Diffusion and Localization in a Dissipative Quantum System

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The motion of a quantum mechanical particle is studied in the presence of a periodic potential and frictional forces. Depending on the parameters, the behavior changes from diffusion to localization.

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Recently, Leggett[1] has drawn attention to the problem of quantum coherence in connection with a macroscopic degree of freedom coupled to a dissipative environment. Subsequently, this problem has been studied for a system with a double-well potential.[2] There, coherence is said to be absent, if the particle—which is short for degree of freedom—is localized in one of the two wells.

In the following, the motion of a particle in a periodic potential is studied and its mobility will be calculated. From a formal point of view, this problem is equivalent to a system of one-dimensional charged particles which interact with a logarithmic potential. An important feature is a duality transformation (methods I and II) which is a mapping of parameters such that diffusive and localized behavior appear interchanged.

A Feynman path-integral formulation in "imaginary" time is of superior advantage in the discussion of dissipative systems.[3] There, the coordinates of the environment can be "integrated out" such that in the end one is left with an effective action $S_{\text{eff}} = S_0 + S_{\text{int}}$,

$$S_0 = \int d\tau \frac{1}{2} m\dot{q}_\tau^{\,2} + \frac{\eta}{4\pi} \int d\tau\, d\tau' \left(\frac{q_\tau - q_{\tau'}}{\tau - \tau'}\right)^2;$$
$$S_{\text{int}} = \int d\tau\, V(q_\tau). \tag{1}$$

The strength of the coupling to the environment is contained in the frictional constant η. The potential is chosen to be $V(q_\tau) = -g\cos q_\tau + F_\tau q_\tau$.

Alternatively, the time-dependent driving force F_τ may act as a source in the generating functional defined by

$$Z[F_\tau] = \int \mathfrak{D} q_\tau \exp(-S_{\text{eff}}). \tag{2a}$$

The functional integral extends over all paths q_τ. The two-point correlation can be calculated as follows:

$$\langle q_\tau q_{\tau'}\rangle = Z^{-1}\, \delta^2 Z/\delta F_\tau\, \delta F_{\tau'}|_{F=0}. \tag{2b}$$

This quantity depends only on the time difference $\tau - \tau'$; its Fourier transform will be written shortly as $\langle qq\rangle_\omega$. Then, the (dimensionless) mobility is given by

$$\mu(\omega) = \eta |\omega| \langle qq\rangle_\omega. \tag{3}$$

Strictly speaking, the analytical continuation of μ in the complex half-plane $\text{Re}\,\omega > 0$ is required. At zero temperature, however, the important limit $\omega \to 0$ can also be obtained from real and positive ω. Thus, it is allowed to conclude that the quantum mechanical particle is diffusing, if $\mu(+0) > 0$; and that is is localized, if $\mu(+0) = 0$.

Method I.—We introduce Fourier transforms and write

$$S_0 = \tfrac{1}{2} \int (d\omega/2\pi) D_\omega^{-1} |q_\omega|^2; \quad D_\omega^{-1} = m\omega^2 + \eta|\omega|.$$

Next, we expand

$$\exp\left(g \int d\tau \cos q_\tau\right) = \sum_{n=0}^{\infty} \int d\tau_1 \ldots d\tau_n \frac{(g/2)^n}{n!} \sum_{\{e_j\}} \exp\left[i \int d\tau \sum_{j=1}^{n} e_j \delta(\tau - \tau_j) q_\tau\right].$$

The quantities $e_j = \pm 1$ may be considered as charges of classical particles located at τ_j. Since $D_{\omega=0}^{-1} = 0$, the functional integral with respect to $[q_\tau]$ can only be performed if the time average of $F_\tau + i\sum e_j \delta(\tau - \tau_j)$ vanishes. This means that the total charge $\sum e_j$ of the particles has to be zero; hence $n = 2N$ and we have a neutral plasma. There are $n!/(N!)^2$ equivalent ways to distribute the charges on the coordinates; I chose

$$\rho_\tau^{\,N} = \delta(\tau - \tau_1) + \ldots + \delta(\tau - \tau_N) - \delta(\tau - \tau_{N+1}) - \ldots - \delta(\tau - \tau_{2N})$$

to be the charge density. Thus, we obtain

$$Z = C\sum_N \int d\tau_1 \ldots d\tau_{2N} [(g/2)^N/N!]^2 \exp\{-\tfrac{1}{2} \int d\tau\, d\tau' [iF_\tau + \rho_\tau^{\,N}] D_{\tau\tau'} [iF_{\tau'} + \rho_{\tau'}^{\,N}]\}, \tag{4}$$

where $C = (\det D)^{-1/2}$. This expression can be interpreted as the grand canonical partition function of a neutral plasma (excepting the source F_τ). The interaction potential between the charges is

$$D_{\tau\tau'} = \int (d\omega/2\pi) D_\omega \exp - i\omega(\tau - \tau') = \begin{cases} -(1/2\eta)r, & r \ll 1, \\ -(1/\pi\eta)\ln r, & r \gg 1, \end{cases} \tag{5}$$

where $r = (\eta/m)|\tau - \tau'|$. At short distances the interaction is Coulomb-like, whereas at large separation, it is dominated by a logarithmic dependence.

