{\text{inst}},$$
(4.16)

and we assume that the distance between the instanton and the antiinstanton greatly exceeds their widths, $\tau_2 - \tau_1 \gg \omega_0^{-1}, |U_{top}''|^{-1/2}$.



Fig. 4.4. Two-instanton composite solution. The integration over the fluctuations in the vicinity of each instanton is performed independently.

If we attempted to formulate the eigenvalue problem linearized about this solution directly, as we did previously for the bounce solution or the single instanton solution, we would discover two soft modes, corresponding to the fact that the action depends very weakly on the positions of the instantons, as long as they are sufficiently far from each other. The associated divergence can be eliminated by dividing the total time interval in two parts, each of them containing a single instanton or antiinstanton, as illustrated in Fig. 4.4. Of course, to make this decomposition exact, we need to integrate over all possible values of the coordinate $q_{\rm int} \equiv q(\tau_{\rm int})$ at

the separation point τ_{int} , and we may write the path integral for the partition function as a convolution

$$\int_{q(0)=q_0}^{q(\beta)=q_0} \mathcal{D}q(\tau) \, e^{-S_E[0,\beta]} = \int dq_{\rm int} \int_{q(0)=q_0}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, e^{-S_E[0,\tau_{\rm int}]} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\beta)=q_0} \mathcal{D}q(\tau) \, e^{-S_E[\tau_{\rm int},\beta]} \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int} \int_{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}} \mathcal{D}q(\tau) \, dq_{\rm int}}^{q(\tau_{\rm int})=q_{\rm int}}^{q(\tau_{\rm int})=q_{\rm$$

where the temporal arguments in S_E indicate that the action is evaluated for the paths that start and end at the corresponding instants of the imaginary time. If the moment τ_{int} is chosen far enough from the centers of the instantons, $|\tau_{1,2} - \tau_{\text{int}}| \gg \omega_0^{-1}$, $|U''_{\text{top}}|^{-1/2}$, the main contribution to the partition function comes from the values of q_{int} close to the bottom of the right well, q_{right} . The solution of Eq. (4.7) in the range $0 \le \tau \le \tau_{\text{int}}$ that satisfies the boundary conditions $q(0) = q_0 \approx q_{\text{left}}, q(\tau_{\text{int}}) = q_{\text{int}} \approx q_{\text{right}}$ is

$$\bar{q}(\tau) = (q_0 - q_{\text{left}}) \exp(-\omega_0 \tau) + (q_{\text{int}} - q_{\text{right}}) \exp(-\omega_0 (\tau_{\text{int}} - \tau)) + Q_{\text{inst}}(\tau - \tau_1), \quad (4.17)$$

and the corresponding part of the Euclidean action is

$$S_E[\bar{q}; 0, \tau_{\text{int}}] = S_{\text{inst}} + \frac{1}{2}\omega_0 \left[(q_0 - q_{\text{left}})^2 + (q_{\text{int}} - q_{\text{right}})^2 \right].$$
(4.18)

To calculate the prefactor of the two-instanton contribution to the partition function, we need to evaluate the determinant of the second functional derivative of the Euclidean action. Now that we factorized the contributions to the partition function from different instantons, the determinant is also factorized into two independent determinants. For the solution (4.17) the associated eigenvalue problem is of the form (4.9a), with the integration limited to the interval $(0, \tau_{int})$ instead of the total interval $(0, \beta)$. Therefore, the zero mode integration, which can be rewritten as the integral over the instanton position τ_1 , will contribute a multiple $A_0 \tau_{int}/(2\pi)^{1/2}$. The non-singular integration over the remaining modes generates the determinant of the second functional derivative of the Euclidean action, which can be written as

$$\det' \left. \frac{\delta^2 S_E}{\delta q(\tau) \,\delta q(\tau')} \right|_{q=\bar{q}} \equiv \prod_{n=1}^{\infty} \tilde{\Lambda}_n(\tau_{\rm int}) \equiv C_r^{-2} \prod_{n=1}^{\infty} \tilde{\lambda}_n(\tau_{\rm int}), \tag{4.19}$$

where the prime means that zero eigenvalue is omitted, the coefficient

$$C_r^{-2} = \prod_{n=1}^{\infty} \tilde{\Lambda}_n(\tau_{\text{int}}) / \prod_{n=1}^{\infty} \tilde{\lambda}_n(\tau_{\text{int}}),$$

and $\tilde{\lambda}_n(\tau_{\text{int}})$ and $\tilde{\Lambda}_n(\tau_{\text{int}})$ are the eigenvalues of the problems (4.9) and (4.9a) respectively, with the boundaries set at $\tau = 0$ and $\tau = \tau_{\text{int}}$. In the limit where τ_{int} is large compared with the instanton width, the eigenvalue spectrum becomes quasicontinuous, and the coefficient C_r has a finite limit *independent* of $\tau_{\text{int}} \gg \omega_0^{-1}$ or the position of the instanton, as long as the instanton does not too close to the boundaries of the interval. For the special case of quartic potential the coefficient C_r is analyzed in more details in Appendix 4.A.

Using the partition function Eq. (4.10) in the absence of instantons to normalize the path integral at the interval $(0, \tau_{int})$, we can write the contribution of non-singular eigenvalues to the prefactor as

$$\tilde{M}(\tau_{\rm int}) \left[\prod_{n=1}^{\infty} \tilde{\Lambda}_n(\tau_{\rm int})\right]^{-1/2} = C_r \left(\frac{\omega_0}{\pi}\right)^{1/2} \exp\left(-\frac{1}{2}\omega_0\tau_{\rm int}\right).$$
(4.20)

Combining the obtained prefactor with the analogous expression evaluated for the interval $(\tau_{\text{int}}, \beta)$, we notice that the separation point τ_{int} enters only through the intervals of positions τ_1 , τ_2 allowed for the two instantons. Adjusting the position of τ_{int} , we can place these points anywhere within the interval $(0, \beta)$, and, therefore, the total contribution Z_1 of a

kink-antikink pair to the partition function can be written as

$$Z_{1} = \int_{0}^{\beta} d\tau_{2} \int_{0}^{\tau_{2}} d\tau_{1} \left(C_{r} \frac{A_{0}}{(2\pi)^{1/2}} \exp(-S_{\text{inst}}) \right)^{2} \exp\left[-\frac{1}{2} \omega_{0} \left(\tau_{\text{int}} + (\beta - \tau_{\text{int}}) \right) \right] \\ \times \frac{\omega_{0}}{\pi} \int dq_{0} \int dq_{\text{int}} \exp\left(-\omega_{0} (q_{0} - q_{\text{left}})^{2} - \omega_{0} (q_{\text{int}} - q_{\text{right}})^{2}) \right)$$
(4.21)
$$= \left(C_{r} \frac{A_{0}}{(2\pi)^{1/2}} \exp(-S_{\text{inst}}) \right)^{2} \frac{1}{2} \beta^{2} \exp\left(-\frac{1}{2} \omega_{0} \beta \right),$$

where we accounted for the cotribution to the exponent (4.18) and to the prefactor (4.20) for each instanton. Clearly, the auxiliary instant τ_{int} drops out safely.

Similarly, it is easy to find the contribution from an arbitrary number of the instantonantiinstanton pairs,

$$Z_n = \left(C_r \frac{A_0}{(2\pi)^{1/2}} \exp(-S_{\text{inst}})\right)^{2n} \frac{1}{(2n)!} \beta^{2n} \exp(-\frac{1}{2}\omega_0\beta),$$
(4.22)

and sum them up to obtain the total partition function

$$Z = 2\exp\left(-\frac{1}{2}\beta\omega_0\right)\cosh\left(\frac{1}{2}\Delta\beta\right), \quad \Delta = 2C_r \frac{A_0}{(2\pi)^{1/2}}\exp(-S_{\text{inst}}), \quad (4.23)$$

where the additional factor 2 comes from the trajectories that start in the vicinity of the right minimum at $\tau = 0$. Therefore, we have reproduced the conjectured form of the partition function, and we see that the tunnelling splitting Δ is indeed associated with the instantons and it is given by the appropriate exponential.

4.4 Instanton gas in a system with Ohmic dissipation

We shall consider now the effect of dissipation on resonant tunnelling, and again we shall limit ourselves to the model where dissipation is due to linear coupling of the system to a phonon bath. Our starting point will be the equation for the Eucledian action (4.1). We shall rewrite the interaction-induced term that describes the nonlocal in time self-action as:

$$S_{i} = \frac{1}{2} \int_{0}^{\beta} \int_{0}^{\beta} d\tau \, d\tau' \, q(\tau) q(\tau') \frac{d^{2} \Upsilon(\tau - \tau')}{d\tau \, d\tau'} \equiv \frac{1}{2} \int_{0}^{\beta} \int_{0}^{\beta} d\tau \, d\tau' \, \frac{dq(\tau)}{d\tau} \frac{dq(\tau')}{d\tau'} \Upsilon(\tau - \tau'), \quad (4.24)$$

where the non-local dissipative coupling

$$\Upsilon(\tau) = \beta^{-1} \sum_{n \neq 0} \omega_n^{-2} \Phi_n e^{-i\omega_n \tau},$$

is defined in terms of the amplitudes (4.1); we have used the fact that there is no zeroth harmonic in this expansion, $\Phi_{n=0} = 0$, and that $q(\tau)$ is periodic: $q(0) = q(\beta)$.

The analysis depends on the interrelation between the characteristic time scales on which the functions $q(\tau)$, $\Upsilon(\tau)$ vary. The most simple and the most interesting results arise in the case where the bath is "slow", *i.e.* the function $\Upsilon(\tau)$ is smooth on the times $\sim \omega_0^{-1}$, $|U''_{top}|^{-1/2}$ (it is clear that if the bath is "fast" it just follows the tunnelling system adiabatically and nothing dramatic would be expected to happen). An important example of coupling to the bath where the low-lying excitations play a substantial role is the coupling that provides Ohmic dissipation. In this case

$$\Upsilon(\tau) = 2\Gamma\beta^{-1}\sum_{n\neq 0}|\omega_n|^{-1}e^{-i\omega_n\tau} = 4\Gamma\beta^{-1}\sum_{n>0}\operatorname{Im}\int_{-i\infty+\tau}^{\tau}d\tau' e^{-i\omega_n\tau'}$$

$$= -\frac{2\Gamma}{\pi}\ln\left|e^{-2\pi i\tau/\beta} - 1\right| = -\frac{\Gamma}{\pi}\ln\left(4\sin^2\left(\frac{\pi\tau}{\beta}\right)\right) \approx -\frac{2\Gamma}{\pi}\ln\left(\frac{|\tau|}{\bar{\tau}}\right),$$
(4.25)

where we assumed $|\tau| \ll \beta$, and introduced an arbitrary constant under the logarithm using the periodicity of the paths $q(\tau)$. The same result can be easily obtained directly from Eq. (4.4). The approximation of the sine by its argument in Eq. (4.25) is based on the fact that the derivatives $dq/d\tau$ in Eq. (4.24) are large in the range of the order of the duration of an instanton, which is $\sim |U''_{top}|^{-1/2} \ll \beta$. If we "coarsen" over the corresponding time scale, the time-derivatives of the instanton solutions become just δ -functions,

$$d\bar{q}/d\tau = -2 \left| q_{\text{left}} \right| \sum_{i} (-1)^{i} \delta(\tau - \tau_{i}),$$

where τ_i are the positions of the antiinstantons (for even is) and instantons (for odd is).

In writing the partition function in the instanton approximation we have to allow for the fact that the "collisions" of the instantons have to be eliminated explicitly to avoid the divergence in the retarded interaction (4.25) for $\tau = 0$. The easiest way to do it "by hand" is to write the partition function of the system (that of the system + the bath divided by the partition function of the bath) as

$$Z = 2\sum_{n=0}^{\infty} \left(\frac{\bar{\tau}\Delta}{2}\right)^{2n} \int_{0}^{\beta} \frac{ds_{2n}}{\bar{\tau}} \int_{0}^{s_{2n}-\bar{\tau}} \frac{ds_{2n-1}}{\bar{\tau}} \cdots \int_{0}^{s_{2}-\bar{\tau}} \frac{ds_{1}}{\bar{\tau}}$$
$$\times \exp\left[2\alpha \sum_{i>j} (-1)^{i-j} \ln\left(\frac{s_{i}-s_{j}}{\bar{\tau}}\right)\right], \quad \alpha \equiv 4\Gamma |q_{\text{left}}|^{2}/\pi.$$
(4.26)

We have set the cutoff in the logarithms to be the same as that in the integrals, and we have used the "bare" instanton solution to evaluate the correction due to the coupling. The latter aproximation is correct provided the strength of the Ohmic coupling of the particle to the bath is not too large so that the characteristic coupling constant $\alpha \ll S_{\text{inst}}$. The action of the instanton determines the exponent in the tunneling splitting, $S_{\text{inst}} \gg 1$, and therefore although the coupling is weak in some sense, the constant α may exceed unity. It is in this case that the interesting features of the behavior of the system come into play.

Formally, Eq. (4.26) is of the form of the classical grand partition function for a Coulomb gas of alternatively positively and negatively charged rods on a circle of circumference β . The strength of the interaction is given by the parameter α . The parameter $\Delta \bar{\tau}/2$ can be interpreted in terms of effective fugacity, $\Delta \bar{\tau}/2 = \exp(\mu/T^*)$. For finite temperatures $T = \beta^{-1}$ the behavior of the system would be expected to be quite simple: various configurations have different energies, and there should be no singularities in a system of a finite length $\beta < \infty$. However, in the limit $T \to 0$ there may occur a phase transition into a degenerate state—the spontaneous symmetry breaking. In terms of the system we are considering the degenerate state corresponds to localization of the particle in either of the potential wells (in contrast to the situation of tunnelling where the ground state is nondegenerate).

The renormalization-group analysis shows that the transition occurs at $\alpha = 1$; the corresponding auxiliary problem was first considered by Anderson and Yuval who investigated the Kondo problem with an anisotropic coupling; this problem looks quite different from the one we have been considering! The similarity between these problems stems from the fact that both systems have a large number of low-lying excitations. In the tunneling problem, the long-range coupling for the auxiliary Coulomb gas arises because of the substantial contribution of the low-frequency modes of the bath into the kernel $\Upsilon(\tau)$; similarly, the Kondo effect arises because of the coupling of an impurity spin to the low-energy electron-hole excitations in Fermi liquid.

4.5 Spin coupled to a thermal bath

So far we have been considering the problem of a dissipating mechanical particle in a symmetric double-well potential, and we limited ourselves to low temperatures where the intrawell vibrations are "frozen" and the high-energy excitations of the bath are frozen, too (coupling to these excitations gives rise to a standard polaronic effect of the renormalization of the parameters of the system, which we assume to be done). In fact, the only "degree of freedom" that the particle had was related to the tunnelling, and in this sence we studied a two-level system. We would expect, therefore, that we can get similar results for a "true" two-level system. The simplest one is just a spin.

We shall prescribe the values $\sigma_z = 1$ and $\sigma_z = -1$ to the particle localized in the left and the right potential well, respectively. The tunnelling corresponds to the mixing of the two states, and thus it may be described by the term $\frac{1}{2}\Delta\sigma_x$ (obviously, the level splitting in this case is Δ). In writing down the coupling to a bath we will allow for the fact that the wave function of the particle in a potential well is localized inside the wells, and it is exponentially small outside. Therefore it may be a good approximation to assume that the matrix elements of the coupling to the thermal bath are diagonal in the localized state representation, *i.e.*, only the σ_z -component of the spin is coupled to the bath.

The described linear coupling of the spin and a thermal bath can be summarized by the Hamiltonian

$$H = H_0 + H_b + H_i;$$

$$H_0 = \frac{1}{2}\Delta\sigma_x; \quad H_i = \frac{1}{2}\sigma_z \sum_{\mu} f_{\mu}q_{\mu} + \frac{1}{8}\sum_{\mu} f_{\mu}^2/\omega_{\mu}^2; \quad H_b = \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right).$$
(4.27)

To evaluate the partition function we shall use the operators rather than the path integral technique. The main difference of the operator formalism is that the operators generally do not commute with each other, and, in order to develop the expansion in powers of a suitably chosen perturbation V, we need first to separate it from the rest of the Hamiltonian. Generally, this can be done by writing

$$e^{-\beta(H'+V)} = e^{-\beta H'} A(\beta),$$

where the operator $A(\beta)$ satisfies the differential equation

$$\frac{dA(\tau)}{d\tau} = -e^{\tau H'} V e^{-\tau (H'+V)} \equiv -V(\tau) A(\tau), \quad A(0) = 1,$$
(4.28)

and the time-dependent operator $V(\tau)$ is the perturbation operator in the interaction representation,

$$V(\tau) \equiv e^{H'\tau} V e^{-H'\tau}$$

If this operator commutes with itself, $[V(\tau), V(\tau')] = 0$ for an arbitrary pair of moments τ and τ' , the solution of the operator equation (4.28) can be trivially found as an exponent. If this is *not* so, we can still find the solution of the discretized version of Eq. (4.28) as a product

$$A(\tau) = \lim_{N \to \infty} \left[1 - V(\tau_N) \,\Delta \tau \right] \left[1 - V(\tau_{N-1}) \,\Delta \tau \right] \dots \left[1 - V(\tau_1) \,\Delta \tau \right],$$

where the time increment $\Delta \tau \equiv \tau_k - \tau_{k-1} = \tau/N$. This product has the property that the operators at later time always stand to the left of those at earlier time; it can be rewritten identically as a *T*-ordered exponent,

$$A(\tau) = \mathcal{T}_{\tau} \left\{ \exp - \int_0^{\tau} V(\tau) \, d\tau \right\},$$

where the time-ordering operator

$$T_{\tau}[A(\tau_1)B(\tau_2)] = \begin{cases} A(\tau_1)B(\tau_2), & \tau_1 > \tau_2 \\ B(\tau_2)A(\tau_1), & \tau_2 > \tau_1 \end{cases}$$

rearranges the operators that depend on the imaginary time from left to right in the decreasing time order .

Choosing the Hamiltonian of the bath as the non-perturbed part of the Hamiltonian, $H' \equiv H_b$, we can write the non-trivial part of the partition function as

$$Z = \left(1/Z^{(b)}\right) \operatorname{Tr} \exp(-\beta H) = \left(1/Z^{(b)}\right) \exp\left(-\frac{\beta}{8} \sum_{\mu} f_{\mu}^{2}/\omega_{\mu}^{2}\right) \operatorname{Tr} T_{\tau} \left\{ \left(4.29\right) \left(-\frac{\beta}{8} \sum_{\mu} f_{\mu}^{2}/\omega_{\mu}^{2}\right) - \left(-\frac{\beta}{8} \sum_{\mu} f_{\mu}^{2}/\omega_{\mu}^{2}\right) \right\} \right\}$$

$$\times \exp\left(-\frac{\Delta}{2}\int_0^\beta \sigma_x(\tau)\,d\tau\right)\,\prod_\mu \exp\left(-\frac{\beta}{2}\left(p_\mu^2 + \omega_\mu^2 q_\mu^2\right)\right)\,\exp\left(-\frac{f_\mu}{2}\int_0^\beta \sigma_z(\tau)\,q_\mu(\tau)\,d\tau\right)\right\},$$

where $Z^{(b)}$ is the partition function of the bath in the absence of the coupling to the system. Typically, the coupling coefficients f_{μ} are small, $|f_{\mu}| \ll 1$, they are inversely proportional to the number of the degrees of freedom of the bath, and the exponentials of the terms $\propto f_{\mu}$ in Eq. (4.29) can be expanded. Keeping the terms up to the second-order in this expansion, and using the expression

$$\prod_{\mu=1}^{N} (1+\epsilon_{\mu}) = \exp\left(\sum_{\mu} \epsilon_{\mu}\right), \quad \epsilon_{\mu} \sim N^{-1} \ll 1,$$

after some algebra we obtain

$$Z = \text{Tr} T_{\tau} \left\{ \exp\left(-\frac{\Delta}{2} \int_{0}^{\beta} d\tau \, \sigma_{x}(\tau) - \frac{1}{4} \int_{0}^{\beta} d\tau_{1} \int_{0}^{\tau_{1}} d\tau_{2} \, \sigma_{z}(\tau_{1}) \, \sigma_{z}(\tau_{2}) \, \kappa(\tau_{1} - \tau_{2}) \right) \right\}, \quad (4.30)$$

where

$$\kappa(\tau_1 - \tau_2) = \sum_{\mu} f_{\mu}^2 \left(\omega_{\mu}^{-1} \,\delta(\tau_1 - \tau_2) - \langle\!\langle q(\tau_1) \, q(\tau_2) \rangle\!\rangle \right),$$

and the irreducible average $\langle\!\langle q_1 q_2 \rangle\!\rangle \equiv \langle q_1 q_2 \rangle - \langle q_1 \rangle \langle q_2 \rangle$. Expressing the coordinates of the oscillators in terms of the creation and annihilation operators,

$$q_{\mu} = (2\omega_{\mu})^{-1/2}(a_{\mu} + a_{\mu}^{+}), \quad \frac{1}{2}\left(p_{\mu}^{2} + \omega_{\mu}^{2}q_{\mu}^{2}\right) = \omega_{\mu}\left(a_{\mu}^{+}a_{\mu} + \frac{1}{2}\right),$$

it is easy to show that thus defined function $\kappa(\tau)$ is identical to that in Eq. (4.1). Clearly, the motivation for the choice of the constant in the Hamiltonian (4.27) was to arrive at the same form of the expression for the partition function Z as we had before in the problem of a continuous system.

The described procedure is usually called the linked cluster approximation. It is clear that the obtained expression (4.30) for the partition function is correct even if the thermal bath is weakly interacting, as long as the coupling of the system to the individual degrees of freedom is weak enough. For the particular realization of the bath as a collection of harmonic oscillators, our result is actually exact, independently of the strength of the coupling f_{μ} with individual oscillators or the number of degrees of freedom in the bath. This can be proven using the cumulant expansion formula,

$$\left\langle e^A \right\rangle = e^{\langle A \rangle + \langle\!\langle A^2 \rangle\!\rangle/2! + \langle\!\langle A^3 \rangle\!\rangle/3! + \dots},$$

since the irreducible averages $\langle\!\langle q(\tau_1) \dots q(\tau_n) \rangle\!\rangle$ of the products of more than two oscillator's coordinates vanish.

The trace in Eq. (4.30) can be evaluated on the eigenfunctions of σ_z , and since the system is symmetrical with respect to the "up" and "down" states, we can find the matrix element of the operator in Eq. (4.30) on the state "down", and then double the result. Because

$$\sigma_x = \sigma_+ + \sigma_-, \quad \sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y),$$

it is clear that the matrix element of the expansion of the exponent $\exp(a\sigma_x)$ on the functions "down" contains only the sequences $\sigma_{-}\sigma_{+}\ldots\sigma_{-}\sigma_{+}$. In the absence of the coupling the contribution from the 2*n*-th order term in the exponent of Eq. (4.30), evaluated on the functions "down" has the familiar form

$$Z_n = \left(\frac{\Delta\bar{\tau}}{2}\right)^{2n} \int_0^\beta \frac{ds_{2n}}{\bar{\tau}} \int_0^{s_{2n}} \frac{ds_{2n-1}}{\bar{\tau}} \cdots \int_0^{s_2} \frac{ds_1}{\bar{\tau}}, \qquad (4.22').$$

The evaluation of the term related to the interaction is easier if one notices that $\sigma_z^2 = I$ and rewrites

$$\sigma_z(\tau_1) \, \sigma_z(\tau_2) \to -\frac{1}{2} \left[\sigma_z(\tau_1) - \sigma_z(\tau_2) \right]^2.$$

The matrix elements of the operator in the brackets differ from zero only when an operator $\sigma_{\pm}(\tau_i)$ (the "kink") is inserted between the operators σ_z , *i.e.* if $\tau_1 < \tau_i < \tau_2$. The further demonstration of the equivalence of the kink and spin-flip models is absolutely straightforward (see Prob. 4.3 at p. 58), and the final answer for the partition function in the case of Ohmic dissipation is of the form (4.26), with $|q_{\text{left}}| = 1$.

