Dissipative quantum transport in a nanowire

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The coherence-to-decoherence transition is studied in a nanowire modeled as a one-dimensional tight-binding lattice in the presence of an external field and in linear interaction with a boson heat bath, characterized by Ohmic dissipation. The focus of attention is the probability propagator which quantifies the likelihood of a quantum particle, such as an electron to end up at an arbitrary site at a time t, given that it was at the origin initially—and from it—the particle-current and the mean-squared displacement. If the bath is absent, the probability operator exhibits quantum coherence as can be captured by say, Bloch oscillation and Wannier-Stark (dynamic) localization. The coupling with the bath—which can be weak or strong—leads to decoherence that will be quantified in the text. The Ohmic model of the spectral function of bath excitations contains a cutoff frequency, which if greater than the temperature (in energy units) defines the "low-temperature" regime, whereas the opposite limit implies "high temperatures." Results will be presented in both these regimes separately.

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I. INTRODUCTION

Recent years have witnessed an upsurge of interest in the physics of nanosystems not merely because of exciting possibilities in applications to quantum technology, but also for exploring nuances of quantum theory. Thus, toy models, such as two-state tunneling centers [1,2] and qubits [3] as well as a one-dimensional harmonic oscillator [4,5] and its variant of cyclotron motion [6], have found their realizations in nanodevices. However, the flip side of size reduction is that small systems are invariably in strong interaction with their quantum environment, even at low temperatures as was dealt with in the references above. Pure quantum evolution which is otherwise coherent is inevitably marred by decoherence—an impediment for protecting quantum information. Therefore, the interplay of coherence and decoherence has become an important area of activity in solid-state physics [1–4,7]. Not surprisingly, the earlier-mentioned textbook systems under the additional influence of quantum dissipation have attracted much interest in recent times [8–10].

Apart from the examples given above, one other system that has been amenable to analytical methods is a dissipative nanowire that can be treated as a one-dimensional tight-binding lattice (TBL). Although a many-site problem, a combination of Wannier (site) representation with Bloch (momentum-space) states—exploiting the periodicity of the underlying lattice—has enabled exact analysis of quantum coherent properties, such as Bloch oscillations—an electron once localized keeps periodically returning under the action of a static electric field to the original site—Wannier-Stark (dynamic) localization, and so on [11–13].

A tight-binding model in coupling with a heat bath finds relevance in several other physical situations, e.g., transfer of excitons in molecular crystals [14], Brownian rectifiers and motors [15–19], electron transport in an array of quantum dots [20], and in molecular wires [21]. Dissipation in a TBL has earlier been studied by us in terms of a set of site-specific classical stochastic forces governed by a telegraph [22] or a Gaussian process [23]. In a related review Kuzemsky studies electron transport in metallic systems (incorporating electron-phonon interactions) using generalized kinetic equations which were derived by the method of the nonequilibrium statistical operator [24]. In this paper we adopt a different and a fully microscopic quantum-mechanical approach in which the forces are viewed as bosonlike excitations, e.g., phonons [25]. The formulation is quite akin to that of Caldeira and Leggett [26] and Leggett [27], and a large number of workers following them [8,9] for treating dissipative tunneling. But, instead of just two sites of a tunneling center, we now have an infinitely large number of sites in a TBL, amongt which tunneling takes place. Such as in the earlier analysis, dissipation is viewed to occur because of a linear coupling between the site-occupancy operator $\hat{N}$ with boson creation and annihilation operators. Thus, in addition to a static field F_0 we have a quantum-mechanically fluctuating field-operator $\hat{F}$ (specified below), acting on $\hat{N}$.

As far as the method of calculation goes, we follow "relaxation" theory [28] that yields a quantum Liouville master equation (QLME) of a density operator as opposed to a functional integral approach of Refs. [26,27]. In particular, our scheme is close on the heels of Silbey and Harris [28], Zwerger [29] and Aslangul *et al.* [30] in which an equation for the reduced density operator is derived by eliminating the bath degrees of freedom.

A few remarks are in order at the outset in order to put into perspective the physical situation at hand. When the external force (F_0) and the heat bath are absent, the tight-binding Hamiltonian is diagonal in the Bloch (momentum) representation. A quantum particle then moves coherently

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in the lattice, such as a free particle with a quantum speed $v_{qu} \sim \Delta d(\hbar = 1)$. When F_0 is imposed on each lattice site the resultant coupling, whereas being diagonal in the Wannier representation, is, however, off-diagonal among the Bloch states. Given that the Bloch states are our basic representation the external field causes dephasing which is still a coherent quantum phenomenon. The result is an effective reduction in the quantum speed quantified by the dimensionless ratio Δ/dF_0, a factor which is reflected in all our expressions in the weak-damping region, underscoring the point that the tunneling and the static force are treated on the same footing.

Before we present the derivation it is pertinent to point out the hierarchy of energy scales in the problem: $\hbar\gamma,\ \Delta,\ dF_0,\ k_BT$, and $\hbar\omega_c$, where Δ is the tunneling energy, dF_0 is the external energy input, γ measures the quantum friction, T is the temperature, and ω_c denotes the cutoff for the frequency spectrum of the bath. In the weak-damping domain $\hbar\gamma \ll dF_0 \sim \Delta$ whereas for strong-damping $\hbar\gamma \ll dF_0 \sim \Delta$, keeping dF_0 fixed. The low-temperature case is defined by $k_BT < \hbar\omega_c$ whereas the opposite inequality characterizes "high temperatures."

The present paper is related with the directed transport of matter in periodic structures, or, more generally, a transmission of information out of unbiased fluctuations. This topical concept is known under labels, such as Brownian rectifiers [15] and Brownian motors [16] and is also applicable for the understanding of intercellular transport along biological polymer filaments. Apart from the biological relevance this concept is enormously fruitful also for the construction of nanoscale and microscale devices, such as pumps, rectifiers, and particle separators [17–19]. By use of a bottom-up approach, such motors have been synthesized even from single chiral molecules [20,21].

