Quantum Ratchets

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We investigate quantum Brownian motion in adiabatically rocked ratchet systems. Above a crossover temperature T_c tunneling events are rare, yet they already substantially enhance the classical particle current. Below T_c, quantum tunneling prevails and the classical predictions grossly underestimate the transport. Upon approaching $T = 0$ the quantum current exhibits a tunneling induced reversal, and tends to a finite limit. [S0031-9007(97)03540-0]

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The quest of extracting usable work from fluctuations has provoked debates ever since the early days of Brownian motion theory [1]. *Prima facie,* periodic structures with broken spatial symmetry (ratchets) seem able to perform the job. Yet, already Smoluchowski and later Feynman [1] point out that an intriguing probabilistic balance prohibits the emergence of directed motion—in reconciliation with the second law of thermodynamics—if only equilibrium fluctuations are acting. As shown with the seminal studies [2,3], this situation changes drastically in the presence of additional unbiased nonthermal forces. Indeed, such classical nonequilibrium models entail a variety of interesting technological applications [3,4], and may be of relevance for intracellular transport as well [5]. The challenge here consists in the study of a *quantum Brownian rectifier* operating in a regime where tunneling and other quantum fluctuation effects become important for the transport properties. Our work opens the possibility of exploiting the ratchet mechanism in physical and biological systems in novel temperature regimes, predicting new qualitative effects such as a *tunneling-induced current reversal*. For example, a new type of superconducting quantum interference device has recently been proposed to investigate the ratchet mechanism [6]. At low temperature, our predictions can be observed *in situ* in these mesoscopic quantum structures. Moreover, using recent technical developments [7], semiconductor superlattices could be designed which, too, exhibit a quantum ratchet effect.

To start out, we consider the *quantum Brownian motion* of a particle with mass m and viscous damping η,

$$m\ddot{x}(t) = -\eta\dot{x}(t) - V'(x(t)) + f(t) + \xi(t), \quad (1)$$

under the simultaneous action of thermal quantum fluctuations $\xi(t)$, and symmetric, unbiased, external driving forces $f(t)$, in an asymmetric, periodic "ratchet"-potential $V(x)$ of period L, such as (cf. Fig. 1)

$$V(x) = V_0[\sin(2\pi x/L) - 0.22\sin(4\pi x/L)]. \quad (2)$$

Equation (1) follows as the exact Heisenberg equation for the coordinate *operator* $x(t)$ from a system-plus-reservoir model with Hamiltonian

$$H(t) = p^2/2m + V(x) - xf(t) + H_B(x,\mathbf{q}). \quad (3)$$

Here, $H_B(x,\mathbf{q})$ describes the heat bath interacting with the particle $x(t)$ and we adopt its usual modelization by an ensemble of harmonic oscillators $\mathbf{q}$ at thermal equilibrium with a coupling bilinear in the bath and particle coordinates [8]. By a suitable choice of the model parameters in $H_B(x,\mathbf{q})$ one recovers the quantum Langevin equation (1) with the operator valued quantum thermal noise $\xi(t)$ being self-adjoint, stationary, and Gaussian. With $\beta = 1/k_BT$, k_B Boltzmann's constant, and $\langle\ \rangle$ the thermal average with respect to H_B, the mean $\langle\xi(t)\rangle$ vanishes and for the symmetrized correlation $\frac{1}{2}\langle\xi(t)\xi(0) + \xi(0)\xi(t)\rangle$ one obtains $k_BT\eta\frac{d}{dt}\coth(\pi t/\hbar\beta)$ (fluctuation dissipation theorem). In the classical limit, i.e., for $\hbar\beta$ much smaller than any characteristic time scale of the deterministic system (1), the symmetrized correlation correctly approaches $2\eta k_BT\delta(t)$ and (1) goes over into the familiar model of a real valued stochastic process $x(t)$ in the presence of Gaussian white noise.