Our next step will be the evaluation of the *kinetics* of tunnelling in the presence of dissipation—the problems of quantum diffusion and of small polarons.

4.A Appendix. Coefficient C_r^{-2} in Eq. (4.19)

Here we analyze the coefficient

$$C_r = \prod_{n=1}^{\infty} \left(\tilde{\lambda}_n(\tau_{\text{int}}) / \tilde{\Lambda}_n(\tau_{\text{int}}) \right)^{1/2}$$

which appeared in Eq. (4.19) as a part of the prefactor resulting from the integration over the paths in the vicinity of the two-instanton solution.

The eigenvalues $\Lambda_n(\tau_{int})$ can be formally obtained by solving the Schrödinger-like equation (4.9a),

$$-\frac{d^2\tilde{q}_n}{d\tau^2} + 2V(\tau)\,\tilde{q}_n = \tilde{\Lambda}_n\,\tilde{q}_n,$$

with the effective potential

$$V(\tau) \equiv U''(Q_{\text{inst}}(\tau)) \tag{4.31}$$

determined by the instanton solution. This potential is different from a constant ω_0^2 only in a narrow range of the coordinate τ , and there may be only a limited number of bound states localized in this region. The corresponding eigenvalues $\tilde{\Lambda}_n^{\text{bound}}(\tau_{\text{int}})$ belong to a discrete spectrum, they do not depend on the size of the region τ_{int} or the position of the instanton. Therefore, the product $\prod \tilde{\Lambda}_n^{\text{bound}}(\tau_{\text{int}})$ is a number of the order of one, independent of τ_{int} .

Now we have to prove that the ratio of the infinite product of the remaining continuous spectrum eigenvalues $\tilde{\Lambda}_n^{\text{cont}}(\tau_{\text{int}})$ and the infinite product of the eigenvalues $\tilde{\lambda}_n(\tau_{\text{int}}) = \omega_0^2 + (n\pi/\tau_{\text{int}})^2$ does not depend on τ_{int} . Away from the instanton position the effective potential (4.31) vanishes, and the wave functions of continuous spectrum can be written as

$$\tilde{q}_n(\tau) = a_{1j} \exp(ip_n \tau) + a_{2j} \exp(-ip_n \tau),$$

where the subscript j = 1 indicates the amplitudes far to the left from the instanton, $\tau_1 - \tau \gg \omega_0^{-1}$, and j = 2 far to the right from the instanton, $\tau - \tau_1 \gg \omega_0^{-1}$; again, we assume $\omega_0 \sim |U_{\text{top}}'|^{1/2}$. The coefficients a_{ij} are related by the transmission matrix,

$$a_{i1} = t_{ij} \, a_{j2}, \tag{4.32}$$

which describes the scattered and the transmitted amplitudes of a plane wave by the localized potential. The quantized values of the momentum p_n can be obtained using the boundary conditions $\tilde{q}_n(0) = \tilde{q}_n(\tau_{\text{int}}) = 0$,

$$\exp(2ip_n\tau_{\rm int}) = \frac{t_{11} + t_{21}}{t_{12} + t_{22}} \equiv \exp(2i\theta(p)), \quad \Rightarrow \quad p_n = \frac{n\pi + \theta(p_n)}{\tau_{\rm int}}, \quad n = 0, \pm 1, \pm 2, \dots \quad (4.33)$$

so that the corresponding eigenvalues of the continuous spectrum

$$\tilde{\Lambda}_n^{\rm cont}(\tau_{\rm int}) = \omega_0^2 + p_n^2.$$

This representation relies on the fact that the absolute value of the ratio of the combinations of the matrix elements t_{ij} in Eq. (4.33) is equal to 1, which follows from the fact that the Schrödinger equation (4.9a) is real, and therefore a complex conjugate solution is also a solution, with the same energy (see Prob. 4.2). Using Eq. (4.33) we can find the ratio of the infinite products of the eigenvalues of quasicontinuous spectrum,

$$\frac{\prod \tilde{\Lambda}_n^{\text{cont}}(\tau_{\text{int}})}{\prod \tilde{\lambda}_n(\tau_{\text{int}})} \approx \exp\left[\sum_n \frac{p_n^2 - (n\pi/\tau_{\text{int}})^2}{\omega_0^2 + (n\pi/\tau_{\text{int}})^2}\right] \approx \exp\left(\frac{2}{\pi} \int dp \, \frac{p \, \theta(p)}{\omega_0^2 + p^2}\right),$$

which is obviously independent of τ_{int} .

Problems

▶ **Problem 4.1** (page 103)

Using the usual Schrödinger equation, find the tunneling energy gap between symmetric and antisymmetric states of a particle in a quartic two-well potential

$$U(q) = -\frac{1}{2}\Omega^2 q^2 \left(1 - \lambda \frac{q^2}{q_0^2}\right).$$

Assume the energy of the particle and other parameters of the problem are such that the quasiclassic approximation applies near the middle of the barrier.

▶ **Problem 4.2** (page 103)

Show that the matrix elements of the transmission matrix (4.32) obey the relationsip

$$|(t_{11} + t_{21})/(t_{12} + t_{22})| = 1.$$

▶ **Problem 4.3** (page 103)

Evaluate the partition function of a spin linearly coupled to a phonon bath, with the Hamiltonian (4.27), and show that at low temperatures this formulation is equivalent to the instanton formulation for a continuous system. For the case of Ohmic dissipation, find the coupling between the spin flips mediated by the bath.

Lecture 5

Quantum kinetic equation

5.1 Relaxation of a spin coupled to a phonon bath

We have to relate the results of the instanton analysis of tunnelling with dissipation to observable properties of a tunnelling system. A simple physical realization of such system is a reorienting defect in a cubic crystal. An example is a two-atomic molecule replacing a host ion at the lattice cite of an alkilehalide crystal; such molecules are usually oriented along one of the symmetry axes, and, therefore, they have several equivalent orientations within a cell.

The resonant tunnelling occurs between the corresponding states (hindered rotation, for higher energies). Another example is the case of so-called off-center impurities: if the ionic radius of an impurity ion is small, the ion often moves away from the lattice cite along one of the symmetry axes, and then, again, it has equivalent positions within a cell, and the resonant tunnelling between these positions may occur (the best known system of this sort is KCl:Li⁺).

Experimentally, the dynamics of a tunnelling centre can be investigated by measuring its absorption spectrum. Because of the tunnelling, the line(s) in the absorption spectrum appear at the frequency(ies) equal to the tunnelling splitting Δ . By applying an electric field, experimentalists can make the orientations of the impurity nonequivalent, and so they have control over the frequencies. The corresponding effect is sometimes called paraelectric resonance, by analogy with paramagnetic resonance (ESR).



Fig. 5.2.

Coupling of the tunnelling system to a bath broadens the spectral lines. It is straight-



Fig. 5.1.

forward to analyse this broadening for weak enough coupling in the model of a spin linearly coupled to a phonon bath that we have discussed before (the results can be immediately generalized to a system with several degenerate states, like an off-center ion in a cubic crystal). The Hamiltonian we have considered was of the form:

$$H = H_0 + H_b + H_i, \quad H_0 = \frac{1}{2}\Delta \sigma_x, \quad H_b = \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right),$$
$$H_i = \frac{1}{2}\sigma_z \sum_{\mu} f_{\mu}q_{\mu} + \frac{1}{8}\sum_{\mu} f_{\mu}^2/\omega_{\mu}^2; \tag{5.1}$$

The symmetric and the antisymmetric states of a two-well system correspond to the eigenstates $|m\rangle$, $m = \pm 1$ of the Pauli matrix, $\sigma_x |m\rangle = m |m\rangle$. The coupling gives rise to the transitions between the states. The width of the corresponding spectral line is determined by the sum of the rates of the transitions "up" and "down", which, in turn, are given by the "golden rule"

$$W \equiv W_{\uparrow} + W_{\downarrow} = 2\pi \sum_{m=\pm 1} \left\langle \left| \left(m, \{n_{\mu}\} | H_{i} | - m, \{n_{\mu}'\} \right) \right|^{2} \delta(m\Delta - \sum_{\mu} \omega_{\mu}(n_{\mu}' - n_{\mu})) \right\rangle, \quad (5.2)$$
$$W = \frac{1}{2} F(\Delta) \coth\left(\Delta/2T\right), \quad F(\omega) = \frac{\pi}{2} \sum_{\mu} \left(f_{\mu}^{2}/\omega_{\mu} \right) \delta(\omega - \omega_{\mu}).$$



The averaging in Eq. (5.2) is performed over the thermal distribution of the vibrations of the bath (the state with a given set $\{n_{\mu}\}$ of the occupation numbers of the modes has the energy $\sum_{\mu} \omega_{\mu}(n_{\mu} + \frac{1}{2})$). In this approximation only the modes with the energy equal to the distance Δ between the levels contribute to the transitions. Notice also that the dimension of the coupling coefficients in the spin Hamiltonian (5.1) differs from that in the coordinate representation, and so does the dimension of the density of states of the bath weighted with the coupling, $F(\omega)$.

In the particular case of Ohmic dissipation the function $F(\omega)$ is proportional to the frequency ω , and

$$W = \pi \alpha \Delta \coth\left(\frac{\Delta}{2T}\right),\tag{5.3}$$

where $\alpha \equiv F(\omega)/2\pi\omega$ is the dimensionless coupling constant introduced in Sec. 4.4. When deriving Eqs. (5.2), (5.3) we assumed that the coupling is weak. This means that the broadening of the levels W is very much smaller than the distance Δ between them. For Ohmic dissipation, this requires the inequality $\alpha \ll 1$; *i.e.*, we are to keep away from the interesting region where the phase transition to a localized state may occur. But even for small values of α , as it is seen from Eq. (5.3), the criterion $W \ll \Delta$ will be violated if the temperature is high enough. For Ohmic dissipation this will happen for $T \gtrsim T_0 = \Delta/\pi\alpha$.

In the range $W \ll \Delta$ the motion of the tunnelling system is simple: if we localize it initially in one of the wells (*i.e.*, $\sigma_z(0) = \pm 1$), it will perform underdamped oscillations between the wells, at the frequency Δ , and, as we shall see in the next section, with the decrement given by W/2. Correspondingly, the absorption spectrum of the system has a peak at the frequency Δ with the halfwidth at the halfmaximum equal to W/2 (the famous result by Weisskopf and Wigner). The questions that we have to answer are: What will happen to the dynamics and to the absorption spectrum if the temperature is raised, or if the coupling is not weak—what will replace the underdamped oscillations? What is the role of other coupling mechanisms, including coupling to electron-hole pairs? What will be the shape of the absorption spectrum if we have more than two levels, even for weak coupling—does the above theory apply to a harmonic oscillator?

5.2 Quantum kinetic equation

The approach we shall use to answer the formulated questions is based on the quantum kinetic equation (QKE). The kinetic equation is an *approximation*. But a good one, and an intuitive one. QKE is formulated for the density operator of a system, $\rho(t)$ (it is often called—and we will often call it that way—the density matrix). The density matrix is a quantum analog of the probability density distribution: it gives the distribution of a system over the quantum states, the probability to find the system in a state with the wave function $|\gamma\rangle$ is given by $(\gamma |\rho| \gamma)$. The time evolution of the density matrix follows from its expansion into the matrix elements on the eigenfunctions of the system $|m\rangle$:

$$(\gamma|\rho(t)|\gamma) = \sum_{m,m'} (\gamma|m(t))\rho_{mm'}(m'(t)|\gamma) \quad \Rightarrow \quad \rho(t) = e^{-iHt}\rho(0)e^{iHt},$$

where H is the Hamiltonian of the system. This implies that the equation for the density matrix can be written in the form:

$$\dot{\rho} = i[\rho, H] \tag{5.4}$$

The average value of any operator \hat{A} is expressed in terms of the density matrix as

$$\langle \hat{A}(t) \rangle = \operatorname{Tr} \left[\hat{A}(t)\rho(0) \right] \equiv \operatorname{Tr} \left[e^{iHt} \hat{A} e^{-iHt} \rho(0) \right] = \operatorname{Tr} \left[\hat{A}(0)\rho(t) \right],$$

therefore, the density operator provides the basic information about the evolution of the observables (notice that the time dependence of $\rho(t)$ is different from the time dependence of the operators in the Heisenberg representation).

The problem is that we need the density operator for the system alone, whereas Eq. (5.4) defines, in the general case of a system coupled to a bath, the time evolution of the density matrix of the system + bath, $\rho_{\rm sb}$. Somehow, we have to eliminate the infinite number of bath's degrees of freedom, and get an equation just for the density operator of the system itself. This equation will be the quantum kinetic equation.

There are several ways to formulate QKE. We shall start with the simplest formulation. Suppose we are interested in the problem of the dynamics of a spin coupled to a bath, and we *assume* that at the initial instant of time t = 0 we know the state of the spin, *i.e.*, we know its density matrix $\rho(0)$. We also *assume* that we know the state of the bath—the bath is in a thermal equilibrium, its density matrix

$$\rho_b(0) \equiv \rho_b^{\text{eq}} = (1/Z^{(b)}) \exp(-\beta H_b), \qquad Z^{(b)} = \text{Tr}_b \exp(-\beta H_b),$$
(5.5)

where Tr_b means the trace over the variables of the bath. Of course, this is an approximation: our assumptions imply that at t = 0 the density matrix of the system + bath is factorized. In other words, we assume that the coupling between the system and the bath is turned on at t = 0. This makes sense provided the coupling is not very strong. We shall see later on what are the actual criteria.

Once we know the initial conditions and the Hamiltonian of the system + bath—it may be of the form (5.1), *e.g.*,—we can write down the density matrix of the system + bath,

$$\rho_{\rm sb}(t) = e^{-i(H_0 + H_b + H_i)t} \rho_{\rm sb}(0) e^{i(H_0 + H_b + H_i)t} \equiv e^{-i(H_0 + H_b)t} U(t) \rho_{\rm sb}(0) U^{\dagger}(t) e^{i(H_0 + H_b)t},$$
$$U(t) = T_t \exp\left(-i \int_0^t dt' H_i(t')\right), \quad H_i(t) = e^{i(H_0 + H_b)t} H_i e^{-i(H_0 + H_b)t}, \tag{5.6}$$

where T_t is the standard operator of chronological ordering. The quantity we are interested in, the density matrix of the system *without* the bath, also called the *reduced* density matrix, is the trace of the matrix $\rho_{sb}(t)$ over the variables of the bath, and we will be evaluating it in the interaction representation:

$$\rho(t) = e^{-iH_0 t} \tilde{\rho}(t) e^{iH_0 t}, \quad \tilde{\rho}(t) = \operatorname{Tr}_b \left[U(t) \rho_{\rm sb}(0) U^{\dagger}(t) \right].$$
(5.7)

The perturbative expansion of the density matrix is obtained by expanding the unitary operators $U(t), U^{\dagger}(t)$,

$$U(t) = 1 - i \int_0^t dt_1 H_i(t_1) - \int_0^t dt_1 \int_0^{t_1} dt_2 H_i(t_1) H_i(t_2) + \dots$$
(5.8)

Each term of this expansion contains some number of operators H_i on both sides from the initial density matrix $\rho_{\rm sb}(0)$. We have to integrate over the positions of these operators, keeping in mind their order, namely, that the terms with larger argument in the expansion of U(t) are on the left, whereas in the expansion of $U^{\dagger}(t)$ they are on the right.



Grafically, every term of the perturbation series can be represented as an appropriate number of dots placed at two horizontal lines as shown in Fig. 5.4. The dots along the upper line represent the terms from the expansion of U(t); they must be arranged in *decreasing* time order as indicated by the arrow. Then, after inserting the initial density matrix $\rho(0)$, follow the terms from the expansion

of $U^{\dagger}(t)$, arranged with *increasing* time; these terms are represented by the dots along the lower line. After this identifications, the subsequent derivation is very similar to the standard Green's function technique, just for a two-particle Green's function.

For the coupling of the form (5.1) (which we assume to be weak at the moment), the first-order term in the constructed expansion vanishes: the average values of the coordinates of the bath $q_{\mu} \equiv (2\omega_{\mu})^{-1/2}(a_{\mu} + a_{\mu}^{\dagger})$ are equal to zero in thermal equilibrium (the factor $\rho_b(0)$ in $\rho_{\rm sb}(0)$ that depends on the variables of the bath is just the equilibrium distribution). The nonzero terms in the expansion of U(t), $U^{\dagger}(t)$ are the ones that contain the pairs $a_{\mu}(t)a_{\mu}^{\dagger}(t')$ with the same μ . Because the parameters f_{μ} are small (they contain the factor $N^{-1/2}$, where N is the number of degrees of freedom of the bath), the Wick's theorem is satisfied, and we have to allow no more than one pair of such terms for each μ . We have three combinations: a pair coming out of U(t), a pair from $U^{\dagger}(t)$, and a pair from the cross-term. Defining the equilibrium correlation function

$$\phi(t) \equiv \langle q(t) \, q(0) \rangle = \sum_{\mu} \frac{f_{\mu}^2}{2\omega_{\mu}} \left[\bar{n}_{\mu} e^{i\omega_{\mu}t} + (\bar{n}_{\mu} + 1)e^{-i\omega_{\mu}t} \right], \quad \bar{n}_{\mu} = \left[e^{\beta\omega_{\mu}} - 1 \right]^{-1}, \tag{5.9}$$

we obtain $\tilde{\rho}(t)$ up to second order:



$$\tilde{\rho}^{(2)}(t) = \rho(0)$$

$$- \frac{1}{4} \int_{0}^{t} dt_{1} \int_{0}^{t_{1}} dt_{2} \sigma_{z}(t_{1}) \sigma_{z}(t_{2}) \phi(t_{1} - t_{2}) \rho(0)$$

$$- \frac{1}{4} \rho(0) \int_{0}^{t} dt_{1} \int_{0}^{t_{1}} dt_{2} \sigma_{z}(t_{2}) \sigma_{z}(t_{1}) \phi(t_{2} - t_{1})$$

$$+ \frac{1}{4} \int_{0}^{t} dt_{1} \sigma_{z}(t_{1}) \rho(0) \int_{0}^{t} dt_{2} \sigma_{z}(t_{2}) \phi(t_{2} - t_{1}). \quad (5.10)$$



The time dependence of the operators $\sigma_z(t)$ in the interaction representation is known,

$$\sigma_z(t) = \frac{1}{2} \left(\sigma_z(0) + i\sigma_y(0) \right) e^{-i\Delta t} + \frac{1}{2} \left(\sigma_z(0) - i\sigma_y(0) \right) e^{i\Delta t}$$

Before evaluating the integrals, let us notice that the density matrix $\tilde{\rho}(t)$ varies in time only because of the coupling, *i.e.*, it varies over the characteristic time of the order of the decay probability W given by Eq. (5.2), and therefore the characteristic time in Eq. (5.10) is $t \sim W^{-1} \gg \Delta^{-1}$. On this time scale the integrands in Eq. (5.10) are rapidly oscillating (or rapidly decaying) functions. The characteristic range of $|t_1 - t_2|$ that contributes to the integrals (5.10) is given by the maximum,

$$t_c = \max\left(\Delta^{-1}, t_{\rm cor}\right),$$

where $t_{\rm cor}$ is the characteristic correlation time of the fluctuations in the bath weighted with the coupling—this is the time over which the function $\phi(t)$ decays.

The time t_c determines the characteristic distance between the dots connected into a pair. This distance is small compared to the total time range, therefore, on the coarsened time scale the dots within a pair merge

together. This tells us immediately that in the fourth order the diagrams that have nested pairs, intersecting lines, or just overlapping pairs are small—their contribution is of the order of t_c/t . So, if we are interested in the main contribution to the higher-order terms of the expansion of $U(t)\rho(0)U^{\dagger}(t)$, we have to keep only the diagrams that consist of pairs of the dots arranged successively. But then we have a simple series, and we can easily evaluate the sum of the diagrams.

It is convenient to write the emerging equation not for the density matrix $\tilde{\rho}(t)$, which depends on the density matrix $\rho(0) \equiv \tilde{\rho}(0)$ of the initially prepared system, but for the Green's function G(t) defined as

$$\tilde{\rho}_{mm'}(t) = G_{mm'}^{nn'}(t)\rho_{nn'}(0), \quad G_{mm'}^{nn'}(0) = \delta_{mn}\delta_{m'n'}.$$
(5.11)



In the following, the upper indices will be often suppressed, and that the two-particle function G will enter the usual operator products in place of the density matrix $\rho_{mm'}$. Graphically, the sum of all diagrams can be represented as



Here the pair of bold lines correspond to G(t), whereas the pair of thin lines is $G^{(0)}(t)$, the Green's function in the absence of the coupling. The box is the polarization operator $\Pi_{ll'}^{nn'}(t,t_1)$; the form of this operator, as well as the limits of the integration in t_1 can be understood by inspecting Eq. (5.10).

Taking the time-derivative of Eq. (5.12), and accounting for the fact that the internal integration in Π requires $t_1 - t_2 \sim t_c \ll t$, we obtain the differential form of the equation for the Green's function

$$\frac{d}{dt}G(t) = -\frac{1}{4}\int_0^t dt\sigma_z(t)\sigma_z(t_1)\phi(t-t_1)G(t) - \frac{1}{4}G(t)\int_0^t dt_1\sigma_z(t_1)\sigma_z(t)\phi(t_1-t) \quad (5.13) \\
+\frac{1}{4}\int_0^t dt_1\sigma_z(t_1)G(t)\sigma_z(t)\phi(t-t_1) + \frac{1}{4}\int_0^t dt_1\sigma_z(t)G(t)\sigma_z(t_1)\phi(t_1-t).$$

It is understood that only the slow-varying terms should be kept here; *e.g.*, the terms oscillating as $\exp(\pm 2i\Delta t)$ that come from the products of the operators σ_z should be dropped—they do not contribute to the integrals in the original integral equation.

Eq. (5.13) is a conventional QKE for the system we are considering. Among other important features, this equation is Markovian: the derivative of the operator G(t) at the instant t is determined by the value G(t) at the same instant. Again, this is similar to what we had in the classical theory. We have obtained this equation in the Born approximation—we have allowed for the second-order terms in H_i only. This limitation can be avoided: the approximation that we have done essentially is that the collisions are short, the dots are grouped in pairs, and the time intervals between the collisions (between the pairs) are very much longer than the distances between the dots within pairs.

An alternative form of the QKE is

$$\frac{d}{dt}G(t) = -\int_0^t dt_1 \operatorname{Tr}_b \{ [H_i(t), [H_i(t_1), G(t)\rho_b^{\text{eq}}]] \}$$
(5.14)

This short equation describes a lot of phenomena!

