A Letters Journal Exploring the Frontiers of Physics

February 2008

EPL, **81** (2008) 30001 www.epljournal.org
doi: 10.1209/0295-5075/81/30001

Decoherence of a particle in a ring

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received 13 July 2007; accepted in final form 21 November 2007
published online 19 December 2007

PACS 03.65.Yz – Decoherence; open systems; quantum statistical methods
PACS 74.40.+k – Fluctuations (noise, chaos, nonequilibrium superconductivity, localization, etc.)
PACS 73.23.-b – Electronic transport in mesoscopic systems

Abstract – We consider a particle coupled to a dissipative environment and derive a perturbative formula for the dephasing rate based on the purity of the reduced probability matrix. We apply this formula to the problem of a particle on a ring, that interacts with a dirty-metal environment. At low but finite temperatures we find a dephasing rate $\propto T^{3/2}$, and identify dephasing lengths for large and for small rings. These findings shed light on recent Monte Carlo data regarding the effective mass of the particle. At zero temperature we find that spatial fluctuations suppress the possibility of having a power law decay of coherence.

Introduction. – The problem of dephasing of a particle coupled to a dissipative environment at temperature T, and in particular in the limit $T\to 0$ has fascinated the mesoscopic community during the last two decades [1–7]. It has been shown [8,9] that the Caldeira-Leggett (CL) framework [10,11] can be generalized and that the proper way to characterize the environment is by its form factor $\tilde{S}(q,\omega)$. Application of the Feynman-Vernon formalism [8,9] and a semiclassical analysis have shown that an interference amplitude P_φ decays with time as $P_\varphi = \exp(-p_\varphi(t))$ with

$$p_\varphi(t)=t\int_{\mathbf{q}}\int_\omega \tilde{S}(\boldsymbol{q},\omega)\,\tilde{P}(-\boldsymbol{q},-\omega), \qquad (1)$$

where the integration measures over the wave vector and the frequency are $\mathrm{d}^3q/(2\pi)^3$ and $\mathrm{d}\omega/2\pi$, respectively. The interference suppression factor P_φ is known in the literature as the *dephasing* [2] or as the *decoherence* factor [12], and in the present work we show that it reflects loss of *purity*. In the semiclassical treatment $\tilde{S}(q,\omega)$ is the *symmetrized* form factor of the environment and $\tilde{P}(q,\omega)$ is the classical *symmetric* power spectrum of the motion. It has been conjectured using *ad hoc* argumentation [13] (see also [2,14]) that "the correct" procedure is to use non-symmetrized spectra. One of our aims is to provide a proper derivation for a corrected eq. (1).

During the last decade the study of a particle in a ring coupled to a variety of environments, has become a paradigm for the study of ground-state anomalies [15–19]. Besides being a prototype model problem it may be realized as a mesoscopic electronic device, and it is also of relevance to experiments with cold atoms or ions that are trapped above an "atom chip" device [20–22], where noise is induced by nearby metal surfaces. A significant progress has been achieved in analyzing the equilibrium properties of this prototype system, in particular the dependence of the ground-state energy on the Aharonov-Bohm flux through the ring.

In the present work we define "dephasing" as the *progressive loss of purity* and find a consistent revised form of eq. (1) that is valid beyond the semiclassical context. We apply this result to the model of a particle on a clean ring that interacts with a dirty-metal environment. At finite temperature we identify the dephasing rate $\Gamma_\varphi = p_\varphi(t)/t$, that vanishes at zero temperature. At $T=0$ we find that *only* in the CL-like limit of our model there is still slow progressive spreading ($p_\varphi(t)\sim \ln t$) which suggests a power law decay of coherence. Our results shed new light on recent Monte Carlo data for the temperature dependence of mass renormalization [23].