For general driving $f(t)$, Eq. (1) gives rise to a highly nontrivial nonequilibrium quantum dynamics. To

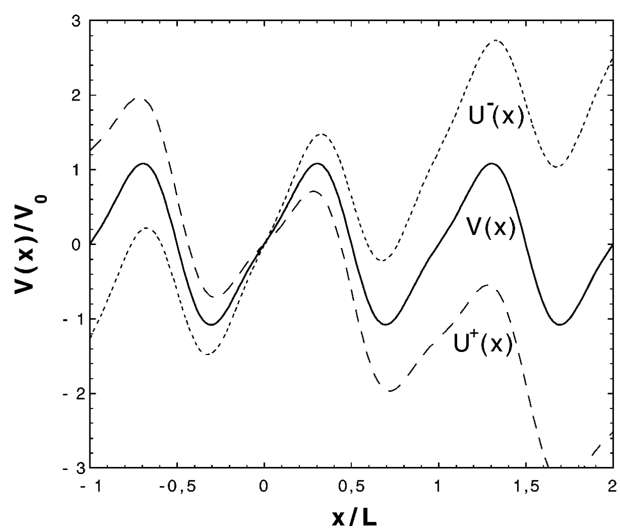

FIG. 1. Solid line: ratchet potential $V(x)$ in (2). Dashed and dotted lines: tilted washboard potentials $U^{\pm}(x)$ in (4) with $Fl = 0.2V_0$, $l = L/2\pi$. Note that the extrema and the separating barriers are *different* for $U^+(x)$ and $U^-(x)$, while the period L is in common.

simplify matters, we restrict ourselves to very slowly varying forces $f(t)$ such that the system can always adiabatically adjust to the instantaneous thermal equilibrium state (accompanying equilibrium). We furthermore assume that $f(t)$ is basically restricted to the values $\pm F$, i.e., the transitions between $\pm F$ occur on a time scale of negligible duration in comparison with the time the particles in (1) are exposed to either of the "tilted washboard" potentials

$$U^{\pm}(x) = V(x) \mp Fx \tag{4}$$

(cf. Fig. 1). As a final assumption we require a positive but not too large F, such that $U^{\pm}(x)$ still display a local maximum and minimum within each period L. Apart from this, the driving $f(t)$ can be either of stochastic or deterministic nature. To fix notations, let us denote by $x_0^{\pm}$ one of the local minima of $U^{\pm}(x)$ and by $x_b^{\pm}$ its neighboring local maximum to the right. The potential barrier which a particle at $x = x_0^{\pm}$ is facing to its right is therefore $\Delta U_r^{\pm} = U^{\pm}(x_b^{\pm}) - U^{\pm}(x_0^{\pm})$ and to its left $\Delta U_l^{\pm} = U^{\pm}(x_b^{\pm} - L) - U^{\pm}(x_0^{\pm})$, implying $\Delta U_l^{\pm} = \Delta U_r^{\pm} \pm FL$; see also Fig. 1.

We focus first on the *classical* motion (1) with m and η values such that a particle starting at rest close to a local maximum of $U^{\pm}(x)$ ends in a neighboring local minimum. So, moderate-to-strong friction dynamics is considered and deterministically "running solutions" excluded. We further assume weak thermal noise, that is, any potential barrier $\Delta U_{r,l}^{\pm}$ is much larger than the thermal energy $k_B T$. Then, the thermally induced escape rate over each such barrier is well approximated by the classical Kramers rate [8]

$$k_{\mathrm{cl}} = \frac{\mu\sqrt{U_0''}}{2\pi\sqrt{|U_b''|}}\, e^{-\beta\Delta U}, \quad \mu = \frac{\sqrt{\eta^2 + 4m|U_b''|} - \eta}{2m}, \tag{5}$$

where indices r, l, and $\pm$ have been dropped, and $U_{0,b}''$ represent the potential curvatures at the extrema. In the fixed potential $U^+(x)$ one thus has a rate $k_{\mathrm{cl},r}^+$ of the form (5) describing thermal hopping to the right, i.e., over ΔU_r^+, and a second rate $k_{\mathrm{cl},l}^+ = k_{\mathrm{cl},r}^+ e^{-\beta FL}$ for hopping to the left over ΔU_l^+, inducing a net particle current $J_{\mathrm{cl}}^+ = L(k_{\mathrm{cl},r}^+ - k_{\mathrm{cl},l}^+)$. The latter is positive in view of $J_{\mathrm{cl}}^+ = Lk_{\mathrm{cl},r}^+(1 - e^{-\beta FL})$ and $F > 0$. Analogously, in the quenched potential $U^-(x)$ one finds the negative current $J_{\mathrm{cl}}^- = -Lk_{\mathrm{cl},l}^-(1 - e^{-\beta FL})$. Because of our assumption of a slowly varying, symmetric driving $f(t)$ the average classical current $J_{\mathrm{cl}} = (J_{\mathrm{cl}}^+ + J_{\mathrm{cl}}^-)/2$ becomes $\frac{L}{2}(1 - e^{-\beta FL})(k_{\mathrm{cl},r}^+ - k_{\mathrm{cl},l}^-)$.