5.3 Kinetics of a two-state system weakly coupled to a bath

To obtain the QKE for a spin linearly coupled to a thermal bath,

$$H_i = \frac{1}{2} \,\sigma_z \sum_{\mu} f_{\mu} q_{\mu},$$

in the explicit *operator* form we have to plug the expressions for the operators $\sigma_z(t)$ into Eq. (5.13), and perform the time integration. The typical "building blocks" are of the form

$$\int_0^t dt_1 \exp\left[i\left(\omega \pm \Delta\right)(t-t_1)\right] = \pi \delta(\omega \pm \Delta) + iP\left(\omega \pm \Delta\right)^{-1}, \ t \gg t_c,$$

where the symbol P means that the principal value of the corresponding integral over ω should be taken. We will also need standard identities for the Pauli matrices,

$$\sigma_{\kappa}^{2} = 1 \ (\kappa = x, y, z), \quad \sigma_{-}\sigma_{+} = \frac{1}{2}(1 - \sigma_{x}), \quad [\sigma_{+}, \sigma_{-}] = \sigma_{x}, \quad \sigma_{\pm} = \frac{1}{2}(\sigma_{z} \mp i\sigma_{y}),$$

and the equilibrium phonon correlator (5.9), which is convenient to express in terms of the function $F(\omega)$,

$$\phi(t) = \frac{1}{\pi} \int d\omega F(\omega) \left[\bar{n}(\omega) e^{i\omega t} + (\bar{n}(\omega) + 1) e^{-i\omega t} \right].$$

The first term in the QKE, corresponding to the first term in Eq. (5.13), is

$$-\frac{1}{4}\int_{0}^{t} dt \,\sigma_{z}(t)\sigma_{z}(t_{1})\phi(t-t_{1})G(t) = -\frac{1}{8}F(\Delta)\left[\coth\left(\frac{\Delta}{2T}\right) + \sigma_{x}(t)\right]G(t)$$

$$+\frac{i}{4\pi}P\int d\omega F(\omega)\left[\frac{\omega}{\omega^{2}-\Delta^{2}} + \sigma_{x}(t)\frac{\Delta}{\omega^{2}-\Delta^{2}}\coth\left(\frac{\omega}{2T}\right)\right]G(t).$$
(5.15)

The structure of the remaining terms is very similar to that of Eq. (5.15). The term where both operators σ_z are on the right is just the Hermitian conjugate to Eq. (5.15). The two terms where G(t) is inserted between the operators σ_z are Hermitian conjugate to each other. The complete QKE for this system is

$$\frac{\partial}{\partial t}G(t) = -\frac{1}{2}WG(t) - \frac{1}{8}F(\Delta)[\sigma_x(t)G(t) + G(t)\sigma_x(t)] - i\frac{1}{2}\mathcal{P}[\sigma_x(t), G(t)] + \frac{1}{2}F(\Delta)\{\bar{n}(\Delta)\sigma_+(t)G(t)\sigma_-(t) + (\bar{n}(\Delta) + 1)\sigma_-(t)G(t)\sigma_+(t)\}, \quad (5.16)$$

where

$$W = \frac{1}{2}F(\Delta)\coth\left(\frac{\Delta}{2T}\right), \quad \mathcal{P} = -2P\int d\omega F(\omega)\frac{\Delta}{\omega^2 - \Delta^2}\coth\left(\frac{\omega}{2T}\right). \tag{5.17}$$

There are terms of the two types in the QKE (5.16), and this is typical for quantum kinetic equations for weakly coupled systems:

- (i) the terms that are proportional to $F(\Delta)$, the weighted density of states of the bath at the frequency of the transitions. These terms describe the decay processes where a transition between the states of the system is accompanied by birth or death of the excitations in the medium. Those of them with the operators on the left or on the right from G correspond to the transitions from a given state of the system due to the scattering and determine the lifetime of the state. The others, with the operators on the both sides of G, describe not just the processes that bring the system to a given state (substantial for the diagonal matrix element of G), but they also allow for the "interference" of the scattering processes. Indeed, we are considering the density matrix ρ_{mn} which refers to two states of the system, m and n, and scattering event involving the same phonon can occur in both states, so, we do have an interference here.
- (ii) The term $\propto \mathcal{P}$ that corresponds to virtual processes. Virtual excitations "dress" the system and renormalize its energy spectrum; the fact that we have just a renormalization here follows from the comparison of the term $\propto \mathcal{P}$ with the term $-\frac{1}{2}i\Delta[\sigma_x,\rho]$ in the initial kinetic equation (*prior* to going to the interaction representation). It is clear that the renormalization comes just to $\Delta \rightarrow \Delta + \mathcal{P}$. In the following discussion this renormalization is assumed to have been done, and the term $\propto \mathcal{P}$ is dropped.



Fig. 5.7. Different states of the spin from the viewpoint of the continuum system.

In order to appreciate the consequences of the derived QKE, we first need to understand very clearly the meaning of the different components of the density matrix

$$\rho = \left(\begin{array}{cc} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{array}\right),$$

where the components are labeled in the usual representation where $\hat{\sigma}_z$ is diagonal. For the tunneling system the probability to find the spin in the position "up", which is characterized by the wavefunction $|z_+\rangle = (1,0)^t$, is

$$P(z_{+}) = (1,0) \left(\begin{array}{c} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{array} \right) \left(\begin{array}{c} 1 \\ 0 \end{array} \right) = \rho_{++}.$$

The probability to find the spin pointing down is, of course,

$$P(z_{-}) = \rho_{--} = 1 - \rho_{++}.$$

Similarly, the probability to find the spin aligned in x-direction, the state characterized by the eigenfunction $|x_+\rangle = (1/\sqrt{2}, 1/\sqrt{2})^t$ of the operator $\hat{\sigma}_x$, is

$$P(x_{+}) = \frac{1}{2} (1,1) \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2} (1+\rho_{+-}+\rho_{-+}).$$

These simple expressions imply that the average

$$\langle \hat{\sigma}_z \rangle \equiv \text{Tr} \{ \hat{\sigma}_z \, \rho \} = \rho_{++} - \rho_{--} = P(z_+) - P(z_-)$$

defines the assymetry of the state, while

$$\langle \hat{\sigma}_x \rangle \equiv \text{Tr} \{ \hat{\sigma}_x \rho \} = \rho_{+-} + \rho_{-+} = P(x_+) - P(x_-)$$

defines the population difference between the symmetric and the antisymmetric states of the quantum well.

The quantum kinetic equation (5.16) was derived in the interaction representation, and it does not account for the evolution associated with the bare system Hamiltonian H_0 . This implies that the average of any operator $\mathcal{O}(t)$ evolves according to the expression

$$\frac{d}{dt} \langle \mathcal{O}(t) \rangle = -i \langle [\mathcal{O}(t), H_0] \rangle + \operatorname{Tr} \{ \mathcal{O}(t) \dot{G}(t) \}, \quad \langle \mathcal{O}(t) \rangle \equiv \operatorname{Tr} \{ \mathcal{O}(t) G(t) \}.$$
(5.18)

It is straightforward to see that Eq. (5.16) results in the following equations for the relaxation of the difference in the populations of the excited and ground states, $\langle \sigma_x(t) \rangle$, and for the off-diagonal matrix element $\langle \sigma_-(t) \rangle \equiv \langle \frac{1}{2} [\sigma_z(t) + i\sigma_y(t)] \rangle$,

$$\frac{d}{dt}\langle\sigma_x(t)\rangle = -W\langle\sigma_x(t)\rangle - \frac{1}{2}F(\Delta), \quad \frac{d}{dt}\langle\sigma_-(t)\rangle = -\left(i\Delta + \frac{1}{2}W\right)\langle\sigma_-(t)\rangle.$$
(5.19)

Both equations look reasonable: earlier we evaluated W as a sum of the reciprocal lifetimes of the system in the ground and excited states, and we noticed that the absorption spectrum (whose shape is determined by the relaxation of the matrix element of the transition from the ground to the excited state) has a halfwidth $\frac{1}{2}W$. The free term in the equation for $\langle \sigma_x(t) \rangle$ is necessary to establish the equilibrium Hibbs distribution. Indeed, in equilibrium the system is characterised by non-zero average

$$\langle \sigma_x \rangle = P(x_+) - P(x_-) = -\frac{F(\Delta)}{2W} = -\tanh\left(\frac{\Delta}{2T}\right) = \frac{\exp(-\Delta/T) - 1}{\exp(-\Delta/T) + 1}$$

which is exactly the expected equilibrium population difference.

The explicit form of QKE is more complicated for more complicated systems. However, for any system with a finite number of states the operator G(t) has a finite number of the matrix elements $G_{nn'}^{mm'}(t)$, and the QKE has a form of a set of linear differential equations for $G_{nn'}^{mm'}(t)$, which is quite straightforward to solve if the parameters are known. The situation is more interesting for systems with an infinite number of levels, as, for example, a harmonic or a weakly anharmonic oscillator. The first question here is how many parameters of relaxation do we have? For a harmonic oscillator linearly coupled to a bath we would expect to have one parameter (there was one parameter in the classical theory). The QKE in this case may be solved in the explicit form by the generating function method, and the solution resolves the "paradoxon" of the harmonic oscillator described in the problem 5.4 at p. 73.

5.4 Quasielastic phonon scattering: diffusion vs tunnelling.

The derived QKE applies to an arbitrary two-level system weakly coupled to a bath, with the coupling linear in phonon operators. The only point where we appealed to the fact that we had in mind a tunnelling system was the discussion of the form of the interaction Hamiltonian. It is straightforward to see that the results hold true if we allow for other terms linear in a_{μ} , a_{μ}^{+} , like $\sigma_y(a_{\mu} + a_{\mu}^{+})$ (in this case we will have the function $F(\omega)$ renormalized) or $\sigma_x(a_{\mu} + a_{\mu}^{+})$ (to the second order of the perturbation theory, the corresponding processes do not affect the slow-time kinetics of the system).

For a realistic tunnelling system it is interesting to investigate the case where the tunnelling splitting Δ is smaller than the relaxation rate: intuitively, one may expect that by making Δ arbitrarily small we will not "switch off" the relaxation. On the other hand, if we apply the above results to the case where the density of states of the bath weighted with coupling $F(\omega)$ falls down *faster* than ω for small ω (which is usually true in the case of coupling to a real phonon bath, but which is not so in the case of Ohmic dissipation, as we shall see below) the effective coupling constant $\alpha_{\Delta} \equiv F(\Delta)/2\pi\Delta$ will fall down with the decreasing Δ , *i.e.* the relaxation will be switching off. The physical reason for this behavior lies in the fact that at $\Delta = 0$ both states $|x_{\pm}\rangle$ evolve coherently in time; the scattering events (after the renormalization of Δ is accounted for) transfer the system between these two states without destroying their coherence. Therefore, even at relatively high temperatures the quantum tunneling is not suppressed, and the coupling of the system to the thermal bath cannot change the spectrum.



An extremely important mechanism of relaxation for tunnelling systems coupled to a phonon bath is the relaxation that occurs when phonons are *scattered* by the system, nearly elastically. The scattering can be viewed as a random modulation of the *phase* of the wave function. The phase of an *n*th state in the absence of interaction is the argument of the exponential $\exp(-iE_nt + i\phi_n)$, with ϕ_n independent of time. When a phonon is scattered by the system, ϕ_n changes, which means that we have a random process $\phi_n(t)$. Now, let us

consider the resonant tunnelling problem. Here, the wave functions of the states with the same energy (in the absence of the tunnelling) are coherent in time, and, therefore, a small perturbation (mixing of the states by the exponentially small tunnelling matrix element) *accumulates* in time. The random modulation of the phase difference between the states breaks their coherence, the interference of the states implied into the concept of resonant tunnelling is no longer there, and thus the tunnelling it suppressed.

The simplest form of the interaction Hamiltonian that describes the quasielastic scatter-

ing by phonons is

$$H_i^{(sc)} = \sum_{\mu,\mu'} \frac{f_{\mu\mu'}}{(\omega_\mu\omega_{\mu'})^{1/2}} a_\mu^+ a_{\mu'} + \frac{1}{2} \sigma_z \sum_{\mu,\mu'} \frac{f_{\mu\mu'}}{(\omega_\mu\omega_{\mu'})^{1/2}} a_\mu^+ a_{\mu'}, \qquad (5.20)$$

where a_{μ}^{+} , a_{μ} are the creation and annihilation operators of the μ th phonon, and we have allowed for the fact that the coupling to phonons is different in the two "intrawell" states of the system that correspond to the eigenvalues $\sigma_{z} = \pm 1$. Clearly, the first term only renormalizes the phonon spectrum, and we shall ignore this term in the following, assuming such renormalization has been done.

The time dependence of all terms in the QKE due to $H_i^{(sc)}$, taken to the second order of the perturbation theory, is the same as that of the term

$$-\frac{1}{4}\sigma_{z}(t)\int_{0}^{t}dt_{1}\sigma_{z}(t_{1})\phi^{(\mathrm{sc})}(t-t_{1}), \quad \phi^{(\mathrm{sc})}(t) = \sum_{\mu,\mu'}\frac{|f_{\mu\mu'}|^{2}}{\omega_{\mu}\omega_{\mu'}}\bar{n}(\omega_{\mu})(\bar{n}(\omega_{\mu'})+1)\exp\left[i\left(\omega_{\mu}-\omega_{\mu'}\right)t\right]$$

In evaluating the integral we shall assume at this point that the temperature greatly exceeds the tunnelling splitting, $T \gg \Delta$. It is the temperature that determines, in the important case of coupling to acoustic phonons, the characteristic frequencies of the phonons that are excited and thus can be scattered. For $T \gg \Delta$ the characteristic phonon frequencies in the integral above greatly exceed the tunnelling splitting Δ , and the time dependence of the operators $\sigma_z(t)$ can be ignored. On the whole, the integral for $t \gg T^{-1}$ is equal just to a constant. The real part of this constant (which corresponds to relaxation processes and which is only substantial in the present problem) is $-\frac{1}{4}W^{(sc)}$, where

$$W^{(sc)} = \pi \sum_{\mu,\mu'} \frac{|f_{\mu\mu'}|^2}{\omega_{\mu}\omega_{\mu'}} \bar{n}(\omega_{\mu})(\bar{n}(\omega_{\mu'}) + 1)\delta(\omega_{\mu} - \omega_{\mu'})$$
(5.21)

Clearly, the scattering is quasielastic: the energy of the scattered phonon is equal to that of the incident one, and the probability of the event is proportional to the number of the phonons "prepared" to be scattered $\bar{n}(\omega_{\mu})$ times the bosonic "emission" factor $\bar{n}(\omega_{\mu'}) + 1$.

The operator in the QKE that describes the scattering processes has the form

$$\left(\frac{dG}{dt}\right)^{(sc)} = -\frac{1}{2}W^{(sc)}G(t) + \frac{1}{2}W^{(sc)}\sigma_z(t)G(t)\sigma_z(t), \quad T \gg W^{(sc)}.$$
 (5.22)

The scattering processes themselves do not give rise to any relaxation of the populations of the intrawell states, the difference in the populations $\langle \sigma_z(t) \rangle$ does not change because of them directly. However, the scattering destroys the coherence of the states, and therefore it affects the interwell transitions (that come into play via tunnelling) which in their turn provide the relaxation of $\langle \sigma_z(t) \rangle$. The equations of motion for the average values of the components of the spin that follow from (5.22) (in the neglect of the decay processes due to the transitions between the tunnel-split states that we considered before) are of the form

$$\frac{d}{dt}\langle\sigma_{-}\rangle = -i\Delta\langle\sigma_{-}(t)\rangle - \frac{1}{2}W^{(\mathrm{sc})}\left(\langle\sigma_{-}\rangle - \langle\sigma_{+}\rangle\right), \quad \frac{d}{dt}\langle\sigma_{x}\rangle = -W^{(\mathrm{sc})}\langle\sigma_{x}(t)\rangle.$$
(5.23)

The quantity $\langle \sigma_x(t) \rangle$ is the measure of the coherence of the intrawell wave functions, *i.e.* of the eigenfunctions $|\uparrow\rangle$, $|\downarrow\rangle$ of the operator σ_z ,

$$\langle \sigma_x(t) \rangle = 2 \operatorname{Re} G_{\uparrow\downarrow}(t)$$

If there were no tunnelling and relaxation, the phase difference between the corresponding up and down states would remain constant. Because of the phonon scattering, the coherence is broken, the phase difference is modulated randomly, and the average $\langle \sigma_x(t) \rangle$ falls down exponentially. This can be interpreted in terms of phase diffusion,

$$\langle \exp\left[i\left(\phi_{\uparrow}(t)-\phi_{\downarrow}(t)\right)\right]\rangle = \exp\left(-W^{(\mathrm{sc})}t\right) \times \exp\left[i\left(\phi_{\uparrow}(0)-\phi_{\downarrow}(0)\right)\right],$$

where $W^{(sc)}$ is the phase diffusion coefficient,

$$\langle \left[\phi_{\uparrow}(t) - \phi_{\downarrow}(t)\right]^2 \rangle - \left[\phi_{\uparrow}(0) - \phi_{\downarrow}(0)\right]^2 = 2W^{(\mathrm{sc})}t.$$

The transport between the two wells is convenient to describe by two coupled real-valued equations that follow from Eq. (5.23),

$$\frac{d}{dt}\langle\sigma_z\rangle = \Delta\langle\sigma_y(t)\rangle, \quad \frac{d}{dt}\langle\sigma_y\rangle = -\Delta\langle\sigma_z(t)\rangle - W^{(\rm sc)}\langle\sigma_y(t)\rangle, \tag{5.24}$$

or an equivalent second-order differential equation for $\langle \sigma_z(t) \rangle$ alone,

$$\frac{d^2}{dt^2} \left\langle \sigma_z(t) \right\rangle + W^{(sc)} \frac{d}{dt} \left\langle \sigma_z(t) \right\rangle + \Delta^2 \left\langle \sigma_z(t) \right\rangle = 0.$$
(5.25)

The general solution for $\langle \sigma_z(t) \rangle$ can be written in the form

$$\langle \sigma_z(t) \rangle = \exp\left(-\frac{1}{2}W^{(\mathrm{sc})}t\right) \left[\sigma_z(0)\cos\tilde{\Delta}t + \tilde{\Delta}^{-1}\left(\dot{\sigma}_z(0) + \frac{1}{2}W^{(\mathrm{sc})}\sigma_z(0)\right)\sin\tilde{\Delta}t\right], \quad (5.26)$$

where the energy gap is renormalized solely because of the damping,

$$\tilde{\Delta} = \left[\Delta^2 - \frac{1}{4} \left(W^{(\mathrm{sc})}\right)^2\right]^{1/2}.$$

It follows from this expression that for $W^{(sc)} < 2\Delta$ the populations of the wells oscillate. In the absence of the dissipation these oscillations persist, as the usual quantum-mechanical oscillations are supposed to, and they decay if the dissipation is present.

An interesting situation arises in the case where the dissipation is strong compared to the tunnelling,

$$W^{(\mathrm{sc})} \gg \Delta.$$
 (5.27)

It is easy to see from Eqs. (5.24)–(5.26) that the kinetics of the system in this regime is characterized by two very different time scales. First, over the time $\sim 1/W^{(sc)}$, the interwell matrix elements of the density matrix $\langle \sigma_x(t) \rangle$, $\langle \sigma_y(t) \rangle$ decay down to their quasistationary values, determined by a given $\langle \sigma_z(t) \rangle$. Then, over a much linger time $\sim \nu_d^{-1}$, where

$$\nu_d = \Delta^2 / W^{(\mathrm{sc})},\tag{5.28}$$

the populations of the wells relax to their equilibrium values,

$$\langle \sigma_z(t) \rangle \approx e^{-\nu_d t} \langle \sigma_z(0) \rangle$$

This relaxation, described by the overdamped form of Eq. (5.25), occurs because of the tunnelling, of course. But this is the tunnelling in the situation of broken coherence, and the relaxation time exceeds strongly both the "initial" relaxation time $1/W^{(sc)}$, and the reciprocal tunnelling splitting $1/\Delta$.

To interpret the rate (5.28) we can think of it in terms of the transition probability as given by the Fermi's golden rule: the product of the squared absolute value of the matrix element of the transition times the density of states. The transition matrix element that mixes the states in the two wells is Δ , whereas the characteristic "density of states" (the reciprocal bandwidth) is the lifetime $1/W^{(sc)}$ within which the states become incoherent, so we get just ν_d . When understood in such terms, it is clear that what we have here is not a coherent tunnelling but hopping, or diffusion over the intrawell states, and ν_d is just the diffusion coefficient.

The picture of hopping that replaces the coherent tunnelling in the range (5.27) applies to systems with an arbitrary number of resonant states, including diffusion of impurities (or muons) over the interstitial positions in crystals, or hopping of an off-center ion over its equivalent orientations. If we limit ourselves to the tunneling between the nearest neighboring sites (just for clarity), we can write the Hamiltonian in the form

$$H_0 = \frac{1}{2} \Delta \sum_m \left(b_{m+1}^+ b_m + b_m^+ b_{m+1} \right), \quad H_i = \frac{1}{2} \sum_m b_m^+ b_m \sum_{\mu,\mu'} \frac{f_{\mu\mu'}^{(m)}}{(\omega_\mu \omega_{\mu'})^{1/2}} a_\mu^+ a_{\mu'}, \tag{5.29}$$

where the operators b_m^+ , b_m create and annihilate the tunnelling (hopping) particle at the site m, and Δ is the tunnelling matrix element.

For temperatures $T \gg \Delta$ we have the same picture of the on-site scattering of the phonons by the particle as we had before, and in the neglect of the shift of the energy level of the system due to the cou-



pling (5.29) (notice that here, as well as in the problem of a spin considered above, the shift arises in the *first* order in H_i) the QKE has a simple form:

$$\frac{dG}{dt} = -\frac{1}{2} \sum_{m} w_{mm} b_m^+(t) b_m(t) G(t) - \frac{1}{2} \sum_{m} w_{mm} G(t) b_m^+(t) b_m(t) + \sum_{mm'} w_{mm'} b_m^+(t) b_m(t) G(t) b_{m'}^+(t) b_{m'}(t), \qquad (5.30)$$

where the transition probability

$$w_{mm'} = \pi \operatorname{Re} \sum_{\mu,\mu'} \frac{f_{\mu\mu'}^{(m)} \left(f_{\mu\mu'}^{(m')}\right)^*}{\omega_{\mu}\omega_{\mu'}} \bar{n}(\omega_{\mu})(\bar{n}(\omega_{\mu'}) + 1)\delta(\omega_{\mu} - \omega_{\mu'})$$
is evaluated in assumption that there is only one particle, $b_m^+ b_m b_{m'}^+ b_{m'} = \delta_{mm'} b_m^+ b_m$. The equations for the average values of the operators are:

$$\frac{d}{dt}\langle b_m^+(t)b_m(t)\rangle = \Delta \operatorname{Im}\left\langle \left(b_m^+(t)b_{m-1}(t) - b_{m+1}^+(t)b_m(t)\right)\right\rangle,\tag{5.31}$$

$$\frac{d}{dt}\langle b_m^+(t)b_{m-1}(t)\rangle = -\frac{1}{2}i\Delta\left\langle \left(b_m^+(t)b_m(t) - b_{m-1}^+(t)b_{m-1}(t)\right)\right\rangle - \frac{1}{2}W^{(\mathrm{sc})}\langle b_m^+(t)b_{m-1}(t)\rangle + \dots$$

where

$$W^{(sc)} = \frac{\pi}{2} \sum_{\mu,\mu'} \frac{\left| f_{\mu\mu'}^{(m)} - f_{\mu\mu'}^{(m-1)} \right|^2}{\omega_\mu \omega_{\mu'}} \bar{n}(\omega_\mu) (\bar{n}(\omega_{\mu'}) + 1) \delta(\omega_\mu - \omega_{\mu'}), \tag{5.32}$$

and the dots in Eq. (5.31) indicate the omitted terms which contain the averages $\langle b_m^+(t)b_{m'}(t)\rangle$ with $|m - m'| \geq 2$. The parameter $W^{(sc)}$ is the diffusion coefficient for the phase difference between the states m and m + 1; this phase diffusion is caused by phonons scattered off the system.