Purity. – Our starting point is the most natural definition for the dephasing factor as related to the purity $\mathrm{trace}(\rho^2)$ of the reduced probability matrix. The notion of purity is very old, but in recent years it has become very popular due to the interest in quantum computation [24]. Assume that the state of the system including the environment is Ψ_{pn}, where p and n label the basis states of the particle and the bath, respectively. Tracing the environment states n defines a reduced probability matrix $[\rho_{\mathrm{sys}}]_{p,p'} = \sum_n \Psi_{pn}\Psi^*_{p'n}$ and the purity is then measured by the dephasing factor $P_\varphi = \sqrt{\mathrm{trace}(\rho^2_{\mathrm{sys}})}$. Assuming a factorized initial preparation as in the conventional Feynman-Vernon formalism, we propose the loss of purity ($P_\varphi < 1$) as a measure for decoherence. A standard reservation applies: initial transients during which the system gets "dressed" by the environment should be ignored as these reflect renormalizations due to the interactions with the high-frequency modes. Other choices of initial state might involve different transients, while the later slow approach to equilibrium should be independent of these transients. In any case, the reasoning here is not much different from the usual ideology of the Fermi golden rule, which is used with similar restrictions to calculate transition rates between levels.

Consider then a factorized initial preparation $\Psi^{(0)}_{pn} = \delta_{p,p_0}\delta_{n,n_0}$, so that within perturbation theory all Ψ_{pn} are small except for $\Psi_{p_0n_0}$. We can relate P_φ to the probabilities $P_t(p,n|p_0,n_0) = |\Psi_{pn}|^2$ to have a transition from the state $|p_0,n_0\rangle$ to the state $|p,n\rangle$ after time t. To leading order we find

$$P_\varphi = P_t(p_0,n_0|p_0,n_0) + \sum_{p\neq p_0} P_t(p,n_0|p_0,n_0) + \sum_{n\neq n_0} P_t(p_0,n|p_0,n_0). \quad (2)$$

The first term in eq. (2) is just the survival probability P_{survival} of the preparation. The importance of the two other terms can be demonstrated using simple examples: For an environment that consists of static scatterers we have $P_{\text{survival}} < 1$ but $P_\varphi = 1$ thanks to the second term. For a particle in a ring that interacts with a $q=0$ environmental mode $P_{\text{survival}} < 1$ but $P_\varphi = 1$ thanks to the third term. Using $\sum_{p,n} P_t(p,n|p_0,n_0) = 1$ we finally obtain

$$p_\varphi = 1 - P_\varphi = \sum_{p\neq p_0}\sum_{n\neq n_0} P_t(p,n|p_0,n_0). \quad (3)$$

This result has the form of a Fermi golden rule (FGR), *i.e.* it is the probability that both the system and the bath make a transition. This differs from the usual FGR treatment [2] in which terms like $P_t(p_0, n\neq n_0|p_0,n_0)$ are included. In the problem that we consider in this paper we can calculate P_φ using a $\mathrm{d}q\mathrm{d}\omega$ integral as in eq. (1). In many examples the $\omega = 0$ transitions have zero measure and therefore P_φ is practically the same as $P_t(p_0,n_0|p_0,n_0)$. Otherwise one has to be careful in eliminating those transitions that do not contribute to the dephasing process. Anticipating the application of eq. (1) for the calculation of the dephasing for a particle in a ring, the integration over q becomes a discrete summation where the $q=0$ related component should be excluded. It is implicit in the derivation of eq. (1) from eq. (3) that at the last step a thermal average is taken over both n_0 and p_0, though in general one may consider non-equilibrium preparations as well.

Dephasing formula. – We would like to apply our revised FGR equation (3) to the general problem of a particle at position $\boldsymbol{R}$ coupled to an environment with electronic density $\mathsf{n}(\boldsymbol{r},t)$. It is implicit that the particle also experiences an external potential that defines the confining geometry. A Hamiltonian $\mathcal{H}_0$ of the particle in the confined geometry defines the states and eigenstates via $\mathcal{H}_0|p\rangle = E_p|p\rangle$. For definiteness we use the Coulomb interaction, though any other interaction may be used, hence the particle-environment interaction is

$$V_{\text{int}} = \int \mathrm{d}^3r\rho(\boldsymbol{r}) \int \mathrm{d}^3r' \frac{e^2\mathsf{n}(\boldsymbol{r}',t)}{|\boldsymbol{r}-\boldsymbol{r}'|} \equiv \int \mathrm{d}^3r\rho(\boldsymbol{r})\,\mathcal{U}(\boldsymbol{r}), \quad (4)$$

where $\rho(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{R}(t))$, with $\boldsymbol{R}(t)$ the position operator of the particle in the Heisenberg (interaction) picture. Our FGR with $P_t(p,n|p_0,n_0) = |\langle p,n|\int_0^t V_{\text{int}}\mathrm{d}t'|p_0,n_0\rangle|^2$ (using $\hbar = 1$ units) yields

$$p_\varphi = e^2 \sum_{p(\neq p_0)}\sum_{n(\neq n_0)} \int_0^t \mathrm{d}t' \int_0^t \mathrm{d}t'' \int_r\int_{r'} \langle p_0|\rho(\boldsymbol{r}'',t'')|p\rangle\langle p|\rho(\boldsymbol{r}',t')|p_0\rangle \times \langle n_0|\mathcal{U}(\boldsymbol{r}'',t'')|n\rangle\langle n|\mathcal{U}(\boldsymbol{r}',t')|n_0\rangle. \quad (5)$$