Next we turn to the *quantum ratchet dynamics* (1). We restrict ourselves to the semiclassical regime, which means that [9,10] $\hbar\mu^{\pm} \ll 2\pi\Delta U_{r,l}^{\pm}$, with $\mu^{\pm}$ as in (5). With moderate-to-strong friction acting, the tunneling dynamics is incoherent. Hence, a quantum rate description holds and the reasoning from the preceding paragraph applies again, except that the classical rates k_{cl} have to be replaced by their *quantum mechanical counterparts* k_{qm} to obtain

$$J_{\mathrm{qm}} = \frac{L}{2}(1 - e^{-\beta FL})(k_{\mathrm{qm},r}^+ - k_{\mathrm{qm},l}^-). \tag{6}$$

Qualitatively, each k_{qm} is governed by a competition between thermal activation up to a certain energy level and tunneling "through" the remaining part of the potential barrier. Quantitatively, a sophisticated line of reasoning has been elaborated during recent years [8] which we will briefly sketch in the following. Starting with the Hamiltonian system-plus-reservoir model (3) and adopting the "imaginary free energy method" [8,10] or, equivalently, the "multidimensional quantum transition state theory" [8,9], it is possible to express the escape rate k_{qm} in terms of functional path integrals. After integration over the bath modes and a steepest descent approximation, one obtains the semiclassical form

$$k_{\mathrm{qm}} = Ae^{-S_B/\hbar}. \tag{7}$$

Here, the exponentially dominating contribution S_B is defined via the nonlocal action

$$S[q] = \int_0^{\hbar\beta} d\tau\left[\frac{m\dot{q}^2}{2} + U(q) + \frac{\eta}{4\pi}\int_{-\infty}^{\infty} d\tau'\left(\frac{q - q'}{\tau - \tau'}\right)^2\right], \tag{8}$$

with the abbreviations $q = q(\tau)$, $q' = q(\tau')$, and omitting indices r, l, and $\pm$ as before. This action has to be extremized for paths $q(\tau)$ under the constraints that $q(\tau + \hbar\beta) = q(\tau)$ for all τ, and that there exists τ with $q(\tau) = x_b$. A trivial such extremizing $q(\tau)$ is always $q(\tau) \equiv x_b$. Among this and the possibly existing further extrema one selects the one that minimizes $S[q]$, say $q_B(\tau)$, to obtain $S_B \coloneqq S[q_B] - \hbar\beta U(x_0)$. The preexponential factor A in (7) accounts for fluctuations about the semiclassically dominating path $q_B(\tau)$.

Closer inspection shows that there exists a crossover temperature

$$T_c = \mu\hbar/2\pi k_B \tag{9}$$

above which $q_B(\tau) \equiv x_b$ is the only admissible extremum in (8), and therefore $S_B/\hbar = \beta\Delta U$. In view of (7) and (4) tunneling thus does not affect the exponentially leading part of the rate in this regime $T \geq T_c$. Moreover, a closed analytical expression for the prefactor A is available [8,10,11], yielding for the quantum rate the result

$$k_{\mathrm{qm}} = k_{\mathrm{cl}}(\lambda_1^0/\Lambda_1^b)\prod_{n=2}^{\infty}(\lambda_n^0/\lambda_n^b), \qquad T \geq T_c. \tag{10}$$

Here, we introduced

$$\lambda_n^{0,b} = m\nu_n^2 + \eta\nu_n + U_{0,b}'', \qquad \nu_n = 2\pi n/\hbar\beta, \tag{11}$$

$$\Lambda_1^b = \sqrt{\mathcal{L}/\pi\beta}\, e^{-\beta[\lambda_1^b]^2/\mathcal{L}}/\mathrm{erfc}\,(\lambda_1^b\sqrt{\beta/\mathcal{L}}), \tag{12}$$

$$\mathcal{L} = \frac{[U_b''']^2}{|U_b''|}\frac{4m\mu^2 + |U_b''|}{2m\mu^2 + |U_b''|} + \frac{d^4U(x_b)}{dx^4}, \qquad (13)$$