In the range of parameters (5.27), where the scattering rate exceeds the tunnelling rate, the off-diagonal (intersite) averages in Eq. (5.31) are small and *fast*: they decay to their quasistationary values (for given occupations of the states) over the time $\sim 1/W^{(sc)}$, whereas the occupations themselves vary over the time $1/\nu_d$, as we expected. These quasistationary values are given by

$$\left\langle b_m^+(t)b_{m-1}(t)\right\rangle \approx -i\frac{\Delta}{W^{(\mathrm{sc})}}\left\langle \left(b_m^+(t)b_m(t) - b_{m-1}^+(t)b_{m-1}(t)\right)\right\rangle$$

By plugging this expression into the equation (5.31) for the populations of the states we arrive at the diffusion equation for the populations:

$$\frac{d}{dt}\langle b_m^+(t)b_m(t))\rangle = \nu_d \left\langle \left(b_{m+1}^+(t)b_{m+1}(t) + b_{m-1}^+(t)b_{m-1}(t) - 2b_m^+(t)b_m(t)\right)\right\rangle$$
(5.33)

with ν_d given by Eq. (5.28). The obtained Eq. (5.33) has a simple form of a diffusion equation. We notice that this equation applies even in the situation of an infinite number of equivalent sites, and is an alternative to the standard notion of the diffusion in the momentum space. The latter occurs if the tunnelling is *strong* and the bandwidth Δ greatly *exceeds* the relaxation rate. In the opposite case we still have a diffusion, but in the *coordinate* space. This process is sometimes called quantum diffusion, and it has been observed in various experiments.

Problems

▶ **Problem 5.1** (page 104)

Small polysterene spheres submerged into water are known to form crystals, for high enough densities. Find the dispersion law for low-lying modes of a crystal formed by Brownian particles. The result applies also, for T exceeding the Debye temperature, to the modes of a 2D Wigner crystal formed by electrons on helium surface: in contrast to Brownian particles

electrons are light, and they are scatterred by low-frequency capillary waves (see Prob. 5.2 below).

▶ **Problem 5.2** (page 104)

Derive the quantum kinetic equation for an electron in a semiconductor which is coupled to acoustic phonons, with the Hamiltonian

$$H = H_0 + H_b + H_i, \quad H_0 = \frac{\mathbf{p}^2}{2m}, \quad H_b = \sum_{\mathbf{q}} \omega_q a_{\mathbf{q}}^+ a_{\mathbf{q}}, \quad H_i = \sum_{\mathbf{q}} f_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} a_{\mathbf{q}} + \text{h.c.}$$

Assume that the temperature (the characteristic energy of an electron) is high—find what it should exceed for (i) the quantum kinetic equation to apply, and (ii) for the scattering to be quasielastic, *i.e.*, for the change of the electron energy to be much less than the energy itself.

▶ **Problem 5.3** (page 106)

Derive the quantum kinetic equation for a harmonic oscillator linearly coupled to a thermal bath, with the Hamiltonian

$$H_0 = \frac{1}{2}(p^2 + \omega_0^2 q^2), \quad H_i = q \sum_{\mu} f_{\mu} q_{\mu}, \quad H_b = \frac{1}{2} \sum_{\mu} (p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2)$$

Assume the coupling to be weak, and the density of states of the bath weighted with coupling to be smooth near ω_0 .

▶ **Problem 5.4** (page 106)

For the harmonic oscillator from the previous problem, evaluate the total lifetime of the *n*th level. What would the absorption spectrum of the oscillator for finite temperatures look like if you considered the oscillator as a set of two-level systems (optical transitions occur between the neighboring levels only)? Does the result agree with what you got for this model before? What is wrong? This is the "paradoxon" of harmonic oscillator.

▶ **Problem 5.5** (page 107)

Large polaron is a self-localized state of a conduction electron in a polar crystal: the electron polarizes the crystal and gets localized in the potential well created by the polarization. The total energy consists of the kinetic energy of the electron $T = \mathbf{p}^2/2m$ (*m* is the effective mass), the potential energy $V(\mathbf{r})$ of the electron in the polarization potential, and the energy of the polarization. The potential energy

$$V(\mathbf{r}) = -e \int d^3 \mathbf{r}_1 \frac{\nabla \cdot \mathbf{P}(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|}, \quad \mathbf{D}[\psi; \mathbf{r}] = -e \int d^3 \mathbf{r}_1 |\psi(\mathbf{r}_1)|^2 \frac{\mathbf{r} - \mathbf{r}_1}{|\mathbf{r} - \mathbf{r}_1|^3}$$
(5.34)

Here, **P**, **D** are the polarization and the electric displacement, respectively; $\psi(\mathbf{r})$ is the electron wave function. It is substantial that the "fast" motion of the localized electrons that form a periodic potential is already incorporated into the effective mass of the conduction electron, and the polarization in (1) is the "slow" part of the total polarization,

$$\mathbf{P}(\mathbf{r}) = \frac{c}{4\pi} \mathbf{D}(\mathbf{r}), \quad c = \epsilon_{\infty}^{-1} - \epsilon^{-1}.$$
(5.35)

 $(\epsilon_{\infty}, \epsilon$ are high- and low-frequency dielectric constants). The full potential energy of the electron and the polarized crystal is given by

$$W = -\frac{1}{2} \int d^3 \mathbf{r} \, \mathbf{P}(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r}) = -\frac{c}{8\pi} \int d^3 \mathbf{r} \, \mathbf{D}^2(\mathbf{r})$$
(5.36)

There is a sort of a virial theorem for the polaron in the ground state: all the energies are multiples of the kinetic energy, T : -W : -E : -V = 1 : 2 : 3 : 4 (here, E = T + V is the total electron energy). Prove this theorem (change $\mathbf{r} \to k\mathbf{r}$ in the wave function of the ground state and allow for the fact that k = 1 provides the minimum to the total energy of the system).

▶ **Problem 5.6** (page 108)

Derive the quantum kinetic equation for a resonantly driven two-level system. Allow for two types of relaxation processes: decay processes (the Hamiltonian H_{i1}), that correspond to the transitions between the states with emission of a phonon, and the processes that correspond to quasielastic scattering of phonons by the system (the Hamiltonian H_{i2} ; this scattering gives rise to random modulation of the phase difference between the states of the system).

$$H = H_0 + H_b + H_{i1} + H_{i2} + H_F, \quad H_0 = \frac{1}{2}\omega_0\sigma_z, \quad H_b = \frac{1}{2}\sum_{\mu} \left(p_{\mu}^2 + \omega_{\mu}^2 q_{\mu}^2\right),$$
$$H_{i1} = \frac{1}{2}\sigma_x \sum_{\mu} f_{\mu}q_{\mu}, \quad H_{i2} = \frac{1}{2}\sigma_x \sum_{\mu,\mu'} f_{\mu\mu'}q_{\mu}q_{\mu'}$$
$$H_F = \frac{1}{2}\sigma_x F \cos \omega t, \quad |\omega - \omega_0| \ll \omega$$

(notice the difference in notations with what we had in Lecture 5.) In deriving the equation keep second-order terms in $H_{i1,2}$, and first-order resonant terms in H_F . Assume $T \ll \omega_0$. Solve the equation for the matrix elements of the density matrix in the stationary regime, and find the dependence of the absorption coefficient on the field amplitude F. This dependence describes what is called absorption saturation.

▶ **Problem 5.7** (page 109)

Find the temperature dependence of the relaxation rate related to the quasielastic phonon scattering in the former problem in the case of an impurity coupled to acoustic phonons. This is the basic broadening mechanism of narrow (zero-phonon) spectral lines of impurities in solids for not too low temperatures.

Lecture 6

Hopping of a strongly coupled system.

6.1 Qualitative arguments.

The kinetics of a tunnelling system coupled to a phonon bath is characterized by several quantities that have the dimension of energy (or frequency):

| tunnelling | frequency | phonon | temperature | two-phonon |
|------------|----------------|--------------------|-------------|---------------------|
| splitting | $_{\rm shift}$ | bandwidth | | scattering rate |
| Δ | \mathcal{P} | $t_{\rm cor}^{-1}$ | T | $W^{(\mathrm{sc})}$ |

(the frequency shift due to the coupling to phonons was considered in Lecture 5). So far the analysis was limited to the case of weak coupling, where the quantities \mathcal{P} , $W^{(sc)}$ that characterize the coupling are small, at least compared to the phonon bandwidth, *i.e.*, to the reciprocal time t_{cor}^{-1} over which the correlations in the bath decay.¹ In this case the coupling linear in the phonon coordinates is not very substantial for the small tunnelling rate Δ , provided the temperature is not too small and the density of states of the bath weighted with coupling decays superlinearly as the frequency goes down to zero.

A qualitatively different physical situation arises in the case where coupling is not weak. Generally speaking, both couplings that are linear and nonlinear in the phonon coordinates may be strong, but usually the strength falls down quite fast with the increasing order of the nonlinearity, and, therefore, we shall limit ourselves to a strong coupling linear in the coordinates. We will first consider the kinetics of a two-state system (*e.g.*, a system moving in a double-well potential), and again we will be using the spin model to describe it. Let us write the Hamiltonian of this model as

$$H = H_0 + H_b + H_i, \quad H_0 = \frac{1}{2} \Delta \sigma_x, \quad H_b = \sum_{\mu} \omega_{\mu} a_{\mu}^+ a_{\mu},$$
$$H_i = \frac{1}{2} \sigma_z \sum_{\mu} (2\omega_{\mu})^{-1/2} \left(f_{\mu} a_{\mu} + f_{\mu}^* a_{\mu}^+ \right), \tag{6.1}$$

¹We shall see later on that $t_{\rm cor}$ should be specified more carefully: we are interested in the correlations at the frequencies that characterize the system and depend on the coupling to it, therefore for certain types of coupling where low-frequency modes are important, like for Ohmic dissipation, $t_{\rm cor}$ may be large for a broad phonon band.

where a_{μ}^{+} , a_{μ} are the phonon creation and annihilation operators.

The matrix element of the coupling Hamiltonian is different depending on whether the system occupies the left or the right well (the states $|\uparrow\rangle$) or $|\downarrow\rangle$, respectively): *e.g.*, if the system is a defect that has two equivalent orientations in an elementary cell, then the different atoms are "more perturbed" when it is in one or the other orientation. Once the phonon bath has adjusted itself to the position of the system (the neighboring atoms have shifted appropriately), the potential for the system is changed, and it is no longer symmetrical: the level in the empty well lies higher than in the occupied one. Resonant tunnelling occurs when both the system and the bath switch simultaneously.

The difference in the energies of the intrawell levels in the absence of the tunnelling $(\Delta \rightarrow 0)$ can be evaluated using a simple perturbation theory. It is characterized by the quantity $P_{\rm st}$ very similar to the Stocks shift in optics:

$$P_{\rm st} = \frac{1}{2} \sum_{\mu} \left(f_{\mu}^2 / \omega_{\mu}^2 \right) \equiv \frac{1}{\pi} \int d\omega \, \omega^{-1} F(\omega) \tag{6.2}$$

Strong coupling occurs when the level shift exceeds both the tunnelling splitting (and thus the tunnelling is suppressed) and the characteristic reciprocal correlation time of the bath:

$$P_{\rm st} \gg \Delta, t_{\rm cor}^{-1}$$
 (6.3)



Further analysis depends crucially on temperature we are interested in. For T = 0 the only way for the system to switch from one well to another is via bringing the whole phonon configuration with it, and therefore there is tunnelling, but the tunnelling rate is exponentially small since it contains the product of the overlap integrals for the wave functions of all the phonons.

We shall consider the situation where T is high enough (but not too high, though). The physical picture of the transitions between the intrawell states in this case is quite simple. Thermal fluctuations in the bath give rise to the fluctuations of the potential in which the system moves and thus of the interlevel spacing. These fluctuations have the characteristic correlation time $t_{\rm cor}$ and are Gaussian. The magnitude of the fluctuations of the level spacing can be estimated if one notices that, for given expectation values of the phonon operators $\bar{a}_{\mu}, \bar{a}_{\mu}^{+}$, the level shift is given by $\sim \text{Re} \sum f_{\mu}\bar{a}_{\mu}$, and therefore in the range of T where the phonon fluctuations are classical the mean square fluctuations of the level spacing are $\sigma \sim P_{\rm st}T$. If $T \ll P_{\rm st}$ (as we assume) the energies of the levels are strongly different for the



Fig. 6.1. When adjusted to the position of the system, oscillators of the thermal bath may shift the position of the occupied level and thus suppress the resonant tunneling.

most of the time. The probability for the levels to cross is given, for Gaussian fluctuations, by $\exp(-P_{\rm st}^2/2\sigma)$, *i.e.*, it is of the activation type, with the exponent ~ $P_{\rm st}/T$. When the levels are crossing there may occur a tunnelling transition, but then the levels are detuned very fast and the system remains localized in a new state. It stays there until the next appropriate large fluctuation occurs. On the whole the switching between the states is of the type of hopping. The idea of hopping of this sort was put forward by Holstein and by Yamashita and Kurosawa in the context of small polaron transport.

6.2 Small-polaron transformation.

The basic tool for the analysis of the transport in the case of strong coupling is the famous small-polaron canonical transformation

$$S = \exp\left[\sigma_z \sum_{\mu} (2\omega_{\mu})^{-3/2} \left(f_{\mu}a_{\mu} - f_{\mu}^* a_{\mu}^+\right)\right], \quad \tilde{a}_{\mu} \equiv S^+ a_{\mu}S = a_{\mu} - (2\omega_{\mu})^{-3/2} \sigma_z f_{\mu}^* \qquad (6.4)$$

The transformed Hamiltonian is of the form

$$\tilde{H} \equiv S^{+}HS = H_{1} + H_{b} - \frac{1}{8}\sum_{\mu}\omega_{\mu}^{-2}|f_{\mu}|^{2}, \qquad (6.5)$$

$$H_{1} = \frac{1}{4}\hat{\Delta}(\sigma_{x} + i\sigma_{y}) + \text{h.c.}, \quad \hat{\Delta} = \Delta \exp\left[-2\sum_{\mu} (2\omega_{\mu})^{-3/2} \left(f_{\mu}a_{\mu} - f_{\mu}^{*}a_{\mu}^{+}\right)\right].$$

The idea of the transformation (6.4) is that it makes the Hamiltonian diagonal in the intrawell representation: it adjusts the equilibrium positions of phonons (*i.e.*, the positions of the atoms surrounding the defects, or, more generally, the expectation values of a_{μ}, a_{μ}^{+}) to the position of the system in each of the wells. But then, since these phonon positions are different in different wells, the operator of the interwell transitions becomes an operator in the space of phonon variables, not in the space of the variables of the system only.

If we were looking for the "coherent" tunnelling transitions where phonons are not created or annihilated, we would have to evaluate the diagonal (in the phonon variables) matrix element of the tunnelling operator,

$$\langle \hat{\Delta} \rangle \equiv \operatorname{Tr}_b \rho_b \hat{\Delta} = \Delta e^{-Q}, \quad Q = \frac{1}{4} \sum_{\mu} \omega_{\mu}^{-3} |f_{\mu}|^2 \left[2\bar{n}(\omega_{\mu}) + 1 \right], \quad Q \gg 1.$$
(6.6)

The factor Q is the famous Debye-Waller factor which arises whenever there are transitions between the states that correspond to different equilibrium positions of phonons. It follows from the inequality (6.3) that the factor Q is parametrically large for strong coupling. The rate of the coherent tunnelling is exponentially small, respectively, with the parametrically large exponent. This rate falls down with the increasing temperature (in general case, there is also an opposite effect of the fluctuational preparation of the barrier for a tunnelling system by a fluctuating bath; we will not consider this effect in what follows).

For not too small T the transitions between the intrawell states occur via the hopping mechanism described above. We may expect that since the duration of the transition is determined by the time over which the fluctuating intrawell levels remain nearly in resonance whereas the transitions themselves occur very occasionally, a transition might play the role of a scattering event from the point of view of kinetics, and for small enough Δ the interval between the "collisions" (switchings) will greatly exceed the duration of a collision. In this case the quantum kinetic equation (QKE) would apply. However, now we have to consider the Hamiltonian H_1 as a perturbation, and we will *neglect* the coherent terms $\sim \langle \hat{\Delta} \rangle$ as given by Eq. (6.6).²

If we skip the terms linear in H_1 , and allow for the second-order terms only, then the QKE for the canonically transformed density matrix takes on the familiar form of Eq. (5.14) of Lecture 6, with the only difference being that $H_i(t)$ should be replaced by $H_1(t)$. The "building block" for the kinetic equation is of the form

$$\int_{0}^{t} dt' \operatorname{Tr}_{b} H_{1}(t) H_{1}(t') = \frac{1}{16} \Delta^{2} \left(\sigma_{x} + i\sigma_{y} \right) \left(\sigma_{x} - i\sigma_{y} \right) \int_{0}^{t} dt' e^{-\left[\psi(0) - \psi(t - t')\right]} + \text{h.c.}, \quad (6.7)$$
$$\psi(t) = \frac{1}{2} \sum_{\mu} \omega_{\mu}^{-3} |f_{\mu}|^{2} \left[\bar{n}_{\mu} e^{i\omega_{\mu}t} + \left(\bar{n}_{\mu} + 1 \right) e^{-i\omega_{\mu}t} \right],$$

In evaluating the integral (6.7) we have to allow for the fact that $\psi(0) = 2Q \gg 1$, and, therefore, the major contribution to the integral comes from the range where t' is close to t—this is just what we need! The function $\psi(t)$ has an extremum at $t_0 = -i/2T$; calculating the integral with the steepest descent method we get the hopping rate

$$W^{(\text{hop})} = \frac{1}{8} \Delta^2 \int_0^t dt' \, e^{-[\psi(0) - \psi(t - t')]} = \frac{1}{8} \Delta^2 t_{\text{hop}} \times \exp(-E_{\text{hop}}/T), \tag{6.8}$$

where

$$E_{\rm hop} = \frac{1}{2}T \sum_{\mu} \frac{|f_{\mu}|^2}{\omega_{\mu}^3} \tanh(\omega_{\mu}/4T), \qquad t_{\rm hop} = 2\pi^{1/2} \left[\sum_{\mu} \frac{|f_{\mu}|^2}{\omega_{\mu} \sinh(\omega_{\mu}/2T)}\right]^{-1/2}$$

The time t_{hop} is the typical time interval that contributes to the integral over time, and, therefore, it gives the characteristic duration of hopping event, an analogue of the duration of the collision. Our analysis applies if this time interval is small compared to the characteristic frequencies of the phonons that contribute to $\psi(t)$,

$$t_{\rm hop} \ll t_{\rm cor}.$$

It is obvious from this inequality, in particular, that we are limited to the range of not too low temperatures.

The QKE for the canonically transformed density matrix takes on the form

$$\frac{\partial \tilde{G}}{\partial t} = -W^{(\text{hop})} \left[\tilde{G}(t) - \frac{1}{4} (\sigma_x + i\sigma_y) \tilde{G}(t) (\sigma_x - i\sigma_y) - \frac{1}{4} (\sigma_x - i\sigma_y) \tilde{G}(t) (\sigma_x + i\sigma_y) \right], \quad (6.9)$$

²A huge amount of work has been done to match the low-T transport of small polarons, that occurs via coherent tunnelling of the system and the bath and is of the band-like diffusion, to the high-T hopping-type transport, and not that the complete solution has been obtained in the closed form; however, the physics is quite clear, and we will not go into the details of the behavior of the system in the crossover region.

where tilde is used to show that the Green's function (and the density matrix) have been subject to the small-polaron canonical transformation (6.4). The matrices $(\sigma_x \pm i\sigma_y)$ raise/lower the system to or from the state $|\uparrow\rangle$, respectively. It is not surprising that, when written for the diagonal matrix elements of \tilde{G} (these matrix elements are not changed as a result of the transformation (6.4)), Eq. (6.9) has the form of a balance equation,

$$\frac{\partial n_{\uparrow}}{\partial t} = -W^{(\text{hop})} \left(n_{\uparrow} - n_{\downarrow} \right), \quad \frac{\partial n_{\downarrow}}{\partial t} = -W^{(\text{hop})} \left(n_{\downarrow} - n_{\uparrow} \right).$$

Clearly, the system is hopping between the wells, *i.e.*, between the states $|\uparrow\rangle$ and $|\downarrow\rangle$, and the probability of hopping is given by $W^{(\text{hop})}$.

The temperature dependence of the rate $W^{(\text{hop})}$ is of the activation type for the temperatures exceeding the phonon frequencies (*i.e.*, the Debye temperature T_D)—again, in agreement with the qualitative arguments discussed above. For $T > T_D$ the activation energy E_{hop} is independent of T, and $E_{\text{hop}} \sim P_{\text{st}}$, as expected. In real systems the activation dependence of $W^{(\text{hop})}$ often extends to the range of temperatures below T_D .

6.3 Ohmic dissipation.

The above arguments should be taken with care in the case of Ohmic coupling to the bath, such that

$$\frac{\pi}{2}\sum_{\mu}\omega_{\mu}^{-1}|f_{\mu}|^{2}\,\delta(\omega-\omega_{\mu})=2\Gamma\omega$$

The high-T small polaron results do not change dramatically in this case: it is obvious that the integrals that give the activation energy E_{hop} and the duration of the hopping t_{hop} converge safely, and the main contribution to these integrals comes from the range of high frequencies.

A different situation occurs for T = 0, and again, we are prepared from our instanton experience that something unusual may happen here (*e.g.*, localization for a strong enough coupling—the phase transition in the instanton "liquid"). For Ohmic dissipation the Debye-Waller factor Q (6.6) diverges logarithmically at low frequencies (there are no problems at high frequencies: there is always a high-frequency cutoff imposed by the change of the coupling, or the change of the density of states of the bath, or presence of higher energy levels of the system, etc). The divergence of Q does not mean localization: it does not depend on the coupling strength, *e.g.*, and it would be strange if the localization happened for an arbitrarily weak coupling. However, this divergence is a sort of the orthogonality catastrophe introduced by Anderson: the overlap integral of the adiabatic intrawell wave functions is equal to zero when the density of states weighted with coupling falls down slowly enough with the decreasing energy of the low-lying excitations (phonons, in the present case).