Given this background the paper is sectionwise divided as follows. In Sec. II, we present the model Hamiltonian H in a system-plus-bath approach in which H is split as a sum of H_S, H_{SB}, and H_B in which H_S describes the subsystem of the TBL, including F_0, H_{SB} the interaction term, and H_B comprises the bath Hamiltonian in terms of free bosons. As stated earlier, the starting point of our method is the expression for the reduced density operator ρ_s for the subsystem wherein the first term is simply the free flow under H_S, that describes coherent evolution. Our initial focus of attention, for both weak and strong dissipations, is the low-temperature domain $k_BT < \hbar\omega_c$ in which quantum effects are expected to be the most prominent. We first consider, in Sec. III, the case of weak dissipation in which H_{SB} is treated perturbatively. Because $\langle H_{SB}\rangle = 0$, by construction where $\langle\cdots\rangle$ denotes an average over the variables in H_B, the nontrivial contribution arises from the second-order term which, as expected, is given in terms of the correlation function of H_{SB}. The latter for a harmonic bath is known exactly [9]. With these second-order perturbation results in hand, we compute the probability $P_m(t)$ of finding the particle at site m at time t given that it had started from the origin and from $P_m(t)$, the particle current and the mean-squared displacement. In Sec. IV, we turn to the case of strong dissipation, which in contrast to Sec. III wherein tunneling is treated to all orders, presupposes tunneling to be small as the latter occurs as a prefactor in a "dressed" interaction Hamiltonian that exponentiates the original coupling via a unitary "polaron" transformation. Tacitly, therefore, the results of Sec. IV cater to the incoherent regime as opposed to Sec. III where weak coupling to the bath helps maintain the system near coherence. Incoherent tunneling is illustrated in this section by means of the particle current and the mean-squared displacement. The plotted results graphically illustrate the distinction between the coherent and the incoherent regimes. Section V is added to physically assess the results for the stationary current at high-temperatures ($k_BT > \hbar\omega_c$) in both the weak- and the strong-dissipation limits in the light of the much studied classical Drude-Kubo formula for the electrical conductivity [30]. We relegate tedious algebraic details to the Appendix. Our principal conclusions are summarized in Sec. VI.

II. MODEL AND METHOD

As a starting point we consider the model Hamiltonian for a charged particle moving on a linear chain of sites n $(-\infty < n < \infty)$ in contact with a bosonic reservoir under the action of a static electric-field $\mathcal{E}_0$ in the direction of the lattice with lattice constant d and of nearest-neighbor intersite overlap integrals $\frac{\Delta}{2}$. The Hamiltonian can be written as

$$\mathcal{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \tag{1}$$

where the subsystem, bath, and interaction Hamiltonians, respectively, are given by

$$\hat{H}_S = \hat{V}_+ + dF_0\hat{N}, \tag{2a}$$

$$\hat{H}_B = \sum_l \omega_l \hat{b}_l^\dagger \hat{b}_l, \tag{2b}$$

$$\hat{H}_{SB} = \hat{N}\sum_l g_l(\hat{b}_l + \hat{b}_l^\dagger) = \hat{N}\hat{F}, \tag{2c}$$

with $F_0 = q\mathcal{E}_0$, charge q, external electric-field $\mathcal{E}_0$, and interaction strength g_l. For the convenience of our calculation we consider the following operators [22,23]:

$$\hat{K} = \sum_{n=-\infty}^{\infty} |n\rangle\langle n+1|, \quad \hat{K}^\dagger = \sum_{n=-\infty}^{\infty} |n+1\rangle\langle n|,$$
$$\hat{N} = \sum_{-\infty}^{\infty} n|n\rangle\langle n|, \quad \hat{V}_+ = -\frac{\Delta}{2}(\hat{K} + \hat{K}^\dagger). \tag{3}$$

In the above equation $|n\rangle$ represents a Wannier state localized on lattice site n and natural units are used ($\hbar = k_B = 1$). These operators also follow the following commutation rules [22,23]:

$$[\hat{K}, \hat{K}^\dagger] = 0; \quad [\hat{K}, \hat{N}] = \hat{K}; \quad [\hat{N}, \hat{K}^\dagger] = \hat{K}^\dagger. \tag{4}$$

Now, our discussion mainly follows the work of Kubo [31,32], van Kampen [33], and Dattagupta and Puri [9] on the QLME. The reduced density operator in the interaction picture obeys the master equation (cf., Eq. (I. A. 37) of Ref. [9]),

$$\tilde{\hat{\rho}}_s(t) = \tilde{\hat{\rho}}_s(0) - \int_0^t dt' \int_0^{t'} d\tau \{\xi^*(\tau)[\hat{N}(t'), \hat{N}(t'-\tau)\tilde{\hat{\rho}}_s(t'-\tau)]$$
$$-\xi(\tau)[\hat{N}(t'), \tilde{\hat{\rho}}_s(t'-\tau)\hat{N}(t'-\tau)]\}. \tag{5}$$

where,

$$\tilde{\hat{\rho}}_s(t) = \hat{U}(t)\hat{\rho}_s(t)\hat{U}^\dagger(t), \quad \hat{U}(t) = \exp(i\hat{H}_S t), \tag{6a}$$

$$\tilde{\hat{\rho}}_s(0) = \hat{\rho}_s(0), \tag{6b}$$

$$\hat{\rho}_s(t) = \mathrm{Tr}_B[\hat{\rho}(t)], \tag{6c}$$

$$\hat{N}(t) = \hat{U}(t)\hat{N}(0)\hat{U}^\dagger(t), \tag{6d}$$

$$\xi(t) = \langle \hat{F}(0)\hat{F}(t)\rangle = \int_0^\infty d\omega\, J(\omega)\left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega t) + i\sin(\omega t)\right], \tag{6e}$$

where $J(\omega)$ is the spectral density of the bath and it can be related with the interaction strength as follows $J(\omega) = \frac{\pi}{2}\sum_l \frac{g_l^2}{\omega_l}\delta(\omega - \omega_l)$. All the dependencies on the bath is now encapsulated within the spectral density $J(\omega)$.