where $\mathrm{erfc}\,(z) = 2\pi^{-1/2}\int_z^\infty e^{-y^2}\,dy$ and $\mathcal{L} > 0$ in (13) has been tacitly assumed. The $\lambda_n^{0,b}$ are the eigenvalues of the action (8) when linearized about the "extremizing paths" $q(\tau) \equiv x_{0,b}$. Close to T_c one has $\lambda_1^b \simeq 0$. Accordingly, the quantity Λ_1^b is obtained by properly including also next to leading order contributions in the steepest descent approximation for A. In the classical limit $T \gg T_c$ all the factors multiplying k_{cl} on the right-hand side of (10) tend to unity, and thus $k_{\mathrm{qm}} \rightarrow k_{\mathrm{cl}}$ [see (5)].

Note that the two rates in the current (6) bring along *two* different crossover temperatures, say $T_c^{\max}$ and $T_c^{\min} < T_c^{\max}$, since $|U_b''|$ in (5) and thus μ in (9) are typically different for $U^\pm(x)$. Similarly, we denote the smaller of the two relevant potential barriers ΔU_r^+ and ΔU_l^- in (6) by $\Delta U^{\min}$.

For a numerical exemplification of our results we use T as control parameter and fix the remaining five model parameters $m,\ \eta,\ V_0,\ F$, and $l := L/2\pi$ in (1), (2), and (4). Without specifying a particular unit system this can be achieved by prescribing the following five dimensionless numbers: First we fix V_0, F, l and thus $U^\pm(x)$ through $Fl/V_0 = 0.2$, $\Delta U^{\min}/V_0 = 1.423$, and $|U_b''^{+}|l^2/V_0 = 1.330$ corresponding to the situation depicted in Fig. 1. Next we choose $\eta/m\Omega_0 = 1$ with $\Omega_0 := [V_0/l^2m]^{1/2}$, meaning a moderate damping as compared to inertia effects. To see this we notice that Ω_0 approximates rather well the true ground state frequency $\omega_0^+ := [U_0''^{+}/m]^{1/2}$ in the potential $U^+(x)$, $\omega_0^+ = 1.153\Omega_0$, and similarly for $U^-(x)$. In particular, $\eta/m\Omega_0 = 1$ strongly forbids deterministically running solutions. Finally, we set $\Delta U^{\min}/k_BT_c^{\max} = 10$ in order to remain in accordance with the weak noise assumption underlying (5) at least up to about $T = 2T_c^{\max}$, and at the same time to meet the semiclassical condition used in (7).

The classical current J_{cl} now readily follows with (5), approaching a straight line for small T in the Arrhenius plot Fig. 2. Its direction is governed by $\Delta U_l^- - \Delta U_r^+$ and is thus positive for our example (cf. Fig. 1). Figure 2 covers the quantum current in the crossover regime $T_c^{\max} \leq T \leq 2T_c^{\max}$ according to (6) and (10). We see that quantum corrections *enhance* the classical transport by more than a factor of 10 near crossover. They become negligible only beyond several $T_c^{\max}$.

For temperatures slightly below crossover the available approximations [10] for the rate (7) turned out as too inaccurate for our purposes. This gap in our data between roughly $T_c^{\max}$ and $T_c^{\min}$ is bridged by the dashes in Fig. 2. For even smaller $T < T_c$ analytical progress is possible only in a few special cases [8], and we have to resort to a numerical evaluation of the rate. We may remark that *only two* numerical studies have previously been available [10,12], both focusing on a cubic potential $U(x)$, and exploiting heavily its special properties. Our

