Quantum Brownian motion in a periodic potential

Matthew P. A. Fisher and Wilhelm Zwerger*
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
(Received 9 May 1985)

We study the statics and dynamics of a quantum Brownian particle moving in a periodic potential and coupled to a dissipative environment in a way which reduces to a Langevin equation with linear friction in the classical limit. At zero temperature there is a transition from an extended to a localized ground state as the dimensionless friction α is raised through one. The scaling equations are derived by applying a perturbative renormalization group to the system's partition function. The dynamics is studied using Feynman's influence-functional theory. We compute directly the nonlinear mobility of the Brownian particle in the weak-corrugation limit, for arbitrary temperature. The linear mobility μ_l is always larger than the corresponding classical mobility which follows from the Langevin equation. In the localized regime $\alpha>1$, μ_l is an increasing function of temperature, consistent with transport via a thermally assisted hopping mechanism. For $\alpha<1$, $\mu_l(T)$ shows a nonmonotonic dependence on T with a minimum at a temperature T^*. This is due to a crossover between quantum tunneling below T^* and thermally assisted hopping above T^*. For low friction the crossover occurs when the particle's thermal de Broglie wavelength is roughly equal to the distance between minima in the periodic potential. We suggest that the regime $\alpha<1$ describes the physics of the observed nonmonotonic temperature dependence of muon diffusion in metals.

I. INTRODUCTION AND MODEL

The study of Brownian motion of a classical particle described by the simple Langevin equation

$$M\ddot{q}+\eta\dot{q}+\frac{\partial V}{\partial q}=\xi(t) \tag{1.1}$$

is one of the basic subjects of nonequilibrium statistical mechanics. Here, η is a phenomenological friction coefficient, $V(q)$ the external potential, M the particles mass, and $\xi(t)$ a fluctuating force which obeys

$$\langle\xi(t)\rangle=0,\quad \langle\xi(t)\xi(t')\rangle=2\eta T\delta(t-t')\ , \tag{1.2}$$

where the angular brackets denote an ensemble average (throughout the paper we take $k_B=1$). In recent years there has been much interest in studying the *quantum* mechanics of a particle, acted on by dissipative forces, which reduces to (1.1) in the classical (i.e., high-temperature) limit.[1-9] The most successful approach has been to couple the quantum particle to an environment or bath of an infinite number of degrees of freedom, which provides both the friction and the fluctuating force. Probably the simplest system-plus-bath Hamiltonian which reduces to (1.1) in the classical regime was recently studied by Caldeira and Leggett.[1] In the Caldeira-Leggett model the coordinate q is coupled *linearly* to an infinite set of harmonic oscillators with a Hamiltonian[10]

$$\hat{\mathscr{H}}=\frac{P^2}{2M}+V(q)+\sum_\alpha P_\alpha^2/2m_\alpha + \tfrac{1}{2}\sum_\alpha m_\alpha\omega_\alpha^2(x_\alpha+q\lambda_\alpha/m_\alpha\omega_\alpha^2)^2\ . \tag{1.3}$$

As far as the properties of the particle are concerned, the coupling constants λ_α and frequencies ω_α are of importance only via the weighted density of states

$$J(\omega)=\frac{\pi}{2}\sum_\alpha\frac{\lambda_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha),\quad \omega>0\ . \tag{1.4}$$

Caldeira and Leggett considered specifically a spectral density of the form

$$J(\omega)=\eta\omega\ . \tag{1.5}$$

With this choice the Hamiltonian (1.3) when treated classically is equivalent, upon elimination of the bath degrees of freedom, to the Langevin equation (1.1). By canonically quantizing (1.3) it is then possible to study the motion of the Brownian particle within the quantum regime.

We emphasize that (1.3) is certainly not the only possible microscopic Hamiltonian which reduces to (1.1) in the classical limit.[2] It is, however, probably the one most amenable to theoretical analysis since all the terms in the Hamiltonian except possibly the external potential are quadratic.[3] For nonlinear potentials $V(q)$ the dynamics is entirely nontrivial,[4-9] and the model (1.3) is expected to share many qualitative features with more complicated system-plus-bath Hamiltonians. As such, the Caldeira-Leggett approach provides us with a generic, yet tractable, model for studying Brownian motion in the quantum regime.

In this paper we use the Caldeira-Leggett model to study the behavior of the quantum Brownian particle in a periodic potential of the form (see Fig. 1)

$$V(q)=-V\cos(2\pi q/q_0)-Fq\ , \tag{1.6}$$

with F a constant externally applied force. As emphasized recently,[8] this model can be generalized easily to arbitrary dimensions and may then be appropriate for describing the motion of a heavy charged particle in the

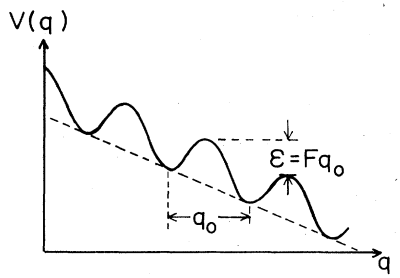

FIG. 1. Periodic potential $V(q)=-V\cos(2\pi q/q_0)-Fq$ with lattice constant q_0 and potential drop $\epsilon=Fq_0$ per period.

interior or at the surface of a metal. The underlying crystal provides the periodic potential, and the coupling to the conduction electrons gives rise to a frictional force (i.e., the dissipated power is proportional to the velocity of the particle squared). Although this reasoning is suggestive, at present there is no detailed justification for replacing the conduction electrons with a bath of harmonic oscillators as in (1.3).[11] Moreover, in a real metal there are additional complications due to the presence of impurities and the effect of phonons. Nevertheless, this model provides an idealized description of the dynamics of charged particles in metals and, as we will see, does in fact show nontrivial behavior which may be compared with real systems.

Caldeira and Leggett[2] originally introduced the Hamiltonian (1.3) to study the macroscopic quantum tunneling of the phase difference q across a Josephson element in an rf SQUID ring. It has also been applied to describe tunneling in a current-biased Josephson junction. Although the washboard potential (1.6) has generally been used to model the current-biased junction,[12] our analysis may not be appropriate in this case. The difficulty is that in the Josephson junction adding 2π to the phase difference (i.e., adding q_0 to q) returns the system to the same state.[13] In our analysis below, however, we treat these states as distinguishable, as is appropriate for a physical particle.

This paper focuses on both the static and dynamic properties of the quantum Brownian particle in the periodic potential (1.6). Firstly we discuss the nature of the particle's ground state in the unbiased periodic potential ($F=0$). In accordance with a suggestion by Schmid[7] and more recent work,[8,14] we find that if the friction exceeds a critical value, the ground state changes from extended to localized. This transition is analyzed by applying a perturbative renormalization-group theory in the weak-corrugation (small V) limit to the system's partition function. The partition function is a one-dimensional (1D) analog of the two-dimensional (2D) sine-Gordon theory[15,16] and the localization transition can in fact be thought of as a 1D version of the roughening transition.[17,18]

The bulk of the paper, however, is devoted to studying directly the *dynamics* of the Brownian particle at finite temperature. In particular, we are interested in the physical dc mobility

$$\mu=v/F\ , \tag{1.7}$$

where v is the particle's steady-state velocity down the washboard potential. We determine μ explicitly in the small corrugation limit (to order V^2) but for arbitrary friction, temperature, and external force. The resulting expression contains the mobility all the way from zero temperature up to the classical limit. The main conclusions we reach are the following.

The linear mobility for the quantum Brownian particle is always larger than the corresponding classical linear mobility which follows from the Langevin equation. This is in accordance with one's intuition that quantum fluctuations allow for tunneling through the barriers of the periodic potential. For large friction, where the particle is localized at $T=0$, the linear mobility is a *monotonically* increasing function of temperature which approaches the classical result as $T\to\infty$. This is consistent with transport via a thermally assisted hopping mechanism, which proceeds at a faster rate with increasing temperature. The most interesting result, however, is for low friction where the particle is delocalized at $T=0$. In this case, the linear mobility is found to have a *nonmonotonic* temperature dependence with a minimum at a crossover temperature T^*. Below T^* the mobility is a *decreasing* function of temperature, whereas above T^* it is *increasing* with T. For $T\ll T^*$ the dominant transport mechanism is "thermally *resisted*" quantum tunneling between adjacent minima in the potential; with decreasing temperature the environment destroys less of the quantum coherence necessary for tunneling and the mobility increases. For $T\gg T^*$, on the other hand, the environment has suppressed the quantum tunneling and the dominant conduction mechanism is thermally *assisted* hopping over the barrier. The crossover temperature is given by[19]

$$T^*=C(\alpha)\hbar^2/Mq_0^2,\quad 0<\alpha<1 \tag{1.8}$$

where $C(\alpha)$ is a monotonically decreasing function of the friction α, which approaches $\pi^2/3$ as $\alpha\to 0$ and zero as $\alpha\to 1$. With *increasing* friction the crossover temperature *decreases,* requiring lower temperatures to reach the quantum tunneling regime ($T<T^*$). For low friction (1.8) can be written

$$\lambda(T^*)\simeq q_0\ , \tag{1.9}$$

where $\lambda(T)=\hbar(MT)^{-1/2}$ is the particle's thermal de Broglie wavelength and q_0 the periodicity in the washboard potential.

Recently several authors[9] have studied the same model in the *strong*-corrugation limit by replacing the system with a tight-binding lattice with one state per site. These authors also find that for low friction the mobility decreases with increasing temperature. However, since thermal activation over the barriers is not present in a tight-binding description, it is not possible to see the crossover from "resisted" quantum tunneling to thermally assisted hopping. The advantage of the present approach is that the results are valid for arbitrary temperature, allowing the crossover to be studied explicitly.

A nonmonotonicity in the diffusive behavior of a Brownian particle has in fact been observed indirectly in

recent experiments probing the spin relaxation of muons in metals.[20–22] Kondo[23] has recently discussed this system in a tight-binding description and argues that the nonmonotonicity is due to a competition between the effects of the electrons and phonons on the nearest-neighbor tunneling rate (computed within Fermi's golden rule). When the temperature approaches the Debye temperature the effect of the phonons is strongly modified, leading to an enhancement in the quantum tunneling rate. In contrast to Kondo, we suggest that the high-temperature regime ($T > T^*$) may in fact correspond to thermal activation over the barriers, rather than a modified quantum tunneling. In our calculation it is these "over-the-barrier" processes which lead to the nonmonotonic diffusive behavior.

The paper is organized as follows: In Sec. II we study the ground-state properties of the particle in the unbiased periodic potential and determine its $T=0$ phase diagram by a renormalization-group calculation. In Sec. III the finite-temperature dynamics is investigated within Feynman's influence-functional theory.[24,25] In particular, it is shown in Sec. III B that there is an exact duality in the time-dependent density matrix between the periodic potential and a tight-binding model. The mobility in the tight-binding lattice is determined in Sec. III C to second order in the hopping matrix element. Using the duality relation, this gives the mobility in the small corrugation limit at arbitrary bias and temperature. The results are discussed in detail in Sec. IV, all the way from zero temperature up to the classical limit.

II. GROUND-STATE PROPERTIES AND LOCALIZATION TRANSITION

In this section we study the ground-state properties of the Hamiltonian (1.3) for a periodic potential with zero bias.[26] By considering the weak-corrugation limit, we argue below that the ground state changes from delocalized to localized in the coordinate q as the dimensionless friction α is raised through a critical value $\alpha=1$. A simple variational calculation suggests that the transition is second order with a localization length diverging as $(\alpha-1)^{-1/2}$. A careful renormalization-group analysis, however, shows that the flows are rather singular, making it difficult to distinguish between a first- or second-order transition.