III. WEAK DISSIPATION AT LOW TEMPERATURES

The second-order perturbation theory, appropriate for weak dissipation, ensues by replacing $\tilde{\hat{\rho}}_s(t)$ in the integrand of Eq. (5) by the zeroth-order first term, namely, $\tilde{\hat{\rho}}_s(0) = \hat{\rho}_s(0)$, which will be denoted as $\hat{\rho}(0)$, henceforth, for brevity. Accordingly, the reduced density operator in this approximation can be rewritten as

$$\tilde{\hat{\rho}}_s(t) \simeq \hat{\rho}(0) - \int_0^t dt' \int_0^{t'} d\tau \{\xi^*(\tau)[\hat{N}(t'), \hat{N}(t'-\tau)\hat{\rho}(0)] - \xi(\tau)[\hat{N}(t'), \hat{\rho}(0)\hat{N}(t'-\tau)]\}. \tag{7}$$

Our principal concern is to derive an explicit expression for the probability propagator $P_m(t)$. In the Wannier space, utilizing Eq. (7), we can identify different order (in order of coupling strength) terms of the probability propagator.

(1) Zeroth order.

The zeroth-order term of the probability propagator $P_m^{(0)}(t)$ is given by

$$P_m^{(0)}(t) = \langle m|e^{-iF_0 dt\,\hat{N}} \exp\left[-i\int_0^t \tilde{\hat{V}}_+(t')dt'\right]\hat{\rho}(0) \times \exp\left[i\int_0^t \tilde{\hat{V}}_+(t')dt'\right] e^{iF_0 dt\,\hat{N}}|m\rangle, \tag{8}$$

where the interaction picture operator $\tilde{\hat{V}}_+(t) = \hat{K}e^{-itF_0 d} +$ H.C.. In the above expression no time ordering is required as $[\hat{K}, \hat{K}^\dagger] = 0$ and the F_0 related term from left and right in Eq. (8) will cancel out (since they are diagonal in the Wannier basis). Considering $\hat{\rho}(0) = |0\rangle\langle 0|$ and going into Bloch representation, we can show [11]

$$P_m^{(0)}(t) = J_m^2\left(\frac{\Delta}{F_0 d}\sqrt{u^2(t) + v^2(t)}\right), \tag{9}$$

with $u(t) = \sin(dF_0 t)$ and $v(t) = [1 - \cos(dF_0 t)]$. The probability propagator at the zeroth order is an oscillatory function of time, known as (coherent) Bloch oscillations. It implies the particle will return back to its initial position repeatedly, i.e., it exhibits Wannier-Stark localization.

Because $\langle \hat{F}\rangle_B = 0$, the first-order term of the probability propagator $P_m^{(1)}(t) = 0$. Thus, we move to the derivation of second-order term of the probability propagator $P_m^{(2)}(t)$.

(2) Second order.

$P_m^{(2)}(t)$ is given by the mth diagonal matrix element of the second term on the right of Eq. (7). That equation contains an operator $G(t)$ defined by

$$\hat{G}(t) = \hat{U}^\dagger(t)\{\xi^*(\tau)[\hat{N}(t'), \hat{N}(t'-\tau)\hat{\rho}(0)] - \xi(\tau)[\hat{N}(t'), \hat{\rho}(0)\hat{N}(t'-\tau)]\}\hat{U}(t). \tag{10}$$

Substituting in Eq. (10), employing Eq. (6) and using the Bloch representation, we have

$$P_m^{(2)}(t) = -\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dk' e^{[im(k-k')]} \times \int_0^t dt' \int_0^{t'} d\tau\, \exp\left[-i\int_0^{(t-t')} dt'' \hat{V}_+^{kk'}(t'')\right] \times (I_1 - I_2 - I_3 + I_4), \tag{11}$$

where

$$I_j(t', \tau) = \langle k|G_j(t', \tau)|k'\rangle, \quad j = 1\text{–}4, \tag{12}$$

and

$$\hat{V}_+^{kk'}(t) = \langle k|\tilde{\hat{V}}_+(t)|k\rangle - \langle k'|\tilde{\hat{V}}_+(t)|k'\rangle = -\Delta[\cos(F_0 dt)(\cos k - \cos k') + \sin(F_0 dt)(\sin k - \sin k')]. \tag{13}$$

Finally, after some tedious algebra (details given in Appendix A), we obtain the second-order term of the probability propagator which is given in Eq. (A28).

At this stage we specify the Ohmic model for the spectral function at low temperatures where it is convenient to use an exponential cutoff [30],

$$J(\omega) = \gamma\omega\,\exp(-\omega/\omega_c), \tag{14}$$

γ parametrizing the damping. The low-temperature limit $\coth(\frac{\beta\omega}{2}) \sim 1$ enables us to employ in Eq. (A28) the approximate expressions,

$$\xi^*(t) + \xi(t) = 4\gamma\int_0^\infty d\omega\,\omega e^{-(\omega/\omega_c)}\cos(\omega t) = \frac{4\gamma[1 - (\omega_c t)^2]}{[1 + (\omega_c t)^2]^2},$$

$$\frac{\xi^*(t) - \xi(t)}{i} = 4\gamma\int_0^\infty d\omega\,\omega e^{-(\omega/\omega_c)}\sin(\omega t) = \frac{8\gamma\omega_c t}{[1 + (\omega_c t)^2]^2}. \tag{15}$$

We use the real and imaginary parts of the bath correlation function in order to calculate the second-order contribution to the mean-squared displacement as in Eqs. (17) and (19) below.

A. Current for weak dissipation at low *T*

The issue of current is of importance in Brownian rectifiers [15] and Brownian motors, which apart from intercellular

