Diffusion and Localization of a Particle in a Periodic Potential Coupled to a Dissipative Environment

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The phase diagram of a Hamiltonian which describes a particle moving in a periodic potential and coupled to an external heat bath has been analyzed in detail. By renormalization-group methods, it is proved that this system exhibits an unusual transition between diffusive behavior and a self-trapped phase. The dynamics along the transition line is shown to be integrable and the order parameter, the mobility, is computed exactly.

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There has recently been a great deal of interest in trying to describe the quantum behavior[1,2] of systems for which the classical motion would be damped due to a dissipative interaction with their environment. The physically particularly interesting situation of a particle moving in a periodic potential has been considered by Schmid.[3] He has shown that the weakly corrugated case is related by a duality transformation to the limit where there are large potential energy barriers between the wells and has conjectured by analogy with the known results for the two-level system[4,5] that a nontrivial phase diagram might occur. This model can be relevant[6] to studies of diffusion of heavy particles, like muons and protons inside metals[7] and at surfaces,[8] hence providing many new experimental realizations where the interplay between quantum effects and dissipation can be studied. Also, as discussed in detail below, it shows an interesting example of self-localization even in the absence of imperfections in the periodic potential, a dynamical effect not discussed before to our knowledge.[9] Here it will be shown that, at zero temperature, there is a transition from diffusive dynamics to a self-trapped situation at a critical value of the coupling to the environment, clarifying and improving the conjecture of a nontrivial phase diagram made earlier.[3] Moreover, we show that the model is solvable along the transition line and we compute exactly the mobility (the order parameter) by making use of the well-known[10] equivalence between fermions and bosons in one dimension.

The model is described by the Hamiltonian

$$H = H_0 + H_{\text{bath}} + H_{\text{int}}, \tag{1}$$

where H_0 describes the motion of a particle (coordinate q) in a periodic potential. The environment is simulated[1] by an appropriate set of harmonic oscillators (a one-dimensional free boson Hamiltonian):

$$H_{\text{bath}} = \sum |k| a_k^\dagger a_k, \quad k = \pm 2\pi m/L \tag{2}$$

with m an integer less than L/ω_c. The coupling of the particle to the environment is linear,

$$H_{\text{int}} = q(2\eta)^{1/2} \sum_k (|k|/2L)^{1/2} i(a_k^\dagger - a_k) + \sum_k (\eta q^2/L), \tag{3}$$

where η is the classical friction coefficient.

We will work in the tight binding limit when the intersite tunneling rates are small as compared with the level spacing within each well. As mentioned earlier, this case can be mapped[3] onto the opposite situation, when the corrugation of the potential is small. In this limit the position operator and the Hamiltonian of the particle alone are then simply

$$q = d \sum_n n c_n^\dagger c_n, \quad H_0 = \Delta \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}), \tag{4}$$

where d is the lattice spacing and n labels the particle site. In the following we will only consider this one-dimensional case. Extension to higher dimensions is straightforward, the main difference being that the environment has to be described by a vector field and the coupling between the position and the field in Eq. (3) has to be replaced by a scalar product. All results discussed below can be extended without difficulty with no qualitative changes.

In order to make the physics more transparent, we will perform a canonical transformation U such that

$$U a_k U^\dagger = a_k - (\eta/|k|L)^{1/2} q. \tag{5}$$

The transformed Hamiltonian is then

$$\tilde{H} = UHU^\dagger = \sum_k |k| a_k^\dagger a_k + \Delta \sum_n \{c_n^\dagger c_{n+1} \exp[-\lambda i \sum_k (2kL)^{-1/2}(a_k^\dagger + a_k)] + \text{H.c.}\} \tag{6}$$

[where the dimensionless parameter $\lambda = (2\eta)^{1/2} d$ has been introduced].