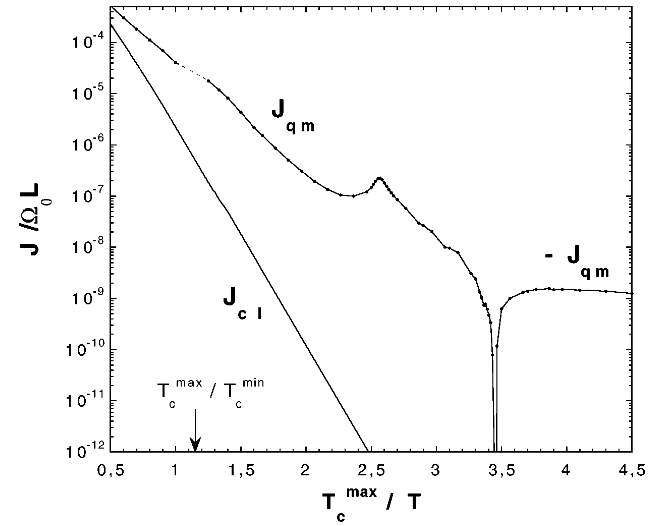

FIG. 2. The classical steady state current J_{cl} and its quantum mechanical counterpart J_{qm} for the ratchet potential from Fig. 1 in dimensionless units $J/\Omega_0 L$. Note the change of sign, the finite $T = 0$ limit, and the nonmonotonicity of J_{qm}. For more details, see main text.

novel numerical method is based on a truncated Fourier series ansatz for $q_B(\tau)$ of the form $\sum_{n=0}^{N} c_n \cos \nu_n\tau + \sum_{n=1}^{N-1} s_n \sin \nu_n\tau$ with the Matsubara frequencies ν_n from (11). This ansatz for the extremization of (8)—suggested by symmetry arguments and the required periodicity of $q_B(\tau)$—leads to a set of $2N$ coupled nonlinear equations for the Fourier coefficients c_n, s_n. The possibility of multiple saddle point solutions requires special care. Once $q_B(\tau)$ is determined, the action follows with (8) and the quantum prefactor A emerges as [8,10,11]

$$A = \left| \frac{\int_0^{\hbar\beta} \dot{q}_B^2(\tau)\,d\tau}{2\pi\hbar} \frac{\prod \lambda_{|n|}^0}{\prod' \lambda_n^B} \right|^{1/2}, \qquad (14)$$

with n running from $-\infty$ to ∞ in the products Π. Similarly as in (10), the λ_n^B here are the eigenvalues of the action (8) when linearized about $q_B(\tau)$. One of them is zero and has to be omitted in the primed product (14). By including sufficiently many Fourier coefficients c_n, s_n in $q_B(\tau)$ and sufficiently many eigenvalues λ_n^B in (14) the uncertainty margin of our numerical rates is at most a few percent for arbitrary $T \geq 0.1T_c$. For $T < 0.1T_c$ reliable extrapolations can be obtained by exploiting known asymptotical analytic results [8].

The quantum current J_{qm} as obtained by the above outlined numerical scheme is depicted for $T < T_c^{\min}$ in Fig. 2. The most remarkable feature is an *inversion* of the quantum current at low temperatures. Further, J_{qm} approaches a finite (negative) limit when $T \rightarrow 0$, implying a finite (positive) stopping force [3,6] also at $T = 0$. In contrast, the classical prediction J_{cl} remains positive but becomes arbitrarily small with decreasing T. A curious detail in Fig. 2 is the nonmonotonicity of J_{qm} around $T_c^{\max}/T \simeq 2.5$, caused via (6) by a similar resonancelike T dependence of the rate $k^{+}_{\mathrm{qm},r}$. While the corresponding action $S^{+}_{B,r}$ remains increasing with decreasing temperature, the prefactor A^{+}_{r} in (7) suddenly grows very fast—much in contrast to the cubic potential case [10]—and so gives rise to the anomalous, resonancelike temperature dependence of $k^{+}_{\mathrm{qm},r}$. A better understanding of this issue is the subject of ongoing work. We also studied other parameter values than those used in Fig. 2 as well as somewhat modified potentials (2). Basically, the same qualitative results are found except that the nonmonotonous temperature dependence disappears for sufficiently large $\Delta U^{\min}/k_B T_c^{\max}$ values.

To explain qualitatively the current reversal, we observe that in the limit $\eta \to 0$, $T \to 0$ (no heat bath), the action S_B from (8) goes over into the familiar Gamow formula

$$S_B \to S_G = 2\left|\int_{x_0}^{x_1} dq \sqrt{2m[U(q) - U(x_0)]}\right|, \qquad (15)$$

where x_1 denotes the first point beyond the potential barrier with $U(x_1) = U(x_0)$ (the absolute value is needed since $x_1 < x_0$ for the escape across ΔU_l^{-}). From (6) and (7) the direction of the quantum current is then governed by the difference $S^{-}_{G,l} - S^{+}_{G,r}$ between the corresponding Gamow actions. The negative sign of this difference is readily verified numerically. With $J_{\mathrm{qm}} \to J_{\mathrm{cl}} > 0$ for large T, the current inversion follows. In this heuristic argument we tacitly ignored the possible occurrence of deterministically running solutions in (1) for the considered small η values.