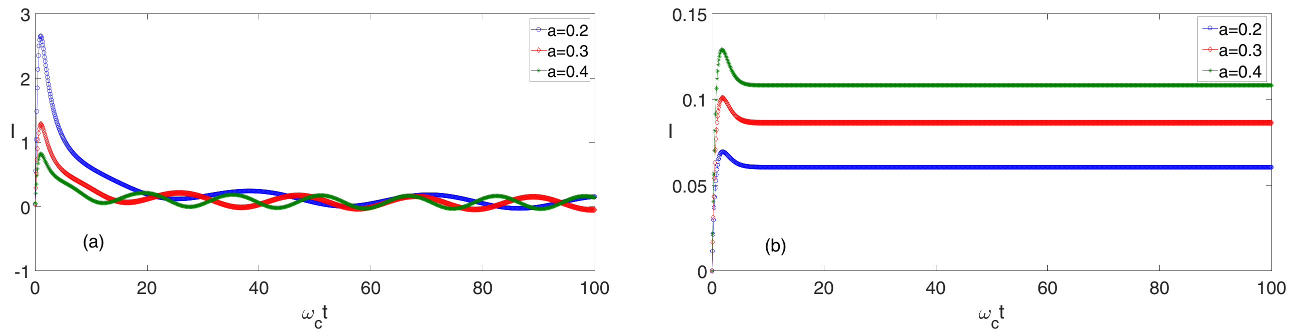

FIG. 1. Plot of current as a function of dimensionless time $\omega_c t$ for three different external bias fields $a = \frac{F_0 d}{\omega_c}$ (electric field) for the weak dissipative regime at (a) low temperatures and (b) at high temperatures. For the plotting purpose, we use $d = \frac{\Delta}{2F_0 d} = 1.0$, $\frac{\gamma}{\omega_c} = 0.005$. Furthermore, we consider $\beta\omega_c = 1.5$ for low temperatures and $\beta\omega_c = 0.05$ for high temperatures. The stationary state current for $a = 0.2,\ 0.3$, and 0.4 are 0.06, 0.09, and 0.11.

transport in biological polymer filaments, are also relevant in nanoscale devices, e.g., pumps and particle rectifiers [16–19]. It is defined by

$$I = q\frac{d\langle\hat{N}(t)\rangle}{dt}. \tag{16}$$

It is evident from the properties of the Bessel functions in Eq. (9) that the zeroth-order current vanishes, implying that there is no current in the purely coherent regime. Thus, we move to the second-order calculation of mean displacement (details can be found in Appendix C),

$$\begin{aligned}\langle\hat{N}_2(t)\rangle &= \sum_{m=-\infty}^{\infty} mP_m^{(2)}(t)\\ &= \left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, W(t',\tau)\left[\frac{\xi^*(\tau)-\xi(\tau)}{i}\right.\\ &\quad \left.\times(z_6+z_7)+[\xi^*(\tau)+\xi(\tau)](z_5+z_4)\right],\end{aligned} \tag{17}$$

The stationary state current is obtained by taking the $t \to \infty$ limit of Eq. (C2). Thus,

$$I_{st} = 2q\pi\gamma\left(\frac{\Delta}{2F_0 d}\right)a\,\sinh(a), \tag{18}$$

where $a = \frac{F_0 d}{\omega_c}$. In Fig. 1, we plot the current as a function of dimensionless time for three different field strengths at low temperatures. Although, the weak dissipation contributes a fluctuating component of current there is a steady oscillation. However, the amplitude as well as the undulation of oscillations discerningly decrease with the growing strength of a implying that the on-site force causes Bloch oscillation. Furthermore, we observe multiple pronounced maxima and minima of current at this weak dissipation at low temperatures. Besides the temporal behavior of current at high temperatures demonstrates a pronounced maxima, but the amplitude of current is much smaller than that of the low-temperature case. In contrast to the low-temperature case, the increase in field helps to delocalize the particle at high temperatures.

B. Mean-squared displacement for weak dissipation at low *T*

The core issue of this subsection is the mean-squared displacement which is defined as follows:

$$S(t) = d^2[\langle\hat{N}^2(t)\rangle - \langle\hat{N}(t)\rangle^2]. \tag{19}$$

The zeroth-order contribution has already been calculated by Dunlap and Kenkre [11] and can be written as

$$S^{(0)}(t) = 2d^2\left(\frac{\Delta}{F_0 d}\right)^2 \sin^2(dF_0 t/2), \tag{20}$$

which once again demonstrates the occurrence of Bloch oscillations in the coherent regime. The effect of weak damping can now be analyzed by considering the second-order probability with the aid of the spectral function at low temperatures as earlier and is given in Eqs. (C1) and (C3): $S(x) = d^2[\langle\hat{N}^2(x)\rangle - \langle\hat{N}(x)\rangle^2]$) of Appendix C. The result is plotted in Fig. 2 that shows an oscillatory behavior viz., Wannier-Stark localization. Weak dissipation, i.e., mild decoherence barely alters the behavior at low temperatures. Again we find quite contrasting behavior (at two different temperature regimes) of MSD of the particle as we increase dimensionless field parameter a. At low temperatures MSD decreases as we increase the parameter a whereas opposite characteristics can be found at high temperatures. But the order of magnitude of MSD is much lower at high temperatures compared to the low-temperature regime.

In the present paper, one of the main aims is to obtain a directed transport of matter or, more generally, a transformation of information out of unbiased fluctuations in a periodic structure. The stationary state current vanishes in the absence of quantum dissipation. However, as a result of a ratchetlike mechanism, a finite current occurs when quantum equilibrium fluctuations interplay with noise [34,35]. To obtain such a Brownian rectifier, such as behavior in periodic structures, the following two conditions are satisfied (i) periodic structure breaks reflection symmetry and (ii) the system must operate far from equilibrium which is implemented by the application of an external dc field. Finally, the use of dissipation is the most natural way to break time-reversal invariance; such a violation presents a necessary element to induce directed current. Thus, one can say that the simplest way to obtain a finite directed current in periodic structure is by the combined use

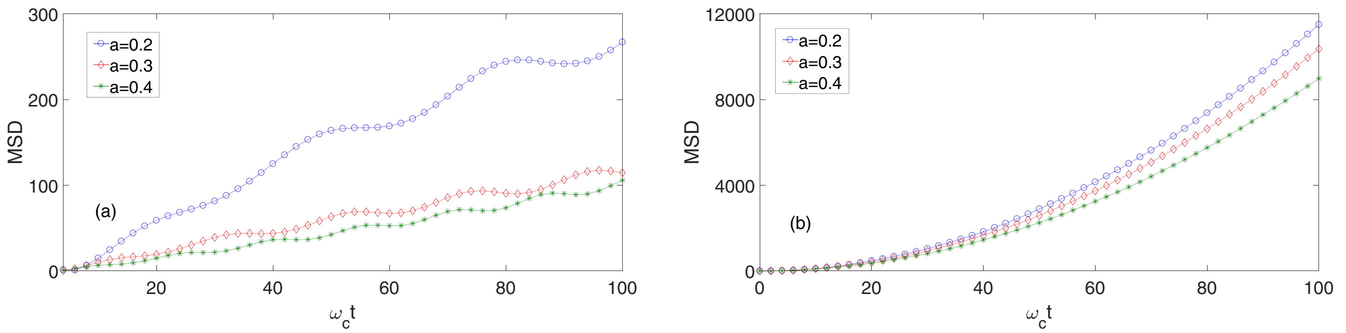

FIG. 2. Plot of the mean-squared displacement (MSD) as a function of dimensionless time $\omega_c t$ for three different external bias fields (electric field) at (a) high temperatures and (b) low temperatures. We also use $\frac{\Delta}{2F_0 d} = 1.0$ and $\frac{\gamma}{\omega_c} = 0.005$. Furthermore, we consider $\beta\omega_c = 1.5$ for low temperatures and $\beta\omega_c = 0.05$ for high temperatures.

