

Dephasing at low temperatures

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We discuss the significance and the calculation of dephasing at low temperatures. The particle is moving diffusively due to a static disorder configuration, while the interference between classical paths is suppressed due to the interaction with a dynamical environment. At high temperatures we may use the white-noise approximation, while at low temperatures we distinguish the contribution of zero-point fluctuations (ZPF) from the thermal noise contribution. We study the limitations of the above semiclassical approach and suggest the required modifications. In particular we find that the ZPF contribution becomes irrelevant for thermal motion. [S0163-1829(99)01917-7]

The application of semiclassical considerations into the analysis of interference and dephasing is as old as the history of quantum mechanics. A particular interest is to apply these considerations to the theory of diffusing electrons in a metal.^{1,2} Dephasing, or the loss of “phase” information, is the consequence of the interaction with some other environmental degrees of freedom, or with some measurement device. The widely accepted dogma is that dephasing is associated with *leaving a trace* in the environment. Lately this dogma has been challenged experimentally³ as well as theoretically,⁴ leading to an intensive debate^{5,6} associated with the question whether zero-point fluctuations (ZPF) of environmental modes may lead to decoherence at the limit of zero temperature. The most physically appealing theoretical considerations are based on the application of Feynman-Vernon (FV) formalism, and simple semiclassical considerations. In particular, the zero-temperature decoherence found within the exactly solvable Caldeira-Leggett (CL) model, is most puzzling. Thus, it is of fundamental importance to address the following: (1) What are the limitations of the semiclassical strategy. (2) What is the applicability of results that are based on the CL model. (3) What are the limitations of the “one-particle” picture when applied to a many-body system. In this paper we are going to explore these questions systematically, using a well controlled strategy. Under consideration is the motion of a particle under the combined influence of static disorder and a dynamical environment. Our reasoning consists of the following three stages: (a) We take the static disorder into account and write the transport probability amplitude as a discrete sum over classical trajectories. (b) We take the stochastic nature of the environment into account by considering the influence of an effective stochastic potential. (c) We take the full dynamical nature of the environment into account by using the FV formalism. Having an environment whose temperature is T , and a particle that is injected with an energy E (not necessarily thermal), one should make a distinction between the cases of high and low temperature T , and analogous distinction between the cases of large and small energy E . We shall argue that the validity of the semiclassical approach is not restricted to high bath temperatures. However, at low bath temperatures, an essential modification is required in the case of motion with small energy E .

It is assumed that the motion of the particle under the influence of the static disorder is diffusive. The transport probability amplitude can be written as a sum $\sum A_a \exp(iS[\mathbf{x}_a]/\hbar)$ over classical trajectories that connect the observation point with the injection point. We shall denote by t the total time of the motion, and $S[\mathbf{x}_a]$ are the corresponding action integrals. The statistical properties of the differences $\mathbf{x}_b(t_2) - \mathbf{x}_a(t_1)$, where a and b are a pair of trajectories, will play a major role in later calculations. These statistical properties can be taken into account via a single function $P(k, \omega)$ that reflects the power spectrum of the motion⁷. For diffusive motion a practical approximation is

$$P(\mathbf{k}, \omega) = 2Dk^2 / [(Dk^2 + 1/t)^2 + \omega^2], \quad (1)$$

where D is the diffusion coefficient. In the large k regime where $k > (Dt)^{-1/2}$ this function is a properly normalized Lorentzian. Note that the collision frequency $\omega \sim v^2/D$, where v is the velocity of the particle, should be used as a cutoff to the slow $1/\omega^2$ power-law decay. Beyond $k \sim v/D$ the above expression is not valid and the power spectrum of the motion is ballisticlike.