The double time integral can be written as a $\mathrm{d}q\mathrm{d}\omega$ integral over Fourier components. For this purpose we define the form factor of the *fluctuations* (as seen by the particle):

$$\tilde{S}(\boldsymbol{q},\omega) = \int \mathrm{d}^3r \int \mathrm{d}\tau\, \langle \mathcal{U}(\boldsymbol{r}',t')\mathcal{U}(\boldsymbol{r},t)\rangle\, \mathrm{e}^{i\omega\tau - i\boldsymbol{q}\cdot\boldsymbol{r}} \quad (6)$$

with thermal average replacing the n_0 state expectation value. $\tilde{S}(q,\omega)$ is related to the dielectric function of the environment $\varepsilon(\boldsymbol{q},\omega)$ via the fluctuation dissipation theorem

$$\tilde{S}(\boldsymbol{q},\omega) = \frac{4\pi e^2}{\boldsymbol{q}^2}\mathrm{Im}\left[\frac{-1}{\varepsilon(\boldsymbol{q},\omega)}\right]\frac{2}{1-\mathrm{e}^{-\omega/T}}. \quad (7)$$

In the semiclassical formulation one replaces the operator $\boldsymbol{R}(t)$ by the classical trajectory $\boldsymbol{R}_{\text{cl}}(t)$, and consequently in eq. (5) the particle-related part of the integrand is replaced by a classical two-point correlation function of the type $\langle f(\boldsymbol{R}_{\text{cl}}(t''))f(\boldsymbol{R}_{\text{cl}}(t'))\rangle$. In the quantum context the particle-dependent part of eq. (5), after Fourier transform, leads to the following definition for the power spectrum of the motion:

$$\tilde{P}(\boldsymbol{q},\omega) = \int \left[\langle \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{R}(\tau)}\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{R}(0)}\rangle - \langle \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{R}}\rangle^2\right]\mathrm{e}^{i\omega\tau}\,\mathrm{d}\tau. \quad (8)$$

Also here, at state of equilibrium, a thermal average should replace the p_0 state expectation value. It is important to realize that this definition, as well as eq. (7), imply that non-symmetrized spectral functions should be used. Our main interest is in very low temperatures, so we set for presentation purpose $p_0 = 0$. Then we get

$$\tilde{P}(\boldsymbol{q},\omega) = \sum_{p\neq 0} |\langle p|\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{R}}|0\rangle|^2\,\delta(\omega - E_p). \quad (9)$$

Using the above *definitions* for $\tilde{S}(\boldsymbol{q},\omega)$ and $\tilde{P}(\boldsymbol{q},\omega)$ we can re-write

$$p_\varphi = \int_0^t \mathrm{d}t' \int_0^t \mathrm{d}t'' \int_q \iint_{\omega',\omega''} \tilde{S}(\boldsymbol{q},\omega')\tilde{P}(-\boldsymbol{q},-\omega'') \times \mathrm{e}^{-i(\omega'-\omega'')(t''-t')} . \tag{10}$$

For practical calculations or for aesthetic reasons we prefer to use soft rather than sharp cutoff for the time integration. Then we get

$$p_\varphi = t \int_q \iint_{\omega,\omega'} \tilde{S}(\boldsymbol{q},\omega)\tilde{P}(-\boldsymbol{q},-\omega') \left[\frac{(2/t)}{(1/t)^2+(\omega-\omega')^2}\right]. \tag{11}$$

This result can be cast into the form of eq. (1) provided $\tilde{P}(\boldsymbol{q},\omega)$ is *re-defined* as the convolution of eq. (8) with the kernel in the square brackets, which is like a time-uncertainty broadened delta function. Equation (11) is our revised form of eq. (1); it provides the dephasing factor $P_\varphi = \exp(-p_\varphi)$ for a general particle-environment interaction.