To obtain information about the nature of the ground state, we study the diagonal elements of the reduced equilibrium density matrix

$$\rho_{\rm eq}(q;\beta)=\sum_n e^{-\beta E_n}\int\prod_\alpha dx_\alpha\,|\psi_n(q,\{x_\alpha\})|^2\,, \quad (2.1)$$

as $\beta\to\infty$. Here ψ_n and E_n are the eigenstates and energies of the full Hamiltonian (1.3). The inverse temperature $\beta=1/k_BT$. It is convenient to write (2.1) as a path integral over paths $q(\tau)$ and $x_\alpha(\tau)$ with the imaginary time τ running from 0 to $\beta\hbar$. After performing the harmonic-oscillator path integrals, the density matrix takes the form

$$\rho_{\rm eq}(q;\beta)=K_0(\beta)\int Dq(\tau)\exp[-H(q)]\,, \quad (2.2)$$

where

$$K_0(\beta)=\prod_\alpha[\tfrac{1}{2}\operatorname{csch}(\beta\hbar\omega_\alpha/2)]$$

is the partition function of the free-oscillator bath. The path integral in (2.2) satisfies the boundary conditions $q(0)=q(\beta\hbar)=q$. The effective Hamiltonian (or effective "action") is given by

$$H=H_0+H_1\,, \quad (2.3)$$

with

$$H_0=\frac{\eta}{4\pi\hbar}\int_0^{\beta\hbar}d\tau\int_{-\infty}^{\infty}d\tau'\left[\frac{q(\tau)-q(\tau')}{\tau-\tau'}\right]^2 +\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\frac{M}{2}\dot q^{\,2}(\tau)\,, \quad (2.4)$$

$$H_1=-\frac{V}{\hbar}\int_0^{\beta\hbar}d\tau\cos\left[\frac{2\pi q(\tau)}{q_0}\right]. \quad (2.5)$$

It is convenient to rewrite H in terms of the dimensionless parameters

$$\phi(\tau)=\frac{2\pi q(\tau)}{q_0}\,, \quad (2.6)$$

$$\alpha=\frac{\eta q_0^2}{2\pi\hbar}\,, \quad (2.7)$$

and

$$V_0=V/E_0\,, \quad (2.8)$$

with the energy E_0 defined by

$$E_0=\frac{(2\pi\hbar)^2}{Mq_0^2}\,. \quad (2.9)$$

Here E_0 is the quantum-mechanical energy necessary to confine a particle of mass M within a lattice spacing. Defining, finally, a corresponding frequency

$$\Lambda=E_0/\hbar\,, \quad (2.10)$$

we have, after taking $\beta\to\infty$ and Fourier transforming (2.4),

$$H=\tfrac{1}{2}\int\frac{d\omega}{2\pi}S_\Lambda(\omega)\,|\phi(\omega)|^2-V_0\Lambda\int d\tau\cos\phi(\tau)\,, \quad (2.11)$$

with

$$S_\Lambda(\omega)=\frac{\alpha}{2\pi}\,|\omega|+\frac{\omega^2}{\Lambda}\,. \quad (2.12)$$

The gradient term proportional to α in (2.11), which arises from integrating out the environmental degrees of freedom, is scale invariant in ω or τ and, as such, is a one-dimensional analog to the Laplacian in two dimensions. Thus, the Hamiltonian (2.11) is essentially a 1D version of the 2D sine-Gordon model.[15,16] The higher-order gradient term due to the kinetic energy simply provides a natural high-frequency cutoff Λ, which is inversely proportional to the particle's mass. By simple power

counting this term is expected to be irrelevant. Thus, in what follows we will drop it,

$$S_\Lambda(\omega)\to S(\omega)=\frac{\alpha}{2\pi}|\omega|\ ,$$

and instead restrict the frequency integrals to $|\omega|<\Lambda$. Equations (2.2), (2.11), and (2.12) are equivalent to the partition function of a classical one-dimensional interface model with "height" variable $\phi(\tau)$ in an external field which favors interfacial positions at integer multiples of 2π. As we will show below, such a model[27] has a roughening transition as α is varied. Since the interfacial width is equivalent, in the original variables, to the width of the ground-state density matrix, this is a transition between a localized and extended eigenstate.

Before we discuss the renormalization-group analysis of this transition, let us first consider a simple variational calculation in a form originally applied by Saito[18] to the sine-Gordon model. This method employs Feynman's variational principle, which states that for any trial Hamiltonian $H_{\rm tr}$ with associated free energy $F_{\rm tr}$, the system's true free energy is bounded above by

$$F\le F_{\rm tr}+\langle H-H_{\rm tr}\rangle_{\rm tr}\ , \tag{2.13}$$

where the average is performed over $H_{\rm tr}$. We choose a quadratic trial Hamiltonian of the form

$$H_{\rm tr}=\tfrac{1}{2}\int_{-\Lambda}^{\Lambda}\frac{d\omega}{2\pi}S_{\rm tr}(\omega)|\phi(\omega)|^2\ , \tag{2.14}$$

$$S_{\rm tr}(\omega)=\frac{\alpha}{2\pi}|\omega|+m\ . \tag{2.15}$$

In the trial Hamiltonian we have replaced the periodic potential by a harmonic potential which constrains the interface to be near the origin. The variational parameter will thus be nonzero for a localized ground state. Minimizing the right-hand side of (2.13) gives the following self-consistent equation:

$$m/\Lambda=V_0\exp(-\tfrac{1}{2}\langle\phi^2\rangle_{\rm tr})=V_0\left[\frac{m}{(\alpha/2\pi)\Lambda+m}\right]^{1/\alpha}\ . \tag{2.16}$$

Since a consistent solution requires that m vanishes in the limit $V_0\to 0$, we obtain

$$m=\begin{cases}0 & \text{for } \alpha<1,\\ \Lambda(2\pi/\alpha)^{1/(\alpha-1)}V_0^{\alpha/(\alpha-1)} & \text{for } \alpha>1\ ,\end{cases} \tag{2.17}$$

which gives a localized ground state if $\alpha>1$. The corresponding interfacial width is

$$\langle\phi^2\rangle_{\rm tr}=\int_{-\Lambda}^{\Lambda}\frac{d\omega}{2\pi}S_{\rm tr}^{-1}(\omega)=(2/\alpha)\ln(\Lambda/m),\quad \Lambda\gg m\ . \tag{2.18}$$

The variational approach thus predicts that for low friction, $\alpha<1$, the interface is rough (i.e., has a width which diverges logarithmically with the size of the system) and the particle is delocalized. For high friction, $\alpha>1$, the particle is localized with a localization length $\xi=q_0\langle\phi^2\rangle^{1/2}$ which, from (2.17) and (2.18), is found to diverge as

$$\xi\sim(\alpha-1)^{-1/2},\quad \alpha\to 1^+\ . \tag{2.19}$$

We now consider a systematic renormalization-group analysis of this transition. Working perturbatively in powers of V_0, we derive scaling equations for α and V_0 using a finite-momentum-shell recursion method.[15] We show below that α is not renormalized to second order in V_0 and argue that this should remain true to all orders. As expected, V_0 is renormalized and a transition at $\alpha=1$ is found. Consider the Hamiltonian (2.11) with $S(\omega)=(\alpha/2\pi)|\omega|$ and a sharp high-frequency cutoff at Λ. As usual, we divide the field into slow and fast modes,

$$\phi(\tau)=\phi_s(\tau)+\phi_f(\tau)\ , \tag{2.20}$$

where

$$\begin{aligned}&\phi(\omega)\approx\phi_s(\omega)\ \text{ for }\ |\omega|\lesssim\mu\ ,\\ &\phi(\omega)\approx\phi_f(\omega)\ \text{ for }\ \mu\lesssim|\omega|<\Lambda\ .\end{aligned} \tag{2.21}$$

Here μ, which separates the slow from the fast modes, is chosen to satisfy $\mu\ll\Lambda$. We now integrate out the fast modes in the density matrix by expanding in powers of V_0,

$$\rho_{\rm eq}\sim\int D\phi\exp(-H_0-H_1)=\int D\phi_s\exp(-\tilde H)\ , \tag{2.22}$$

where $\tilde H$ is given by

$$\tilde H=\frac{\alpha}{4\pi}\int\frac{d\omega}{2\pi}|\omega|\,|\phi_s(\omega)|^2+\langle H_1\rangle -\tfrac{1}{2}\langle(H_1-\langle H_1\rangle)^2\rangle+O(V_0^3)\ . \tag{2.23}$$

The averages in (2.23) are over the fast modes with a two-point correlation function

$$G(\tau)=\langle\phi_f(\tau)\phi_f(0)\rangle=\int_{|\omega|<\Lambda}\frac{d\omega}{2\pi}S^{-1}(\omega)e^{i\omega\tau}W(\omega/\mu)\ , \tag{2.24}$$

where $W(x)$ is a smoothing function with $W(x)\to 0$ for $x\ll 1$ and $W(x)\approx 1$ for $x\gg 1$. To avoid the generation of spurious long-ranged behavior in $G(\tau)$, $W(x)$ must be chosen sufficiently smoothly.[28] For example, with

$$W(x)=\frac{|x|}{(1+x^2)^{1/2}}\ , \tag{2.25}$$

we have, for $\Lambda\gg\mu$,

$$\begin{aligned}&G(\tau)=(2/\alpha)K_0(\mu\tau)\ \text{ if }\ \Lambda\tau\gg 1\ ,\\ &G(0)=(2/\alpha)\ln(\Lambda/\mu)\ ,\end{aligned} \tag{2.26}$$

where K_0 is the modified Bessel function of the second kind which falls off exponentially for large argument.[29] The averages in (2.23) can be expressed entirely in terms of $G(\tau)$,

$$\langle H_1 \rangle = -V_0 \Lambda \exp[-\tfrac{1}{2}G(0)] \int d\tau \cos\phi_s(\tau) , \tag{2.27}$$

$$\langle (H_1 - \langle H_1 \rangle)^2 \rangle = \frac{(V_0\Lambda)^2}{2} \exp[-G(0)] \int d\tau \int d\tau' \{ \cos[\phi_s(\tau)+\phi_s(\tau')](e^{-G(\tau-\tau')}-1) + \cos[\phi_s(\tau)-\phi_s(\tau')](e^{G(\tau-\tau')}-1) \} . \tag{2.28}$$

To complete the renormalization-group transformation, we must rescale, $\tau \to \tau' = (\Lambda/\mu)\tau$, to bring $\tilde{H}$ back into its original form. No rescaling of ϕ (i.e., wave-function renormalization) is needed, since the theory has an underlying $\phi \to \phi + 2\pi$ symmetry. Consider first the renormalization of V_0 generated by odd powers in (2.23). After rescaling in (2.27) we have, to lowest order,

$$V_0(\mu) = V_0(\Lambda)(\Lambda/\mu)\exp[-\tfrac{1}{2}G(0)] = V_0(\Lambda)(\mu/\Lambda)^{1/\alpha - 1} . \tag{2.29}$$

To obtain the differential flow equations, we differentiate $V_0(\mu)$ with respect to μ, keeping the bare parameters Λ and $V_0(\Lambda)$ fixed. Defining $dl = -d\mu/\mu$, we then have

$$\frac{\partial V_0}{\partial l} = -\left[\frac{1}{\alpha} - 1\right] V_0(l) + O(V_0^3) , \tag{2.30}$$

which shows that to lowest order V_0 scales to zero if $\alpha < 1$ and grows if $\alpha > 1$.