In order to understand how the hopping parameter is changed by the interaction with the bath at $T=0$, let us first suppose that the high-energy oscillators follow instantaneously the motion of the particle. Then Δ is reduced by a usual overlap integral[11] (computed by simple normal ordering of the exponential):

$$\Delta_r = \Delta \exp[-(\lambda^2/4L)\sum_k 1/|k|]. \tag{7}$$

The sum over k is cut off in the ultraviolet by an upper frequency ω_c and self-consistently[11] in the low frequencies by Δ_r. Hence

$$\Delta_r \sim \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)} \text{ for } \alpha=\lambda^2/4\pi < 1, \tag{8a}$$

$$\Delta_r = 0 \text{ for } \alpha = \lambda^2/4\pi > 1. \tag{8b}$$

Alternatively, one can write directly[12] from Eq. (7)

$$\frac{d}{d\ln\omega_c}\left[\frac{\Delta(\omega_c)}{\omega_c}\right] = (\alpha-1)\frac{\Delta(\omega_c)}{\omega_c}. \tag{9}$$

These naive calculations give a vertical transition line at $\alpha=\lambda^2/4\pi=1$ between diffusive motion and localization of the particle. In a previous paper[5] we showed how the same argument applied to the two-level system had to be corrected in a full treatment of the transition around $\alpha=1$ to take into account other divergent contributions. The corrected transition line is no longer vertical for the two-level system. Here the very surprising result is that there is no such correction because of the translation invariance of the problem, and that the naive result is the true one.

Let us write the Hamiltonian $\tilde{H}$ [Eq. (6)] in a continuum notation to ease the discussion of its symmetries:

$$\tilde{H} = \int dx \left\{ [\tfrac{1}{2}\pi^2(x) + (\nabla_x\phi)^2] + \delta(x)\Delta\left[\sum_{n=1}^{N} c_n^\dagger c_{n+1}\exp[-\lambda i\phi(x)] + \text{H.c.}\right]\right\}; \tag{10}$$

we put periodic boundary conditions on the lattice ($c_{N+1}=c_1$). It is possible to do this on $\tilde{H}$ without breaking invariance by translation. For $N=2$ (N is the number of sites) this makes our system essentially different from the two-level system[4,5] but the physics should not be changed when $N >> 1$ (as can be checked in the free-particle case by use of the results of Ref. 13). Following the strategy of Refs. 5 and 12 we analyze the model in perturbation theory around the point $\alpha=1$, $\Delta=0$ using $\alpha-1$ and Δ/ω_c as small parameters. The divergences that appear then are constrained by the symmetries of our Hamiltonian: $x \to -x$ parity in real space ($c_n \to c_{-n}$, $\phi \to -\phi$), and the translation invariance already mentioned,

$$c_n \to \exp\left(i\frac{2\pi n}{N}\right)c_n, \quad \phi(n) \to \phi(n) + \frac{2\pi}{\lambda N}.$$

These divergences should also vanish when there is no hopping particle. What are the corresponding local relevant terms compatible with these constraints? We have the renormalization of Δ already mentioned, a renormalization of the particle wave function, and a global shift of energy. The counterterm that was responsible for the nontrivial renormalization of λ (CT1 of Ref. 5) is given by

$$\delta\lambda\, \partial_t\phi(0)(c_n^\dagger c_n - c_{n+1}^\dagger c_{n+1}),$$

but it identically vanishes when we sum over n. There could also appear higher charges ($l > 1$) of the form

$$\Delta_l\delta(x)\sum_{n=1}^{N}\{c_n^\dagger c_{n+m}\exp[-i\lambda l\phi(x)] + \text{H.c.}\},$$

but their scale dimension at $\alpha=1$ is l^2 in the free field theory. [This can be simply verified by normal ordering of the operators in the exponential as in Eq. (7).] Therefore, they are irrelevant around $\alpha=1$ (see the similar discussion in Ref. 12 for harmonic perturbation around the Kosterlitz-Thouless transition).

The above argument indicates that the transition line is vertical in all orders of perturbation theory around $\Delta=0$ and $\alpha=1$. It can be checked to first order in two ways. First, we have verified that in a diagrammatic analysis similar to that of Ref. 5, an explicit cancellation occurs between the diagrams which were responsible for the renormalization of λ in the two-level system, and new diagrams that occur in the present problem, because the operator $e^{i\lambda\phi}$ (positive charge) need not be followed by $e^{-i\lambda\phi}$ (negative charges). The fact that the charges are not forced to alternate destroys the screening effect. Alternatively, the partition function can be expressed[3] as a disordered gas of charges along a line, interacting with a logarithmic potential. Cardy gave a general analysis of such systems to lowest order in the fugacity (Δ in our case) along lines similar to the original analysis of Anderson and Yuval.[14] Translating his results[15] to our problem, we obtain again a vertical flow.