An insight into the localization of a tunnelling system due to its coupling to a bath can be gained and the critical value of the coupling parameter Γ can be obtained from the following arguments: the factor $\exp(-Q)$ describes renormalization of the tunnelling matrix elements due to phonons that follow the system adiabatically, and can adjust themselves to the intrawell position before the system switches to another position. The frequencies of such phonons should exceed some quantity $\bar{\omega}$ which, in its turn, exceeds the tunnelling splitting,

$$\bar{\omega} = p\Delta, \quad p \gg 1,$$

The adiabatically renormalized tunnelling matrix element is given by

$$\Delta' = \Delta \exp\left[-Q\left(\bar{\omega}\right)\right], \quad Q(\bar{\omega}) = \frac{1}{4} \sum_{\omega_{\mu} \ge \bar{\omega}} \omega_{\mu}^{-3} \left|f_{\mu}\right|^{2}.$$
(6.10)

After the tunneling splitting Δ has been reduced according to Eq. (6.10), even slower modes of the bath can adjust to the position of the system, and we can further reduce the minimal cut-off frequency $\bar{\omega}$, find a new Δ' , further reduce $\bar{\omega}$, and so on, until at the end we arrive at the self-consistent expression for the renormalized tunneling rate of the form

$$\bar{\Delta} = \Delta \exp\left[-Q\left(p\bar{\Delta}\right)\right] \tag{6.11}$$

The solution of this equation in the case of Ohmic dissipation reads

$$\bar{\Delta} = \Delta \left(\frac{p\Delta}{\omega_{\rm cut}}\right)^{\alpha/(1-\alpha)}, \quad \alpha = \frac{1}{\pi}\Gamma, \tag{6.12}$$

where $\omega_{\rm cut}$ is the high-frequency cutoff frequency, *e.g.*, the Debye frequency.

For the dimensionless coupling constant $\alpha < 1$ the value of $\overline{\Delta}$ remains finite, but as α approaches 1 it falls down to zero. This is an indication of the disappearance of tunnelling for strong enough coupling in the case of Ohmic dissipation, even for zero temperature.

A physically interesting situation where Ohmic dissipation is relevant, and the orthogonality catastrophe arises, is the situation of coupling to the electron-hole bath,

$$H_{i} = \frac{1}{2} \sigma_{z} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k} \mathbf{k}'} a_{\mathbf{k}}^{+} a_{\mathbf{k}'}, \quad H_{b} = v_{F} \sum_{\mathbf{k}} (k - k_{F}) a_{\mathbf{k}}^{+} a_{\mathbf{k}}.$$
(6.13)

Here, $a_{\mathbf{k}}^+$, $a_{\mathbf{k}}$ are electron creation and annihilation operators (the spin index has been dropped); v_F is the Fermi velocity, and k_F is the Fermi momentum (the energy is counted off from the Fermi surface). In the case of s-scattering by a tunnelling system with the wells at the distance **R** away from each other, the matrix elements $V_{\mathbf{k}\mathbf{k}'} \propto 1 - \exp(-i(\mathbf{k} - \mathbf{k}')\mathbf{R})$.

The quantity that characterizes the renormalization of the tunnelling matrix elements and the kinetics of the system coupled to the bath on the whole is, as we know, given by the correlator ∞

$$\Xi(\omega) = \int_{-\infty}^{\infty} dt \langle H_i(t) H_i(0) \rangle e^{i\omega t}.$$
(6.14)

In the case of Ohmic coupling to a phonon bath for T = 0, and in the neglect of tunnelling (the case of the utmost interest at the moment), this correlator is just equal to $\Gamma\omega$. In the case of coupling (6.13),

$$\Xi(\omega) = \Gamma_{el} v_F^2 \int_{-\infty}^0 dk \int_0^\infty dk' \delta \left[\omega + v_F \left(k - k'\right)\right] = \Gamma_{el} \,\omega, \quad \Gamma_{el} = \frac{1}{2} \pi \overline{\left|V_{\mathbf{k}\,\mathbf{k}'}\right|^2} \rho_F^2, \tag{6.15}$$

where the overbar means the average over the directions of momenta \mathbf{k} , \mathbf{k}' on the Fermi surface, $k = k' = k_F$, and ρ_F is the density of states on the Fermi surface.

It follows from Eq. (6.15) that the density of states of the electron-hole bath weighted with coupling is the same as in the case of Ohmic dissipation due to phonons, and all the effects considered in the latter case arise in the model (6.13). This model is very general, the only assumption is *s*-scattering of the electrons. This is one of the major reasons why the model of Ohmic dissipation is so interesting and has attracted so much attention.

Appendix A

Solutions to all exercises

► Solution 1.1 (p. 17)

Follow the standard variational procedure to find equations of motion. Substituting $q \longrightarrow q + \delta q$, one gets in the linear order by δq

$$0 = \delta R = \int \left[\ddot{q} + 2\Gamma\dot{q} + U'(q)\right] \left[\delta\ddot{q} + 2\Gamma\delta\dot{q} + U''(q)\delta q\right] dt.$$
(A.1)

Integrating by parts several times with boundary conditions $\delta q = \delta \dot{q} = 0$ both at t = 0 and $t = -\infty$ yields

$$\frac{d^{2}L}{dt^{2}} - 2\Gamma \frac{dL}{dt} + U''(q)L = 0 \quad \text{with} \quad L = \ddot{q} + 2\Gamma \dot{q} + U'(q)$$
(A.2)

The first integral of this non-linear equation ("Energy") can be found by exactly the same procedure as used for the second order Lagrange equations in classical mechanics. Namely, multiplying Eq. (A.2) by \dot{q} , after some transformations

$$0 = \frac{d^2L}{dt^2}\dot{q} - 2\Gamma\frac{dL}{dt}\dot{q} + U''(q)L\dot{q}$$

$$= \frac{d}{dt}\left(\dot{q}\frac{dL}{dt} - \ddot{q}L\right) + L \ddot{q} + \frac{d}{dt}\left(-2\Gamma L\dot{q}\right) + 2\Gamma L\ddot{q} + LU''(q)\dot{q}$$

$$= \frac{d}{dt}\left(\dot{q}\frac{dL}{dt} - \ddot{q}L - 2\Gamma L\dot{q}\right) + L\frac{dL}{dt}$$

$$= \frac{d}{dt}\left(\dot{q}\frac{dL}{dt} - \ddot{q}L - 2\Gamma L\dot{q} + L^2/2\right);$$

we see that the expression in parenthesis is a constant. The boundary conditions at $t = -\infty$ restricts this constant to be zero, leaving us with the *third* order differential equation

$$\dot{q}\frac{dL}{dt} - \ddot{q}L - 2\Gamma L\dot{q} + L^2/2 = 0.$$
 (A.3)

Defining $v = \dot{q}/L$, we note that $\dot{v} = (\ddot{q}L - \dot{q}\dot{L})/L^2$, and the above equation can be written as

$$L^2\left(\dot{v} + 2\Gamma v - \frac{1}{2}\right) = 0.$$

Since L = 0 obviously does not satisfy our boundary conditions, our equation is just

$$\dot{v} + 2\Gamma v = 1/2$$

with the solution

$$v = \frac{1 + C_1 e^{-2\Gamma t}}{4\Gamma},$$

where C_1 is yet another integration constant. Substituting back for q, we obtain

$$\ddot{q} + 2\Gamma\left(1 - \frac{2}{1 + C_1 e^{-2\Gamma t}}\right)\dot{q} + U'(q) = 0.$$

This equation is already of the desired second order, but it turns out that it is possible to make further simplification as the initial conditions require $C_1 = 0$. Indeed, for any non-zero C_1 the system has a *positive* friction at $t = -\infty$ and, therefore, would never come out of the equilibrium. If, however, $C_1 = 0$, the equation is just

$$\ddot{q} - 2\Gamma \dot{q} + U'(q) = 0. \tag{A.4}$$

This is the equation of motion for the original system moving backward in time (check the sign of the friction!). Clearly, this equation always has the required solution: reverting the direction of time once again, we obtain the equation for a particle starting at $t = -t_0$ with $q = q_0$ and $p = -p_0$, with *positive* friction. Our experience tells us that the particle will eventually end up in the bottom of the well with zero velocity. Moreover, we know that there exists only one such solution!

After deriving the second-order equation of motion (A.4), it is easy to find the value of the functional (1.8),

$$\mathcal{R} = \int \left[\ddot{q} + 2\Gamma \dot{q} + U'(q) \right] \left[\ddot{q} + 2\Gamma \dot{q} + U'(q) \right] dt$$

Adding and subtracting $0 = \ddot{q} - 2\Gamma \dot{q} + U'(q)$ to the first and from the second multiples respectively, one obtains

$$\mathcal{R} = \int 2 \left[\ddot{q} + U'(q) \right] 4\Gamma \dot{q} \, dt = 8\Gamma \left(\dot{q}^2 / 2 + U(q) \right) \Big|_{t=-\infty}^{t_0},$$

or, finally,

$$\mathcal{R} = 8\Gamma \left(p^2/2 + U(q) - U(q_{\rm st}) \right)$$

If we substitute this value in Eq. (1.4) and account for the relation (1.7), we obtain precisely the Boltzmann distribution for the probability of finding the particle with a given total energy. The fact that the trajectory of the most probable "uphill" motion, driven by the bath fluctuations, coinsides with that of sliding back under the influence of the friction force, is consistent with the principle of detailed equilibrium, which states that in thermal equilibrium every process must have its counterprocess happening with equal rate.

▶ Solution 1.2 (p. 17)

The average of the product p(t)f(t) can be found by multiplying the expansion of Eq. (1.14)

$$p(t) \approx p(t - \delta t) - \delta t \left[2\Gamma p(t - \delta t) + U'(q(t - \delta t))\right] + \mathcal{O}(\delta t^2) + \int_{t - \delta t}^t f(t') dt'$$

by f(t). In the r.h.s., the only contribution to the average will come from the last term, and Eq. (1.3) leads directly to the intermediate result $\langle f(t) p(t) \rangle = D$.

The averaged product of Eq. (1.5) and $p(t) = \dot{q}(t)$, which can be rewritten as

$$\frac{d}{dt} \langle E(t) \rangle + 2\Gamma \langle p^2(t) \rangle = \langle f(t) \, p(t) \rangle, \quad E(t) \equiv \frac{p^2}{2} + U(q(t)),$$

obviously determines the energy balance in the system. In the stationary regime the average energy does not change, and we immediately obtain $2\Gamma \langle p^2(t) \rangle = D$.

► Solution 1.3 (p. 17)

After separating the variables with the substitution

$$w(Q,t) = \sum_{\lambda} C_{\lambda} e^{-\lambda t} e^{-U(Q)/2D} \phi_{\lambda}(Q),$$

we obtain the time-independent Schrödinger-like equation of the form

$$\phi_{\lambda}'' + [E_{\lambda} - V(Q)] \phi_{\lambda} = 0, \qquad V(Q) = \left(\frac{U'}{2D}\right)^2 - \frac{U''}{2D}.$$
 (A.5)

Physically, the eigenvalue $E_{\lambda} \equiv \lambda/2D$ determines the speed with which the particular density profile is returning to the equilibrium. The function

$$\phi_0(Q) = \operatorname{Const} \exp\left(-U/2D\right)$$

obeys Eq. (A.5) with the eigenvalue $E_0 = 0$; it corresponds to the equilibrium Boltzmann probability distribution. This function has no nodes and, therefore, it is the ground state solution of the Schrödinger equation (A.5). This is, of course, consistent with the statement that any



initial distribution must eventually come to the equilibrium one. In this problem we need to find the smallest positive eigenvalue λ_1 with the associated eigenfunction $\phi_1(Q)$, corresponding to the exponentially slow process of equilibration between the two wells.

To find a very small value E_1 we will employ a special perturbation theory, ordinarily used for finding the level-splitting associated with quantum-mechanical tunneling. Specifically, we know that the two wavefunctions must obey the equations

$$0 = \phi_1'' + [E_1 - V(Q)]\phi_1, \qquad 0 = \phi_0'' - V(Q)\phi_0$$

We multiply the first equation by ϕ_0 and the second one by ϕ_1 , and subtract the results

$$0 = \phi_0 \phi_1'' - \phi_1 \phi_0'' + E_1 \phi_1 \phi_0 = (\phi_0 \phi_1' - \phi_1 \phi_0)' + E_1 \phi_1 \phi_0.$$

Integrating over one of the wells, we obtain

$$E_1 \int_{-\infty}^{Q} \phi_1(Q') \phi_0(Q') \, dQ' = \phi_1(Q) \, \phi_0'(Q) - \phi_0(Q) \, \phi_1'(Q). \tag{A.6}$$

Normally, we would find the approximate value of the energy from this expression using the quasiclassical wavefunctions in the region between the wells. However, it is easy to check that the effective potential V(Q) has a third minimum near the top of the original barrier U(Q), and the quasiclassic approximation fails. We shall use a different way of finding an approximate wavefunctions, utilizing our knowledge of the exact ground state function ϕ_0 , and the fact that the eigenvalue λ_1 is exponentially small. This approach is similar to that used in deriving the Kramers solution.

The density equilibration within each well happens much faster than that between the wells, and we expect the distribution inside each well to be very close to an (independent) equilibrium. The approximate wavefunction can be found by connecting these quasiequilibrium solutions using the general zero-energy solution of Eq. (A.5). In general, we can write

$$\phi_1(x) = \begin{cases} A_1 \phi_0(Q), & Q_0 - Q \gg L_0, \\ \phi_0(Q) \left\{ A_0 + B_0 \int_{Q_0}^Q e^{[U(Q') - U(Q_0)]/D} dQ' \right\}, & Q_1 \ll Q \ll Q_2, \\ A_2 \phi_0(Q), & Q - Q_0 \gg L_0, \end{cases}$$

where the characteristic length L_0 is defined by the potential profile near the top of the barrier, and the solution in the middle region provides a constant flow of particles. The coefficients A_1 , A_2 can be found from the normalization condition of ϕ_1 and the required orthogonality between ϕ_1 and ϕ_0 (which directly follows from Eq. (A.6) if we set $Q = \infty$), while the coefficients A_0 , B_0 must be chosen by matching the wavefunctions between the regions. After some algebra Eq. (A.6) yields

$$\lambda_1 = \frac{D}{M} \left\{ N_1^{-1} + N_2^{-1} \right\},$$

where

$$N_1 \approx \int_{-\infty}^{Q_0} e^{-U(Q)/D} dQ, \quad N_2 \approx \int_{Q_0}^{\infty} e^{-U(Q)/D} dQ, \quad M \approx \int_{Q_1}^{Q_2} e^{U(Q)/D} dQ$$

Unlike the Kramers solution, the above expressions are valid for any form of the potential U(Q) at small enough D. For the potential quadratic both near the bottoms of the wells and the top of the barrier, the characteristic length is $L_0^2 = D/|U_0''|$, and

$$\lambda_1 = \frac{1}{2\pi} e^{-U_0/D} \sqrt{|U_0''|} \left\{ \sqrt{U_1''} e^{U_1/D} + \sqrt{U_2''} e^{U_2/D} \right\},$$

where the indices 0, 1, 2 correspond to the values in the points Q_0, Q_1, Q_2 respectively.

▶ Solution 1.4 (p. 18)

This problem is a simpler version of Prob. 1.1; in this case

$$\mathcal{R} = \int dt \, (2\Gamma \dot{q} + U'(q))^2, \quad q(-\infty) = q_{\rm st}; \quad q(t) = q.$$

The Lagrange equation can be written as

$$2\Gamma \frac{d}{dt} \left[2\Gamma \dot{q} + U'(q) \right] = \left[2\Gamma \dot{q} + U'(q) \right] U''(q),$$

or, after some algebra

$$4\Gamma^2 \ddot{q} - U'(q) \, U''(q) = 0.$$

Multiplying this expression by \dot{q} , we notice that the obtained equation is the total time derivative; therefore

$$2\Gamma^2(\dot{q})^2 - [U'(q)]^2/2 = \text{Const}$$

To satisfy the condition at $t = -\infty$ the arbitrary constant must vanish, Const = 0, and the equation of motion along the extremal path becomes

$$2\Gamma \dot{q} = U'(q). \tag{A.7}$$

Here the positive sign was chosen to enable the particle to go out of the stable equilibrium position. The obtained equation of motion describes an overdamped particle moving "backward" in time. The value of the functional \mathcal{R} along this trajectory is

$$\mathcal{R} = \int_{-\infty}^{t} dt \left(4\Gamma \dot{q}\right) 2U'(q) = 8\Gamma \left[U(q) - U(q_{\rm st})\right]$$

▶ Solution 1.5 (p. 18)

As usual, the extremal solution gives the transition probability with an exponential accuracy. The preexponent can be evaluated by accounting for quadratic fluctuations around the saddle-point solution. Since we did not calculate the corresponding functional determinant, we would have exceeded the accuracy of the method by including the Jacobian in the optimal path functional.

The complete path integral over the particle's trajectory q(t), however, must include the Jacobian of the transformation from f(t) to q(t). This functional determinant can be found by writing the equation of motion (1.7) linearized near the extremal solution $q_0(t) =$ $q(t) - \delta q(t)$ in the finite difference form

$$\frac{2\Gamma}{\Delta t}(\delta q_{i+1} - \delta q_i) + U''(q_0(t_i))\delta q_i = f(t_i), \tag{A.8}$$

with the time interval $\Delta t = t_{i+1} - t_i$. The determinant of the corresponding matrix is

$$\frac{\partial[\delta q_1,\ldots,\delta q_{N-1}]}{\partial[\delta f_1,\ldots,\delta f_{N-1}]} = \prod_{i=1}^{N-1} \left(\frac{2\Gamma}{\Delta t} + U''[q_0(t_i)]\right) \approx \left(\frac{2\Gamma}{\Delta t}\right)^{N-1} \exp\left\{\frac{1}{2\Gamma}\sum_i \Delta t \, U''[q_0(t_i)]\right\}.$$

In the limit $\Delta t \to 0$ the sum becomes an integral, and, up to an overall constant, the required Jacobian of the transformation from f(t) to q(t) can be written as

$$\frac{\partial [\delta f(t)]}{\partial [q(t)]} = \exp\left\{-\frac{1}{2\Gamma}\int U''[q(t)]\,dt\right\}.$$

This implies that the probability distribution for the trajectories of an overdamped particle in the potential U(q) is given by the following path integral

$$P[q(t)] \sim \int \mathcal{D}[q(t)] e^{-\mathcal{R}/4D} e^{-(1/2\Gamma) \int U''[q(t)] dt},$$

where \mathcal{R} is defined by Eq. (1.8).

▶ Solution 1.6 (p. 18)

In this problem we just need to perform the momentum integration of the Kramers solution (1.20). After integrating by parts the total current over the top of the barrier is

$$j = \int_{-\infty}^{\infty} p w(p,q) dp = \lambda T \int_{-\infty}^{\infty} dp \exp\left[-\frac{p^2}{2T}\left(1 + \frac{\lambda\Omega^2}{2\Gamma}\right)\right] = \frac{T \lambda}{\Omega^3} \sqrt{4\pi\lambda\Gamma T},$$

where we set and arbitrary constant to one, and used the relationship $\lambda(\lambda\Omega^2 + 2\Gamma) = 1$. Similarly, the right-going current at q = 0

$$\begin{aligned} j_{+} &= j - j_{-} = \int_{0}^{\infty} p \, w(p,q) dp \\ &= T \int_{0}^{\infty} d\xi \, \exp - \frac{\Omega^{2} \xi^{2}}{4\lambda \Gamma T} + \lambda T \int_{0}^{\infty} dp \, \exp \left[-\frac{p^{2}}{2T} \left(1 + \frac{\lambda \Omega^{2}}{2\Gamma} \right) \right] \\ &= \frac{j}{2} \left(1 + \frac{1}{\lambda \Omega} \right). \end{aligned}$$

As a result, the ratio $j_+/j_- = (1 + \lambda \Omega)/(1 - \lambda \Omega)$.

► Solution 1.7 (p. 18)

WKB-approach. The potential is assumed to be smooth enough, so that the Schrödinger equation

$$\psi'' + \frac{2m}{\hbar^2} (E - U(q))\psi = 0$$
(A.9)



can be solved approximately,

$$\psi(q) = \sum_{\pm} \frac{C_{\pm}}{\sqrt{|k|}} e^{\pm i \int k \, dq}, \qquad (A.10)$$

where $k^2 = 2m(E - U)/\hbar^2$. This solution is correct as long as

$$\frac{k''}{k} \sim \left(\frac{k'}{k}\right)^2 \ll k^2; \tag{A.11}$$

it definitely fails in the vicinity of the turning points of the classical motion (these regions are circled in Fig. A.2). In order to connect the wavefunctions found in different regions, we need to continue these solutions analytically beyond the turning points.

In the region (i) the wavenumber k is purely imaginary, and the solution decays to the left exponentially,

$$\psi_{(i)} = \frac{C_0}{\sqrt{|k|}} \exp \int_a^q k \, dx$$

In the vicinity of the turning point a, but far enough from it so that Eq. (A.11) is still satisfied, we expand

$$-k^{2} = \frac{2m}{\hbar^{2}}(U(q) - E) = \frac{2mU'(a)}{\hbar^{2}}(q - a) + \dots$$

Denoting $\alpha^2 = 2mU'(a)/\hbar^2$, we can write after an explicit integration in the exponent

$$\underbrace{\overset{\mathbf{i}}{\underset{q=a}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}}}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset{\mathbf{i}}{\overset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Fig. A.3. The immediate vicinity of the turning point a can be avoided by moving around it in the complex plane where the WKB approximation holds. Moving above the point q = a we obtain

 $\begin{aligned} (a-x) &\to (x-a)e^{-i\pi}, \quad (a-x)^{3/2} \to (x-a)^{3/2}e^{-i3\pi/2}, \\ \psi_{(i)} &\to \frac{C_0}{\alpha\sqrt{q-a}} \exp\left[i\pi/4 + \frac{2i\alpha}{3}(a-q)^{3/2}\right], \end{aligned}$

whereas moving below this point

$$\psi_{(i)} \longrightarrow \frac{C_0}{\alpha \sqrt{q-a}} \exp\left[-i\pi/4 - \frac{2i\alpha}{3}(a-q)^{3/2}\right].$$

These are precisely the two solutions of Eq. (A.9) in the region (ii). Each time the analytic continuation gives only one part of the solution; the other part is lost, because, compared to the terms we keep, it is exponentially small off the real axis. The correct solution in the region (ii) is

$$\psi_{(ii)} = \frac{2C_0}{\sqrt{|k|}} \cos\left(\pi/4 + \int_a^x k(x)dx\right).$$
 (A.12)

Instead of doing complicated transformations in the vicinity of the right edge of the well, let us start over again with the outgoing flow of the particles in the region (iv),

$$\psi_{(\mathrm{iv})} = \frac{C_1}{\sqrt{|k|}} \exp i \int_a^x k(x) dx.$$

Going around the turning point in the complex plane as before, it is easy to see that this single solution transforms to the sum of two exponents,

$$\psi_{\text{(iii)}} = \frac{C_1}{\sqrt{|k|}} \left(e^{-i\pi/4 + \int_c^x |k| dx} + e^{i\pi/4 - \int_c^x |k| dx} \right).$$

Close to the left edge of the barrier the first term becomes exponentially bigger than the second one, and we may discard the second term. Therefore, the corresponding solution inside the well is

$$\psi_{(ii)} = \frac{2C_1}{\sqrt{|k|}} \cos\left(-\pi/4 + \int_x^b k(x) \, dx\right),\tag{A.13}$$

and in order for Eqs. (A.12) and (A.13) match each other, we require

$$C_0 = C_1$$
, and $-\frac{\pi}{2} + \int_a^b k(x) \, dx = n \, \pi$,

which is the usual Bohr-Sommerfeld quantization condition.