of both dissipation and nonequilibrium asymmetric driving forces. Although dissipation breaks time-reversal symmetry in an obvious way thereby breaking also detailed balance symmetry, it is not sufficient to yield finite transport. The key additional element is a source of dynamical asymmetry introduced by an external dc field.

Before concluding this section, we can infer our results on the temporal behavior of current (I) and MSD for the weak dissipative regime in the context of coherence-to-decoherence transition. The oscillatory behavior of current at very low temperatures clearly indicates Bloch oscillation of the particle which is completely quantum and coherent phenomena. As we move to the high temperatures the oscillation dies down and clearly indicates a transition from coherence-to-decoherence regime. Furthermore, the coherent motion of the charged particle in the weak dissipative regime as depicted in the probability propagator Eq. (A28) reflects in the temporal behavior of MSD: $S(t) \propto t^2$. This kind of dependence $S(t) \propto t^2$ is also observed in the context of coherent motion of exciton transfer in molecular crystals [14,36,37].

IV. STRONG DISSIPATION AT LOW TEMPERATURES

In Sec. III we dealt with weak dissipation, that is, we restricted our analysis to a small deviation from quantum coherence. Here we turn attention to the opposite limit of strong coupling with the bath which renders tunneling to be incoherent. Examples in which the system-bath interaction is comparable to the system's energy terms abound in quantum dots [38,39], photosynthetic complexes [40–42], and certain nanostructures [43–45]. Several nonperturbative numerical techniques have been developed, such as in the hierarchy master equations [46,47], the quasiadiabatic propagator approaches [48], the density matrix renormalization group [49], the numerical renormalization group [50], the multiconfiguration time-dependent Hartree method [51,52], stochastic path integrals [53,54], etc. However, all these techniques are computationally challenging and difficult to implement for large systems. Hence, we need methods that are straightforward, physically transparent and easy to execute.

Given this motivation we resort to a modified polaron transformation which exponentiates the original coupling and, therefore, any perturbation treatment of the new interaction Hamiltonian, would automatically incorporate the coupling to all orders, albeit the tunneling that occurs as a prefactor in the transformed coupling, is effectively taken to be small [36,55]. For this reason, the underlying scheme is dubbed the noninteracting blip approximation (NIBA) [56]. The latter has been shown to be equivalent to relaxation treatments [2,9].

The modified polaron transformation is defined by the unitary operator,

$$\hat{S}(t) = \exp\left[\hat{N}\left\{i\,dF_0 t - \frac{g_l}{\omega_l}(\hat{b}_l - \hat{b}_l^\dagger)\right\}\right], \tag{21}$$

which transforms the Hamiltonian in Eq. (1) to a time-dependent form

$$\hat{H}'(t) = \frac{\Delta}{2}[\hat{K}\hat{B}_+ \exp(-i\,dF_0 t) + \text{H.c.}] + \chi\hat{N}^2 + \hat{H}_B. \tag{22}$$

Thus, comparing with the decomposition in Eq. (2), the system Hamiltonian and the interaction term now have new forms

$$\hat{H}_S = \chi\hat{N}^2, \quad \hat{H}_{SB} = \frac{\Delta}{2}[\hat{K}\hat{B}_+ \exp(-idF_0 t) + \text{H.c.}], \tag{23}$$

with $\chi = \sum_l \frac{g_l^2}{\omega_l}$ and $\hat{B}_\pm = \exp[\pm\sum_l \frac{g_l}{\omega_l}(\hat{b}_l - \hat{b}_l^\dagger)]$.

At this stage it is pertinent to point out a couple of important differences between our method here and earlier applications of NIBA [2,9,30]: The effect of the external static force F_0 is incorporated (in the interaction picture) within the modified time-dependent polaron transformation and, hence, is exactly accounted for; (b) the employed master equation for the reduced density operator [56], uses the "time-convolution" form [57] as opposed to the "convolutionless" form [30,58]. The differences show up in the mean-squared displacement as indicated in the text below.

With this proviso the Eq. (I. A. 37) of Ref. [9] can be adapted to

$$\begin{aligned}\frac{d\hat{\rho}_s(t)}{dt} &= -i[\hat{H}_s, \hat{\rho}_s(t)] - 2\int_0^t d\tau\,\text{Re}[\phi(\tau)]\cos(F_0 d\tau)\\ &\quad\times\{2\hat{\rho}_s(t-\tau) - [\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K} + \hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]\}\\ &\quad - 2\int_0^t d\tau\,\text{Im}[\phi(\tau)]\sin(F_0 d\tau)[\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K}\\ &\quad - \hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger].\end{aligned} \tag{24}$$

Now, the bath correlation function, in view of the dressed interaction Hamiltonian takes a form distinct from $\xi(t)$ of the weak-dissipation case and can be written as [2,9]

$$\Phi(t) = \frac{\Delta^2}{4} \exp\left[-\int_0^\infty d\omega \frac{J(\omega)}{\omega}\left\{\coth\left(\frac{\beta\omega}{2}\right)[1 - \cos(\omega t)] - i\sin(\omega t)\right\}\right]. \quad (25)$$

A. Current for strong dissipation at low *T*

Using the definition of the current given in Eq. (22) and some algebra involving the commutation properties of the operators $\hat{K}$, $\hat{K}^\dagger$, and $\hat{N}$, we can show

$$I(t) = -q\,d\,\Delta^2 \int_0^t d\tau\, \mathrm{Im}[\phi(\tau)]\sin(F_0 d\tau). \quad (26)$$

It may be stressed again that Eq. (26) is a perturbative result in which the tunneling has been treated to second order. One can easily verify that the right-hand side of Eq. (26) vanishes for either $F_0 = 0$ or in the limit of vanishing coupling (i.e., $g_l = 0$) as expected physically. It is to be noted that Eq. (26) is identical with Aslangul *et al.* (Eq. (18) of Ref. [30]), if we can identify $\mathrm{Im}[\Phi(\tau)] = \exp[-A_2(\tau)\sin[A_1(\tau)]]$ and $F_0 = \epsilon$, although the results start to deviate from the second moment of $P_m(t)$ onwards, as mentioned earlier.