We now take the stochastic nature of the environment into account by introducing into the Hamiltonian a stochastic potential that satisfies

$$\langle \mathcal{U}(\mathbf{x}'', t'') \mathcal{U}(\mathbf{x}', t') \rangle = \phi(t'' - t') \cdot w(\mathbf{x}'' - \mathbf{x}'). \quad (2)$$

It is assumed that $w(\mathbf{r})$ depends only on $|\mathbf{r}|$. The intensity of the noise is characterized by the parameter

$$\nu \equiv \int_{-\infty}^{\infty} \phi(\tau) d\tau \cdot |w''(0)|. \quad (3)$$

The power spectrum of the noise $\phi(\omega)$ is the Fourier transform of $\phi(\tau)$. We shall assume *Ohmic environment*, meaning that at the classical limit $\phi(\omega) = \nu$ up to some cutoff frequency $1/\tau_c$ which is assumed to be larger than any other relevant frequency scale. Thus, in the classical limit we can use the white-noise approximation (WNA), namely $\phi(\tau) = \nu \delta(\tau)$. For the quantum-mechanical case see Eq. (10). Without loss of generality we shall assume the normalization $w''(0) = -1$. The d -dimensional Fourier transform of $w(\mathbf{r})$ will be denoted by $\tilde{w}(\mathbf{k})$. The mode density (after angular

integration) is $g(k) = (C_d/(2\pi)^d)k^{d-1}\tilde{w}(k)$, where C_d is the total solid angle. We shall assume that

$$g(k) = Cl^{2+\sigma}k^{\sigma-1} \quad \text{for } k < 1/l, \quad (4)$$

where l characterize the spatial scale of the correlations, and C is a dimensionless constant. In the case of short-range Gaussian-type correlations σ equals simply d . For the long-range Coulomb interaction to be discussed later it equals $d-2$. In order to have a well-defined model we must have $|w''(0)| < \infty$, therefore only $-2 < \sigma$ is meaningful. The regime $-2 < \sigma \leq 0$ is well defined but it requires special treatment since $w(0)$ diverges.

The path-integral expression for the probability to propagate from the injection point to the observation point constitutes a double sum $\int \int \mathcal{D}\mathbf{x}' \mathcal{D}\mathbf{x}''$ over the path variables $\mathbf{x}'(\tau)$ and $\mathbf{x}''(\tau)$. Averaging over realizations of \mathcal{U} one obtains the influence functional $\exp(-S_N/\hbar^2)$. See Ref. 8 for details. The noise action functional is

$$S_N[\mathbf{x}', \mathbf{x}''] = \frac{1}{2} \int_0^t \int_0^t dt_1 dt_2 \phi(t_2 - t_1) \times [w(\mathbf{x}_2'' - \mathbf{x}_1'') + w(\mathbf{x}_2' - \mathbf{x}_1') - 2w(\mathbf{x}_2'' - \mathbf{x}_1')], \quad (5)$$

where \mathbf{x}_i is a shorthand notation for $\mathbf{x}(t_i)$. The corresponding semiclassical expression for that probability is

$$\sum_{ab} A_a A_b^* \exp\left(-\frac{S_N[\mathbf{x}_a, \mathbf{x}_b]}{\hbar^2}\right) \exp\left(i\frac{S[\mathbf{x}_a] - S[\mathbf{x}_b]}{\hbar}\right). \quad (6)$$

It is obvious that the interference contribution (the terms $a \neq b$) is suppressed due to the noise, while the classical (diagonal) contribution survives.⁹ This is the *dephasing* effect. See the general discussion in Ref. 2. We are interested here in the computation of these dephasing factors, as well as in illuminating their physical significance. For the purpose of calculating the typical value of the dephasing factor, Eq. (5) can be replaced by

$$\langle S_N \rangle \approx t \int_0^\infty g(k) dk \int_0^\infty \frac{d\omega}{\pi} \phi(\omega) P(k, \omega). \quad (7)$$

If the integral on the right-hand side is independent of t , then the typical dephasing factor in Eq. (6) can be written as a simple exponential $\exp(-t/\tau_\varphi)$.