Schmid[3] has proposed to differentiate the different phases of the model by the mobility μ of the particle, defined as the coefficient of the logarithmic growth of a suitably normalized two-point function, i.e.,

$$A(t)=\langle q(t)q(0)-q(0)q(0)\rangle=(\mu/2\pi^2\alpha)\ln t+O(1),\quad t\to\infty. \tag{11}$$

It is interesting to note that the mobility can be expressed in terms of boson operators only, although it is initially a property of the external particle. First we rewrite $\tilde{H}$ [Eqs. (6) and (10)] using momentum operators:

$$\tilde{H}=\sum_k |k|\, a_k^\dagger a_k+2\Delta\sum_p c_p^\dagger c_p\cos[p-\lambda\sum_k (2kL)^{-1/2}(a_k^\dagger+a_k)]. \tag{12}$$

It is now obvious that the momentum p is conserved and can be treated as a number. For each p we can write an effective Hamiltonian for the bath as [using the continuum notation Eq. (10)]

$$\tilde{H}_p=\tfrac{1}{2}\int[\pi^2(x)+(\partial_x\phi)^2]dx+2\Delta\cos[p-\lambda\phi(0)]. \tag{13}$$

The free boson Hamiltonian has the symmetry $\phi(x)\to\phi(x)+\phi_0$, so that there is a set of canonical transformations which relate Hamiltonians for different values of k, and their eigenenergies do not depend on k. Note that these features make the problem qualitatively different from the polaron case, where the band is parabolic and an effective mass can easily be defined. This is very similar to what happens when there is no potential (free particle with friction[13,16]). In fact, the expansion of the cosine to second order gives us exactly the effective Hamiltonian for the bath in the free-particle case.[13] As shown below the mobility depends only on this effective Hamiltonian for $p=0$. Therefore, it is equal to 1 (the value for the case of free particle with friction) to second order in λ, and we have checked that it is not affected by the λ^4 term in first order of perturbation theory.

In order to obtain an expression for the mobility in terms of boson operators we will use the following periodic representation of the position operator in a box of size S ($S=Nd$) with periodic boundary conditions:

$$\tilde{Q}_S=(S/2\pi i)[\exp(2\pi iq/S)-1]. \tag{14}$$

The two-point correlation function $A(t)$ [Eq. (11)] is then written

$$A(t)=\lim_{S\to\infty}\langle\tilde{Q}_S^*(t)\tilde{Q}_S(0)-\tilde{Q}_S^*(0)\tilde{Q}_S(0)\rangle. \tag{15}$$

After insertion of a complete set of momentum eigenstates for the particle this is expressed as

$$A(t)=\lim_{p\to 0}p^{-2}\langle 0_{p=0}|\exp(-i\tilde{H}_p t)-1|0_{p=0}\rangle, \tag{16}$$

where $|0_{p=0}\rangle$ is the ground state of $\tilde{H}_{p=0}$.[17] As mentioned above, $\tilde{H}_p$ is related to $\tilde{H}_{p=0}$ by the canonical transformation which shifts ϕ to $\phi-p/\lambda$ [see Eq. (13)]. This transformation can be written as $\exp(ip\Pi/\lambda)$, where Π is the total momentum of the field. Making use of this and taking the limit $p\to 0$ in Eq. (16), we have

$$A(t)=\lambda^{-2}\langle 0_{p=0}|\Pi(t)\Pi(0)-\Pi(0)\Pi(0)|0_{p=0}\rangle, \tag{17}$$

which is the expression of the mobility in terms of phonon operators. This expression [or directly Eq. (16)] allows us to compute exactly the mobility along the transition line $\lambda^2/4\pi=1$. For this particular value of λ the long-time dynamics of $\tilde{H}_p$ ($t>>1/\omega_c$) is completely integrable in terms of Fermi fields. Using the well-known boson-fermion equivalence in one dimension[10] we can write[18]