Consider next the renormalization of α coming from even powers in V_0, i.e., Eq. (2.28). Since $G(\tau)$ is short ranged and falls off exponentially with the renormalized "lattice spacing" μ^{-1}, we may perform a gradient expansion in (2.28). As in the sine-Gordon model, the first term generates a $\cos(2\phi)$ contribution which is irrelevant[30] near the transition at $\alpha = 1$. The most relevant operator generated by the gradient expansion in the second term is of the form $\int d\tau (\partial\phi/\partial\tau)^2$. In the 2D sine-Gordon theory this renormalizes the temperature.[15,16] However, in the one-dimensional theory considered here, such a term is irrelevant by simple power counting and clearly does not modify α, the coefficient of $\int d\omega \, |\omega| \, |\phi(\omega)|^2$. Thus, we conclude that α is not renormalized to second order in V_0. In fact, we believe that α will remain unchanged to all orders. To argue this, we first observe that the friction η is the coefficient of an operator which is nonlocal in τ [i.e., the first term in Eq. (2.4)]. In our momentum-shell recursion method, however, only local operators can be generated, and thus η cannot be modified. Moreover, since $q \to q + q_0$ is a symmetry of the Hamiltonian, q_0 is not renormalized either (there is no need for wave-function renormalization), and thus the dimensionless friction coefficient $\alpha = \eta q_0^2/2\pi\hbar$ remains unchanged under the full renormalization-group transformation.[31]

The flows we have deduced are shown in Fig. 2. Since α is not renormalized, the flows are all vertical.[32] We have also drawn the flows near $V_0 = \infty$ by exploiting a self-duality between the weak corrugation and the tight-binding limit $V_0 \to \infty$. Specifically, Schmid[7] demonstrated that the equilibrium density matrix in an imaginary-time path-integral representation is self-dual under $\alpha \to 1/\alpha$ and $V_0 \to \Delta(V_0)$, with Δ the hopping matrix element in the tight-binding limit, which goes to zero as $V_0 \to \infty$. As in the variational calculation, the flows indicate a transition as a function of the dimensionless friction α. For $\alpha < 1$ and V_0 small, V_0 scales to zero, implying that at long imaginary timescales the system's behavior is described by the Gaussian fixed line $V_0 = 0$. Thus, the interface is rough and the particle delocalized. When $\alpha > 1$ and V_0 small, V_0 is increased by the flows outside the range of the weak-corrugation expansion. The behavior of the system is then determined by the fixed point which attracts these flows.

It is tempting to connect the flows between the two perturbative regimes of large and small V_0, implying that for $\alpha > 1$ all flows terminate at the localized fixed line $V_0 = \infty$. This is reasonable only if the coefficients of all the higher powers in V_0, in the flow equation (2.30), vanish at $\alpha = 1$ as the linear term does. For example, if, as in the 2D sine-Gordon theory,[15,16] the coefficient of the cubic term were nonzero and, say, negative at $\alpha = 1$, then a parabolic line of fixed points $V_0 \sim (\alpha - 1)^{1/2}$ would terminate the flow lines for $\alpha > 1$ in Fig. 2. To rule out this possibility, we have demonstrated explicitly[33] that the coefficient of the V_0^3 term does indeed vanish at $\alpha = 1$. We believe that, in fact, the coefficients vanish at $\alpha = 1$ to all orders in V_0. Thus, $\alpha = 1$ would represent a fixed line. This suggests that it is not unreasonable to connect the flows as shown in Fig. 2. At any rate it seems extremely likely that for $\alpha > 1$ they will terminate at a localized fixed point. We thus conclude, in agreement with the variational calculation, that when $\alpha > 1$ the particle is localized for arbitrarily small V_0.

Even if the flows for $\alpha > 1$ are as depicted in Fig. 2, it is still impossible within perturbation theory to discern

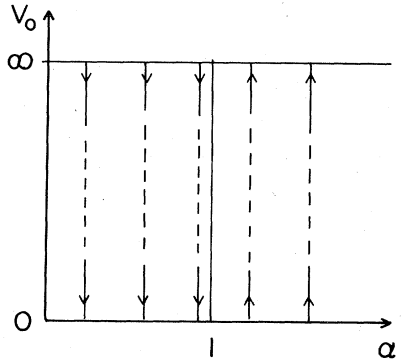

FIG. 2. Scaling flows at zero temperature in the unbiased potential. The dashed lines are the expected flows for intermediate corrugation strength V_0. For any V_0 the ground state is delocalized if $\alpha < 1$ and localized if $\alpha > 1$.

whether the transition is second or first order (in the sense that the localization length diverges smoothly or with a discontinuous jump as $\alpha \to 1^+$). Normally, the correlation length would be determined by integrating the flow equations from small V_0 out to a reference state, say $V_0 \simeq 1$, where it is argued to be of order 1 (in units of the lattice spacing). This method cannot be applied here, since a flow which starts near $\alpha = 1$ and small V_0 arrives at a reference state that is still near the transition $\alpha = 1$ and, thus, might not have a correlation length of order 1. Consequently, from the perturbative flow equations, we can neither confirm nor refute the prediction from the variational treatment (2.19) that the localization length for small V_0 diverges smoothly as $(\alpha - 1)^{-1/2}$ when $\alpha \to 1^+$.

We would like to point out that, through the simple extension

$$H = H(q_x) + H(q_y) + H(q_z) , \tag{2.31}$$

the analysis above can trivially be extended to two or three dimensions without any change in the phase diagram and scaling behavior.

Finally, we emphasize that the nature of the ground state, and, in particular, the existence of the localization transition, is rather sensitive to the precise form of the coupling in the original Hamiltonian (1.3). For example, suppose this coupling was modified in such a way that the nonlocal term in the effective Hamiltonian (2.4) took the form

$$\int d\tau \int d\tau' \frac{g(q(\tau) - q(\tau'))}{(\tau - \tau')^2} , \tag{2.32}$$

with some non-negative function g, satisfying $g(0) = 0$. The nature of the ground state is then exceedingly sensitive to the behavior of $g(q)$ for large argument. If, for example, $g \sim aq^4$ for $q \to \infty$, then the particle would be localized regardless of the magnitude of a (since this term renormalizes α, the coefficient of the quadratic term, leading to flows which always scale to large V_0). On the other hand, if g decays to zero as $q \to \infty$, then the particle will be delocalized. This is because, in this case, it is always possible to find a quadratic theory of the form (2.4) with $\alpha < 1$, which nevertheless suppresses the interfacial fluctuations *more* than (2.32).

III. DYNAMICS AT FINITE TEMPERATURE

A. Statement of the problem

In this section we study the dynamics of the quantum particle with coordinate q which is generated by the Hamiltonian (1.3). Our aim is to calculate the response to a time-independent external force F. In particular, we analyze the nonlinear dc mobility μ defined by

$$\mu = v/F , \tag{3.1}$$

where v is the velocity of the particle moving down the ("washboard") potential

$$V(q) = -V\cos(2\pi q/q_0) - Fq . \tag{3.2}$$

Due to the external force F, subsequent minima in this potential differ in energy by an amount $\epsilon = Fq_0$. Of interest is the dependence of the mobility on the dimensionless friction α, the corrugation strength V, the bias ϵ, and, in particular, the temperature T. The analysis is based on the influence-functional formalism developed by Feynman and Vernon.[24] Initially the system is prepared with the particle in a localized wave packet near the origin and the harmonic oscillators in a thermal distribution at temperature T. The probability density $P(x,t)$ for finding the particle at x at a later time t is expressed as a double path integral. The particle's mobility is then obtained directly by averaging x over the probability density

$$\mu = \lim_{t \to \infty} \left[\frac{\langle x(t) \rangle}{tF} \right] . \tag{3.3}$$

Our calculation of μ is, for the sake of clarity, divided into two steps. In Sec. III B the general Feynman-Vernon theory is introduced and applied specifically to the Hamiltonian (1.3). Since the potential energy (3.2) enters in the exponent of the path integral and is nonlinear in q, the probability density cannot be computed exactly. However, by expanding the exponential and retaining all terms, we derive a formally exact expression for the nonlinear mobility μ as an infinite series in powers of V^2. Using this result, the system's mobility μ is, in turn, related to the mobility for a particle hopping on a one-dimensional tight-binding (TB) lattice with matrix element V. The tight-binding model is at the same temperature T, but has a dimensionless friction $1/\alpha$ and energy drop ϵ/α between nearest-neighbor sites. In particular, we show that the mobilities are related by

$$\frac{\mu(\epsilon,\alpha)}{\mu_0} = 1 - \frac{\mu_{\rm TB}(\epsilon/\alpha, 1/\alpha)}{\mu_0} , \tag{3.4}$$

at arbitrary T and ϵ. Here $\mu_0 = 1/\eta$ is the mobility for a free particle, $V = 0$, with friction (which is independent of ϵ or T and also whether the particle is quantum or classical in nature). Equation (3.4) is a generalization to *real times* and finite T and ϵ of the duality between the periodic potential and a tight-binding model, discussed by Schmid for the $T = 0$ equilibrium density matrix.[7]

In Sec. III C the formal power-series expression for the mobility is analyzed in the weak-corrugation limit. In particular, μ is obtained to second order in V at arbitrary temperatures, friction, and external force. The calculation is most easily discussed in the language of the dual tight-binding system which, in this limit, has a very small hopping matrix element.

B. Feynman-Vernon theory and duality

In this section we derive a formal expression for the nonlinear mobility in the periodic potential (3.2) and relate it to the corresponding quantity in a tight-binding model with hopping matrix element V. To study the dynamics

generated by the Hamiltonian (1.3), we use the influence-functional formalism developed by Feynman and Vernon.[24,25] This theory considers directly the time-dependent reduced density matrix

$$\hat{\rho}(t)=\mathrm{Tr}_B\hat{\rho}_{\mathrm{tot}}(t)\ , \tag{3.5}$$

traced over the bath coordinates. The probability density $P(x,t)$, which is necessary to obtain the mobility via Eq. (3.3), is simply the diagonal matrix element of $\hat{\rho}$,

$$P(x,t)=\langle x\,|\,\hat{\rho}(t)\,|\,x\rangle\ . \tag{3.6}$$

Under the assumption that the initial total density matrix factorizes,[34] the time evolution of $\hat{\rho}(t)$ in the coordinate representation can be written as

$$\langle q\,|\,\hat{\rho}(t)\,|\,q'\rangle=\int dq_0\int dq_0'\langle q_0\,|\,\hat{\rho}(0)\,|\,q_0'\rangle \times J(q,q',t;q_0,q_0',0)\ . \tag{3.7}$$

Here, J is given by the double path integral

$$J(q,q',t;q_0,q_0',0)=\int_{q_0}^{q}Dq\int_{q_0'}^{q'}D^*q'\exp\{(i/\hbar)[S(q)-S(q')]+i\Phi(q,q')\}\ , \tag{3.8}$$

where

$$S(q)=\int_0^t\left[\frac{M}{2}\dot{q}^2-V(q)\right]dt' \tag{3.9}$$

is the classical action of the uncoupled particle and $\Phi[q(t'),q'(t')]$ the influence phase. In this formulation the environment has been eliminated completely from the problem and reveals itself through an effective coupling between the paths $q(t')$ and $q'(t')$ described by Φ. If the bath of harmonic oscillators is assumed initially in thermodynamic equilibrium at temperature T, Φ has the form[1]

$$\begin{aligned}i\Phi(x,y)=&-(i/\hbar)\int_0^t dt'\int_{t'}^t ds\,2x(t')y(s)\alpha_I(s-t')\\&-(1/\hbar)\int_0^t dt'\int_0^{t'}ds\,y(t')\alpha_R(t'-s)y(s)\\&-(i/\hbar)M(\Delta\omega)^2\int_0^t dt'\,x(t')y(t')\ ,\end{aligned} \tag{3.10}$$

where for later convenience we have introduced center-of-mass and relative coordinates

$$x=\tfrac{1}{2}(q+q'),\quad y=q-q'\ . \tag{3.11}$$

The functions α_I and α_R, as well as the counter term in the original Hamiltonian (1.3) which we have included in Φ, may be expressed in terms of the environment density of states $J(\omega)$ introduced in (1.4) by

$$\alpha_I(t)=-\int_0^\infty\frac{d\omega}{\pi}J(\omega)\sin(\omega t)\ , \tag{3.12}$$

$$\alpha_R(t)=\int_0^\infty\frac{d\omega}{\pi}J(\omega)\cos(\omega t)\coth(\tfrac{1}{2}\beta\hbar\omega)\ , \tag{3.13}$$

$$\tfrac{1}{2}M(\Delta\omega)^2=\int_0^\infty\frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\ . \tag{3.14}$$