The lifetime is defined as the ratio of a probability

$$W = \int_{a}^{b} |\psi|^{2} \approx \hbar |C_{0}|^{2} 2 \int_{a}^{b} \frac{dx}{\sqrt{2m(E-U)}} \equiv \hbar |C_{0}|^{2} \frac{T}{m}$$

to find the particle inside the well, and the current out of the well,

$$I = \frac{\hbar}{2mi} \left(\psi_{iv}^* \frac{d}{dx} \psi_{iv} - \psi_{iv} \frac{d}{dx} \psi_{iv}^* \right) = \frac{\hbar |C_0|^2}{m} \exp\left(-2\int_b^c |k(x)| \, dx\right).$$

Therefore the lifetime is simply

$$\tau = T/D,$$

where $T = 2 \int_a^b dx [2(E-U)/m]^{-1/2}$ is the classical period of oscillations of a particle with energy E in the potential U(x), and

$$D = \exp{-\frac{2}{\hbar} \int_{b}^{c} \sqrt{2m(U-E)} \, dx}$$

is the transparency of the barrier.

Even though we used the quasiclassical approximation to find the wavefunction, the obtained answer is quite accurate for all states. For example, the lifetime of the ground state in a nearly harmonic potential well is

$$\tau = \frac{T}{D\sqrt{\pi}},$$

which is only $\sqrt{\pi} \approx 1.7$ smaller then our WKB result.

► Solution 1.8 (p. 18)

The non-local term L[q(t)] can be cast in the desired form after integrating Eq. (1.26) by parts,

$$L[q(t)] = 2 \int_0^t \dot{q}(t') \,\kappa(t - t') \,dt' + 2\kappa(t) \,q(0), \tag{A.14}$$

where

$$\kappa(t) = \frac{1}{\pi} \int_0^\infty \frac{d\omega}{\omega} F(\omega) \, \cos(\omega t).$$

This function decays with the characteristic time $t_c \sim \omega_c^{-1}$ defined in Sec. 1.B; after sufficiently long time $t \gg t_c$ the term with initial conditions in Eq. (A.14) can be dropped.

Averaging the random force f(t) defined by Eq. (1.25) over the initial conditions, we obtain Eq. (1.30). With the definition (1.27) we finally obtain

$$\langle f(t)f(t')\rangle = T \frac{2}{\pi} \int \frac{d\omega}{\omega} F(\omega) = 2T \kappa(t-t').$$

This is the classical version of the fluctuation-dissipation theorem for the considered system.

► Solution 1.9 (p. 18)

In this problem we essentially have to rewrite Sec. 1.B, using non-commuting operators as the Hamiltonian variables. Begin with the Hamiltonian (1.22) modified for the quantum oscillator case

$$H = H_0 + H_b + H_i, H_0 = \omega_0 \left(a^{\dagger} a + \frac{1}{2} \right), H_b = \frac{1}{2} \sum_{\mu} \omega_{\mu} \left(b^{\dagger}_{\mu} b_{\mu} + \frac{1}{2} \right),$$
$$H_i = \sum_{\mu} \left(f_{\mu} q \, q_{\mu} + \frac{1}{2} (f_{\mu} / \omega_{\mu})^2 q^2 \right), \text{ where } q = \frac{a + a^{\dagger}}{\sqrt{2\omega_0}}, q_{\mu} = \frac{b_{\mu} + b^{\dagger}_{\mu}}{\sqrt{2\omega_{\mu}}}.$$

The Heisenberg equations of motion for the oscillator operators are

$$-i\dot{a}^{\dagger} = \omega_0 a^{\dagger} + \frac{1}{\sqrt{2\omega_0}} \sum_{\mu} \left(f_{\mu} q_{\mu} + \frac{f_{\mu}^2}{\omega_{\mu}^2} q \right), \qquad (A.15)$$

$$-i\dot{b}^{\dagger}_{\mu} = \omega_{\mu} b^{\dagger}_{\mu} + \frac{f_{\mu}}{\sqrt{2\omega_{\mu}}} q.$$
 (A.16)

The self-consistent equation for the operators a, a^{\dagger} can be obtained by substituting the solution of the second equation,

$$b^{\dagger}_{\mu} = b^{\dagger}_{\mu 0} e^{i\omega_{\mu}t} + \frac{i f_{\mu}}{\sqrt{2\omega_0}} \int_0^t q(t-\tau) e^{i\omega_{\mu}\tau} d\tau,$$

in Eq. (A.15). We obtain, in perfect analogy with Eq. (1.35),

$$-i\dot{a}^{\dagger} = \omega_0 a^{\dagger} - \frac{1}{\sqrt{2\omega_0}} \{ L[q(t)] + f(t) \},\$$

where L[q(t)] is given exactly by Eq. (1.26) with the coupling density of states (1.27), and the operator of the environmental force

$$f(t) = -\sum_{\mu} \frac{f_{\mu}}{\sqrt{2\omega_{\mu}}} \left(b_{\mu 0}^{\dagger} e^{i\omega_{\mu}t} + b_{\mu 0} e^{-i\omega_{\mu}t} \right).$$

By introducing the *slow* variables $a^{\dagger}(t) \rightarrow a^{\dagger}(t) \exp i\omega_0 t$, we obtain the equations of motion that look exactly like Eq. (1.35). Therefore, we can perform the expansion (1.36) and, keeping only the resonant terms in the limit $\tau \rightarrow \infty$, obtain the quantum form of the Langevin equations

$$\dot{a}^{\dagger} = -a^{\dagger} \Gamma + i a^{\dagger} \mathcal{P} - \tilde{f}(t), \qquad (A.17)$$

where Γ and \mathcal{P} are given by Eqs (1.38), and the slow part of the random force

$$\tilde{f}(t) = i \sum_{\mu} \frac{f_{\mu}}{2\sqrt{\omega_0 \omega_{\mu}}} b_{\mu_0} e^{i(\omega_0 - \omega_{\mu})t}.$$

The corresponding correlation function

$$\left\langle \tilde{f}^{\dagger}(t)\,\tilde{f}(t')\right\rangle = \frac{1}{2\omega_0}\sum_{\mu}\frac{f_{\mu}^2}{2\omega_{\mu}}\,e^{i(\omega_0-\omega_{\mu})\,(t-t')}\left\langle b_{\mu}^{\dagger}\,b_{\mu}\right\rangle = \frac{1}{2\pi\omega_0}\int d\omega F(\omega)\,n_{\omega}\,e^{i(\omega_0-\omega)\,(t-t')},\quad(A.18)$$

where $n_{\omega} = (e^{\beta\omega} - 1)^{-1}$ is the usual bosonic occupation number. The correlator (A.18) is essentially non-zero only in the vicinity of t = t'; in the coarsened time

$$\int e^{i(\omega-\omega_0)t} dt = 2\pi\delta(\omega-\omega_0),$$

which leads to

$$\left\langle \tilde{f}^{\dagger}(t) \, \tilde{f}(t') \right\rangle = 2\Gamma \, n_{\omega_0} \, \delta(t - t').$$
 (A.19)

Similarly, the other correlator

$$\left\langle \tilde{f}(t)\,\tilde{f}^{\dagger}(t')\right\rangle = 2\Gamma\,\left(n_{\omega_0}+1\right)\,\delta(t-t').\tag{A.20}$$

The solution of the quantum Langevin equation (A.17) and its conjugate can be written as

$$a^{\dagger}(t) = a_0^{\dagger} e^{-z^* t} + \int_0^t \tilde{f}^{\dagger}(\tau) e^{-z^*(t-\tau)} d\tau, \quad a(t) = a_0 e^{-zt} + \int_0^t \tilde{f}(\tau) e^{-z(t-\tau)} d\tau, \quad z \equiv \Gamma + i\mathcal{P}.$$

This implies the averages

$$\left\langle a^{\dagger}(t) \right\rangle = \left\langle a_{0}^{\dagger} \right\rangle e^{-z^{*}t}, \quad \left\langle a(t) \right\rangle = \left\langle a_{0} \right\rangle e^{-zt},$$
 (A.21)

$$\left\langle a^{\dagger}(t) a(t) \right\rangle = \left\langle a_{0}^{\dagger} a_{0} \right\rangle e^{-2\Gamma t} + n_{\omega_{0}} \left(1 - e^{-2\Gamma t} \right) \to n_{\omega_{0}}, \quad t \to \infty$$
 (A.22)

and, in generall, for $n \ge m$,

$$\left\langle a^{\dagger^{n}}a^{m}\right\rangle = \sum_{k=1}^{m} \frac{n!\,m!}{k!\,(n-k)!\,(m-k)!} \left\langle a_{0}^{\dagger^{n-k}}a_{0}^{m-k}\,e^{-(n+m-2k)\,\Gamma\,t+i(n-m)\,\mathcal{P}\,t}\right\rangle \,n_{\omega_{0}}^{k}\left(1-e^{-2\Gamma\,t}\right)^{k}.$$

Clearly, in the stationary case, the averages do not resemble those for an oscillator. Instead, the Wick theorem is satisfied,

$$\left\langle a^{\dagger^n}(t) a^m(t) \right\rangle \stackrel{t \to \infty}{=} m! \, \delta_{nm} \left(2\Gamma \, n_{\omega_0} \right)^k$$

► Solution 1.10 (p. 18)

This is a linear dissipative system; the Langevin equation is



$$L \ddot{Q} + R \dot{Q} + \frac{Q}{C} = \mathcal{E}(t),$$

where L is the inductance, C is the capacitance and R is the total resistance of the RCL cirquit, and $\mathcal{E}(t)$ is the e.m.f. of the thermal noise. It is possible to solve this problem directly using the results of the previous one. Here we give an alternative solution,

Fig. A.4. based only on the knowledge of the thermal averages for a weakly dissipative oscillator, and the assumption that thermal e.m.f. generated on the resistor is independent of the presence of other elements, so that the weakly-dissipative oscillator works as the spectrum analyzer.

The average thermal energy in the cirquit,

$$\frac{L\langle I^2 \rangle}{2} = \frac{\langle Q^2 \rangle}{2C} = \frac{\hbar\omega_0}{2} \left(n_{\omega_0} + \frac{1}{2} \right), \tag{A.23}$$

is sustained by the fluctuations of the thermal e.m.f. with the correlator

$$\langle \mathcal{E}_{\omega} \mathcal{E}_{\omega'} \rangle = A(\omega) \, \delta(\omega + \omega'),$$

where $A(\omega)$ is so far an unknown function. Assuming this function varies slowly at the scale of Γ , the equilibrium energy (A.23) can be written as

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\langle |Q_{\omega}|^2 \rangle}{2C} = \frac{1}{2L^2C} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\omega)}{(\omega_0^2 - \omega^2)^2 + 4\Gamma^2\omega^2} \approx \frac{A(\omega_0)}{2L^2C} \frac{1}{4\Gamma\omega_0^2} = \frac{A(\omega_0)}{4R},$$

where $\Gamma = R/2L$ and $\omega_0^2 = (LC)^{-1}$. Comparing this result with Eq. (A.23), we obtain

$$A(\omega) = R\,\omega\,(2n_\omega + 1).$$

This is the quantum version of the fluctuation-dissipation theorem for this system. In the classical limit $\hbar\omega \ll T$ we, of course, recover the usual form $A(\omega) \to 2 R T$.

Alternative solution Defining the canonical parameters $2\Gamma \equiv R/L$, $\omega_0^2 = (LC)^{-1}$, the coordinate $q = Q/\sqrt{C}$ and the force $f = \sqrt{C}\mathcal{E}/L$, we can rewrite this equation in the canonical Langevin form

$$\ddot{q} + 2\Gamma\dot{q} + \omega_0^2 q = f(t),$$

with $\langle f(t) f(t') \rangle = 2\Gamma T \,\delta(t-t')$. The corresponding quantum Langevin equations can be written as Eq. (A.17) with $\mathcal{P} = 0$. The operator of the environmental force f(t) expressed in terms of operators \tilde{f} , \tilde{f}^{\dagger} is

$$f(t) = \sqrt{\frac{\omega_0}{2}} \left[\tilde{f}^{\dagger}(t) + \tilde{f}(t) \right].$$

With these definitions, and using the Ohmic form (1.28) of the function $F(\omega)$, the power spectrum of the fluctuations of the random force can be obtained from the correlators Eq. (A.18) and its counterpart for $\langle \tilde{f}(t) \tilde{f}^{\dagger}(t') \rangle$.

► Solution 2.1 (p. 32)

The equations of motion for pair operators are obtained by commuting them with the Hamiltonian,

$$-i\dot{\psi}_l = [H,\psi_l] = -t\,\psi_r + 2eV\psi_l,\,\ldots$$

The pair tunneling current can be written as

$$\frac{I}{2e} = \frac{d}{dt} \left(\psi_l^{\dagger} \psi_l \right) = i \left[H, \psi_l^{\dagger} \psi_l \right] = it \left(\psi_r^{\dagger} \psi_l - \psi_l^{\dagger} \psi_r \right).$$

Introducing the classical degrees of freedom,

$$\psi_{l,r} = n_{l,r}^{1/2} \exp(i\phi_{l,r}), \quad n_l \approx n_r \equiv n_0, \quad \phi_r = \phi_l + \theta, \tag{A.24}$$

we obtain the Josephson current

$$I = 2i e n_0 t \left[e^{i(\phi_l - \phi_r)} - \text{c.c.} \right] = -4 n_0 e t \sin \theta.$$

Similarly, the phase evolution equation

$$\dot{\theta} = 2eV$$

is derived from the definitions (A.24) by taking a difference of the following equations

$$\dot{\psi}_l^{\dagger}\psi_l - \psi_l^{\dagger}\dot{\psi}_l = -2i\dot{\phi}_l n_l = it \left(\psi_r^{\dagger}\psi_l + \psi_l^{\dagger}\psi_r\right) - 2ieV\psi_l^{\dagger}\psi_l,$$

$$\dot{\psi}_r^{\dagger}\psi_r - \psi_r^{\dagger}\dot{\psi}_r = -2i\dot{\phi}_r n_r = it \left(\psi_r^{\dagger}\psi_l + \psi_l^{\dagger}\psi_r\right) + 2ieV\psi_r^{\dagger}\psi_r.$$

For the circuit shown in Fig. A.5, $I_1 = C \dot{V}$, $I_2 = V/R$, and the total current

$$I = I_1 + I_2 = C \dot{V} + V/R,$$

or, in terms of the phase difference θ ,

$$\ddot{\theta} + 2\beta \,\dot{\theta} + \omega_0^2 \sin \theta = 0,$$



Fig. A.5.

where $2\beta \equiv (RC)^{-1}$, $\omega_0^2 \equiv 8 n_0 e^2 t/C$. The Langevin equation for this system can be obtained by adding the e.m.f. of the Nyquist noise generated on the resistor (See Prob. 1.10 at p. 18).

► Solution 2.2 (p. 32)

Let us measure the energy E down from the top of the barrier. Then Eq. (2.4) becomes

$$W = Z^{-1} \int_0^{\Delta U} dE \, \exp(-2S(E) + E/T), \qquad (2.4')$$

where the tunneling action

$$S[E] = \int_0^E \tau_p(E) \, dE.$$

is expressed in terms of the period $\tau_p(E)$ of oscillations in the inverted potential. If this period is a linear function of energy, $\tau_p(E) = \tau_p(0) + \tau'_p(0)E$, then

$$W(E) \approx Z^{-1} e^{-\Delta U/T} \int_0^\infty dE \exp\left[(T^{-1} - T_0^{-1}) E - E^2 / \tau_p'(0) \right] = A(T) e^{-R(T)},$$

where the exponent

 T_0^{-1}

 T_{1}^{-1}

$$R(T) = \frac{\Delta U}{T} - \frac{1}{4\tau'_p(0)}(T^{-1} - T_0^{-1})^2.$$

Similarly, if the period has a non-monotonic form,

$$\tau_p(E) = \tau_p(0) - |\tau'_p(0)| E + \tau''_p(E) E^2/2,$$

as illustrated in Fig. A.6, the extremum equation $\tau_p(E) = T^{-1}$ has two solutions in the region of temperatures

$$\frac{1}{\tau_p(0)} \equiv T_0 < T < T_1 \equiv \frac{1}{\tau_{\min}}.$$

Fig. A.6.

E \rightarrow In this case the escape exponent will be determined by the minimum of the action, which can be reached either in the endpoint E = 0 or in one of the roots

$$E_{\pm} = \frac{|\tau_p'(0)| \pm \sqrt{[\tau_p'(0)]^2 + 2(T^{-1} - T_0^{-1})}}{\tau_p''(0)}$$

of the extremum equation. This situation, which is characterized by competition between different minima, is somewhat analogous to first order phase transitions. Conversely, the analogy to to second-order phase transitions can be drawn in the usual case, where the fluctuations in the vicinity of the bounce solution diverge (see Sec. 3.1) as the temperature approaches the crossover.

▶ Solution 2.3 (p. 32)

The bounce solution corresponds to the motion of a particle in the inverted potential with zero energy,

$$\frac{1}{2}\dot{q}^2 - U(q) = \frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2 + \frac{1}{4}q^4 = 0,$$
(A.25)

which can be integrated as usual,

$$(\tau - \tau_0) = \int \frac{dq}{\sqrt{q^2 - q^4/2}} = \left\{ \begin{array}{l} q = \sqrt{2}\sin\alpha\\ dq = \sqrt{2}\cos\alpha\,d\alpha \end{array} \right\} = -\int \frac{d\alpha}{\sin\alpha} = \ln\left|\tan\frac{\alpha}{2}\right|,$$

with the result

$$q = \sqrt{2} \sin \alpha = \pm \frac{\sqrt{2}}{\cosh(\tau - \tau_0)}$$

The corresponding action

$$S[q] = \int \left(\frac{\dot{q}^2}{2} + U(q)\right) d\tau = 2 \int_0^{\sqrt{2}} dq \sqrt{2U(q)} = 2 \int_0^{\sqrt{2}} dq \, q \sqrt{1 - q^2/2} = \frac{4}{3},$$

where we used the energy equation (A.25) to express the time differential $d\tau = dq/\sqrt{2U}$.

▶ Solution 2.4 (p. 32)

We need to evaluate the prefactor

$$C = \frac{A_1}{(2\pi)^{1/2}} \left[\frac{\det\left(-\frac{d^2}{d\tau^2} + 1 - 3q^2\right)_{q=0}}{\left|\det'\left(-\frac{d^2}{d\tau^2} + 1 - 3q^2\right)_{q=Q(\tau)}\right|} \right]^{1/2},$$
(2.28')

for the bounce solution $Q(\tau)=\sqrt{2}/\cosh\tau$ found in the previous problem. Here the zero mode normalization term

$$A_1 \stackrel{(2.23)}{=} \left\{ \int_{-\infty}^{\infty} d\tau \left[\dot{Q}(\tau - \tau_0) \right]^2 \right\}^{1/2} = \left\{ \int d\tau \left[\frac{1}{2} \dot{Q}^2 + U(Q) \right] \right\}^{\frac{1}{2}} = \frac{2}{\sqrt{3}}$$

The numerator of Eq. (2.28') is trivial,

$$\Delta_0 \equiv \det \left(-\frac{d^2}{d\tau^2} + 1 - 3q^2 \right)_{q=0} = \prod_{n=1}^{\infty} \left(1 + 4\pi^2 \beta^2 n^2 \right),$$

but we have to work much harder to find the denominator.

We need to find all eigenvalues Λ_n and the corresponding eigenfunctions $q_n(\tau)$ for the equation

$$-\ddot{q}_n + (1 - 3Q^2) q_n = \Lambda q_n,$$

with the boundary conditions $q(-\beta/2) = q(\beta/2)$, $\dot{q}(-\beta/2) = \dot{q}(\beta/2)$ in the limit of large $\beta \to \infty$. After the transformation $\tanh \tau = \xi$, $q(\tau) = \phi(\xi)$ the differential equation acquires a hypergeometric form,

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{d\phi}{d\xi}\right] + \left[\frac{2\Lambda}{1-\xi^2} + 6\right]\phi = 0,$$

with the solution [See L&L III, §23, Prob. 5]

$$\phi = (1 - \xi^2)^{\epsilon/2} F[\epsilon - 2, \epsilon + 3, \epsilon + 1, (1 - \xi)/2],$$

where

$$F(\alpha,\beta,\gamma,z) = 1 + \frac{\alpha\beta}{\gamma}\frac{z}{1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\frac{z^2}{2!} + \cdots,$$

with s = 2 and $\epsilon = \sqrt{1 - \Lambda}$.

Using the property [L&L III, Eq. (E.5)]

$$F(\alpha, \beta, \gamma, z) = (1-z)^{-\alpha} F\left(\alpha, \gamma - \beta, \gamma, \frac{z}{z-1}\right)$$
$$= (1-z)^{2-\epsilon} F\left(\epsilon - 2, -2, \epsilon + 1, -\frac{1-\xi}{1+\xi}\right),$$

we obtain

$$\begin{split} \phi &= \operatorname{Const} \frac{e^{-\epsilon\tau}}{(1+e^{-2\tau})^2} \, F(\epsilon-2,-2,\epsilon+1,-e^{-2x}) \\ &= \operatorname{Const} \frac{e^{-\epsilon\tau}}{(1+e^{-2\tau})^2} \, \left\{ 1 + \frac{(\epsilon-2)(-2)}{\epsilon+1} \frac{(-e^{-2\tau})}{1!} + \frac{(\epsilon-1)(\epsilon-2)(-2)(-1)}{(\epsilon+1)(\epsilon+2)} \frac{e^{-4\tau}}{2!} + \dots \right\} \\ &= \operatorname{Const} \frac{e^{-\epsilon\tau}}{(1+e^{-2\tau})^2} \, \left\{ 1 + \frac{2(\epsilon-2)}{\epsilon+1} e^{-2\tau} + \frac{(2-\epsilon)(1-\epsilon)}{(2+\epsilon)(1+\epsilon)} e^{-4\tau} \right\} \end{split}$$

This wavefunction is obviously zero at $\tau \to +\infty$, and it also vanishes at $\tau \to -\infty$ if the term $\sim e^{-4\tau}$ is absent, therefore $\epsilon = 1$ or $\epsilon = 2$ are the only allowed values. The value $\epsilon = 1$ corresponds to $\Lambda_1 = 0$ and the wavefunction $\psi_1 = \sinh \tau / \cosh^2 \tau$ —this is the solution we already know. Similarly, for $\epsilon = 2$, we obtain $\Lambda_0 = 2E + 1 = -3$ and $\psi_0 = 1/\cosh^2 \tau$.

