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’ (WNA), while at low temperatures we distinguish the contribution of ‘zero point fluctuations’ (ZPF) from the ‘thermal noise contribution’ (TNC). 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.

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 [32]. 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 experimentally [33] as well as theoretically [34], leading to an intensive debate [35] associated with the question whether 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 letter 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 consist 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 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 \( \sum A_n \exp(iS_n|x_0|/\hbar) \) over classical trajectories that connect the observation point with the injection point. We shall denote by \( t \) the total time of the motion, and \( S_n|x_0| \) are the corresponding action integrals. The statistical properties of the differences \( x_b(t_2)-x_a(t_1) \), where \( a\&b \) is 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 motion [36]. For diffusive motion a practical approximation is

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

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 \( \omega\sim\nu^2/D \), where \( \nu \) is the velocity of the particle, should be used as a cutoff to the slow \( 1/\omega^2 \) power-law decay. Beyond \( k\sim\nu/D \) the above expression is not valid and the power spectrum of the motion is ballistic-like.

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

\[
\langle \mathcal{U}(x''',t''')\mathcal{U}(x',t') \rangle = \phi(t''-t') \cdot w(x''-x')
\]

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

\[
\nu \equiv \int_{-\infty}^{\infty} \phi(\tau)d\tau \cdot |w''(0)|
\]

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 \( 1/\tau_0 \), which is assumed to be larger than any other relevant frequency scale. Thus, in the classical limit we can use the WNA, namely \( \phi(\tau) = \nu \delta(\tau) \). For the quantum mechanical see [37]. Without loss of generality we shall assume the normalization \( w''(0) = -1 \). The
$d$-dimensional Fourier transform of $w(r)$ will be denoted by $\tilde{w}(k)$. 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

$$g(k) = C\ell^{2+\sigma}k^{\sigma-1} \quad \text{for} \quad k < 1/\ell$$

(4)

where $\ell$ characterize the spatial scale of the correlations, and $C$ is a dimensionless constant. In case of short range Gaussian-type correlations $\sigma$ 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 $-2 < \sigma < 0$ 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 $\int \int D\mathbf{x}'D\mathbf{x}''$ over the path variables $\mathbf{x}'(\tau)$ and $\mathbf{x}''(\tau)$. Averaging over realizations of $\mathcal{U}$ one obtains the influence functional $\exp(-S_N/h^2)$. See [8] for details. The noise action functional is

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

$$[w(\mathbf{x}_2' - \mathbf{x}_1') + w(\mathbf{x}_2'-\mathbf{x}_1') - 2w(\mathbf{x}_2'' - \mathbf{x}_1'')]$$

(5)

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

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

(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 $\dagger$. This is the the dephasing effect. See general discussion in [4]. 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, [3] can be replaced by

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

(7)

If the integral on the right hand side is independent of $t$, then the typical dephasing factor in [3] can be written as a simple exponential $\exp(-t/\tau_\phi)$.

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 $\exp(iS_F/h - S_N/h^2)$. 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 [8] and lead to the introduction of the DLD model $\dagger$. The interaction with the bath-oscillators is

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

(8)

Here $x_\alpha$ is the (fixed) location of the $\alpha$ oscillator and $Q_\alpha$ 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 $\ell$, and $c_\alpha$ are coupling constants. For an ohmic bath the following expression (generalized here for any dimension) has been derived:

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

(9)

where $\eta$ 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 $\ell$, such that the classical trajectories are well separated with respect to this microscopic scale. Under such circumstances it has been observed in [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 [3] the limit $\ell \to \infty$, which is equivalent to the formal substitution $w(r) = -r^2/2$. Averaging the factor $\exp(iS_F/h)$ over diffusive trajectories one obtains, as in [3], a non-generic factor $\exp(-t/\tau_\phi)$ where $1/\tau_\phi = \eta D/h$. 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 [3] 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.(8) 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 ohmic bath the symmetrized power spectrum of the noise is

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

(10)

For high temperatures $1/\tau_\phi < k_B T/\hbar$, one can use the WNA. Substituting $\phi(\tau) = 2\eta k_B T$ into (8), one obtains [8] the universal high temperature result.
\[
\left( \frac{1}{\tau^*} \right)_{\text{WNA}} = \frac{2\eta k_B T \ell^2}{\hbar^2} \quad \text{for } 0 < \sigma .
\]

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 \(S_N = 2\eta k_B T \ell^2 (Dt)^{-\sigma/2} t\), leading to a dephasing factor of the type \(\exp\left(-\left(t/\tau^*\right)^{(2-\sigma)/2}\right)\), where \(1/\tau^* \propto T^{2/(2-\sigma)}\) in agreement with the well known results [4].

\[
\frac{1}{\tau^*} \approx \frac{C}{\ell^{2+\sigma}} \left(\frac{k_B T}{\hbar D}\right)^{\sigma/2} \frac{2\eta k_B T}{\hbar^2},
\]

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 \(k \sim 1/\ell\), and \([13]\) should be modified by the replacement \(\sigma \rightarrow 2\).