Dephasing rate. – At finite temperatures, if t is larger compared with dynamically relevant time scales, and in particular $t \gg 1/T$, we can replace the square brackets in eq. (11) by $2\pi\delta(\omega-\omega')$. Consequently we get linear growth $p_\varphi \approx \Gamma_\varphi t$ with the rate

$$\Gamma_\varphi = \int_q \int_\omega \tilde{S}(\boldsymbol{q},\omega)\tilde{P}(-\boldsymbol{q},-\omega). \tag{12}$$

Following standard arguments one conjectures that the long time decay is exponential, *i.e.* $P(t)=\exp(-\Gamma_\varphi t)$, as in the analysis of Wigner's decay. In terms of the dielectric function $\varepsilon(q,\omega)$ we obtain the following general result:

$$\Gamma_\varphi = \sum_{p\neq 0} \int_q \frac{4\pi e^2}{q^2} \mathrm{Im}\left[\frac{1}{\varepsilon(q,-E_p)}\right] \frac{2|\langle p|\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{R}}|0\rangle|^2}{\mathrm{e}^{E_p/T}-1}. \tag{13}$$

Our assumption $t \gg (1/T)$ implies that (13) can be trusted only if $\Gamma_\varphi \ll T$ which implies a weak-coupling condition (see below).

Dirty metal. – So far we kept the derivation general, without specifying either the particle states $|p\rangle$ or the dielectric function $\varepsilon(q,\omega)$. We consider now a particle of mass M on a ring of radius R so that $\mathcal{H}_0 = -(2MR^2)^{-1}\partial_\theta^2$, where θ is the angle variable. The particle eigenstates are then $|p_m\rangle \propto \mathrm{e}^{im\theta}$ with energy eigenvalues $E_m = m^2/(2MR^2)$. We study the effect of low-frequency fluctuations ($|q| \lesssim 1/\ell, |\omega| \lesssim \omega_c$) due to a dirty-metal environment for which $\varepsilon(q,\omega) = 1+4\pi\sigma(-i\omega+Dq^2)^{-1}$, where σ is the conductivity, D is the diffusion constant, and ℓ is the mean free path. Below we identify the renormalized value of the high-frequency cutoff ω_c as the classical damping rate $\gamma_r = 2\pi\alpha/M\ell^2$, where the dimensionless interaction strength is $\alpha = e^2/(8\pi^2\sigma\ell) = 3/(8(k_F\ell)^2)$ and k_F is the Fermi wave vector. We first consider the case of a large ring with $r = R/\ell \gg 1$. Using the Fourier expansion [16,17]

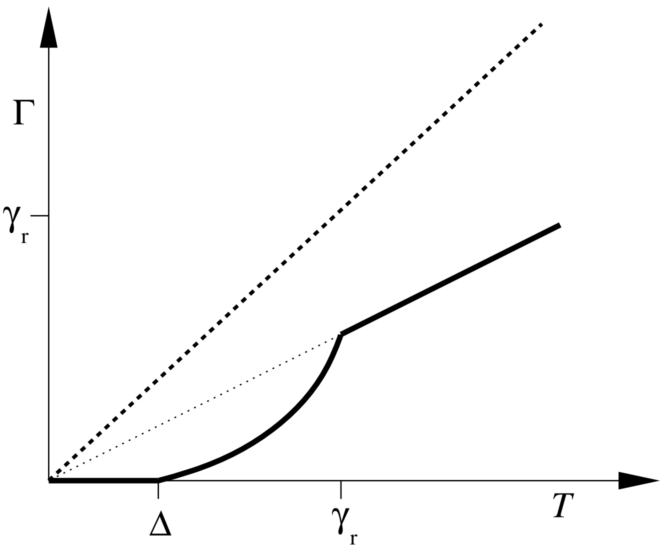

Fig. 1: Illustration of the dependence of the dephasing rate Γ on the temperature T. The dephasing rate is well defined for $t > (1/T)$, and hence the self-consistency requirement is $\Gamma \ll T$. This condition is demonstrated by a comparison with the dashed line. The illustration assumes weak coupling $\alpha \ll 1$ and large rings $\alpha r^2 \gg 1$ so that the energy cutoff is $\gamma_r = 2\pi\alpha/M\ell^2 \gg \Delta = 1/MR^2$. For extremely low temperatures, such that T is smaller compared with the spacing Δ, the probability to excite the system is exponentially small and the familiar two-level modeling becomes applicable.