Next, we calculate

$$\langle g_\tau g_{\tau'} \rangle = D_{\tau\tau'} - \int d\bar{\tau}\, d\bar{\tau}'\, D_{\tau\bar{\tau}} \langle \rho_{\bar{\tau}} \rho_{\bar{\tau}'} \rangle D_{\bar{\tau}'\tau'},$$

where $\langle \rho_\tau \rho_{\tau'} \rangle$ is the charge-density correlation function of the plasma. Again, it depends only on the coordinate difference $\tau - \tau'$; its Fourier transform will be written as $\langle \rho\rho \rangle_\omega = S_\omega$. Then the mobility assumes the form

$$\mu(\omega) = 1 - D_\omega S_\omega \tag{6}$$

[with an unimportant prefactor $(1 + m|\omega|/\eta)^{-1}$ omitted]. Note the similarity of $\mu(\omega)$ with the inverse static dielectric function $1/\epsilon(q)$ of a Coulomb plasma.[4]

Method II.—The second method (instanton technique[5]) is correct asymptotically if

$$s = 8(mg)^{1/2} \gg 1; \quad s \gg \eta. \tag{7}$$

One argues that in this limit, the tunneling of the quantum mechanical particle between adjacent minima of the potential $-g\cos q$ (that is, $q = 2\pi n$) can well be described in WKB approximation. There, the path q_τ^{cl} which corresponds to the classical motion of the undamped particle in the "inverted" potential leads to a predominant contribution to the path integral. Hence, $m\ddot{g}_\tau^{\text{cl}} - g\sin q_\tau^{\text{cl}} = 0$, and there are kinklike solutions (instantons), where q_τ^{cl} just changes by $\pm 2\pi$ in a lapse of time $\omega_0^{-1} = (\lambda/m)^{-1/2}$. For instance, there is a solution $f(\tau) = 4 \arctan \exp(\omega_0 \tau)$. Furthermore, one can construct a sequence of kinks ($e_j = +1$) and antikinks ($e_j = -1$) located at the positions $\tau_1, \ldots, \tau_n$:

$$\hat{q}_\tau = \sum_{j=1}^{n} e_j f(\tau - \tau_j), \tag{8a}$$

which are approximate solutions of the classical equation of motion, $\hat{q}_\tau \simeq q_\tau^{\text{cl}}$, provided that $|\tau_j - \tau_k| \gg \omega_0^{-1}$. Of importance will be the Fourier transform

$$-i\omega \hat{q}_\omega = h_\omega \sum_j e_j \exp(i\omega\tau_j), \tag{8b}$$

where h_ω is the Fourier transform of $\dot{f}(\tau)$; $h_0 = 2\pi$.

Next, we calculate $S_{\text{eff}}[\hat{q}]$. In order to remove a constant (yet infinite) term, we replace $-g\cos q$ by $g[1 - \cos q]$. Then, we obtain

$$S_{\text{eff}}[\hat{q}] = ns + \tfrac{1}{2}\sum_{jk} e_j e_k \Delta_{\tau_j \tau_k} + i\int (d\omega/2\pi)(F_{-\omega} h_\omega/\omega) \sum_j e_j \exp(i\omega\tau_j). \tag{9}$$

One recognizes an effective interaction between kinks and antikinks which involves an interaction potential

$$\Delta_{\tau\tau'} = \int (d\omega/2\pi) h^2(\omega)(\eta/|\omega|) \exp - i\omega(\tau - \tau') = \begin{cases} -\alpha\eta\rho^2, & \rho \ll 1, \\ -4\pi\eta\ln\rho, & \rho \gg 1, \end{cases} \tag{10}$$

where $\rho = \omega_0|\tau - \tau'|$ and α is of order unity. It is important to note that the above result can only be obtained if $\sum e_j = 0$; otherwise, the action is infinitely large. This means that $n = 2N$.

A few steps in the ensuing procedure should be explained. The functional integral is reduced to integrations with respect to the positions of the kinks such that $\tau_1 < \tau_2 < \ldots < \tau_{2N}$ (summation with respect to N included). Further, the Gaussian fluctuation around $\hat{q}_\tau$ can be included if one replaces $e^{-s} \to \gamma/2 = \omega_0(2s/\pi)^{1/2} e^{-s}$. Eventually, one arrives at an expression for $Z[F]$ very similar to Eq. (4) except for two differences: (i) the trivial replacement $D_{\tau\tau'} \to \Delta_{\tau\tau'}$, $g \to \gamma$; and (ii) different functional form in which the source F_τ enters. Note that (ii) leads to an expression for the mobility,

$$\mu(\omega) = \Delta\omega\Sigma_\omega, \tag{11}$$

which differs formally from Eq. (6). On the other hand, Σ_ω differs from S_ω only by the replacement (i).