Specializing to Ohmic dissipation with spectral density $J(\omega)=\eta\omega$, the influence phase (3.10) becomes

$$\begin{aligned}i\Phi(x,y)=&(i/\hbar)\eta\int_0^t dt'\,x(t')\dot{y}(t')\\&-(i/\hbar)\eta x(t)y(t)-S_2(y)\ ,\end{aligned} \tag{3.15}$$

with

$$S_2(y)=\frac{1}{\hbar}\int_0^t dt'\int_0^{t'}ds\,y(t')\alpha_R(t'-s)y(s)\ . \tag{3.16}$$

Due to the nonlinearities which enter into $S(q)$, it is clear that a direct evaluation of the double path integral for J is not possible. In order to make progress, we expand the cosine term of the potential and write

$$\exp\left[\frac{i}{\hbar}V\int_0^t dt'\cos(2\pi q/q_0)\right]=\sum_{n=0}^\infty\frac{(iV/\hbar)^n}{n!}\int_0^t dt_1\int_0^t\cdots\int_0^t dt_n\prod_{i=1}^n\cos[2\pi q(t_i)/q_0]\ . \tag{3.17}$$

Since each cosine has two Fourier components, it is convenient to introduce n variables, $e_i=\pm1$, which we refer to as charges. Then (3.17) may be written in the form

$$\sum_{n=0}^\infty\left[\frac{iV}{2\hbar}\right]^n\sum_{\{e_i\}}\int dt_1\int dt_2\cdots\int dt_n\exp\left[-\frac{i}{\hbar}\int_0^t dt'\rho(t')q(t')\right]\ , \tag{3.18}$$

where $\sum_{\{e_i\}}$ denotes the summation over all possible configurations of the e_i, and

$$\rho(t)=\frac{2\pi\hbar}{q_0}\sum_{i=1}^n e_i\delta(t-t_i) \tag{3.19}$$

is the corresponding charge density. The time integration in (3.18) is over the range $0<t_1<\cdots<t_n<t$. Since we need to calculate a double path integral for the time-dependent density matrix, this procedure has to be repeated for the conjugate variable q'. A new set of charges $\sigma_j=\pm1$ are introduced with corresponding charge density

$$\rho'(t)=\frac{2\pi\hbar}{q_0}\sum_{j=1}^{n'}\sigma_j\delta(t-t_j')\ . \tag{3.20}$$

Inserting these expansions into (3.7) and expressing everything in terms of the coordinates x and y, we find that the probability density can be written in the following form:

$$P(x,t)=\sum_{n,n'=0}^{\infty}\left[\frac{iV}{2\hbar}\right]^n\left[\frac{-iV}{2\hbar}\right]^{n'} \times\sum_{\{e_i,\sigma_j\}}\int dt_1\int dt_2\cdots\int dt'_{n'}\int dx_0\int dy_0\langle x_0+\tfrac{1}{2}y_0\,|\,\hat{\rho}(0)\,|\,x_0-\tfrac{1}{2}y_0\rangle G(\rho,\rho';x_0,y_0)\,, \tag{3.21}$$

with

$$G=\int_{x_0}^{x}Dx\int_{y_0}^{0}Dy\exp\left[(i/\hbar)\int_0^t dt'[M\dot{x}\dot{y}+\eta x\dot{y}+Fy-x(\rho-\rho')-\tfrac{1}{2}y(\rho+\rho')]-S_2(y)\right]. \tag{3.22}$$

The advantage of this representation is that the path integrals over x and y are now Gaussian and can be done exactly. Performing these integrations, we obtain

$$G=\frac{M}{2\pi\hbar d(t)}\exp\left[\frac{i}{\hbar}Mx\dot{y}\Big|_0^t+\frac{i}{\hbar}\int_0^t dt'[F-\tfrac{1}{2}(\rho+\rho')]y(t')-S_2(y)\right], \tag{3.23}$$

where $d(t)=\gamma^{-1}(1-e^{-\gamma t})$ ($\gamma=\eta/M$), and the path $y(t')$ is the solution of the differential equation

$$\ddot{y}-\gamma\dot{y}=(\rho'-\rho)/M\,, \tag{3.24}$$

with boundary conditions $y(0)=y_0$ and $y(t)=0$. Taking the Fourier transform of (3.24) and inserting it into $S_2(y)$, it is easy to see that at long times $t\to\infty$ the only configurations which contribute are those for which

$$\int_0^t(\rho-\rho')dt'=0\,. \tag{3.25}$$

Thus, we can restrict the sum over n and n' in Eq. (3.21) to $n+n'=$even, which leads to a series containing only even powers in V.

The general solution of (3.24) may be written as a sum of a particular and a homogeneous solution, $y=y_p+y_h$. It is convenient to define a function

$$h(t)=e^{\gamma t}H(-t)+H(t)\,, \tag{3.26}$$

where $H(t)$ is the usual Heaviside step function. Then a particular solution may be written as

$$y_p(t')=\frac{q_0}{\alpha}\left[\sum_{i=1}^{n}e_i h(t'-t_i)-\sum_{j=1}^{n'}\sigma_j h(t'-t'_j)\right], \tag{3.27}$$

which has the form shown in Fig. 3. Due to condition (3.25), y_p satisfies $y_p(t)=\dot{y}_p(t)=0$, and up to exponentially small terms of order $\exp[-\gamma\min(t_1,t'_1)]$ we also have that $y_p(0)=\dot{y}_p(0)=0$. The homogeneous solution which fulfills the required boundary conditions is therefore

$$y_h(t')=\frac{y_0}{\gamma d(t)}\{1-\exp[-\gamma(t-t')]\}\,. \tag{3.28}$$

We are now in a position to obtain our formal expression for the mobility μ. Consider the average position of the particle at time t

$$\langle x(t)\rangle=\int_{-\infty}^{\infty}dx\,xP(x,t)\,, \tag{3.29}$$

which gives the mobility directly by using (3.3). For a finite dc mobility μ, $\langle x(t)\rangle$ will grow linearly with time for $t\to\infty$. Thus, we need only keep those terms which scale linearly with time. As is shown in Appendix A, the mobility μ may be written in the form

$$\frac{\mu}{\mu_0}=1-\frac{1}{F}\lim_{t\to\infty}\left\langle\frac{1}{t}\int_0^t dt'\tfrac{1}{2}(\rho+\rho')\right\rangle. \tag{3.30}$$

Here we have defined an average by

$$\langle A\rangle=\sum_{\substack{n,n'=0\\ n+n'\text{ even}}}^{\infty}\left[\frac{iV}{2\hbar}\right]^n\left[\frac{-iV}{2\hbar}\right]^{n'}\sum_{\{e_i,\sigma_j\}}\int dt_1\int dt_2\cdots\int dt'_{n'}A\exp\Omega(\dot{y}_p)\,, \tag{3.31}$$

with

$$\Omega(y_p)=\frac{i}{\hbar}\int_0^t dt'[F-\tfrac{1}{2}(\rho+\rho')]y_p(t')-S_2(y_p)\,, \tag{3.32}$$

and y_p given by (3.27). Equation (3.30) is our formally exact expression for the nonlinear mobility at arbitrary temperature. The first term gives the mobility $\mu_0=1/\eta$ in the absence of a periodic potential $V=0$. The second nontrivial term is an infinite series in powers of V^2 and describes the deviation from μ_0 due to the presence of the corrugation.

In view of the complexity of the average (3.31), this expression does not seem very useful for explicitly calculat-

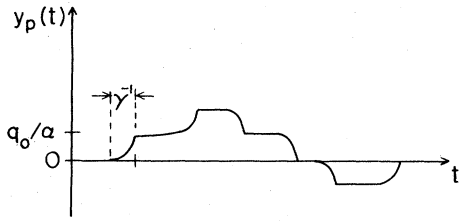

FIG. 3. Typical particular solution of Eq. (3.24). The step heights are of size $\pm q_0/\alpha$ and are rounded on the timescale γ^{-1}.

ing the mobility for nonzero V. However, as will be shown in the following, the nontrivial part is, apart from changes in the parameters, identical to the mobility in a tight-binding model with hopping matrix element V. This result will then be used in Sec. III C to evaluate explicitly the nonlinear mobility in the small corrugation limit at arbitrary temperature and friction.

Consider a tight-binding model consisting of a lattice of discrete sites connected by some nearest-neighbor hopping matrix element. The continuous coordinate q then becomes a discrete variable with values $n\tilde{q}_0$, $n=0, \pm 1, \pm 2, \ldots$, where $\tilde{q}_0$ is the distance between lattice sites. The paths which have to be summed over in the influence-functional theory consist of successive steps of size $\pm\tilde{q}_0$ (see Fig. 4). The central idea underlying the transcription of (3.31) into a tight-binding model is to associate the charges e_i and σ_j with the possible nearest-neighbor hops $\pm\tilde{q}_0$ of the paths $q_s(t)$ and $q_s'(t)$ on the tight-binding lattice. Thus, we define tight-binding trajectories

$$q_s(t)=\tilde{q}_0 \sum_{i=1}^{n} e_i H(t-t_i) , \tag{3.33}$$

$$q_s'(t)=\tilde{q}_0 \sum_{j=1}^{n'} \sigma_j H(t-t_j') . \tag{3.34}$$

Since $y_p(t)$ which enters into (3.32) looks like a smoothed-out tight-binding trajectory with step size q_0/α [see (3.27) and Fig. 3], it is natural to choose the lattice spacing $\tilde{q}_0$ in the tight-binding model as

$$\tilde{q}_0=q_0/\alpha . \tag{3.35}$$

The trajectories $x_s=\frac{1}{2}(q_s+q_s')$ and $y_s=q_s-q_s'$ may be expressed in terms of our old charge densities as

$$\begin{aligned} x_s(t)&=\eta^{-1}\int_0^t dt'[\tfrac{1}{2}(\rho+\rho')] , \\ y_s(t)&=\eta^{-1}\int_0^t dt'(\rho-\rho') . \end{aligned} \tag{3.36}$$

In order to make the interpretation of (3.30) and (3.31) in terms of a tight-binding model complete, we reexpress Ω in (3.32) in terms of the sharp tight-binding trajectories x_s and y_s rather than the smooth particular solution y_p and the charge densities ρ and ρ'. Inserting y_p from (3.27) into (3.32), and using (3.36), it is straightforward to show that, apart from exponentially small boundary terms, Ω takes the form

$$\Omega=\frac{iF}{\hbar}\int_0^t dt' y_s(t')+i\Phi^{(\gamma)}(x_s,y_s) , \tag{3.37}$$

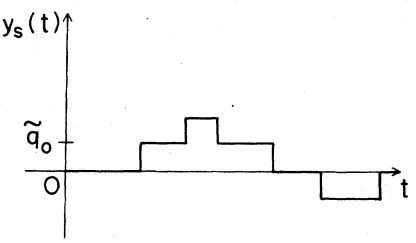

FIG. 4. Typical tight-binding hopping trajectory $y_s=q_s-q_s'$ with lattice constant $\tilde{q}_0$.

where Φ is the influence phase defined in (3.10). The superscript γ, however, indicates that the spectral density which enters Φ is now of the form

$$J^{(\gamma)}(\omega)=\frac{\eta\omega}{1+(\omega/\gamma)^2} , \tag{3.38}$$

with a soft cutoff at frequency γ. Formally, this is due to the smoothness of $y_p(t)$ which is smeared out on a scale γ^{-1}, compared to the sharp tight-binding trajectory $y_s(t)$. Physically, it means that the finite mass of the particle provides a natural cutoff for the bath oscillators in the tight-binding model.