For $\Lambda > 1$, the parameter $\epsilon = \sqrt{1 - \Lambda} \equiv ik$ is purely imaginary. Our solution becomes

$$\begin{split} \psi(\tau) &= \frac{e^{-ik\tau}}{(1+e^{-2\tau})^2} \left\{ 1 + \frac{2(ik-2)}{1+ik} e^{-2\tau} + \frac{2-ik}{2+ik} \frac{1-ik}{1+ik} e^{-4\tau} \right\} \\ &= \left\{ \begin{array}{ll} e^{-ik\tau}, & \tau \to +\infty, \\ \frac{2-ik}{2+ik} \frac{1-ik}{1+ik} e^{-ik\tau}, & \tau \to -\infty. \end{array} \right. \end{split}$$

Clearly, this potential does not scatter linear waves. We can meet the periodicity requirements by demanding

$$\frac{2-ik}{2+ik}\frac{1-ik}{1+ik}e^{i\,k\,\beta} = e^{-2\pi\,i\,n}, \quad n = 0, \pm 1, \pm 2, \dots$$

This is equivalent to $\beta k_n = 2\pi n + \delta(k_n)$, where $\delta(k) = 2 \arctan(k) + 2 \arctan(k/2)$ is the phase shift associated with the potential well. Obviously, $\Lambda_n = 1 + k_n^2$, and we now have everything to compute the determinant

$$\left| \frac{\Delta_0}{\Delta_1'} \right|^{\frac{1}{2}} = \frac{1}{\sqrt{3}} \frac{\prod_{n=1}^{\infty} \left(1 + 4n^2 \pi^2 T^2 \right)}{\prod_{n=1}^{\infty} \left(1 + [2\pi n + \delta(k_n)]^2 T^2 \right)} \\ \approx \frac{1}{\sqrt{3}} \exp\left\{ \frac{1}{\pi} \int_0^\infty \frac{k \left(2\pi - \delta(k) \right) dk}{k^2 + 1} \right\}$$

where the approximation of the sum by the integral is valid because only large values $n \sim \beta$ contribute to this sum.

Performing the integration, we obtain the prefactor associated with the bounce solution,

,

$$C_1 = \frac{2}{3\sqrt{2\pi}} \exp(\ln 6) = \frac{4}{\sqrt{2\pi}}.$$

The full prefactor for the tunneling rate is twice as large, because there exists another, symmetric classical solution $\bar{q}(\tau) = -Q_0(\tau)$, responsible for the particles escaping to the left. Therefore, the tunneling rate from the quartic potential well (2.36) can be written as

$$W = \frac{8}{\sqrt{2\pi}\hbar} \exp\left(-4/3\hbar\right),$$

where the Planck constant \hbar was restored to provide a small parameter for the quasiclassical expansion.

▶ Solution 2.5 (p. 33)

In the lowest order in powers of the coupling to the thermal bath, we can neglect any corrections to the bounce solution

$$Q(\tau - \tau_0) = \beta \sum_n Q_n e^{i\omega_n(\tau - \tau_0)}, \quad \omega_n = 2\pi \, n \, T.$$

Since $Q(\tau)$ is real, $Q_n = Q_{-n}^*$. Let us write the correction to the Euclidean action

$$\Delta S_E = \sum_{\mu} \int_0^{\beta} d\tau \left[\left(\frac{dq_{\mu}}{d\tau} \right)^2 + \omega_{\mu}^2 q_{\mu}^2 + f_{\mu} q q_{\mu} + \frac{f_{\mu}^2}{2\omega_{\mu}^2} q^2 \right] \\ = \frac{\beta}{2} \sum_{n,\mu} (\omega_n^2 + \omega_{\mu}^2) \left| q_{\mu,n} + \frac{f_{\mu}q_n}{\omega_n^2 + \omega_{\mu}^2} \right|^2 + \frac{\beta}{2} \sum_{n,\mu} f_{\mu}^2 \left(\frac{1}{\omega_{\mu}^2} - \frac{1}{\omega_n^2 + \omega_{\mu}^2} \right) |q_n|^2.$$

The first term contributes to the partition function of the *non-perturbed* phonon bath, while the second term constitutes the correction to the exponent of the tunneling probability,

$$\Delta S_E = \frac{\beta}{2} \sum_{n,\mu} |Q_n|^2 f_\mu^2 \left(\frac{1}{\omega_\mu^2} - \frac{1}{\omega_n^2 + \omega_\mu^2} \right) > 0.$$
 (A.26)

Note, that this is just a different form of the correction in Eq. (3.7) with the coefficients (3.9). The correction to the Euclidean effective action is obviously positive, and we conclude that, in the lowest order approximation, the thermal bath coupling suppresses the quantum tunneling.

▶ Solution 3.1 (p. 41)

The classical partition function is given by the integral

$$Z = \int e^{-\beta H(p,q)} dp dq = \sqrt{2\pi T} \int e^{-\beta U(q)} dq,$$

where $H(p,q) = p^2/2 + U(q)$ is the classical Hamiltonian of the particle. For negative $\lambda = -|\lambda|$, the potential energy is positive only in the regions

$$|\arg q - n\pi/2| < \pi/4, \quad n = 0, 1, 2, 3,$$

which are shaded in Fig. A.7, and the integration along the real axis q formally diverges. The integration can converge only if the integration contour begins and ends in shaded regions.



To evaluate the imaginary part of the partition function, we have to do the analytic continuation as explained in Sec. 2.4. Introduce the continuously varying $\lambda = |\lambda| e^{i\phi}$. As ϕ changes from zero to π , in order to preserve the convergence of the integral, the integration contour which originally was aligned with the real axis is gradually deformed into the dashed line. The saddle-point integration the contour shown with the solid line, which passes through the extremum points $q_{\pm} = \pm |\lambda|^{-1/2}$ of the potential energy, gives the imaginary part of the partition function

Fig. A.7.

$$\operatorname{Im} Z = \frac{2\pi T}{\Omega} \exp(-\beta \,\Delta U),$$

where $\Omega^2 \equiv |U''(q_{\pm})| = 2$, and $\Delta U \equiv U(q_{\pm}) - U(0) = 1/4\lambda$. The contribution of each saddle point to the imaginary part of the free energy is, therefore,

$$\beta \operatorname{Im} F_{\pm} \approx \frac{\operatorname{Im} Z}{Z} = \frac{\omega}{2\Omega} e^{-\beta \Delta U}$$

$$W_{\pm} = (\omega/2\pi) \exp(-\beta \Delta U) = (T_0/T) \, 2 \operatorname{Im} F_{\pm},$$

with $T_0 = \Omega/2\pi$. The total escape rate is, of course, twice as large, because we need to add the contributions of both stationary points, which reflects the fact that the particle can escape in either direction.

► Solution 3.2 (p. 41)

Start with Eq. (3.10) where the function

$$\kappa(\tau) = \beta^{-1} \sum_{n} \Phi_n e^{-i\omega_n \tau},$$

and the coefficients are given by Eq. (3.9) [See also Prob. 2.5 at p. 33]. Because $\Phi_{n=0} = 0$,

$$\int_0^\beta \kappa(\tau - \tau') \, d\tau = 0$$

the action does not change after the addition of the quantity

$$0 = -\frac{1}{4} \int_0^\beta d\tau \int_0^\beta d\tau' \kappa(\tau - \tau') \left[q^2(\tau) + q^2(\tau') \right].$$

Therefore, the non-local term can be written as

$$\Delta S_E = -\frac{1}{4} \int_0^\beta d\tau \int_0^\beta d\tau' \,\kappa(\tau - \tau') \,[q(\tau) - q(\tau')]^2. \tag{A.27}$$

The dependence of the function $\kappa(\tau - \tau')$ on the imaginary time τ is determined by the sum

$$A(\omega,\tau) = \sum_{n} \frac{\omega_n^2}{\omega_n^2 + \omega^2} e^{-i\omega_n\tau}$$

which is convenient to transform using the Poisson summation formula,

$$A(\omega,\tau) = \frac{1}{2\pi} \sum_{m} \int d\nu \left[1 - \frac{\omega^2}{\omega^2 + \nu^2} \right] e^{i\nu(\tau - m\beta)} = \sum_{m} \delta(\tau - m\beta) - \frac{|\omega|}{2} e^{-|\omega(\tau - m\beta)|}.$$

Eq. (A.27) becomes

$$\Delta S_E = -\frac{1}{2\pi} \int_0^\beta d\tau \int_0^\beta d\tau' [q(\tau) - q(\tau')]^2 \sum_m \int_0^\infty \frac{d\omega}{\omega} F(\omega) \left\{ \delta(\tau - \tau' - m\beta) - \frac{\omega}{2} e^{-\omega |\tau - \tau' - m\beta|} \right\}.$$

The term with δ -function vanishes because of the periodicity of $q(\tau)$, while the remaining part can be transformed by changing $\tau \to \tau - m\beta$ in the *m*'th term, so that the summation over *m* is replaced by extending the integration interval in τ ,

$$\Delta S_E = \frac{1}{2} \int_{-\infty}^{\infty} d\tau \int_0^{\beta} d\tau' [q(\tau) - q(\tau')]^2 \underbrace{\frac{1}{2\pi} \int d\omega F(\omega) e^{-\omega|\tau - \tau'|}}_{\alpha(\tau - \tau')}.$$

This is the expression we needed to prove. For the special case of Ohmic dissipation, $F(\omega) = 2\Gamma\omega e^{-\epsilon\omega}$, $\epsilon \to +0$, and we easily obtain

$$\alpha(\tau) = \frac{\Gamma}{\pi} \int_0^\infty d\omega \,\omega \, e^{-\epsilon\omega + \omega|\tau - \tau'|} = \frac{\Gamma}{\pi} \frac{1}{(\epsilon + |\tau - \tau'|)^2} \stackrel{\epsilon \to 0}{=} \frac{\Gamma}{\pi(\tau - \tau')^2}$$

As promiced, the non-local coupling function has a long-range tail.

► Solution 3.3 (p. 41) Suggested solution

Use the action in the form (3.7), with no kinetic energy term, and

$$\Phi_n = \frac{2\omega_n^2}{\pi} \int_0^\infty \frac{d\omega}{\omega} \frac{F(\omega)}{\omega^2 + \omega_n^2} = \begin{pmatrix} \text{Ohmic} \\ F(\omega) = 2\Gamma \omega \end{pmatrix} = \frac{4\Gamma\omega_n^2}{\pi} \int_0^\infty \frac{d\omega}{\omega^2 + \omega_n^2} = 2\Gamma |\omega_n|_{\mathcal{H}}$$

which corresponds to the Ohmic dissipation case,

$$S_E = \int_0^\beta U(q) \, d\tau + \beta \, \Gamma \sum_n |\omega_n| \, q_n \, q_{-n}, \qquad U(q) = 3U_0 \, \left(\frac{q}{q_0}\right)^2 \left(1 - \frac{2q}{3q_0}\right). \tag{A.28}$$

Using the Fourrier expansion $q(\tau) = \sum_{n} a_n \exp(i\omega_n \tau)$, we can write the equations of motion in the form

$$s q_m + |\omega_m| q_m = \frac{s}{q_m} \sum_l q_{m-l} q_l, \quad \text{where} \quad s \equiv \frac{3U_0}{\Gamma q_0^2}. \tag{A.29}$$

This is an infinite set of quadratic algebraic equations, which is, of course, impossible to solve in general. Luckily, the form of the solution can be guessed as $q_m = A \exp(-B|m|)$, and the convolution in the r.h.s. of Eq. (A.29) can be evaluated as

$$(q^2)_m \equiv \sum_l q_{m-l} q_l = |A|^2 e^{-B|m|} (|m| + \coth B) = A |m| q_m + A q_m \coth B.$$

The coefficients here can be mached with those in Eq. (A.29), with the result

$$2q_0 = A \coth B, \qquad \coth B = \frac{\beta s}{2\pi}.$$
 (A.30)

The partition function can be evaluated after some more algebra,

$$S_E = 2\Gamma\beta \sum_{m\geq 0} (s+\omega_m) |q_m|^2 - \frac{\Gamma\beta s}{3q_0} \sum_{m=-\infty}^{\infty} q_{-m}(q^2)_m$$

= $\frac{2\Gamma\beta}{3} \sum_{m\geq 0} (\omega_m + s) |q_m|^2 = 4\pi \Gamma q_0^2 \left[1 - \frac{1}{3} \left(\frac{2\pi}{\beta s}\right)^2\right]$
= $4\pi \left(\Gamma q_0^2\right) \left[1 - \frac{4\pi^2}{27} \frac{T^2}{U_0^2} \left(\Gamma q_0^2\right)^2\right].$

Alternative solution

We had to use the Fourrier representation of the extremum equation for the Euclidean action functional (A.28) because the dissipative term is non-local in the time representation. Here we shall write a *differential* equation for $q(\tau)$, by using a trick similar to the Wiener-Hopff method of solving ordinary differential equations. Let us decompose the function $q(\tau) = q_{+}(\tau) + q_{-}(\tau)$, where

$$q_{+}(\tau) = \sum_{n} ' q_{n} e^{i\omega_{n}\tau} \equiv \frac{q_{0}}{2} + \sum_{n>0} q_{n} e^{i\omega_{n}\tau},$$

is the part of the function $q(\tau)$ analytic in the upper half-plane of complex τ , and $q_{-} \equiv q_{+}^{*}$ as follows from the reality of $q(\tau)$. Now the effective action (A.28) can be written in a completely local form,

$$S_E = 2\Gamma \int_0^\beta \left\{ -i \, q_+^* \frac{\partial q_+}{\partial \tau} + s \, |q_+|^2 - \frac{3 \, s}{2q_0} \, q^3 \right\} \, d\tau. \tag{A.31}$$

Performing the variation over $q_{-} = q_{+}^{*}$, we obtain an integro-differential equation

$$-i\frac{dq_{+}}{d\tau} + s q_{+} = \frac{s}{2q_{0}} (q^{2})_{+}, \qquad (A.32)$$

with the integration hidden in the r.h.s.: $(q^2)_+$ denotes the part of the function q^2 which is analytic in the upper half plane of comlex τ .

Let us assume that the function $q_{+}(\tau)$ has only power-like singularities,

$$q_{+}(\tau) = C_0 (\tau - \tau_0)^{\alpha}, \quad \tau \to \tau_0 \equiv \tau'_0 - i\tau''_0.$$

By construction, these singularities can only be below the real axis, $\tau_0'' > 0$. For negative α the most singular part of $(q^2)_+$ is $(q_+)^2$, and, writing the equation for q_+ near the singularity, by power counting it is easy to conclude that the only possibility is $\alpha = -1$, *i.e.* $q_+(\tau)$ may have only single poles and no other singularities.

Generally, at zero temperature, $\beta = \infty$, the obtained variational equations admit solutions with different number of poles,

$$q_+(\tau) = \sum_{k=1}^N \frac{C_k}{\tau - \tau_k}.$$

For such functions, it is easy to calculate the quantity $(q^2)_+$ by expanding the square into irreducible fractions, and discarding the terms with singularities in the wrong half of the complex plane. The simplest is the function with only one pole, N = 1, which corresponds to the usual bounce solution. For this case, the variational equation has the form

$$\frac{iC_1}{s\left(\tau-\tau_1\right)^2} + \frac{C_1}{\tau-\tau_1} = \frac{1}{2q_0} \left[\frac{C_1^2}{(\tau-\tau_1)^2} + \frac{2C_1 C_1^*}{(\tau-\tau_1)(\tau_1-\tau_1^*)} \right],$$

and we immediately obtain

$$C_1 = \frac{2iq_0}{s}, \quad \tau_1'' = \frac{1}{s}$$

The position of the single pole is defined uniquely, up to a translation along the real axis. As a result, the overdamped bounce solution at zero temperature can be written as

$$q(\tau) = \frac{8q_0}{1 + 4s^2 (\tau - \tau_0')^2},$$

and the corresponding action evaluates to $S_E = 4\pi q_0^2 \Gamma$.

At non-zero temperatures the construction is similar, but we have to account for the periodicity of the functions $q_{\pm}(\tau)$. The simplest periodic solution of variational equations has a single pole per period,

$$q_{+}(\tau) = \sum_{k} \frac{C}{\tau - \tau_{0} - \beta k} = \pi C T \cot[(\tau - \tau_{0}) \pi T], \quad q(\tau) = 2 \operatorname{Re} q_{+}(\tau), \quad (A.33)$$

and in the vicinity of the point $\tau_k \equiv \tau_0 + \beta k$ we obtain the equation

$$\frac{iC}{s(\tau-\tau_k)^2} + \frac{C}{\tau-\tau_k} = \frac{1}{2q_0} \left[\frac{C^2}{(\tau-\tau_k)^2} + \frac{2\pi i T |C|^2 \coth(2\pi T \tau_0'')}{(\tau-\tau_k)} \right],$$

which implies

$$C = \frac{2iq_0}{s}, \quad \tanh(2\pi \, \tau_0'' \, T) = \frac{2\pi \, T}{s}.$$

Of course, these relations are equivalent to Eqs. (A.30). However, the easiest way to calculate the corresponding action is by performing the Fourrier representation. Therefore, the only advantage of this more complicated approach is that we managed to solve the extremum equations directly, and thus eliminated the "guessing" part of the solution.

▶ Solution 3.4 (p. 41)

It is important that the coupling H_i is linear in the variables of the bath, so that we can integrate out its degrees of freedom. The functions $q(\tau)$ and $f_{\mu}(q(\tau))$ are periodic with the period β . Denoting

$$\phi_n^{\mu} = \beta^{-1} \int_0^\beta f_{\mu}(q(\tau)) \, e^{-i\omega_n \tau} \, d\tau,$$

where ω_n are the usual Matsubara frequencies, we can write the part of the Euclidean action depending on the coordinates of phonons

$$S_E = \frac{\beta}{2} \sum_{n,\mu} \left\{ (\omega_{\mu}^2 + \omega_n^2) |q_n^{\mu}|^2 + \phi_n^{\mu} q_{-n}^{\mu} + \phi_{-n}^{\mu} q_n^{\mu} \right\}$$
$$= \frac{\beta}{2} \sum_{n,\mu} (\omega_{\mu}^2 + \omega_n^2) \left| q_n^{\mu} + \frac{\phi_n^{\mu}}{\omega_{\mu}^2 + \omega_n^2} \right|^2 - \frac{\beta}{2} \sum_{n,\mu} \phi_n^{\mu} \frac{1}{\omega_n^2 + \omega_{\mu}^2} \phi_{-n}^{\mu}.$$

After the shift of the oscillator coordinates, the first term evaluates to the non-perturbed action of the bath. The effect of the thermal bath on the system is entirely due to the second term, which can be written as

$$\delta S[q] = -\frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\mu f_\mu(q(\tau)) f_\mu(q(\tau')) \,\alpha_\mu(\tau - \tau'),$$

where

$$\alpha_{\mu}(\tau) \equiv \beta^{-1} \sum_{n} \frac{e^{i\omega_{n}\tau}}{\omega_{n}^{2} + \omega_{\mu}^{2}} = \frac{e^{-\omega_{\mu}\tau} + e^{-\omega_{\mu}(\beta-\tau)}}{2\omega_{\mu} \left(1 - e^{-\omega_{\mu}\beta}\right)}.$$

Note that this coupling does not vanish at $\tau = 0$; in addition to the dissipation induced by the bath it accounts for the renormalization of the potential U(q).

► Solution 4.1 (p. 58)

See L&L "Quantum Mechanics".

► Solution 4.2 (p. 58)

Consider the wavefunction which is equivalent to a plane wave $\phi(\tau) = e^{ik\tau}$ in the asymptotic region $\tau \to +\infty$. The asymptotic form of this solution in the region $\tau \to -\infty$ can be obtained with the scattering matrix t_{ij} , which relates the amplitudes of the waves far from the potential barrier, $a_{i1} = t_{ij} a_{j2}$, so that

$$\phi(\tau) = t_{11} e^{ik\tau} + t_{21} e^{-ik\tau}, \quad \tau \to -\infty$$

Since the potential is real, the complex-conjugate function $\phi^*(\tau)$ is also a solution,

$$\phi^*(\tau) = \begin{cases} e^{-ik\tau}, & \tau \to +\infty, \\ t_{11}^* e^{-ik\tau} + t_{21}^* e^{ik\tau}, & \tau \to -\infty. \end{cases}$$

On the other hand, we can use the transmission matrix to find the $\tau \to -\infty$ asymptotics of the same solution as

$$\phi^*(\tau) = t_{12} e^{ik\,\tau} + t_{22} e^{-ik\,\tau}, \quad \tau \to -\infty.$$

The two forms of the same asymptotic must be equal, which implies

$$t_{12} = t_{21}^*, \quad t_{22} = t_{11}^*, \quad \text{and, therefore,} \quad \left| \frac{t_{11} + t_{21}}{t_{12} + t_{22}} \right| = \left| \frac{t_{11} + t_{21}}{t_{11}^* + t_{21}^*} \right| = 1.$$

▶ Solution 4.3 (p. 58)

Rewrite the partition function (4.30) in the form

$$Z = \operatorname{Tr} T_{\tau} \left\{ \exp\left(-\frac{\Delta}{2} \int_0^\beta \sigma_x(\tau) \, d\tau + \frac{1}{8} \int_0^\beta d\tau' \int_0^{\tau'} d\tau'' \, \kappa(\tau' - \tau'') \left[\sigma_z(\tau') - \sigma_z(\tau'')\right]^2 \right) \right\},$$

where $\kappa(\tau)$ is given by Eq. (4.2), or Eq. (4.4) for the special case of Ohmic dissipation. Expanding this expression in powers of Δ , we insert the spin flip operators at different moments of imaginary time τ_k . These operators affect the value of the integrand in the second term in the exponent, which becomes a piecewise continuous function with values 0 or $4\kappa(\tau' - \tau'')$ depending on the number of spin flips inserted between the moments τ' and τ'' . Because of the trace, only an even number of spin flips is allowed every term of this expansion, and the exponent of the 2n-th term can be written as

$$\frac{1}{2} \left(\int_{\tau_1}^{\tau_2} d\tau' \int_0^{\tau_1} d\tau'' + \int_{\tau_2}^{\tau_3} d\tau' \int_{\tau_1}^{\tau_2} d\tau'' + \int_{\tau_3}^{\tau_4} d\tau' \int_0^{\tau_1} d\tau'' + \int_{\tau_3}^{\tau_4} d\tau' \int_{\tau_2}^{\tau_3} d\tau'' + \dots \right) \kappa(\tau' - \tau'').$$

Defining

$$\gamma(\tau_1 - \tau_2) \equiv \int_0^{\tau_1} d\tau' \int_0^{\tau_2} d\tau'' \,\kappa(\tau' - \tau'') \stackrel{\bar{\tau} \ll |\Delta \tau| \ll \beta}{=} -\frac{\Gamma}{\pi} \ln|\tau_1 - \tau_2| + \text{Const},$$

where $\bar{\tau}$ is some high-frequency cut-off, we can rewrite the sum of integrals as

$$\frac{\Gamma}{\pi} \sum_{i>j} (-1)^{i-j} \ln \left| \frac{\tau_i - \tau_j}{\bar{\tau}} \right|,\,$$

where the contribution of the end points $\tau = 0, \beta$ cancel because of the periodicity of the function $\gamma(\tau)$, and the self-interaction terms contribute to the definition of the cut-off time $\bar{\tau}$. The partition function becomes

$$Z = 2\sum_{n\geq 0} \left(\frac{\Delta\bar{\tau}}{2}\right)^{2n} \int_0^\beta \frac{d\tau_{2n}}{\bar{\tau}} \int_0^{\tau_{2n}} \frac{d\tau_{2n-1}}{\bar{\tau}} \dots \int_0^{\tau_2} \frac{d\tau_1}{\bar{\tau}} \exp\left\{2\alpha \sum_{i>j} (-1)^{i-j} \ln\left|\frac{\tau_i - \tau_j}{\bar{\tau}}\right|\right\},$$

where $\alpha \equiv \Gamma/\pi$ and the overall factor 2 is due to the trace over the spin values. Comparing this expression with Eq. (4.26), we conclude that, indeed, the spin system is equivalent to a continuous two-level system with $q_{\text{left}} = 1/2$.