The FV path-integral expression is \textit{exact} in principle. On the other hand, our semiclassical expression \([4]\) involves the stationary-phase \textit{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 \(kcb\) of real classical trajectories that correspond to the motion of a fictitious \textit{classical test particle}. Let us assume for simplicity that \(kcb\) are loops related by time-reversal. It is also essential in the following argumentation that the interaction with the environment is \textit{short range}, as in the \(0 < \sigma\) DLD model with \(\ell\) 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 \textit{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 \([4]\) includes only one term. It is well known \([\ref{footnote4}]\) 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 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 \(\omega_\alpha\) 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 “re-normalization” 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 \(c^2\). At the same time \(P\) is proportional to \(c^2\) 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 \( \ell \) becomes large compared with the distance that is explored by the particle. In case of the CL model (\( \ell \rightarrow \infty \)) the decoherence process is no longer determined by the scattering mechanism. Rather, we have a crossover to a non-perturbative spreading mechanism. See detailed discussion of this point in [4].

The semiclassical strategy cannot be trusted if some of the effective bath-oscillators are such that \( E/\hbar < \omega_{\tau} \). For diffusive motion such a situation will occur if \( E/\hbar < D/\ell^2 \). 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 [8] should be modified for small-energy motion, let us obtain it using an elementary perturbative calculation. This is straightforward for short range interaction (0<\( \sigma \)) since it is plausible that \( 1/\tau_{\phi} \) 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 \( P = (1 - |\langle n\psi|S|n\psi \rangle|^2)_\beta \). The subscript \( \beta \) implies thermal average over the quantum-mechanical states \( n \) of the bath-oscillators. The incoming particle is described by the wavefunction \( \psi \). Note that the precise definition of ‘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

\[
\langle n\psi|S|n\psi \rangle = 1 - \frac{1}{\hbar^2} \int_0^t \int_0^{t_2} dt_2 dt_1 \langle n\psi|\mathcal{H}_1(t_2)\mathcal{H}_1(t_1)|n\psi \rangle
\]

Standard manipulations which are based on the definition of the ohmic DLD model lead to the result \( P = 1/\tau_{\phi} \) where

\[
\frac{1}{\tau_{\phi}} = \frac{1}{\hbar^2} \int \frac{dk}{(2\pi)^d} \int \frac{d\omega}{2\pi} \tilde{\psi}(k)\Phi(\omega) P_{qm}(-k, -\omega)
\]

Here \( \Phi(\omega) = \hbar |\langle n\psi|n\psi \rangle| = \frac{\hbar(\omega)}{\omega} \) is the non-symmetrized version of \( \Phi(\omega) \), where \( n(\omega) = 1/(\exp(\hbar\omega/k_B T) - 1) \) for \( \omega > 0 \), and \( n(\omega) = (1 + n(\omega)) \) for \( \omega < 0 \). At zero temperature \( \Phi(0) = 0 \). The quantum-mechanical power spectrum of the motion is defined as the (complex) Fourier transform of \( P_{qm}(k, \tau) \) which is the correlator of the operator \( \exp(ikx) \). Using the semiclassical estimate \( P_{qm}(k, \omega) \approx P(k, \omega) \) one obtains again the integral expression in [8] for the dephasing rate. The validity of the semiclassical estimate for \( P_{qm}(k, \omega) \) 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:

\[
P_{qm}(k, \omega) = \frac{\hbar |\omega|}{k_B T} n(\omega) P(k, \omega)
\]

Thus, it is suggested that for thermal motion \( k_B T/\hbar \) should serve as an effective cutoff in the \( \omega \) integration of Eq.(6). Consequently the ZPF contribution for the dephasing rate should be omitted. For non-thermal 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 Fermi sea. Here we consider ballistic-like motion as a test case. The average scattering rate can be calculated by using a kinetic picture. The transition rate for unit volume is \( \mathcal{W}(p'|p) = \tilde{\omega}(k)\Phi(\omega)/\hbar^2 \), where \( k=(p'-p)/\hbar \) and \( \omega=(E(p')-E(p))/\hbar \). The average scattering rate is proportional to \( \int \mathcal{W}(p'|p) \). Standard manipulations lead to Eq.(14) with (13). Note that for the ballistic-like motion under consideration one should substitute \( P(k, \omega) = 1/(v|k|) \) 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 \( \sigma > 0 \)).

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