From (3.37) it is clear that $\exp\Omega$ is identical to the complete influence functional for the tight-binding paths x_s and y_s in the presence of an external force F. Moreover, the remaining pieces in (3.31) can be interpreted as the nearest-neighbor transition amplitudes per unit time $\pm iV/2\hbar$ for hopping on the lattice, integration over all possible locations of the hops, and a summation over all possible paths. Thus, the average defined in (3.31) is equivalent to an average over the diagonal time-dependent density matrix of a corresponding tight-binding model. Therefore, using (3.36), Eq. (3.30) may be written as

$$\frac{\mu}{\mu_0}=1-\frac{1}{\mu_0}\lim_{t\to\infty}\left[\frac{\langle x_s(t)\rangle}{Ft}\right] , \tag{3.39}$$

where $\langle x_s(t)\rangle$ is the average position of a particle hopping on a tight-binding lattice with hopping matrix element V and lattice constant $\tilde{q}_0=q_0/\alpha$. The tight-binding model is at the original temperature T and subject to the same external force F. Since the lattice spacing in the tight-binding theory enters only through the dimensionless friction constant $\tilde{\alpha}$, we have

$$\tilde{\alpha}=\frac{\eta\tilde{q}_0^2}{2\pi\hbar}=\frac{1}{\alpha} \tag{3.40}$$

with η remaining fixed. In terms of the energy drop $\epsilon=Fq_0$ per period in the original washboard potential, the energy drop $\tilde{\epsilon}=F\tilde{q}_0$ between nearest-neighbor lattice sites in the tight-binding model is now

$$\tilde{\epsilon}=\epsilon/\alpha . \tag{3.41}$$

Denoting the mobility in the tight-binding model as $\mu_{\rm TB}(\tilde{\epsilon},\tilde{\alpha})$, we finally obtain from (3.39) the desired result

$$\frac{\mu(\epsilon,\alpha)}{\mu_0}=1-\frac{\mu_{\rm TB}(\epsilon/\alpha,\,1/\alpha)}{\mu_0} . \tag{3.42}$$

We have thus demonstrated an exact duality between the nonlinear mobility of a particle in a periodic potential and in a corresponding tight-binding model. It is most important to stress that no restrictions were placed on T or ϵ in our derivation. The relation (3.42) is therefore valid at *arbitrary* temperature and *arbitrary* bias. This goes far beyond a previous investigation of the problem by Schmid,[7] where a $\tilde{\mu}\to 1-\tilde{\mu}$ duality was found by a formally similar analysis of the partition function at zero temperature. In particular, $\tilde{\mu}$—which should correspond to our linear mobility at $T=0$—is defined there as the prefactor in the logarithmic growth of $\langle q(\tau)q(0)\rangle$ at

large imaginary times. In contrast, we have worked at finite T and within a real-time formulation from the beginning and have defined μ in the usual way as the ratio between current and field.

It should be kept in mind that the dual tight-binding model has a soft cutoff γ in the environment spectrum (3.38) which was not present in the original continuum problem. This cutoff will play a crucial role in the analysis of Sec. III C. Finally, we remark that the duality between the periodic potential and the tight-binding model actually holds for the full time-dependent density matrix. The mapping is, thus, not confined to $\langle x(t)\rangle$ alone, but can be extended to different kinds of averages.

$$\langle x_s(t)\rangle = \sum_{\substack{n,n'=0 \\ n+n' \text{ even}}}^{\infty} \left[\frac{iV}{2\hbar}\right]^n \left[\frac{-iV}{2\hbar}\right]^{n'} \sum_{\substack{\{e_i,\sigma_j\} \\ \sum_i e_i = \sum_j \sigma_j}} \int dt_1 \int dt_2 \cdots \int dt'_{n'} x_s(t) \exp\Omega \tag{3.44}$$

and

$$\Omega = \frac{iF}{\hbar}\int_0^t dt' y_s(t') + i\Phi^{(\gamma)}(x_s,y_s)\ , \tag{3.45}$$

where Φ is the influence phase defined in (3.10). The x_s and y_s are sharp tight-binding trajectories with transitions of size $\pm\tilde{q}_0 = \pm q_0/\alpha$ at times t_i $(i=1,2,\ldots,n)$ and t'_j $(j=1,2,\ldots,n')$ (see Fig. 4). The double summation and integrations in (3.44) are simply a representation of the functional integral over the paths $q_s(t)$ and $q'_s(t)$, which hop on a one-dimensional tight-binding lattice with hopping matrix element V. These paths can be most easily visualized in terms of the walk of a fictitious particle on an infinite matrix, whose elements correspond to the discrete values of (q,q') (see Fig. 5). At $t=0$ the walker starts at the origin and then performs vertical or horizontal steps with weight $\pm iV/2\hbar$, returning at time t to the main diagonal at some arbitrary position $x_s(t)=\frac{1}{2}(q_s+q'_s)$. Equation (3.44) is then simply a sum over all possible paths the walker can take which return to the main diagonal. As in the corresponding two-state calculation,[4,6] we refer to the times that the walker is on the main diagonal $y_s=q_s-q'_s=0$ as "sojourns" and denote as "blips" the periods spent in either of the first off diagonals $y_s=\pm\tilde{q}_0$. All other locations on the matrix apart from the tridiagonal will be referred to collectively as "higher-order blips."

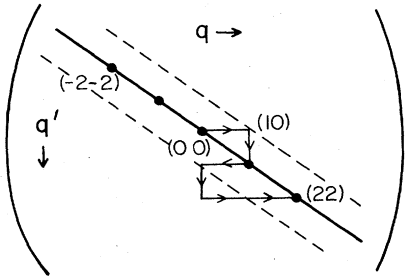

FIG. 5. Matrix representation of the discrete density matrix $\langle q\,|\,\hat{\rho}(t)\,|\,q'\rangle$ in a tight-binding model. The average in (3.44) corresponds to a random walk on this matrix, with amplitudes $\pm i(V/2\hbar)$ per unit time for horizontal or vertical hops and an additional factor $\exp\Omega$. To lowest order in V the walks may be restricted to the tridiagonal indicated by the dashed lines.

C. Mobility in the weak-corrugation limit

In this section the formal power-series expression derived in Sec. III B for the nonlinear mobility is analyzed in the weak-corrugation limit. In particular, we calculate the mobility to second order[35] in V, but at arbitrary friction, temperature, and bias. Our general results from Sec. III B (3.39), (3.31), and (3.37), were

$$\frac{\mu}{\mu_0} = 1 - \frac{1}{\mu_0}\lim_{t\to\infty}\left[\frac{\langle x_s(t)\rangle}{Ft}\right], \tag{3.43}$$

with

We now analyze the general expression in the weak-corrugation limit $V\to 0$. The most naive approach is to simply retain only those terms in the series (3.44) which are proportional to V^2. In terms of our walker, we then need only consider the four paths which start at (0,0) and take one vertical and one horizontal step, ending at $x_s(t)=\pm 1$. We need not consider the paths which take two steps and return to $x_s(t)=0$, since they carry no weight in the average (3.44). In the language of blips and sojourns, the four paths consist each of a single blip between the original and final sojourns. Since $y_s=0$ during the sojourns, the only contribution to the weight $\exp\Omega$ comes from the blip. It is convenient to label the four possible blips by $\xi=\pm 1$, if the blip is above or below the main diagonal, and $\zeta=\pm 1$, if x_s changes by $\pm\tilde{q}_0/2$ upon entering the blip from the previous sojourn. The weight of a single blip obtained by inserting the trajectories into (3.45) is denoted by

$$B(\xi,\zeta) = \exp\Omega\,|_{\text{blip}}\ . \tag{3.46}$$

For a blip starting at t_1 and ending at t'_1, it is straightforward to show that

$$B(\xi,\zeta,t_1-t'_1) = \exp\left[i\xi\left[\frac{\epsilon}{\alpha\hbar}(t_1-t'_1) - \zeta(2/\alpha)\tilde{Q}_1(t_1-t'_1)\right] - (2/\alpha)\tilde{Q}_2(t_1-t'_1)\right], \tag{3.47}$$

where

$$\tilde{Q}_1(t) = \int_0^\infty d\omega \frac{J^{(\gamma)}(\omega)}{\eta\omega^2}\sin(\omega t)\ , \tag{3.48}$$

$$\tilde{Q}_2(t) = \int_0^\infty d\omega \frac{J^{(\gamma)}(\omega)}{\eta\omega^2}[1-\cos(\omega t)]\coth(\tfrac{1}{2}\beta\hbar\omega)\ , \tag{3.49}$$

and $J^{(\gamma)}(\omega)$ is the spectral density (3.38) with a soft cutoff

γ. The contribution to $\langle x_s(t)\rangle$ from these four blips is then

$$\langle x_s(t)\rangle = \left[\frac{V}{2\hbar}\right]^2 \sum_{\xi,\zeta=\pm 1} \int_0^t dt_1 \int_0^{t'_1} dt'_1\, \zeta\tilde{q}_0 \times B(\xi,\zeta,t_1-t'_1)\,. \tag{3.50}$$

Since B only depends on $t_1-t'_1$, it is clear that $\langle x_s(t)\rangle$ grows linearly with time. As $t\to\infty$ we obtain

$$\lim_{t\to\infty}\left[\frac{\langle x_s(t)\rangle}{t}\right] = 4\frac{q_0}{\alpha}\left[\frac{V}{2\hbar}\right]^2 \times \int_0^\infty dt \sin(\epsilon t/\alpha\hbar)\sin[(2/\alpha)\tilde{Q}_1(t)] \times \exp[-(2/\alpha)\tilde{Q}_2(t)]\,. \tag{3.51}$$

Inserting this into (3.43) gives, within our naive perturbation theory, the final result for the mobility to order V^2.

To justify this result, it is necessary to check whether the neglected higher-order terms in (3.44), proportional to $V^4, V^6, \ldots$, are indeed small in comparison to those terms retained. Since the general structure of the series (3.44) for long times is actually of the form

$$\langle x_s(t)\rangle = a_1 V^2 t + a_2 (V^2 t)^2 + \cdots\,, \tag{3.52}$$

these terms would eventually dominate the V^2 terms as $t\to\infty$ no matter how small we choose V. The correct procedure for obtaining the mobility to order V^2—as opposed to the naive perturbation theory above—therefore really involves a summation of the whole series, letting $t\to\infty$ and then extracting the coefficient of V^2 as $V\to 0$. It is not obvious that this will give the same answer as the coefficient a_1 in (3.52), i.e., it is not clear that we can interchange the limits $V\to 0$ and $t\to\infty$. By summing an infinite class of terms, however, we show in Appendix B that the two limits can indeed be interchanged and the naive approach (3.51) gives the correct answer to order V^2.