▶ Solution 5.1 (p. 72)

Without going into complicated matters of the inter-particle forces, let us assume the particles in a crystal interact by a pairwise potential, quadratic near the minimum at some distance a, and short-range enough so that we can restrict ourselves to the nearest-neighbor coupling. The energy assocuated with small displacements from the equilibrium position **a** is

$$\delta_{\mathbf{r}} U \equiv U(|\mathbf{a} + \mathbf{r}|) - U(a) = \frac{m \,\omega_0^2}{2} \,(|\mathbf{a} + \mathbf{r}| - a)^2 \approx \frac{m \,\omega_0^2}{2} \,(\hat{\mathbf{a}} \cdot \mathbf{r})^2, \qquad \hat{\mathbf{a}} \equiv \frac{\mathbf{a}}{a}.$$

Therefore, the equation for the displacement \mathbf{r}_i of *i*-th particle in the crystal can be written as

$$\ddot{\mathbf{r}}_i + \eta \dot{\mathbf{r}}_i = -\omega_0^2 \sum_j (\mathbf{r}_i - \mathbf{r}_j \cdot \hat{\mathbf{a}}_j) \, \hat{\mathbf{a}}_j,$$

where the summation is performed over the nearest neighbors of the chosen particle, and η is the coefficient of viscous friction.

For an infinite uniform crystal the solutions of this infinite system of linear differential equations are plane waves, $\mathbf{r}_j = \mathbf{u}_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{a}_j - i\omega t)$, where the frequency ω , the momentum \mathbf{k} and the amplitude $\mathbf{u}_{\mathbf{k}}$ satisfy the equation

$$-\omega^2 \mathbf{u}_{\mathbf{k}} - i\omega \,\eta \,\mathbf{u}_{\mathbf{k}} + \omega_0^2 \sum_j \left(1 - e^{i\mathbf{k}\cdot\mathbf{a}_j}\right) \hat{\mathbf{a}}_j \left(\hat{\mathbf{a}}_j \cdot \mathbf{u}_{\mathbf{k}}\right) = 0.$$

In the absence of the dissipation the low-lying modes of this equation are characterized by the sound speed s, $\omega_k = s k$; for the solid in d dimensions there are exactly d different sound modes. The corresponding dispersion equation for the dissipative modes can be written as

$$-\omega^2 - i\eta\,\omega + s^2\,k^2 = 0.$$

For $s k \ll \eta$ the corresponding frequences are $\omega_+ \approx i\eta$, $\omega_- \approx 2is^2 k^2/\eta$. There are exactly two overdamped modes for each original sound mode. However, only one of these modes is a true Goldstone mode: the mode ω_- which describes the diffusion. The presence of such mode is granted by the translational invariance.

▶ Solution 5.2 (p. 73)

Let us begin with Eq. (5.14), which is applicable for long enough times,

$$t^{-1} \sim W \ll t_{\text{corr.}}^{-1} \sim \min(T, T_D),$$

where T_D is the Debye temperature associated with the bath. After some algebra one can show that the interaction Hamiltonian in the interaction representation is given by the expression

$$H_i(t) \equiv e^{it(H_0 + H_b)} H_i e^{-it(H_0 + H_b)} = \sum_q f_q e^{i\mathbf{q}\mathbf{r}} e^{it\Delta_p^+} + \text{h.c.} = \sum_q f_q e^{it\Delta_p^-} e^{i\mathbf{q}\mathbf{r}} + \text{h.c.}$$

where $\Delta_p^+ = \varepsilon_{p+q} - \varepsilon_p - \omega_q$, $\Delta_p^- = \varepsilon_p - \varepsilon_{p-q} - \omega_q$, and $\varepsilon_p \equiv p^2/2m$. Now it is easy to evaluate the phonon average of the double commutator in Eq. (5.14), with the result

$$\begin{aligned} -\frac{dG}{dt} &= \sum_{q} |f_{q}|^{2} \int_{0}^{t} dt' \Big\{ e^{i(t-t')\Delta_{p}^{-}} G(n_{q}+1) + n_{q} G e^{i(t-t')\Delta_{p}^{+}} - n_{q} e^{it\Delta_{p}^{-}} e^{i\mathbf{q}\mathbf{r}} G e^{-i\mathbf{q}\mathbf{r}} e^{-it'\Delta_{p}^{-}} \\ &- (n_{q}+1) e^{-it\Delta_{p}^{+}} e^{-i\mathbf{q}\mathbf{r}} G e^{i\mathbf{q}\mathbf{r}} e^{it'\Delta_{p}^{-}} \Big\} + \text{h.c.}, \end{aligned}$$

where the density matrix is, of course, Hermitian, $G^{\dagger} = G$. In the derived expression the exponent $e^{i\mathbf{qr}}$ serves as the momentum boost operator; taking the matrix elements between the states with momenta \mathbf{p} and \mathbf{p}' , we get

$$\begin{aligned} -\frac{d\tilde{\rho}_{\mathbf{p},\mathbf{p}'}}{dt} &= \sum_{q} \left| f_{q} \right|^{2} \int_{0}^{t} dt' \\ &\times \Big\{ \Big[(n_{q}+1) \left(e^{i(t-t')\Delta_{p}^{-}} + e^{-i(t-t')\Delta_{p'}^{-}} \right) + n_{q} \left(e^{i(t-t')\Delta_{p'}^{+}} + e^{-i(t-t')\Delta_{p}^{+}} \right) \Big] \tilde{\rho}_{\mathbf{p},\mathbf{p}'} \\ &- n_{q} \left[e^{it\Delta_{p}^{-} - it'\Delta_{p'}^{-}} + (t\leftrightarrow t') \right] \tilde{\rho}_{\mathbf{p}-\mathbf{q},\mathbf{p}'-\mathbf{q}} - (n_{q}+1) \Big[e^{it'\Delta_{p'}^{+} - it\Delta_{p}^{+}} + (t\leftrightarrow t') \Big] \tilde{\rho}_{\mathbf{p}+\mathbf{q},\mathbf{p}'+\mathbf{q}} \Big\}. \end{aligned}$$

Ignoring the principal value parts generated by the time integration (as before, these terms renormalize the kinetic energy of the particle), we obtain the final form of the quantum kinetic equation for the particle in a thermal bath

$$-\frac{d\tilde{\rho}_{\mathbf{p},\mathbf{p}'}}{dt} = W\tilde{\rho}_{\mathbf{p},\mathbf{p}'} - \pi \sum_{q} |f_{q}|^{2} n_{q} e^{it \mathbf{q}(\mathbf{p}-\mathbf{p}')/m} \left[\delta(\Delta_{p'}^{-}) + \delta(\Delta_{p}^{-})\right] \tilde{\rho}_{\mathbf{p}-\mathbf{q},\mathbf{p}'-\mathbf{q}} -\pi \sum_{q} |f_{q}|^{2} (n_{q}+1) e^{-it \mathbf{q}(\mathbf{p}-\mathbf{p}')/m} \left[\delta(\Delta_{p}^{+}) + \delta(\Delta_{p'}^{+})\right] \tilde{\rho}_{\mathbf{p}+\mathbf{q},\mathbf{p}'+\mathbf{q}}, W = \pi \sum_{q} |f_{q}|^{2} \left\{ n_{q} \left[\delta(\Delta_{p}^{+}) + \delta(\Delta_{p'}^{+})\right] + (n_{q}+1) \left[\delta(\Delta_{p'}^{-}) + \delta(\Delta_{p}^{-})\right] \right\}.$$
(A.34)

The usual (quasiclassical) kinetic equation can be obtained from the derived quantum kinetic equation by defining the Wigner distribution function

$$f(\mathbf{p}, \mathbf{r}) = \int e^{i\mathbf{k}\mathbf{r}} \,\hat{\rho}_{\mathbf{p}+\mathbf{k}/2, \mathbf{p}-\mathbf{k}/2} \,\frac{d\mathbf{k}}{(2\pi)^d}, \quad \hat{\rho} = e^{-itH_0} \tilde{\rho} e^{itH_0}. \tag{A.35}$$

It is easy to check that this function gives correct averages for any operator depending either on momenta or on coordinates. However, unlike the classical distribution function, the function (A.35) may have complex values, and it preserves complete information about the quantum correlations. Ignoring a small difference between \mathbf{p} and \mathbf{p}' in the arguments of δ -functions (which amounts to suppressing the quantum interference of the scattered particles), from Eq. (A.34) it is easy to obtain the usual form of kinetic equation,

$$\frac{\partial \mathbf{f}_{\mathbf{p},\mathbf{r}}}{\partial t} + \frac{\mathbf{p}}{m} \frac{\partial \mathbf{f}_{\mathbf{p},\mathbf{r}}}{\partial \mathbf{r}} = -W \,\mathbf{f}_{\mathbf{p},\mathbf{r}} + 2\pi \sum_{q} |f_{q}|^{2} \left[(n_{q}+1) \,\mathbf{f}_{\mathbf{p}+\mathbf{q},\mathbf{r}} \,\delta(\Delta_{p}^{+}) + n_{q} \,\mathbf{f}_{\mathbf{p}-\mathbf{q},\mathbf{r}} \,\delta(\Delta_{p}^{-}) \right].$$

The second term in the l.h.s. comes from the commutator with the bare Hamiltonian.

The quasielastic scattering approximation works if the phonon frequency $\omega_q = q s \leq \min(T, T_D)$, where s is the sound speed, is much smaller then a typical electron's energy, $p^2/m \sim \max(T, \epsilon_F)$. It always works for degenerate electrons, $T \leq \epsilon_F$, at the temperatures much below the Debye temperature, $T \ll T_D$, and for non-degenerate electrons if $T \gg T_D$. This approximation can also work for degenerate electrons above the Debye temperature (in this case electrons' momenta are of the same order of magnitude as those of phonons) if $qs \sim ps \ll p^2/m$, or $m s^2 \ll \epsilon_F \sim m v_F^2$.

► Solution 5.3 (p. 73)

See the following problem for the treatment in terms of quantum Langevin equation; the QKE description is not ready yet.

▶ Solution 5.4 (p. 73)

First, let us find the correct absorption spectrum of the system. Ignoring the double frequency terms, the coupling to the external field is

$$H_{\mathcal{E}} = \mathcal{E} e^{i\omega t} a(t) + \text{h.c.},$$

and in the lowest order approximation the absorption rate is given by the Fermi's golden rule

$$W = 2\pi \left| \mathcal{E} \right|^2 \left\{ \overline{\left[a^{\dagger}(t) \, a(t') \right]}_{\omega} + \overline{\left[a(t) \, a^{\dagger}(t') \right]}_{\omega} \right\},$$

where the averaging is performed over the equilibrium state of the bath. The equilibrium evolution of the system is governed by the quantum Langevin equations (See Prob. 1.9 at p. 18), with the solution

$$a^{\dagger}(t) = e^{i\omega_0 t} \left\{ a_0^{\dagger} e^{-z^* t} + \int_0^t \tilde{f}^{\dagger}(t') e^{-z^*(t-t')} dt' \right\},$$

where $z^* = \Gamma - i\mathcal{P}$ is the combination of the line broadening Γ and the oscillator frequency shift \mathcal{P} associated with the bath coupling, and $\tilde{f}(t)$ is the quantum operator of the random force with the correlators

$$\left\langle \tilde{f}^{\dagger}(t) f(t') \right\rangle = 2\Gamma n_{\omega_0} \delta(t-t'), \quad \left\langle \tilde{f}(t) f^{\dagger}(t') \right\rangle = 2\Gamma (n_{\omega_0}+1) \delta(t-t').$$

Now it is easy to find the correct absorption probability,

$$W = 2\pi \left| \mathcal{E} \right|^2 \frac{\Gamma \coth(\beta \omega_0/2)}{\Gamma^2 + (\omega - \omega_0)^2}, \quad \Gamma \equiv F(\omega_0)/2\omega_0.$$

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The decay rate associated with *m*-th oscillator level can be found considering the operator $H_i = q \sum_{\mu} f_{\mu} q_{\mu}$ as a perturbation to the oscillator $H_0 = \omega_0 (a^{\dagger}a + 1/2)$ in *m*-th excited state. We have

$$\Gamma_{m} = 2\pi \sum_{\mu} |f_{\mu}|^{2} \,\delta(\omega_{0} - \omega_{\mu}) \left\{ \frac{(a^{\dagger}a)_{m}}{2\omega_{0}} \,\overline{\frac{b_{\mu}b_{\mu}^{\dagger}}{2\omega_{\mu}}} + \frac{(aa^{\dagger})_{m}}{2\omega_{0}} \,\overline{\frac{b_{\mu}b_{\mu}}{2\omega_{\mu}}} \right\} \\ = 2\Gamma \left\{ m \left(n_{\omega_{0}} + 1 \right) + (m+1) \, n_{\omega_{0}} \right\}, \quad \Gamma = \frac{F(\omega_{0})}{2\omega_{0}}.$$
(A.36)

An obviously wrong result for the absorption spectrum of the system can be obtained by considering the oscillator as a collection of two-level systems with an appropriate equilibrium population and the transition rate (A.36). We have

$$W = 2\pi \left| \mathcal{E} \right|^2 \sum_{m=0}^{\infty} \frac{\Gamma_m e^{-\beta m \omega_0} \left(1 + e^{-\beta \omega_0}\right)}{\Gamma_m^2 + (\omega - \omega_0)^2} \quad (\text{WRONG!}).$$

The problem with this approach is, obviously, that it ignores the correlations between the levels of the oscillator other than neighboring; these correlations are important because the spectrum is equidistant and all states evolve with commensurate frequencies. Note, however, that in the limit of small temperatures the higher excited states are not populated, correlations between them vanish, and the approximation of the oscillator in terms of a two-level system is basically correct.

▶ Solution 5.5 (p. 73)

The localized electron obeys the following non-linear Schrödinger equation

$$-\frac{1}{2}\nabla^2\psi + \psi V_{[\psi]}(\mathbf{r}) = E\psi.$$

The electron's potential energy can be integrated by parts,

$$V = \int |\psi(\mathbf{r}_1)|^2 V_{[\psi]}(\mathbf{r}) d^3 \mathbf{r}_1 = -e \int |\psi(\mathbf{r}_1)|^2 \frac{d^3 \mathbf{r}_1}{|\mathbf{r} - \mathbf{r}_1|} (\nabla \cdot \mathbf{P}(\mathbf{r})) d^3 \mathbf{r}$$

= $e \int |\psi(\mathbf{r}_1)|^2 d^3 \mathbf{r}_1 \frac{\mathbf{r} - \mathbf{r}_1}{|\mathbf{r} - \mathbf{r}_1|} \cdot \mathbf{P}(\mathbf{r}) d^3 \mathbf{r} = -\int d^3 \mathbf{r} \mathbf{D}(\mathbf{r}) \cdot \mathbf{P}(\mathbf{r}) \equiv 2W$

which proves the relationship V = 2W.

The potential energy entering the Schrödinger equation can be written as a variational derivative,

$$V_{[\psi]}(\mathbf{r}) = \frac{1}{2} \frac{\delta}{\delta \psi^*} V = \frac{\delta}{\delta \psi^*} W,$$

which implies that the ground state solution $\psi_1(\mathbf{r})$ of the Schrödinger equation minimizes the functional

$$E = \int \left\{ \frac{1}{2} (\nabla \psi)^2 + |\psi(\mathbf{r})|^2 V_{[\psi]}(\mathbf{r}) \right\} d^3 \mathbf{r} = T + W.$$

Let us consider the scaled wavefunction $\psi_k(\mathbf{r}) \equiv k^{3/2}\psi_1(k\mathbf{r})$. Clearly, the associated kinetic energy is $T_k = k^2 T$, and the Coulomb potential energy is $W_k = k W$. The functional

$$E_k = k^2 T + k W$$
must have a minimum at k = 1, which implies W = -2T. Therefore, -V = 2(-W) = 4T, and the total energy E = T + V = -3T, and we can write the "long" fraction

$$T: -W: -E: -V = 1:2:3:4.$$

▶ Solution 5.6 (p. 74)

Begin by writing the interaction Hamiltonian in the interaction representation. The terms H_{i1} and H_{i2} are transformed as discussed in Sec. 5.2 and Sec. 5.4 respectively, while the Hamiltonian H_F responsible for the interaction with the external field can be written as

$$H_F(t) = \frac{F}{2} \left[\sigma_+(t) + \sigma_-(t) \right] \cos(\omega t), \quad \sigma_\pm(t) = e^{\mp i\omega_0 t} \left(\sigma_x \pm i\sigma_y \right) / 2.$$

In the lowest order the r.h.s. of the quantum kinetic equation can be written as a sum of independent terms due to different processes defined by the interaction Hamiltonian,

$$\frac{dG}{dt} = \left(\frac{dG}{dt}\right)_{i1} + \left(\frac{dG}{dt}\right)_{i2} + \left(\frac{dG}{dt}\right)_F, \quad \left(\frac{dG}{dt}\right)_F = -i\left[H_F(t), G(t)\right]$$

The remaining two terms were considered before, they are particularly simple at high temperatures, $T \gg \omega_0$,

$$\left(\frac{dG}{dt}\right)_{i1} = -\frac{W}{2} \left[G(t) - \sigma_+(t) G(t) \sigma_-(t) - \sigma_-(t) G(t) \sigma_+(t)\right]$$
$$\left(\frac{dG}{dt}\right)_{i2} = -\frac{W^{(sc)}}{2} \left[G(t) - \sigma_x(t) G(t) \sigma_x(t)\right],$$

with W and $W^{(sc)}$ being the probabilities associated with the phonon emission and quasielastic scattering as defined by Eqs. (5.17) and (5.21) respectively. The corresponding evolution equations for the averages $\langle \sigma_z \rangle$, $\langle \sigma_{\pm} \rangle$ are easily obtained using Eq. (5.18),

$$\left[\frac{d}{dt} + W + W^{(sc)}\right] \langle \sigma_z \rangle = -iF \left[\sigma_+(t) - \sigma_-(t)\right] \cos(\omega t), \qquad (A.37)$$

$$\left[\frac{d}{dt} + i\omega_0 + \frac{W + W^{(sc)}}{2}\right] \langle \sigma_+ \rangle = \frac{W^{(sc)}}{2} \langle \sigma_- \rangle - \frac{iF}{2} \langle \sigma_z \rangle \cos(\omega t), \quad (A.38)$$

At lower temperatures the zero mode oscillations can no longer be ignored, and we have to restore a few more additional terms in the r.h.s. of the kinetic equation. For the evolution equations (A.37), (A.38), it is easy to guess the form of additional terms from the known equilibrium solution of the QKE

$$\rho_{\rm eq} = \frac{1}{2} \left[1 - \sigma_z \tanh\left(\beta \omega_0/2\right) \right],$$

which implies that the averages

$$\langle \sigma_z \rangle_{\rm eq} = -\tanh(\beta \omega_0/2), \quad \langle \sigma_{\pm} \rangle_{\rm eq} = 0.$$

Such values can be obtained by adding a term $-(W + W^{(sc)}) \tanh(\beta \omega_0/2)$ to the r.h.s. of Eq. (A.37); of course, the same result can be obtained by a direct calculation. For a twolevel system, the density matrix has only three independent parameters, and it is uniquely determined by the averages $\langle \sigma_{\mu} \rangle$. Now that we have a complete set of equations for these averages, it is straighforward to find their time-dependence, and then restore the timedependence of the density matrix.

To solve the evolution equations for $\langle \sigma_{\mu}(t) \rangle$, we separate the real and imaginary parts of Eq. (A.38),

$$\begin{aligned} \frac{d}{dt} \langle \sigma_x \rangle - \omega_0 \langle \sigma_y \rangle + \frac{W}{2} \langle \sigma_x \rangle &= 0, \\ \frac{d}{dt} \langle \sigma_y \rangle + \omega_0 \langle \sigma_x \rangle + \frac{W + 2W^{(sc)}}{2} \langle \sigma_x \rangle &= -\frac{F}{2} \langle \sigma_z \rangle \cos(\omega t), \end{aligned}$$

express the average $\langle \sigma_y \rangle$ in terms of $\langle \sigma_z \rangle$, and substitute the result into the corrected Eq. (A.37). In the resonant approximation, and with an additional assumption that all kinetic coefficients are small, $W, W^{(sc)} \ll \omega_0$, we obtain

$$\frac{d}{dt}\langle \sigma_z \rangle + \Gamma \langle \sigma_z \rangle + \frac{\Gamma}{16} \frac{|F|^2}{\Delta^2 + \Gamma^2/4} \langle \sigma_z \rangle = -\Gamma \tanh(\beta \omega_0/2),$$

where the total linewidth $\Gamma \equiv W + W^{(sc)}$ and frequency mismatch $\Delta \equiv \omega_0 - \omega$. The derived equation describes the evolution of the population difference between the levels; the term proportional to the field intensity $|F|^2$ is proportional to the radiation absorption rate. The radiation with large enough intensity greatly enhances the interlevel transition rate, thus reducing the population difference $\langle \sigma_z \rangle$. As a result, the processes of radiation emission and absorption compensate each other, and the absorption rate saturates at exactly one half of its zero-temperature value.

▶ Solution 5.7 (p. 74)

In this problem we just have to evaluate the scattering probability (5.21) for the case of phonons coupled to a bistable impurity. Typically, one can expect that shifting the impurity can modify the local potential, which would modify one or more pairwise elasticity constants, or an effective mass localized in the given lattice cell. This implies that the coupling coefficients $f_{\mathbf{kk}'}$, where \mathbf{k} is the momentum of acoustic phonons, will be typically proportional to the square of the momentum, $f_{\mathbf{kk}'} \sim \alpha k^2$. As a result, the expression (5.21) can be astimated as following

$$W^{(sc)} \sim \pi \alpha^2 \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \frac{k^4}{\omega_k \omega_{k'}} \bar{n}(\omega_k) (\bar{n}(\omega_{k'}) + 1) \,\delta(\omega_k - \omega_{k'}).$$

At small temperatures, the momentum integration can be extended to infinity, and, after introducing the dimensional momentum $\mathbf{q} = s\mathbf{k}/T$, the scattering probability acquires the form

$$W^{(\mathrm{sc})} \sim \frac{\pi \alpha^2}{16\pi^3} \frac{T^7}{s^{10}} \int_0^\infty \frac{q^6 \, dq}{\sinh^2(q/2)} \sim \frac{\alpha^2 \, T^7}{s^{10}}, \quad T \ll T_D.$$

At larger temperatures the cutoff at the Debye momentum k_D comes into play, and the scattering probability crosses over to a much slower quadratic temperature dependence

$$W^{(\rm sc)} \sim \frac{\pi \, \alpha^2 T^2}{s^5 \, a^5} \sim \frac{\alpha^2 T^2}{a^5 s^5}, \quad T \gg T_D,$$

where $a \sim \pi/k_D$ is the typical lattice spacing. It is now clear that the scattering can be an important mechanism only at sufficiently high temperatures.