The full analysis should take into account the dynamical nature of the environment. Namely, one should consider an Hamiltonian $\mathcal{H} = \mathcal{H}_0(\mathbf{x}, \mathbf{p}) + \mathcal{H}_{\text{env}}(\mathbf{x}, Q_\alpha, P_\alpha)$, where the latter term incorporates the interaction with environmental degrees of freedom. It is possible in principle (but generally not in practice) to use the FV formalism in order to derive an appropriate influence functional $\exp(iS_F/\hbar - S_N/\hbar^2)$. The fluctuation-dissipation theorem (FDT) implies that if S_N is known, and the temperature of the bath is further specified, then also some of the dissipative properties of the environment are determined uniquely. Therefore, it is plausible that the CL procedure of constructing an effective harmonic bath, is useful in order to derive an actual expression for the friction functional S_F . Indeed, this strategy has been adapted in

Ref. 8 and leads to the introduction of the ‘‘diffusion localization and dissipation’’ (DLD) model.¹⁰ The interaction with the bath oscillators is

$$\mathcal{H}_I = \sum_\alpha c_\alpha Q_\alpha u(\mathbf{x} - \mathbf{x}_\alpha). \quad (8)$$

Here \mathbf{x}_α is the (fixed) location of the α oscillator and Q_α is its dynamical coordinate. The bath oscillators are distributed uniformly all over space. The interaction of the particle with each of the oscillators is described by $u(r)$. The range of the interaction is l , and c_α are coupling constants. For an Ohmic bath the following expression (generalized here for any dimension) has been derived:

$$S_F = \eta \int_0^t d\tau \nabla w(\mathbf{r}) \cdot \dot{\mathbf{R}}, \quad (9)$$

where η is a friction parameter, and the path variables are $\mathbf{r} = \mathbf{x}'' - \mathbf{x}'$ and $\mathbf{R} = (\mathbf{x}'' + \mathbf{x}')/2$. From FDT it follows that if an Ohmic environment is characterized by a temperature T then the friction parameter should be $\eta = \nu/(2k_B T)$. We shall assume an environment that is characterized by a short spatial autocorrelation scale l , such that the classical trajectories are well separated with respect to this microscopic scale. Under such circumstances it has been observed in Ref. 8 that S_F will have no effect on the interference contribution. This statement does not hold in case of the CL model. The CL version for S_F is obtained by taking in Eq. (9) the limit $l \rightarrow \infty$, which is equivalent to the formal substitution $w(\mathbf{r}) = -r^2/2$. Averaging the factor $\exp(iS_F/\hbar)$ over diffusive trajectories one obtains, as in Ref. 5, a nongeneric factor $\exp(-(t/\tau_\varphi)^2)$ where $1/\tau_\varphi = \eta D/\hbar$. This particular result turns out to be identical, up to a logarithmic factor, with the genuine result (12), to be discussed later. However, it is not consistent to use the CL version for S_F in the present circumstances, and therefore the approach of Ref. 5 does not apply. With the above observations, our semiclassical strategy implies that S_F of a generic environment has no consequence on the analysis of dephasing, and Eq. (6) is still valid. Our main conclusion below will be that this (semiclassically based) statement *fails* for a low-energy particle.

We turn now to discuss some actual results for the dephasing rate. For the Ohmic bath the symmetrized power spectrum of the noise is

$$\phi(\omega) = \eta |\omega| \hbar \coth\left(\frac{\hbar |\omega|}{2k_B T}\right) \quad \text{for } |\omega| < 1/\tau_c. \quad (10)$$

For high temperatures $1/\tau_c < k_B T/\hbar$, one can use the WNA. Substituting $\phi(\tau) = 2\eta k_B T$ into Eq. (5), one obtains⁸ the universal high-temperature result

$$\left(\frac{1}{\tau_\varphi}\right)_{\text{WNA}} = \frac{2\eta k_B T l^2}{\hbar^2} \quad \text{for } 0 < \sigma. \quad (11)$$