IV. DISCUSSION: DEPENDENCE OF THE MOBILITY ON TEMPERATURE

A. Classical and zero-temperature limits

In the following we will discuss in detail the actual behavior of the mobility in the weak-corrugation limit using the general expression derived in Sec. III C. From Eqs. (3.43), (3.51), and (B13) the nonlinear mobility to order V^2 is given by

$$\frac{\mu(\epsilon,\alpha)}{\mu_0} = 1 - \frac{2\pi V^2}{\epsilon\hbar\gamma} I \tag{4.1}$$

with

$$I = \gamma \int_0^\infty dt \sin(\epsilon t/\alpha\hbar)\sin[(2/\alpha)\tilde{Q}_1(t)] \times \exp[-(2/\alpha)\tilde{Q}_2(t)]\,, \tag{4.2}$$

or alternatively

$$I = \tanh(\epsilon/2\alpha T)\gamma \int_0^\infty dt \cos(\epsilon t/\alpha\hbar) \times \cos[(2/\alpha)\tilde{Q}_1(t)] \times \exp[-(2/\alpha)\tilde{Q}_2(t)]\,. \tag{4.3}$$

The functions $\tilde{Q}_1$ and $\tilde{Q}_2$ are defined by

$$\tilde{Q}_1(t) = \int_0^\infty d\omega \frac{\sin(\omega t)}{\omega} f(\omega/\gamma)\,, \tag{4.4}$$

$$\tilde{Q}_2(t) = \int_0^\infty d\omega \frac{1-\cos(\omega t)}{\omega} \coth(\tfrac{1}{2}\beta\hbar\omega) f(\omega/\gamma)\,, \tag{4.5}$$

with a cutoff function $f(x)=(1+x^2)^{-1}$. It is important to emphasize that the result (4.1) is valid only perturbatively for small V; thus, V must always be chosen sufficiently small that μ/μ_0 remains close to 1. This is always possible, except when $\alpha>1$ and both T and ϵ tend to zero. In this limit the coefficient of V^2 diverges and the perturbation expansion is invalid.

We start with a discussion of the high-temperature limit, where a comparison with results from the classical Langevin equation is possible. In the classical limit the temperature must be taken sufficiently large that all the $\hbar$ dependence in (4.1) cancels out. In particular, by taking

$$T \gg \hbar\gamma\,, \tag{4.6}$$

we may replace the $\coth(\frac{1}{2}\beta\hbar\omega)$ in $\tilde{Q}_2$ by $2T/\hbar\omega$. To leading order in $\hbar\gamma/T$ the factor $\exp[-(2/\alpha)\tilde{Q}_2(t)]$ then takes the form

$$\exp[-K(\gamma t + e^{-\gamma t} - 1)]\,, \tag{4.7}$$

where we have introduced the purely classical dimensionless quantity

$$K = \frac{2\pi T}{\alpha\hbar\gamma} = \frac{T}{V}\left[\frac{\omega_0}{\gamma}\right]^2\,, \tag{4.8}$$

with ω_0 the small undamped oscillation frequency around the minima of the unbiased periodic potential. Notice that (4.7) is now independent of $\hbar$. The only remaining $\hbar$ dependence in (4.2) is in the argument of the second sine, since $\alpha\sim\hbar^{-1}$. Provided that in addition to (4.6) we take

$$T \gg E_0 = \frac{(2\pi\hbar)^2}{Mq_0^2}\,, \tag{4.9}$$

it is straightforward to show that irrespective of the value of K, the integral (4.2) is cut off at values of t such that $(2/\alpha)\tilde{Q}_1(t) \ll 1$. Thus, to leading order in E_0/T and $\hbar\gamma/T$, the $\sin[(2/\alpha)\tilde{Q}_1(t)]$ may be replaced by its argument and we obtain the classical result

$$\frac{\mu^{\rm cl}(\epsilon)}{\mu_0} = 1 - \pi\left[\frac{V}{T}\right]^2 \frac{T}{\epsilon} K \int_0^\infty dx \sin\left[\frac{K\epsilon}{2\pi T}x\right](1-e^{-x}) \times \exp[-K(x+e^{-x}-1)]\,. \tag{4.10}$$

As required, all the $\hbar$ dependence has now dropped out. The linear mobility follows with $\epsilon \to 0$,

$$\frac{\mu_l^{\rm cl}}{\mu_0} = 1 - \frac{1}{2}\left[\frac{V}{T}\right]^2 e^K K^{-K+1}\gamma(K,K) , \tag{4.11}$$

where $\gamma(K,K)$ is the incomplete γ function.[29] These classical results can be checked by performing perturbation theory directly on the Langevin equation (1.1). Inserting the expansion

$$q(t) = q^{(0)}(t) + Vq^{(1)}(t) + V^2 q^{(2)}(t) + \cdots \tag{4.12}$$

into (1.1) and comparing powers of V, we find that to second order in V^2 the corresponding ratio $\mu(\epsilon)/\mu_0$ is exactly equal to (4.10).

To complete the analysis of the high-temperature limit, we examine the form of the quantum corrections to the classical mobility. These can be generated in a straightforward fashion by retaining the next-to-leading terms in the expansion in powers of E_0/T of the $\coth(\frac{1}{2}\beta\hbar\omega)$ in $\tilde{Q}_2$ and the $\sin[(2/\alpha)\tilde{Q}_1]$ in Eq. (4.2). To lowest order we find that the linear mobility has quantum corrections proportional to $\hbar^2$ of the form

$$1 - \frac{\mu_l(T,\alpha)}{\mu_0} = \left[1 - \frac{\mu_l^{\rm cl}}{\mu_0}\right][1 - W(K)(E_0/T) + O((E_0/T)^2)] , \tag{4.13}$$

where $W(K)$ is a smoothly varying, positive function of K which approaches $\frac{1}{12}$ as $K \to 0$ and $\frac{1}{4}$ as $K \to \infty$. It is of interest to note that the sign of the quantum corrections is such that they *enhance* the mobility compared to the classical prediction. This is in accord with one's intuition that inclusion of quantum fluctuations allow the particle to tunnel between the minima of the washboard potential, thus increasing the mobility. Of course, as $E_0/T \to 0$ the coherence necessary for tunneling is completely suppressed and the classical result is obtained. Using the inequalities $\tilde{Q}_2 > \tilde{Q}_2$ (classical) [see (4.7)], and

$$\sin[(2/\alpha)\tilde{Q}_1] < (2/\alpha)\tilde{Q}_1 ,$$

it is easy to see from (4.1) and (4.2) that quite generally for arbitrary $T \neq 0$ we have

$$\mu_l(T) > \mu_l^{\rm cl}(T) , \tag{4.14}$$

with $\mu_l^{\rm cl}$ defined in (4.11). Although we have proven (4.14) only to order V^2, it is likely to hold to any order in V.

After discussing the high-temperature limit, we now turn to the opposite extreme of zero temperature. In this limit we recall that the renormalization-group treatment in Sec. II indicated a $T=0$ localization transition as a function of α, with the particle localized for $\alpha > 1$ and delocalized for $\alpha < 1$. Consequently, we expect that the linear mobility for $\alpha > 1$ should vanish at zero temperature. This is clearly a nonperturbative result[36] and cannot be deduced from our expansion to order V^2. For $\alpha < 1$, on the other hand, the weak-corrugation expansion is valid all the way down to zero temperature. To facilitate the computation of the nonlinear mobility at $T=0$, we replace the smooth cutoff $f(x) = (1+x^2)^{-1}$ by an exponential one, $f(x) = e^{-x}$. With this choice the integrals for $\tilde{Q}_1$ and $\tilde{Q}_2$ in (4.4) and (4.5) can be performed explicitly:

$$\tilde{Q}_1(t) = \tan^{-1}(\gamma t) , \tag{4.15}$$

$$\exp[-(2/\alpha)\tilde{Q}_2(t)] = [1+(\gamma t)^2]^{-1/\alpha} \times \left[\frac{|\Gamma(1+\tilde{T}+i\tilde{T}\gamma t)|^2}{|\Gamma(1+\tilde{T})|^2}\right]^{2/\alpha} , \tag{4.16}$$

with $\tilde{T} = T/\hbar\gamma$ as the reduced dimensionless temperature. Inserting these in (4.2) we find that at zero temperature

$$\frac{\mu(\epsilon, T=0)}{\mu_0} = 1 - \frac{\pi^2}{\alpha\Gamma(2/\alpha)}\left[\frac{V}{\hbar\gamma}\right]^2 \times \left[\frac{\epsilon}{\alpha\hbar\gamma}\right]^{2(1/\alpha-1)} \exp\left[-\frac{\epsilon}{\alpha\hbar\gamma}\right] . \tag{4.17}$$

This shows explicitly that for $\alpha > 1$ our perturbation expansion breaks down for the linear mobility $\epsilon \to 0$. However, it is still valid as long as $\epsilon/\alpha\hbar\gamma$ is large enough such that μ/μ_0 is near 1. For $\alpha < 1$, setting $\epsilon = 0$, we see that the linear mobility is identical to μ_0, independent[37] of the corrugation strength V. The potential is only felt through the non-Ohmic corrections, varying as $\epsilon^{2(1/\alpha-1)}$. This strange result is related to the fact that for $\alpha < 1$ the particle in the dual tight-binding lattice [see Eq. (3.42)] is localized at $T=0$ since $\tilde{\alpha} = 1/\alpha > 1$, and a finite current only arises in the nonlinear response $\mu_{\rm TB} \sim \epsilon^{2(\tilde{\alpha}-1)}$. For $\epsilon \gg \alpha\hbar\gamma$ the nonlinear mobility approaches μ_0 as expected, although the detailed asymptotic behavior may depend on the choice of the cutoff $f(x)$. At any rate it can be inferred from (4.1) and (4.3) that this remains valid at arbitrary temperature, since for $\epsilon \to \infty$, $1 - \mu/\mu_0$ goes to zero faster than $1/\epsilon$.

B. Linear mobility

For the remainder of the discussion we will confine ourselves to the linear mobility μ_l, but consider arbitrary temperature. Using Eq. (4.3) and taking $\epsilon \to 0$ gives for the linear mobility

$$\frac{\mu_l(\alpha,T)}{\mu_0} = 1 - \frac{\pi V^2}{\alpha\hbar\gamma T} R(\alpha,\tilde{T}) , \tag{4.18}$$

with the dimensionless integral R defined by

$$R(\alpha,\tilde{T}) = \gamma \int_0^\infty dt \cos[(2/\alpha)\tilde{Q}_1(t)] \times \exp[-(2/\alpha)\tilde{Q}_2(t)] , \tag{4.19}$$

which depends on temperature only through the dimensionless combination $\tilde{T} = T/\hbar\gamma$. Let us first discuss the case $\alpha > 1$. In the limit $T \ll \hbar\gamma$ the integral (4.19) can be

evaluated explicitly using the exponential cutoff and gives

$$R(\alpha,\tilde{T})=\frac{\sqrt{\pi}}{2}\frac{\Gamma(1/\alpha)}{\Gamma(1/\alpha+\frac{1}{2})}\left[\frac{\pi T}{\hbar\gamma}\right]^{2/\alpha-1}, \quad T\ll\hbar\gamma \tag{4.20}$$

so that $1-\mu_I/\mu_0$ varies as $\tilde{T}^{-2(1-1/\alpha)}$. Thus, for $T\ll\hbar\gamma$, μ_I is an *increasing* function of temperature as it is in the high-temperature limit $T\gg\hbar\gamma$. Since we were unable to find a closed-form expression for R at arbitrary temperatures, we have evaluated the integral numerically. The result is shown in Fig. 6, where μ_I/μ_0 is plotted versus the reduced temperature $T/\hbar\gamma$ for the specific value $\alpha=\frac{3}{2}$. This demonstrates that $\mu_I(T)$ is a monotonically increasing function at all temperatures (solid line in Fig. 6). As the temperature approaches zero, however, $R/T\to\infty$, indicating that in this limit the perturbative expansion breaks down and the mobility cannot be determined from (4.18). Thus, we have terminated the solid line in Fig. 6 such that μ_I/μ_0 remains close to 1. As mentioned earlier, however, at $T=0$ the renormalization-group calculation in Sec. II demonstrates that, for $\alpha>1$, the ground state is localized, implying that the linear mobility vanishes identically. We have used a dashed line in Fig. 6 to interpolate between these two results.