In conclusion, we have studied quantum Brownian motion in a ratchet potential when rocked by slowly varying, symmetric driving forces $f(t)$. Significant quantum corrections of the classically predicted particle current set in already well above the crossover temperature T_c, where tunneling processes are still rare. With decreasing temperature, quantum transport is greatly enhanced as compared to the classical adiabatic results [2(b),2(e)] and eventually even takes the opposite direction. Another remarkable consequence of the intriguing interplay between thermal noise and quantum tunneling is a finite current at $T = 0$, yielding a finite stopping force. Moreover, the quantum Brownian rectifier exhibits a "resonancelike" temperature dependence. All these novel features appear to be typical for a large class of quantum ratchet systems. Such effects clearly become of paramount importance for applications in mesoscopic systems at low temperatures. Note that T_c can reach values larger than 100 K in some physical and chemical systems [8], while it is in the mK region in Josephson systems [8,10].

The quantum-induced current reversal in slowly rocked ratchets may be used as a diagnostic tool to detect the role of quantum tunneling in a ratchet dynamics. Moreover, our dissipative quantum ratchet study implicitly reports on the behavior of one of the first ratchets with finite inertia [13]. Whether or not biological processes in ratchet systems in the deep quantum regime utilize the phenomenon of tunneling-induced directed motion remains to be explored.

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[1] M. von Smoluchowski, Phys. Z. **XIII**, 1069 (1912); R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley, Reading, MA, 1966), Vol. **I**, Chap. 46; J. M. R. Parrondo and P. Espanol, Am. J. Phys. **64**, 1125 (1996).

[2] (a) A. Ajdari and J. Prost, C. R. Acad. Sci. Paris **315**, 1635 (1992); (b) M. O. Magnasco, Phys. Rev. Lett. **71**, 1477 (1993); (c) R. D. Astumian and M. Bier, Phys. Rev. Lett. **72**, 1766 (1994); (d) C. R. Doering, W. Horsthemke, and J. Riordan, Phys. Rev. Lett. **72**, 2984 (1994); (e) R. Bartussek, P. Hänggi, and J. G. Kissner, Europhys. Lett. **28**, 459 (1994).

[3] For a review, see P. Hänggi and R. Bartussek, *Lecture Notes in Physics*, edited by J. Parisi *et al.* (Springer-Verlag, Berlin, 1996), Vol. **476**, pp. 294–308.

[4] J. Rousselet, L. Salome, A. Ajdari, and J. Prost, Nature (London) **370**, 446 (1994); L. P. Faucheux, L. S. Bourelieu, P. D. Kaplan, and A. J. Libchaber, Phys. Rev. Lett. **74**, 1504 (1995).

[5] R. D. Astumian and M. Bier, Biophys. J. **70**, 637 (1996).

[6] I. Zapata, R. Bartussek, F. Sols, and P. Hänggi, Phys. Rev. Lett. **77**, 2292 (1996).

[7] B. J. Keay *et al.*, Phys. Rev. Lett. **75**, 4098 (1995); **75**, 4102 (1995).

[8] For a review, see P. Hänggi, P. Talkner, and M. Borkovec, Rev. Mod. Phys. **62**, 251 (1990).

[9] P. Hänggi and W. Hontscha, J. Chem. Phys. **88**, 4094 (1988); E. Freidkin, P. S. Riseborough, and P. Hänggi, Z. Phys. B **64**, 237 (1986); **67**, 271(E) (1987).

[10] H. Grabert, P. Olschowski, and U. Weiss, Phys. Rev. B **36**, 1931 (1987).

[11] A. I. Larkin and Yu. N. Ovchinikov, Sov. Phys. JETP **59**, 420 (1984); H. Grabert and U. Weiss, Phys. Rev. Lett. **53**, 1787 (1984); P. S. Riseborough, P. Hänggi, and E. Freidkin, Phys. Rev. A **32**, 489 (1985).

[12] L. D. Chang and S. Chakravarty, Phys. Rev. B **29**, 130 (1984); **30**, 1566(E) (1984).

[13] P. Jung, J. G. Kissner, and P. Hänggi, Phys. Rev. Lett. **76**, 3436 (1996).