This result does not apply for $-2 < \sigma \leq 0$ (for electrons $d \leq 2$), because $w(0)$ diverges. Still, using the WNA and doing some simple manipulations, one obtains $S_N = 2\eta k_B T l^{2+\sigma} (Dt)^{-\sigma/2}$, leading to a dephasing factor of the type $\exp(-(t/\tau_\varphi)^{(2-\sigma)/2})$, where $1/\tau_\varphi \propto T^{2/(2-\sigma)}$ in agreement with the well-known results.^{1,2}

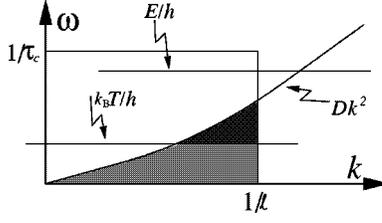


FIG. 1. The (k, ω) plane. The shaded regions indicate those environmental modes that are effective in the dephasing process. The darker region indicates a possible excess contribution due to ZPF.

We are interested in going beyond the WNA. It is useful to use Eq. (7) in order to perform the actual calculation. The domain of integration is illustrated in Fig. 1. If the temperature is *high* enough, such that $D/l^2 < k_B T/\hbar$, then one can still use the WNA result. As the temperature becomes *low*, such that $k_B T/\hbar < D/l^2$, the dephasing rate $1/\tau_\varphi$ becomes larger than the value which is predicted by the WNA. This is due to the ZPF in the frequency zone $k_B T/\hbar < \omega$ where $\phi(\omega) = \hbar \eta \omega$. Later we shall see that E/\hbar should be used as a cutoff for the ω integration. Therefore, *the present analysis, and Eq. (12) below, does not apply to a low-energy particle*. Considering the ZPF contribution, the integral in Eq. (7) is dominated by (k, ω) modes that are concentrated along the curve $\omega = Dk^2$. Moreover, most of the contribution comes from modes with large wave number, namely $k \sim 1/l$. Thus the ZPF contribution to the dephasing rate is essentially as in Ref. 4 and applies to low temperatures to any $-2 < \sigma$

$$\left(\frac{1}{\tau_\varphi}\right)_{\text{ZPF}} = \frac{C}{(2+\sigma)\pi} \ln\left[1 + \left(\frac{lv}{D}\right)^4\right] \times \frac{1}{\hbar} \eta D. \quad (12)$$

At low but finite temperatures, meaning $1/l < k_B T/\hbar \ll D/l^2$, one should consider the thermal noise contribution (TNC) that comes from the lower shaded region of Fig. 1. For $-2 < \sigma \leq 0$ the TNC dephasing factor is determined by $k \sim (Dt)^{-1/2}$ modes. For these modes $Dk^2 < k_B T/\hbar$, and therefore the previously discussed WNA applies. On the other hand, for $0 < \sigma$ one obtains

$$\left(\frac{1}{\tau_\varphi}\right)_{\text{TNC}} = C' l^{2+\sigma} \left(\frac{k_B T}{\hbar D}\right)^{\sigma/2} \frac{2 \eta k_B T}{\hbar^2} \quad (13)$$

where C' is a numerical factor. The above expression is valid for $0 < \sigma < 2$, where the dephasing process is dominated by modes with $k \sim (k_B T/\hbar D)^{1/2}$. For $2 < \sigma$ the dephasing process is dominated by modes with $k \sim 1/l$, and Eq. (13) should be modified by the replacement $\sigma \rightarrow 2$.