$$\ell \int_q \mathrm{e}^{-i\boldsymbol{q}\cdot(\boldsymbol{R}(\theta)-\boldsymbol{R}(\theta'))} \frac{4\pi}{q^2} = \frac{1}{\sqrt{4r^2\sin^2(\frac{\theta-\theta'}{2})+1}} = 1 - \sum_m a_m \sin^2\left(\frac{m(\theta-\theta')}{2}\right) \tag{14}$$

with

$$a_m \approx \begin{cases} \frac{2}{\pi r}\ln\frac{r}{m}, & 1 \leqslant m \leqslant r, \\ 0, & \text{otherwise}, \end{cases} \tag{15}$$

we have

$$\int_q \frac{4\pi}{q^2} |\langle 0|\mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{R}}|p_m\rangle|^2 = \frac{1}{4}a_{|m|} \tag{16}$$

and therefore

$$\Gamma_\varphi = 2\pi\alpha \sum_{m\neq 0} a_m \frac{E_m \mathrm{e}^{-|E_m|/\omega_c}}{\mathrm{e}^{E_m/T}-1} \approx 2\pi\alpha T \sum_{0<|m|<r_{\text{eff}}} a_m , \tag{17}$$

where $r_{\text{eff}} \equiv \min\{r, (2MR^2T)^{1/2}, (2MR^2\omega_c)^{1/2}\}$ is determined by the conditions $m < r$ and $E_m < T$ and $E_m < \omega_c$. At high temperatures, $T > \omega_c$, r_{eff} is temperature independent and therefore $\Gamma_\varphi \propto T$, while at low temperatures (but still $T > 1/(2MR^2)$) we get, as shown schematically in fig. 1,

$$\Gamma_\varphi = 4\alpha T\sqrt{2M\ell^2T}\,|\ln\sqrt{2M\ell^2T}| \sim T^{3/2}|\ln T|. \tag{18}$$

From these results it follows that the self-consistency requirement $\Gamma_\varphi \ll T$, as discussed after eq. (13), is globally satisfied for any temperature if $\alpha \ll 1$, or equivalently if $k_F\ell \gg 1$; in the regime of eq. (18) the constraint $\Gamma_\varphi \ll T$ is satisfied also with stronger α. We note that if the $m=0$ Fourier component were included in the summation, then the low-T form would change to $\Gamma_\varphi \propto T$, in contrast with the proper result eq. (18).

Though the derivation of eq. (11) refers to the one particle problem, it turns out that the treatment of dephasing in the many-body problem is not much different. Namely, the effect of the "Pauli principle" in the low-temperature Fermi sea occupation can be incorporated via an appropriate modification of the cutoff scheme for the spectral functions involved. On the heuristic level it involves a T-dependent momentum cutoff as in [12], while more recently it has been formulated and established using more advanced methods [25].

Zero temperature. – We would like to discuss the "zero-temperature" regime. If the temperature were extremely low, such that $T \ll \Delta$ where $\Delta \sim 1/(MR^2)$ is the ground-state level spacing, we could treat the problem using a "two-level approximation", which is a very well-studied model [12]. We do not further discuss this regime. From here on we assume $T \gg \Delta$. Thus, we can treat the dω integration as if the levels of the ring form a continuum. But we still can define "zero temperature" as such for which the practical interest is in the time interval $t \ll 1/T$, which can be extremely long. Then one realizes that eq. (11) gives a non-zero result even at "zero temperature":

$$p_\varphi \approx \alpha \sum_m a_m \ln \frac{\omega_c}{E_m + (1/t)}, \tag{19}$$

where ω_c is the high-frequency cutoff of the environmental modes. Assuming $\ell \ll R$ we get after a transient

$$p_\varphi \approx \alpha\ell \int_0^{1/\ell} \mathrm{d}q \; \ln\left[\frac{1}{q\ell}\right] \ln\left[\frac{M\omega_c}{q^2}\right] \approx \alpha, \tag{20}$$