In the low-temperature regime along with the long-time limit $\omega_c t \gg 1$, one can find

$$A_1(t) = \mathrm{Im}[\ln\phi(t)] = 2\gamma\,\tan^{-1}(\omega_c t) \simeq \pi\gamma\,\mathrm{sgn}(t),$$
$$A_2(t) = \mathrm{Re}[\ln\phi(t)] \simeq 2\gamma\,\ln\left[\omega_c\tilde{\tau}\sinh\left(\frac{\pi t}{\beta}\right)\right]. \quad (27)$$

Employing this low-temperature form of the spectral density [as in Eq. (27)] we can show [30]

$$I(t) = q\,d\,\Delta_{\mathrm{eff}}^2 \int_0^t d\tau\,\sin(F_0 d\tau) \times \exp\left[-2\gamma\,\ln\left(\frac{\omega_c\beta}{\pi}\right)\sinh\left(\frac{\pi\tau}{\beta}\right)\right], \quad (28)$$

with $\Delta_{\mathrm{eff}}^2 = \Delta^2\sin(\pi\gamma)$. It is instructive to examine at $T = 0$ the closed-form expressions for the stationary ($t \to \infty$) current for $\gamma < 1/2$,

$$I_{st} = q\,d\,\Delta_{\mathrm{eff}}^2 \frac{\sin[\pi(1-2\gamma)/2]\Gamma(1-2\gamma)}{\omega_c^{2\gamma}(F_0 d)^{1-2\gamma}}. \quad (29)$$

On the other hand, for $\gamma = 1/2$, we obtain the stationary current,

$$I_{st} = \frac{q\,d\,\Delta_{\mathrm{eff}}^2\pi}{2\omega_c}\mathrm{sgn}(F_0 d). \quad (30)$$

The behavior of the current as a function of time ($x = \omega_c t$) at zero temperature is shown in Fig. 3 . It is interesting to note that the current is more or less insensitive to the noise strength γ. This is in contrast to the high-temperature characteristic, akin to the classical situation as will be demonstrated in Sec. V below. On the other hand, the temporal behavior of stationary current at high temperatures for three different external fields is shown in Fig. 4(a). Furthermore, one may note that the current is sensitive to the external field at low temperatures as well as at the high-temperature regime.

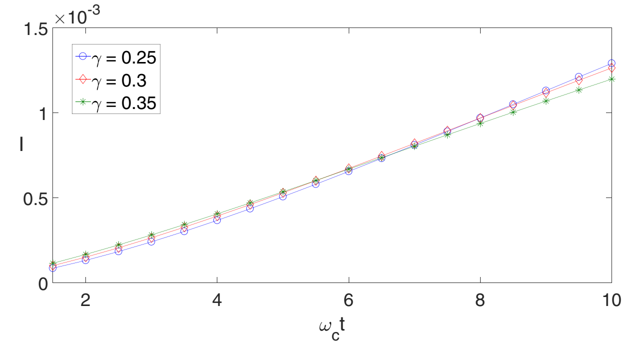

FIG. 3. Plot of current as a function of dimensionless time $x = \omega_c t$ at long times for three different noise strengths at zero temperature. For the plotting purpose we use $F_0 = 0.1$, $\Delta = 0.1$, $d = 1.0$, $\omega_c = 1$, $T = 1.5$.

B. Mean-squared displacement for strong dissipation at low *T*

The mean-squared displacement is defined in Eq. (19). In order to calculate this from the master equation (24) we employ the commutation relations among $\hat{K}$, $\hat{K}^\dagger$, and $\hat{N}$ and the cyclic property of the trace to obtain the following equalities:

$$\mathrm{Tr}_s[(\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K})\hat{N}^2] = \langle\hat{N}^2(t-\tau)\rangle + 2\langle\hat{N}(t-\tau)\rangle + 1,$$
$$\mathrm{Tr}_s\{[\hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]\hat{N}^2\} = \langle\hat{N}^2(t-\tau)\rangle - 2\langle\hat{N}(t-\tau)\rangle + 1. \quad (31)$$

As before we follow Ref. [30] for evaluating the correlation function $\Phi(t)$ at low temperatures ($k_B T < \hbar\omega_c$) to arrive at $S(t)$, which differs from the one in Ref. [30] for reasons of employing the time-convolution master equation as alluded to above (for details see Appendix D). Here we simply quote the analytically derivable result for $\gamma = 1/2$ in the long-time region ($\omega_c t \gg 1$) which exhibits the expected diffusive behavior,

$$S(t) = 2Dt, \quad (32)$$

with $D = \frac{(\pi\Delta)^2}{(\omega_c\beta)^2}\ln[\mathrm{sech}(\frac{F_0 d\beta}{2})]$. The temporal behavior of MSD is plotted in Fig. 5 which demonstrates the diffusive behavior at low temperatures. The low-*T* behavior is not sensitive to the change in the external field. The high-temperature behavior is quite sensitive to the change in the external field, and it also shows a diffusive kind of behavior.

Unlike the weak-dissipative regime, the absence of oscillatory nature in the temporal behavior of the current and MSD in the strong-dissipative system clearly indicates a transition from coherent-to-incoherent motion as we increase the dissipation. Furthermore, the diffusive nature of MSD $S(t) \propto t$ [Eq. (32)] confirms Brownian-like motion of the particle.