Considering Eqs. (6) and (11), we conclude that $0 \leq \mu \leq 1$. Essentially, $\mu(+0)$ depends only on η and s (the scale in the time variable is irrelevant). For the sake of definitiveness, I will use the terminology of phase transitions in the discussion of this dependence. Possible candidates for different phases are (A_1) $\mu \equiv 0$, (A_2) $\mu \equiv 1$, and (B) $0 < \mu < 1$.

The two representations for μ can be mapped onto each other if one is allowed to neglect differences in the core regions of the interaction potential $D_{\tau\tau'}$ and $\Delta_{\tau\tau'}$. Then, we may use the substitution $\mu \to 1 - \mu$; $2\pi\eta \to 1/2\pi\eta$; $mg/\eta \to \gamma/\omega_0$

(this also takes care of the difference in the time scale). The fixed point of this mapping is $2\pi\eta^* = 1$; $s^* = 1.5$ [unfortunately, Eq. (7) is not strongly satisfied]. At this point, there is either a transition between phases A_1 and A_2, or there is phase B with $\mu = \frac{1}{2}$.

A renormalization technique has been developed by Anderson and Yuval[6] for the problem of a one-dimensional plasma with logarithmic interaction. They consider only the case of ordered charges $(+-+-+-\ldots)$; the difference may be relevant, but it will be neglected in the following. According to their result, g scales to zero if g is small and $\eta < \eta^*$. The same is true for γ, if $\eta > \eta^*$. The most plausible interpretation of this result is that $\mu \equiv 0$ and $\mu \equiv 1$, respectively, in these two regions.

A phase diagram is shown in Fig. 1. Accordingly, one expects the particle to be localized[7] only in region A_1, where $\eta > \eta^*$ and where s is sufficiently large. In regions A_2 and B, the particle is expected to show diffusive behavior. Considering the differences between B and A_2, one may speculate that in region B, diffusion will be incoherent or stochastic, whereas in region A_2, diffusion is a coherent and regular process.[8]

The results of Ref. 2 on the behavior of a damped particle in a bistable potential are contained in the upper part ($s \to \infty$) of Fig. 1. The interpretation of their results is unambiguous in region A_1 where the particle is localized in one of the two wells. However, it is not clear whether in region B the tunneling is coherent (in the sense of a beat phenomenon) or incoherent (in a stochastic sense).

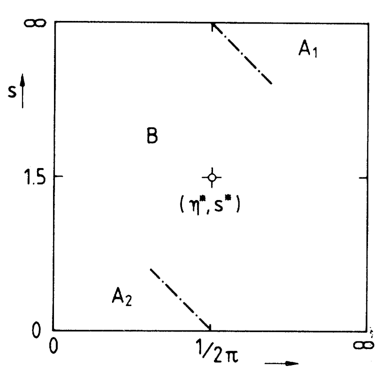

FIG. 1. Phase diagram in (η, s) plane. Phases A_1 and A_2 have $\mu \equiv 1$ and $\mu \equiv 0$, respectively. In B, we have $0 < \mu < 1$. At the fixed point (circle) of the duality transformation, $\mu = \frac{1}{2}$. The phase boundaries (dash-dotted lines) are drawn according to Anderson and Yuval (Ref. 6). The quantum mechanical particle is localized only in region A_1.

The above statements apply only to the case of zero temperature (which corresponds to the thermodynamic limit in the system of charged particles). No phase transition occurs at finite temperature.

I wish to stress that the most important feature of the present model is a frictional force on the particle proportional to its velocity. Formally, this means that $D_\omega^{-1} \to \eta|\omega|$ for sufficiently small $|\omega|$. In the analogous systems of charged particles this property corresponds to the logarithmic behavior of the interaction at large distances. Other properties of D_ω^{-1} are irrelevant, at least in the limits $s \to 0$ and $s \to \infty$, respectively.

One expects that such a type of frictional force can only be found for a particle which is macroscopic in comparison with its environment. Furthermore, it seems that macroscopic quantum systems with $D_\omega^{-1} \to \eta|\omega|$ represent cases on a borderline which separates systems of qualitatively different behavior depending on whether D_ω^{-1} decreases faster or slower than the first power of $|\omega|$ in the limit $|\omega| \to 0$.

In an experimental realization of the present model by a resistively shunted Josephson junction, one has $\eta = \hbar/4e^2R$, $s = (8\hbar C I_0 e^{-3})^{1/2}$, where R, C, and I_0 are the resistivity (for small voltages; see preceding paragraph), the capacitance, and the maximal Josephson current of the device. With tunnel junctions, one is most likely in region A_1. In such a case, it would be most interesting to observe the incipient localization as the temperature is lowered to absolute zero.[9]

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[7]The self-trapping effect of a polaron [Y. Toyozawa, Prog. Theor. Phys. 26, 29 (1961)] is not related to the localization effect here: The environment provides only a frictional force and no energy renormalization; furthermore, continuous translational symmetry has to be broken strongly ($s\rightarrow\infty$).

[8]If μ is interpreted as $1/\epsilon$, then the transition $A_1 \rightarrow B \rightarrow A_2$ corresponds to the transition metal$\rightarrow$insulator $\rightarrow$ vacuum.

[9]Further theoretical investigations will be devoted to this problem.