The monotonicity of $\mu_I(T)$ for $\alpha>1$ is physically very reasonable. As the temperature is raised from zero, we expect that the localized (at $T\equiv0$) particle will be transported via a thermally activated hopping mechanism. Since the friction is large enough to suppress much of the quantum tunneling and localize the particle even at zero temperature, this thermal hopping is in some sense rather classical in nature. In any case, with increasing temperature the hopping proceeds at a faster rate, giving a larger mobility.

Finally let us consider the case $\alpha<1$. Using (4.18) and (4.20) we find that, for $T\ll\hbar\gamma$, μ_I is given by

$$\frac{\mu_I(\alpha<1,T\ll\hbar\gamma)}{\mu_0}=1-\frac{\pi^{2/\alpha+1/2}\Gamma(1/\alpha)}{2\alpha\Gamma(1/\alpha+\frac{1}{2})}\times\left[\frac{V}{\hbar\gamma}\right]^2\left[\frac{T}{\hbar\gamma}\right]^{2(1/\alpha-1)}. \tag{4.21}$$

Thus, μ_I approaches μ_0 with a power law as $T\to0$. Since μ_I also approaches μ_0 in the opposite limit $T\to\infty$, which is described by (4.11), there must exist a crossover temperature T^* where $\mu_I(T)$ has a minimum. Below T^* the mobility is a *decreasing* function of temperature, whereas above T^* it is *increasing* with T. This behavior is shown in Fig. 7, where for $\alpha=\frac{1}{4}$ we have plotted the mobility as a function of temperature by evaluating (4.19) numerically. We have determined the crossover temperature numerically (and analytically for $\alpha\to0$) and find

$$T^*=C(\alpha)\hbar^2/Mq_0^2, \tag{4.22}$$

where $C(\alpha)$ is a monotonically decreasing function of the friction α which approaches $\pi^2/3$ as $\alpha\to0$ and zero as $\alpha\to1^-$. In the low-friction limit, (4.22) can be written alternatively as

$$\lambda(T^*)\simeq q_0, \tag{4.23}$$

with $\lambda(T)=\hbar/\sqrt{MT}$ the particle's thermal de Broglie wavelength. We emphasize that (4.22) and (4.23) are only valid in the small corrugation limit; with increasing V we expect that T^* will increase.

The physics of this interesting crossover behavior may be explained in the following way. At zero temperature and $\alpha<1$, the perturbation of the environment is sufficiently weak to allow the particle to tunnel quantum mechanically between neighboring minima in the periodic potential (i.e., the particle is delocalized). However, with increasing temperature the random fluctuations of the environment are more effective at destroying the quantum coherence necessary for tunneling and consequently reduce the mobility. We refer to this as thermally *resisted* quantum tunneling. Thus, for $T<T^*$ the mobility is a

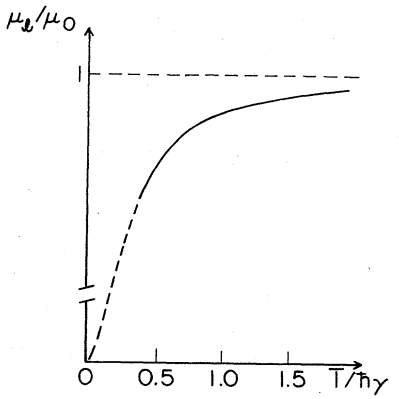

FIG. 6. The solid line is the linear mobility for $\alpha=\frac{3}{2}$ computed numerically from (4.18) and (4.19). The vertical scale is left in arbitrary units since the deviation of the solid line from 1 is proportional to the square of the corrugation strength V which can be varied at will (so long as μ/μ_0 remains close to 1). At $T=0$ the linear mobility vanishes identically. The dashed line is an interpolation between these two results.

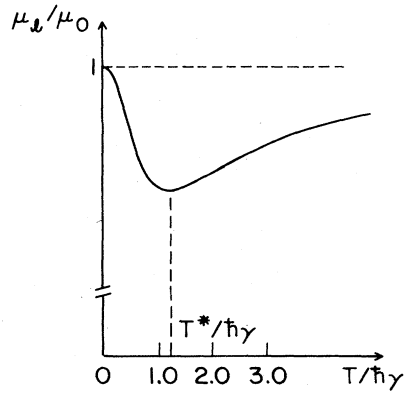

FIG. 7. The linear mobility (solid line) for $\alpha=\frac{1}{4}$ computed numerically from (4.18) and (4.19). The crossover temperature T^* separates regimes dominated by thermally *resisted* quantum tunneling and thermally *assisted* hopping.

decreasing function of temperature. There is, of course, an additional competing effect arising from transport via an "over-the-barrier" thermally *assisted* hopping process. When $T > T^*$, the environment has suppressed quantum tunneling and the assisted hopping mechanism becomes dominant. For $T > T^*$ the transport is thus enhanced by the finite-temperature bath and becomes an *increasing* function of temperature.

We emphasize that the crossover temperature decreases with increasing friction. Thus, the quantum tunneling regime ($T < T^*$) is most accessible when the particle is only weakly coupled to its environment.

A nonmonotonic temperature dependence in the diffusive behavior of a Brownian particle has in fact been observed recently in experiments on muons in metals.[20–22] In these experiments the diffusion is inferred indirectly by observing the muon's spin relaxation. We believe that the crossover behavior present in the simplified Caldeira-Leggett Hamiltonian describes the same physics as occurs in these systems. It is not appropriate to compare our results with these experiments in a quantitative fashion, however, since the model studied here offers at best an idealized description. Nevertheless, we emphasize that our results demonstrate certain generic features which should be common to many systems. Specifically, for a particle localized[38] at $T=0$ the linear mobility is a monotonically increasing function of temperature. When the ground state is delocalized, on the other hand, $\mu_l(T)$ is nonmonotonic with a minimum around T^*, where the transport crosses over from thermally constrained quantum tunneling to thermally assisted hopping. In the weak-corrugation and low-friction limit the crossover temperature occurs when the thermal de Broglie wavelength is roughly equal to q_0, the lattice constant in the periodic potential.

ACKNOWLEDGMENTS

It is a pleasure to thank A. T. Dorsey, E. Fradkin, and, in particular, A. J. Leggett for stimulating discussions. We are also indebted to D. S. Fisher and D. Huse for helpful suggestions and clarifying discussions. One of us (W.Z.) has been supported in part by the Deutsche Forschungsgemeinschaft (Bonn, Germany). The other of us (M.P.A.F.) is grateful to AT&T Bell Laboratories for support during the course of this work. This research was also supported by the John D. and Catherine T. MacArthur Foundation at the University of Illinois under Grant No. 0-6-40129.

APPENDIX A

In this appendix we use the formal result (3.21) for the probability distribution $P(x,t)$, to obtain the final expression for the mobility (3.30)—(3.32). It is convenient to introduce a generating functional

$$\tilde{P}(\lambda,t)=\int dx\, e^{i\lambda x}P(x,t)\ , \tag{A1}$$

which is normalized to 1, $\tilde{P}(\lambda=0,t)=1$, for all t. Then the first moment $\langle x(t)\rangle$, used to obtain the mobility in (3.3), may be calculated from

$$\langle x(t)\rangle=-i\frac{\partial\tilde{P}(\lambda,t)}{\partial\lambda}\bigg|_{\lambda=0}\ . \tag{A2}$$

To abbreviate the notation, we define an average by

$$\langle A\rangle=\sum_{\substack{n,n'=0\\(n+n'\ \text{even})}}^{\infty}\left[\frac{iV}{2\hbar}\right]^n\left[\frac{-iV}{2\hbar}\right]^{n'}\times\sum_{\{e_j,\sigma_j\}}\int dt_1\int dt_2\cdots\times\int dt'_{n'}A\exp[\Omega(y)]\ , \tag{A3}$$

with

$$\Omega(y)=(i/\hbar)\int_0^t dt'[F-\tfrac{1}{2}(\rho+\rho')]y(t')-S_2(y)\ . \tag{A4}$$

Then from (3.21) the generating function may be written as

$$\tilde{P}(\lambda,t)=\frac{M}{2\pi\hbar d(t)}\int dx\int dx_0\int dy_0\langle x_0+\tfrac{1}{2}y_0\,|\,\hat{\rho}(0)\,|\,x_0-\tfrac{1}{2}y_0\rangle\langle\exp\{i[\lambda+(M/\hbar)\dot{y}(t)]x-(i/\hbar)M\dot{y}_0x_0\}\rangle\ . \tag{A5}$$

Integrating over x gives a δ function of argument $\dot{y}(t)+\hbar\lambda/M$. This can be transformed into a δ function of argument y_0, if we use the condition (3.25), which leads to $\dot{y}(t)=\dot{y}_0-\gamma y_0$. Since $\dot{y}_0$ from (3.28) is given by $\dot{y}_0=-y_0e^{-\gamma t}/d(t)$, we find $\delta(y_0-\hbar\lambda d/M)$, with $d=d(t)$. The integral over y_0 can now be done, giving

$$\tilde{P}(\lambda,t)=\int dx_0\left\langle x_0+\frac{\hbar\lambda d}{2M}\,\middle|\,\hat{\rho}(0)\,\middle|\,x_0-\frac{\hbar\lambda d}{2M}\right\rangle\times\exp(i\lambda e^{-\gamma t}x_0)\langle 1\rangle_\lambda\ . \tag{A6}$$

For times $t\gg\gamma^{-1}$ we may set $\exp(i\lambda e^{-\gamma t}x_0)$ equal to 1, and if we define

$$\rho_0(y_0)=\int dx_0\langle x_0+\tfrac{1}{2}y_0\,|\,\hat{\rho}(0)\,|\,x_0-\tfrac{1}{2}y_0\rangle\ , \tag{A7}$$

the generating functional then becomes

$$\tilde{P}(\lambda,t\gg\gamma^{-1})=\rho_0\left[\frac{\hbar\lambda d}{M}\right]\langle 1\rangle_\lambda\ . \tag{A8}$$

The average $\langle 1\rangle_\lambda$ depends on λ, since the path $y(t')$ which occurs in the functional $\exp[\Omega(y)]$ is given by

$$y(t')=\frac{\hbar\lambda}{M\gamma}(1-e^{-\gamma(t-t')})+y_p(t')\ . \tag{A9}$$

For any initial distribution, which has zero average momentum

$$\langle p(t=0)\rangle=-i\hbar\frac{\partial\rho_0(y)}{\partial y}\bigg|_{y=0}=0\ ,$$

there is no contribution to $\langle x(t)\rangle$ which depends on the initial condition. Then, due to the normalization condition $\rho_0(0)=1$, the first term in (A8) may be replaced by 1. The only contribution to $\langle x\rangle$ then comes from differentiating the first term in $\Omega(y)$ with respect to λ. We obtain

$$\langle x(t)\rangle=(1/\eta)\left\langle \int_0^t dt'\{1-\exp[-\gamma(t-t')]\} \times[F-\tfrac{1}{2}(\rho+\rho')]\right\rangle , \tag{A10}$$

where the average on the right-hand side is now defined with $y(t')$ replaced by $y_p(t')$ since $\lambda=0$. The contribution which arises from $\exp[-\gamma(t-t')]$ is exponentially small away from the right endpoint $t'=t$ and does not scale linearly with t. For $\gamma t\to\infty$ we find, therefore, that

$$\langle x(t)\rangle=\frac{F}{\eta}t-\frac{1}{\eta}\left\langle \int_0^t dt'[\tfrac{1}{2}(\rho+\rho')]\right\rangle , \tag{A11}$$

where we have used the fact that $\langle 1\rangle_{\lambda=0}=\tilde{P}(\lambda=0)=1$. According to (3.3), $\langle x(t)\rangle$ has to be divided by Ft to obtain the physical mobility μ. Remembering that $\mu_0=\eta^{-1}$, this gives precisely (3.30).