$$\exp[i2\sqrt{\pi}\phi(x)]=(2\pi/\omega_c L)\sum_{k,k'}c_{1,k}^\dagger c_{2,k'}\exp[ix(k'-k)], \tag{18}$$

$$\tilde{H}_{p=0}=\sum_k k(c_{1k}^\dagger c_{1k}-c_{2k}^\dagger c_{2k})+2(\tilde{\Delta}/L)\sum_{k,k'}(c_{1k}^\dagger c_{2k'}+c_{2k}^\dagger c_{1k'}),\quad \tilde{\Delta}=(\pi/\omega_c)\Delta. \tag{19}$$

Equation (19) is a Hamiltonian for independent fermions and hence exactly soluble.[19] Translating $A(t)$ into fermion operators, we get

$$A(t)=\tfrac{1}{4}\langle S(t)S(0)-S(0)S(0)\rangle,\qquad S=\sum_k(c_{1k}^\dagger c_{1k}-c_{2k}^\dagger c_{2k}). \tag{20}$$

After some algebraic manipulations, we obtain finally

$$A(t)\sim 2[\tilde{\Delta}/\pi(1+\tilde{\Delta}^2)]^2\ln t,\qquad \mu=4\tilde{\Delta}^2/(1+\tilde{\Delta}^2)^2. \tag{21}$$

The mobility changes continuously along the transition line with $\tilde{\Delta}$, the dimensionless ratio between the hopping parameter and the high-energy cutoff needed to define the phonon bath, and μ goes to zero as $\tilde{\Delta}\to 0$.

Our whole analysis is summarized by the phase diagram presented in Fig. 1. We have studied the tight-binding limit of the model proposed by Schmid. This is the upper part of Fig. 1. We have shown that there is a transition in the behavior of the particle when $\alpha=1$, where α is a dimensionless parameter [Eqs. (6) and (8)] measuring the coupling of the particle to its en-

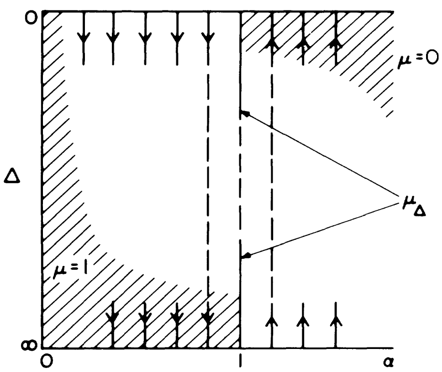

FIG. 1. Phase diagram of the model; μ is the mobility. Dashed lines are conjectured flow in the intermediate-coupling regime.

vironment. For $\alpha > 1$, the dimensionless hopping parameter $\tilde{\Delta}$ is renormalized to zero (upward-pointing arrows in the upper right corner of the phase diagram) and the particle is self-trapped by the combined effects of the potential and the friction. The mobility is therefore zero in this region. This part of the phase diagram is well under control (which we have indicated by shading the corresponding area) because $\tilde{\Delta}$ decreases as we lower the cutoff. For a typical $\alpha < 1$, Δ remains finite leading to a diffusive behavior of the particle. We can only present a conjecture for the value of the mobility (see below) since $\tilde{\Delta}$ grows outside the range of validity of our perturbation theory. For a small α we are again on safer ground since the Hamiltonian reduces to the one for the free particle with friction for which the mobility is 1 (shaded upper left corner). Finally, we can translate those results for the lower part of the diagram by using the duality transformation of Schmid (upper right $\leftrightarrow$ lower left, upper left $\leftrightarrow$ lower right, $\mu \leftrightarrow 1-\mu$). In the middle of the phase diagram we do not expect the appearance of new physical effects and only a smooth crossover between the $\Delta=0$ repulsive fixed line to the "free particle with friction" line at the bottom of the diagram for $\alpha < 1$, and the opposite flow for $\alpha > 1$. This physical argument lets us conjecture (dashed lines) that the phase diagram is divided into two parts: $\mu=1$ to the left of the vertical line $\alpha=1$ and $\mu=0$ to its right.[20]

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