V. DRUDE-KUBO FORMULA

The Kubo formula for the electrical conductivity (or for that matter, for any transport property) is a cornerstone of nonequilibrium statistical mechanics and irreversible processes. It relates the steady-state response of a charge particle system to an applied electric field in terms of a time integral

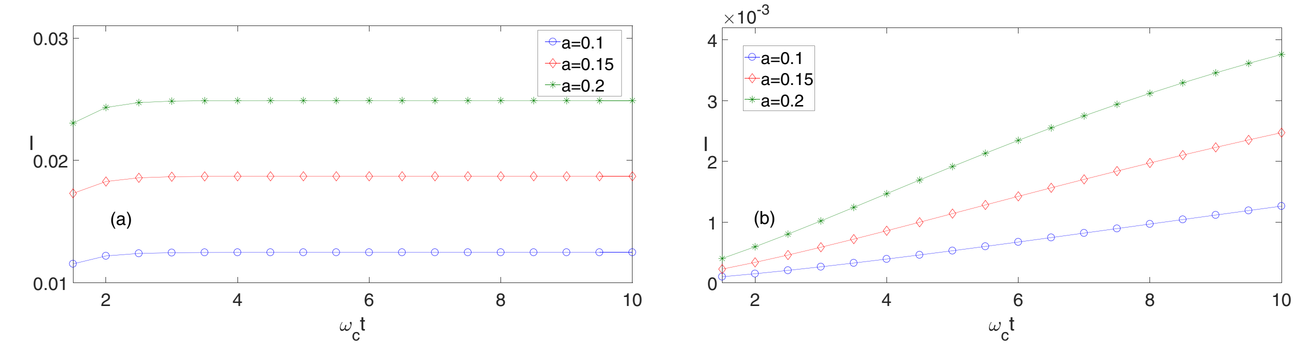

FIG. 4. Plot of the current as a function of dimensionless time $\omega_c t$ for three different external bias fields $a = \frac{F_0 d}{\omega_c}$ (electric field) for the strong dissipative regime at (a) high temperatures and (b) at low temperatures. For the plotting purpose we use $d = \frac{\Delta}{2F_0 d} = 1.0,\ \frac{\gamma}{\omega_c} = 0.5$. Furthermore, we consider $\beta\omega_c = 1.5$ for low temperatures and $\beta\omega_c = 0.05$ for high temperatures. At high temperatures, the stationary current magnitudes are 0.012, 0.018, and 0.025 for $a = 0.1, 0.15,$ and 0.2, respectively.

of the velocity-correlation function in equilibrium in terms of the conductivity σ [59],

$$\sigma = n\beta q^2 \int_0^\infty dt \langle \hat{v}(0)\hat{v}(t)\rangle_0, \tag{33}$$

where n is the number density of charges and $\hat{v}$ is the velocity operator for a quantum system. Here the subscript 0 emphasizes that the fluctuations belong to a system in thermal equilibrium. In writing Eq. (33) we have tacitly used the high-temperature limit in which $\hbar\beta \sim 0$. Note that in the completely classical case of, e.g., Brownian motion [10], the velocity correlation is governed by a single relaxation rate, say λ, in which case,

$$\langle \hat{v}(0)\hat{v}(t)\rangle_0 = \langle \hat{v}^2(0)\rangle \exp[-\lambda t]. \tag{34}$$

Substituting Eq. (34) into Eq. (33) and employing the standard equipartition theorem result for the mean-squared velocity in thermal equilibrium, we retrieve the celebrated Drude formula,

$$\sigma = nq^2/m\lambda. \tag{35}$$

In our case, $\hat{v}$ is an operator, defined by the equation of motion,

$$\hat{v}(t) = d\frac{d\hat{N}(t)}{dt} = id[\hat{H}(t), \hat{N}] = -id\frac{\Delta}{2}[\hat{K}(t) - \hat{K}^\dagger(t)]. \tag{36}$$

In the rotated frame under the unitary transformations, the velocity operator becomes

$$\hat{v}(t) = -i\,d\Delta[\hat{K}\hat{B}_+(t)\exp(-iF_0 dt) - \hat{K}^\dagger\hat{B}_-(t)\exp(iF_0 dt)]. \tag{37}$$

From Eq. (33), then,

$$\sigma = n\beta\left(\frac{q\,d\Delta}{2}\right)^2 \int_0^\infty dt[\langle \hat{B}_+(0)\hat{B}_-(t)\rangle e^{iF_0 dt} + \text{H.c.}], \tag{38}$$

where we have used the fact that $\hat{K}^\dagger\hat{K} = \hat{K}\hat{K}^\dagger = I$ and $\langle \hat{B}_+(0)\hat{B}_+(t)\rangle = \langle \hat{B}_-(0)\hat{B}_-(t)\rangle = 0$ in the Ohmic dissipation model.

In order to make contact with the high-temperature results for the steady-state current, we will have to transcribe

$$I_{st} = \frac{F_0}{qnd}\sigma, \tag{39}$$

and use for the bath correlations the classical-like expressions,

$$\langle \hat{B}_-(0)\hat{B}_+(t)\rangle = \langle \hat{B}_+(0)\hat{B}_-(t)\rangle = \exp(-\lambda t). \tag{40}$$

We then have from Eqs. (38)– (40),

$$I_{st} = \frac{q\beta\,dF_0\Delta^2}{2}\frac{\lambda}{[\lambda^2 + (dF_0)^2]}. \tag{41}$$

This result can be identified with high-temperature results, and this can be shown as below.

(3) High temperature and weak dissipation.