APPENDIX B

In this appendix we rederive our naive perturbation-theory result (3.51) by summing an infinite class of terms in the general expression (3.44). It is clearly impossible to sum up the whole series (3.44) to all orders. In the following we thus make two simplifying approximations which will enable us to sum the series. From the definition of the influence phase Φ in (3.10) we see that the real part of Ω in (3.45) is proportional to y_s^2. Thus, paths taken by the walker which wander far away from the main diagonal $y_s=0$ are largely suppressed. Moreover, a segment of a path which starts on the main diagonal wanders out to, say, $y_s=\pm n\tilde{q}_0$, and then returns to the diagonal contributes at least a term of order V^{2n} in (3.44). Since we are interested in the mobility to order V^2, we thus consider only those paths which stay on the tridiagonal. These restricted paths consist solely of sojourns, $y_s=0$, and blips, $y_s=\pm\tilde{q}_0$. In addition, as can be seen from (3.47), a blip of length t contains a contribution $\exp[-(2/\alpha)\tilde{Q}_2(t)]$ in its weight factor. Since $\tilde{Q}_2(t)$ grows large with time, this factor suppresses long blips. The sojourns, on the other hand, do not have such a suppression factor and as a result will typically be much longer than the blips. It is then appropriate to treat the system as a noninteracting gas of blips separated by long sojourns. Within this approximation a given path is built up from successive blips, and its weight is simply a product of the weights (3.46) of the individual blips. Consequently, the entire series can be summed. The consistency of this procedure must be checked at the end of the calculation; in particular, the typical blip times [which can be estimated from their weights B in (3.47)] must be much smaller than the time of a blip and its neighboring sojourn (which is the characteristic time emerging from the calculation). This technique was originally applied to the two-state problem[4] and is referred to as the noninteracting-blip approximation.

All the possible paths on the tridiagonal elements of the matrix in Fig. 5 can be conveniently labeled by three quantities: the times $\{t_i\}$, $i=1,\ldots,2m$, at which the hops take place, a set of integers $\{N_i\}$, $i=1,\ldots,m$, which correspond to the position $N_i=x_s/\tilde{q}_0$ that the fictitious particle occupies during the ith sojourn, and a set $\{\xi_i=\pm1,\zeta_i=\pm1\}$, $i=1,\ldots,m$, specifying the types of blips which separate the sojourns. Here m denotes the number of blips in a given path. Since a blip can only move the walker at most one unit along the main diagonal, we have that $\Delta N_i=N_{i+1}-N_i=0,\pm1$. The summation over all allowed paths can then be carried out in three stages. First we consider a summation over the allowed blips for a given set of sojourn positions $\{N_i\}$ and times $\{t_i\}$. There are two types of blips which can separate sojourns with $\Delta N=\pm1$. We denote their total weight by $f_\pm$. Between sojourns with $\Delta N=0$ four blips are possible which carry a weight f_0. Using the single-blip weight factor (3.47), we find

$$f_\pm(t)=\left[\frac{V}{2\hbar}\right]^2\sum_{\xi=\pm1}B(\xi,\pm) =\frac{V^2}{2\hbar^2}\cos[(\epsilon t/\alpha\hbar)\mp(2/\alpha)\tilde{Q}_1(t)] \times\exp[-(2/\alpha)\tilde{Q}_2(t)] , \tag{B1}$$

$$f_0(t)=-\left[\frac{V}{2\hbar}\right]^2\sum_{\xi,\zeta=\pm1}B(\xi,\zeta)=-f_+(t)-f_-(t) , \tag{B2}$$

where t is the length of the blip under consideration. Next we integrate over the times $\{t_i\}$, i.e., the locations and lengths of the blips, again for fixed $\{N_i\}$. In the noninteracting-blip approximation this can be easily done by a Laplace transformation. For a given set of $\{N_i\}$ the contribution to the Laplace transform of $x_s(t)$ then becomes

$$\frac{1}{\lambda}\left[\frac{f_0(\lambda)}{\lambda}\right]^{n_0}\left[\frac{f_+(\lambda)}{\lambda}\right]^{n_+}\left[\frac{f_-(\lambda)}{\lambda}\right]^{n_-} , \tag{B3}$$

where $f_0(\lambda)$ and $f_\pm(\lambda)$ are Laplace transforms of $f_0(t)$ and $f_\pm(t)$, respectively. The $n_\pm$ and n_0 are the number of adjacent pairs of sojourns in the set $\{N_i\}$ which differ in position by ±1 or 0. Finally, we must perform a sum over all possible sojourn sets $\{N_i\}$, which can be generated by the fictitious particle starting at the origin $N=0$ and walking up and down the diagonal. To perform this final summation it is convenient to introduce a generating functional

$$G(s,t)=\sum_{N=-\infty}^{\infty}s^N W_N(t) , \tag{B4}$$

where $W_N(t)$ is the weight for the sum over all paths [as in (3.44)] which end at site N at time t. The average $\langle x_s(t)\rangle$ then follows by differentiating G,

$$\langle x_s(t)\rangle=\tilde{q}_0\langle N(t)\rangle=\tilde{q}_0\frac{\partial G(s,t)}{\partial s}\bigg|_{s=1} . \tag{B5}$$

Since the final position N of a path is equal to n_+-n_-, the factor s^N in the generating function may be absorbed

in the weights of the trajectories by simply changing f_+ into sf_+ and f_- into f_-/s. The total number of trajectories with given $\{n_0,n_\pm\}$ is

$$C=(n_0+n_++n_-)!/n_0!n_+!n_-!\ .$$

Thus the Laplace transform of the generating functional is given by

$$\lambda G(s,\lambda)=\sum_{n_0,n_\pm=0}^{\infty} C\left[\frac{f_0(\lambda)}{\lambda}\right]^{n_0} \times\left[\frac{sf_+(\lambda)}{\lambda}\right]^{n_+}\left[\frac{f_-(\lambda)}{\lambda s}\right]^{n_-}, \tag{B6}$$

which can be written in the simple final form

$$\lambda G(s,\lambda)=[\lambda-f_0(\lambda)-sf_+(\lambda)-f_-(\lambda)/s]^{-1}\ . \tag{B7}$$

Differentiating with respect to s and using (B2) we find

$$\langle N(\lambda)\rangle=\frac{f_+(\lambda)-f_-(\lambda)}{\lambda^2}\ . \tag{B8}$$

If $f_\pm(\lambda)$ have well-defined limits as $\lambda\to 0$, the Laplace inversion is straightforward and gives

$$\lim_{t\to\infty}\left[\frac{\langle N(t)\rangle}{t}\right]=f_+(\lambda=0)-f_-(\lambda=0)\ . \tag{B9}$$

Using the definition of $f_\pm(t)$ in (B1), it is easy to see that this agrees precisely with (3.51). Thus, we have rederived the naive perturbation-theory result by an explicit summation of all possible paths on the discrete density matrix (see Fig. 5) restricted to the tridiagonal and within the noninteracting-blip approximation.

A particularly simple interpretation of our result (B7) may be obtained by taking the limit $\lambda\to 0$ and defining $\Gamma=-f_0(\lambda=0)$ and $\Gamma_\pm=f_\pm(\lambda=0)$. Then the generating function becomes identical to one for a nearest-neighbor hopping model described by a master equation

$$\dot P_N=-\Gamma P_N+\Gamma_+P_{N-1}+\Gamma_-P_{N+1}\ , \tag{B10}$$

with rates $\Gamma_\pm$ to the right or left and $\Gamma=\Gamma_++\Gamma_-$. The Γ introduced in this way is in fact identical to the relaxation rate of a two-state system with Ohmic dissipation in the regime where exponential relaxation holds.[6,39]

We must now check the self-consistency of the noninteracting-blip approximation, which requires that a typical blip time be small compared to a blip and its neighboring sojourn. The typical sojourn time is essentially the mean residence time on a particular diagonal site, and from (B10) it is clear that this is equal to Γ^{-1}. An average blip length $\langle t\rangle$ can be obtained by taking the first moment of the blip weight (3.47) or, equivalently, $f_0(t)$,

$$\langle t\rangle=\frac{\int_0^\infty dt\, tf_0(t)}{\int_0^\infty dt\, f_0(t)}=[f_0(\lambda=0)]^{-1}\left|\frac{\partial f_0(\lambda)}{\partial\lambda}\right|_{\lambda=0}\ . \tag{B11}$$

The validity of the noninteracting-blip approximation requires that $\langle t\rangle\ll\Gamma^{-1}$ or

$$\left|\frac{\partial f_0(\lambda)}{\partial\lambda}\right|_{\lambda=0}\ll 1\ . \tag{B12}$$

Since, according to (B2), we have $f_0\sim V^2$, it appears that we can always satisfy the inequality (B12) by choosing V small enough. This is in fact the case except when $\alpha>1$ and $T=\epsilon=0$, since then the integral multiplying V^2 in (B12) is divergent. Thus, caution must be exercised in using (3.51) when $\alpha>1$ and T and ϵ are both tending to zero.

Finally, we note that there is a detailed balance condition between forward and backward hopping $\Gamma_+/\Gamma_-=\exp(\beta\tilde\epsilon)$. To prove this, we observe that the function $C(t)=\tilde Q_2(t)+i\tilde Q_1(t)$ can be analytically continued to the lower complex t plane and satisfies

$$C(t-i\beta\hbar)=C^*(t)=C(-t)\ .$$

Using this we may also express the final result (3.51) in the alternate form

$$\lim_{t\to\infty}\left[\frac{\langle x(t)\rangle}{t}\right]=\frac{q_0}{\alpha}\left[\frac{V}{\hbar}\right]^2\tanh(\epsilon/2\alpha T) \times\int_0^\infty dt\cos(\epsilon t/\alpha\hbar)\cos[(2/\alpha)\tilde Q_1(t)] \times\exp[-(2/\alpha)\tilde Q_2(t)]\ . \tag{B13}$$

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*Present address: Physik Department, Technische Universität München, D-8046 Garching, Federal Republic of Germany.

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[34]Since we are interested in long-time properties like the dc mobility, this assumption concerning the initial condition should not be crucial.

[35]Since the mobility is symmetric under $V \to -V$, it does not contain a term linear in V.

[36]If in the strong-corrugation limit the periodic potential is replaced by a tight-binding model, then the vanishing mobility can be derived explicitly by working perturbatively to second order in the hopping matrix element.

[37]Although (4.17) only demonstrates the independence of the linear mobility (at $T=0$) on the corrugation strength to order V^2, we believe that this will remain true for arbitrary large V. This belief is based on the exact duality (3.42) relating μ to the mobility in a tight-binding lattice with $\tilde{\alpha} = 1/\alpha$. For $\alpha < 1$, $\tilde{\alpha}$ is larger than one and the renormalization-group flow diagram indicates that the tight-binding particle will be localized and thus have a vanishing linear mobility. Via the duality, this implies that the linear mobility in the washboard potential will be identically equal to μ_0, even for strong corrugation.

[38]As discussed at the end of Sec. II, whether or not the particle is localized (at $T=0$) is sensitive to the details of the coupling to the environment.

[39]This equivalence to the master equation has been suggested also by U. Weiss and H. Grabert (Ref. 9).