The FV path-integral expression is *exact* in principle. On the other hand, our semiclassical expression (6) involves the stationary-phase *approximation*. Therefore, it is important to understand, physically as well as mathematically, the validity limits of the semiclassical strategy. Each stationary-phase point of the exact FV path integral is a pair a and b of real classical trajectories that correspond to the motion of a fictitious *classical test particle*. Let us assume for simplicity that a and b are loops related by time reversal. It is also essential

in the following argumentation that the interaction with the environment is *short range*, as in the $0 < \sigma$ DLD model with l which is a small scale. It follows from the definition of the influence functional that under such circumstances $P = 1 - \exp(-S_N[a])$ is the probability for a fictitious test particle to *leave a trace* along the way (i.e., to change the quantum-mechanical state of at least one bath oscillator along the loop). For simplicity one may consider the restricted problem of a particle that travels across a single bath oscillator, meaning that Eq. (8) includes only one term. It is well known¹¹ that the semiclassical approximation is equivalent to a self-consistent mean-field scheme, where it is assumed that the wave function for the particle-oscillator system can be written as a product of a scattered particle and driven oscillator. Such an ansatz implies that for weak scattering we can treat the particle as moving with constant velocity v and solve for the oscillator. It turns out that this reduction requires the assumption of small energy transfer. Therefore, one should anticipate problems once an oscillator with ω_α larger than E is involved. In the latter case, there is no justification to think of the particle as decoupled from the bath, moving with some constant velocity, capable of exciting the oscillator along the way. Therefore, the corresponding probability P loses its physical significance. Still, the interference contribution of the specified loop will be suppressed. It is true that a low-energy particle ($\omega_\alpha < E$) is not capable of exciting the oscillator, but there is a finite probability to be scattered elastically, and consequently the original interference contribution is suppressed. However, this suppression does not have the meaning of genuine decoherence. Rather, it reflects a coherent “renormalization” of the bare dynamics. One wonders whether $\exp(-S_N[a])$ gives an estimation for the suppression of the original interference contribution due to these elastic scattering events. Unfortunately this is not the case. The elastic scattering off an oscillator involves a second-order process of virtual emission followed by absorption of a quanta $\hbar \omega_\alpha$. Therefore, the elastic scattering probability is proportional to c_α^4 . At the same time P is proportional to c_α^2 in leading order. Therefore, under such circumstances, $\exp(-S_N[a])$ does not reflect any physically meaningful quantity. It should be emphasized that the above argumentation *does not apply* once l becomes large compared with the distance that is explored by the particle. In case of the CL model ($l \rightarrow \infty$) the decoherence process is no longer determined by the *scattering mechanism*. Rather, we have a cross-over to a nonperturbative *spreading mechanism*. See detailed discussion of this point in Ref. 7.

The semiclassical strategy cannot be trusted if some of the effective bath oscillators are such that $E/\hbar < \omega_\alpha$. For diffusive motion such a situation will occur if $E/\hbar < D/l^2$. Note that the notion of large/small energy is in complete analogy with the notion of high/low temperature. For thermal motion $E \sim k_B T$ and the two notions coincides. In order to see how expression (7) should be modified for small-energy motion, let us obtain it using an elementary perturbative calculation. This is straightforward for the short-range interaction ($0 < \sigma$), since it is plausible that $1/\tau_\varphi$ has then the significance of inelastic scattering rate. The leading-order inelastic scattering probability is expressed in terms of the diagonal matrix elements of the scattering matrix, namely $P = \langle 1 - |\langle \mathbf{n} \psi | S | \mathbf{n} \psi \rangle|^2 \rangle_\beta$. The subscript β implies thermal average

over the quantum-mechanical states \mathbf{n} of the bath oscillators. The incoming particle is described by the wave function ψ . Note that the precise definition of the ‘‘dephasing rate’’ becomes vague once the semiclassical approach is abandoned. It seems plausible that P should be averaged over eigenstates of the disordered potential. Using second-order perturbation theory

$$\langle \mathbf{n}\psi | S | \mathbf{n}\psi \rangle = 1 - \frac{1}{\hbar^2} \int_0^t \int_0^{t_2} dt_2 dt_1 \langle \mathbf{n}\psi | \mathcal{H}_I(t_2) \mathcal{H}_I(t_1) | \mathbf{n}\psi \rangle.$$