where, for clarity of presentation, we converted the m summation into a $\mathrm{d}q \equiv (1/R)\mathrm{d}m$ integral. Accordingly, we deduce that for $r \gg 1$ coherence is maintained if $k_F\ell \gg 1$. This should be contrasted with the CL limit ($\ell \to \infty$) where the integral has a singular $q \sim 0$ contribution from the lowest fluctuating mode ($m=1$), and consequently $p_\varphi \approx 2\alpha r^2 \log(\omega_c t)$, which is a well-known expression [6,15]. But once $r<1$ the condition for using our perturbation result is replaced by $\alpha r^2 \ll 1$, which is an ℓ-independent condition. In this CL limit the quantization of the energy spectrum is important and the renormalized cutoff frequency becomes $\omega_c \sim \Delta$ instead of $\omega_c \sim \gamma_r$. Accordingly, in the latter circumstances, the time during which the log spreading prevails diminishes.

Effective mass. – It can be shown [9] that the mass renormalization in the inertial (polaronic) sense is $\Delta M = \eta/\omega_c$. However, in recent works [16–18], the mass renormalization concept appears in a new context. The free energy $\mathsf{F}(T,\Phi)$ of a particle in a ring is calculated, where Φ is the Aharonov-Bohm flux through the ring. Then the coherence is characterized by the "curvature", which is a measure for the sensitivity to Φ. The curvature can be parameterized as

$$\left.\frac{\partial^2 \mathsf{F}}{\partial \Phi^2}\right|_{\Phi=0} = \frac{e^2}{M^* R^2} f(M^* R^2 T), \tag{21}$$

where in the absence of environment $M^* = M$ is the bare mass of the particle, and the T-dependence simply reflects the Boltzmann distribution of the energy. In the presence of coupling to the environment $M^* > M$ and M^* depends on both α and T. At $T=0$, for fixed $\alpha \ll 1$, Monte Carlo data show [22] that the ratio M^*/M is independent of the radius provided $r > r_c$, where r_c is a critical radius. As the radius becomes smaller compared with r_c, the ratio M^*/M rapidly approaches unity. In the regime of "large R" the mass renormalization effect diminishes with temperature and depends on the scaled variable RT, while for "small R" the ratio M^*/M depends on the scaled variable R^4T. The natural question is whether we can shed some light on the physics behind this observed temperature dependence. Making the conjecture that the temperature dependence of M^*/M is determined by dephasing it is natural to suggest the following measure of coherence:

$$x(T,R) = p_\varphi\left(t = \frac{1}{\Delta_{\text{eff}}}\right) \approx \frac{\Gamma_\varphi}{\Delta_{\text{eff}}} \approx 2\pi\alpha\bar{a}MR^2T, \tag{22}$$

where $\bar{a}$ is an average value of a_n. Equation (22) describes dephasing at time $t = 1/\Delta_{\text{eff}}$, where $\Delta_{\text{eff}} \sim r_{\text{eff}} \times (MR^2)^{-1}$ is the energy scale that characterizes the "effective" transitions; hence the variable x measures the level sharpness. For a dirty metal with $\ell \ll R$ the typical value of the Fourier components is $\bar{a} \sim 1/r$ as implied by eq. (15). On the other hand, for a dirty metal with $\ell \gg R$ there is only one effective mode with $\bar{a} \sim r^2$. Accordingly, we get the RT and the R^4T dependence, respectively, in agreement with the Monte Carlo simulations. The condition $x < 1/2$ can serve as a practical definition for having coherence. It can be translated either as a condition on the temperature, or optionally it can be used in order to define a coherence length that depends on the temperature. The conjecture is that M^*/M is a function of x.

Summary. – In this paper we derive a new perturbative expression for the dephasing factor $P_\varphi(t)$ and apply it to a particle in a ring coupled to fluctuations of a dirty-metal environment. We find that the dephasing rate vanishes at $T=0$. We also define a coherence criterion that identifies a dephasing length. The latter diverges as T^{-1} for large radius and as $T^{-1/4}$ for small radius, in agreement with Monte Carlo data on mass renormalization. The renormalized mass is an equilibrium property which affects temporal correlation functions.

But we see that it reflects non-equilibrium features of the dynamics which are expressed in the dephasing factor calculation. We find this relation between equilibrium and non-equilibrium scales an intriguing phenomena.

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We thank F. Marquardt and J. Imry for helpful communications. This research was supported by a grant from the DIP, the Deutsch-Israelische Projektkooperation.

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