Standard manipulations which are based on the definition of the Ohmic DLD model lead to the result $P = 1/\tau_\varphi$ where

$$\frac{1}{\tau_\varphi} = \frac{1}{\hbar^2} \int \frac{d\mathbf{k}}{(2\pi)^d} \int \frac{d\omega}{2\pi} \tilde{w}(k) \Phi(\omega) P_{qm}(-\mathbf{k}, -\omega). \quad (14)$$

Here $\Phi(\omega) = \hbar \eta |\omega| n(\omega)$ is the nonsymmetrized version of $\phi(\omega)$, where $n(\omega) = 1/[\exp(\hbar\omega/k_B T) - 1]$ for $0 < \omega$, and $n(\omega) = [1 + n(|\omega|)]$ for $\omega < 0$. At zero temperature $\Phi(0 < \omega) = 0$. The quantum-mechanical power spectrum of the motion is defined as the (complex) Fourier transform of $P_{qm}(\mathbf{k}, \tau)$ which is the correlator of the operator $\exp(i\mathbf{k}\mathbf{x})$. Using the semiclassical estimate $P_{qm}(\mathbf{k}, \omega) \approx P(\mathbf{k}, \omega)$ one obtains again the integral expression in Eq. (7) for the dephasing rate. However, the validity of the semiclassical estimate for $P_{qm}(\mathbf{k}, \omega)$ is restricted to the frequency range $|\omega| < E/\hbar$. Quantum mechanics cannot support larger frequencies. For thermal motion the result of the quantal FDT is related to the result of the classical FDT as follows:

$$P_{qm}(\mathbf{k}, \omega) = \frac{\hbar |\omega|}{k_B T} n(\omega) P(\mathbf{k}, \omega). \quad (15)$$

Thus, it is suggested that for thermal motion $k_B T/\hbar$ should serve as an effective cutoff in the ω integration of Eq. (7). Consequently the ZPF contribution for the dephasing rate *should be omitted*. For nonthermal motion E/\hbar is the proper cutoff and some (or all) of the ZPF contribution should be included.

Finally, one wonders whether additional modifications are required once we turn to treat (semiclassically) the problem of dephasing of electrons in a metal, taking into account the presence of the Fermi sea. Here we consider ballisticlike motion as a test case. The average scattering rate can be calculated by using a kinetic picture. The transition rate for unit volume is $W(p'|p) = \tilde{w}(k) \Phi(\omega)/\hbar^2$, where $k = (p' - p)/\hbar$ and $\omega = [E(p') - E(p)]/\hbar$. The average scattering rate is proportional to $\int \int d\mathbf{p}' d\mathbf{p} [1 - f(E')] f(E) W(p'|p)$. Standard manipulation leads to Eq. (14) with Eq. (15). Note that for the ballisticlike motion under consideration one should substitute $P(\mathbf{k}, \omega) = 1/(v|k|)$ for $|\omega| < v|k|$ and zero otherwise. This calculation implies that the dephasing rate is similar to the inelastic scattering rate also for the many-body case (provided $0 < \sigma$).

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⁹It is always true that $0 \leq S_N$. However, the concept of dephasing implies that $S_N \rightarrow \infty$ for long trajectories. The assumption of having short τ_c is important here. If we take $\phi(\tau) = \text{const}$, then some important interference contribution will not be suppressed in the $t \rightarrow \infty$ limit. See Ref. 8 for details. This observation is essential in order to understand, within the path-integral approach, why *static* disorder leads to either weak or strong localization effect.

¹⁰Obviously, these three effects come out naturally from the solution of the DLD model. Note, however, that localization effect is out of the scope of the preset application.

¹¹We thank Uzy Smilansky for pointing this out.