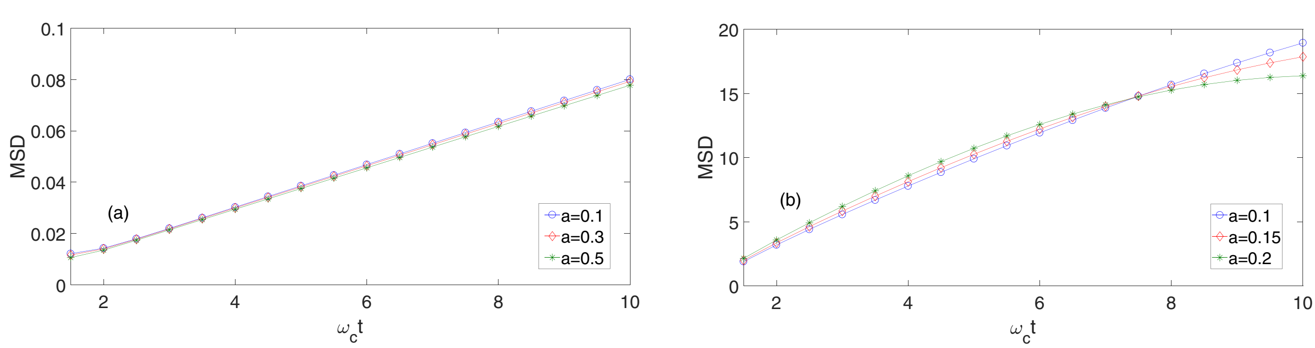

FIG. 5. Plot of MSD as a function of dimensionless time $\omega_c t$ for three different external bias fields (electric field) for the strong dissipative regime at (a) high temperatures and (b) at low temperatures. We also use $\frac{\Delta}{2F_0 d} = 1.0$ and $\frac{\gamma}{\omega_c} = 0.5$. Furthermore, we consider $\beta\omega_c = 1.5$ for low temperatures and $\beta\omega_c = 0.05$ for high temperatures.

At high temperatures, we have

$$\xi(\tau)+\xi^*(\tau)=\frac{4\pi\gamma}{\beta\omega_c}e^{-\omega_c\tau},\quad \xi(\tau)-\xi^*(\tau)=2i\gamma\pi e^{-\omega_c\tau}. \tag{42}$$

Now, utilizing these relations for the bath spectrum in Eq. (17) and performing a double integral one can obtain mean displacement which is explicitly shown in Appendix C [Eq. (C4)]. After taking the time derivative of it and then multiplying by charge q, one can obtain the expression of the current. Finally taking the long-time limit of it one can obtain the steady-state current at weak dissipation and high temperatures,

$$I_{st}^{\text{weak}}=\frac{q\pi\gamma}{\beta}\left(\frac{\Delta}{2F_0d}\right)\frac{(F_0d)}{\left[\omega_c^2+(F_0d)^2\right]}. \tag{43}$$

(4) High temperature and strong dissipation.

Although, we are in the high-temperature regime, i.e., $T\gg\omega_c$, we are well below the Kramers region. Using the Lorentzian cutoff function, one can obtain [60]

$$\text{Im}[\ln\phi(t)]=A_1(t)=\pi\gamma[1-e^{-\omega_c t}],$$
$$\text{Re}[\ln\phi(t)]=A_2(t)\simeq\frac{2\gamma\pi}{\omega_c\beta}[\omega_c t+e^{-\omega_c t}-1], \tag{44}$$

where γ is the dissipation parameter. In the long-time limit $\omega_c t\gg 1$, one can approximate

$$A_1(t)\simeq\pi\gamma,\quad A_2(t)\simeq\frac{2\gamma\pi}{\beta}t. \tag{45}$$

Hence, we derive the particle current,

$$\begin{aligned}I(t)&=q\,d\Delta_{\text{eff}}^2\int_0^t d\tau\ \sin(F_0d\tau)\exp\left(-2\gamma\frac{\pi\tau}{\beta}\right)\\&=\frac{1}{2}\frac{qF_0d\beta\Delta_{\text{eff}}^2}{\pi}\left[\frac{2\gamma\pi/\beta}{(F_0d)^2+\left(\frac{2\gamma\pi}{\beta}\right)^2}\right.\\&\quad\left.-\frac{e^{-(2\gamma\pi t/\beta)}[(2\gamma\pi/\beta)\sin(F_0dt)+F_0d\ \cos(F_0dt)]}{(F_0d)^2+(2\gamma\pi/\beta)^2}\right],\end{aligned} \tag{46}$$

where $\Delta_{\text{eff}}^2=\Delta^2\sin(\pi\gamma)$. One may evaluate the stationary state current from Eq. (46) by taking long-time limit $t\to\infty$,

$$I_{st}=\frac{1}{2}\frac{qF_0d\beta\Delta_{\text{eff}}^2}{\pi}\frac{2\gamma\pi/\beta}{(F_0d)^2+(2\gamma\pi/\beta)^2}. \tag{47}$$

Equation (47) can be rewritten as follows:

$$I_{st}=\frac{1}{2}\frac{q\beta\,dF_0}{\pi}\Delta_{\text{eff}}^2\frac{(2\gamma\pi/\beta)}{[(2\gamma\pi/\beta)^2+(dF_0)^2]}, \tag{48}$$

and setting λ as $(2\gamma\pi/\beta)$ with the tunneling frequency Δ is now replaced by a dressed tunneling frequency Δ_{eff} in the strong-dissipation regime.

The treatment given in this section not only puts our theory in the perspective of the Kubo analysis of irreversible processes, but also—concomitantly—lays stress on the fact that our method, in general, goes beyond the steady-state theory of Kubo and extends it to a region in which a time-dependent conductivity can be investigated. Furthermore, it is apparent that as far as the steady-state current is concerned, there exists an analogy with the classical Drude relation for the electrical conductivity both in the weak- and strong-dissipation regimes, although in the latter case, the tunneling is effectively reduced because of quantum noise.

VI. CONCLUSIONS

We have performed here a perturbative analysis of quantum dissipation in a nanowire, modeled as a one-dimensional tight-binding lattice. By assuming the coupling with the environment of bosons to be weak, we have calculated the current and diffusivity in order to illustrate the competition between coherence and decoherence. Our method of calculation has been a treatment of an underlying master equation for the density operator, in a "subsystem-bath" approach. Because the subsystem is handled exactly, quantum coherence properties are taken care of *in toto*. How these properties—characterized, for example, by the particle current and mean-squared displacement—are influenced by the bath-induced decoherence, has been the principal concern of this paper.

The transport, which is otherwise coherent, becomes highly incoherent, when the coupling to the environment is strong. The analytical results, backed up by graphical illustrations of particle current and mean-squared displacement, present a contrasting picture with the case of weak dissipation for which the dynamics remain weakly incoherent. Expressions are presented in both the steady-state and the non-steady-state situations, thus, making contact with the classical Kubo-Drude analysis of electrical conductivity.

The profound differences in the nature of the motion depicted, respectively, by the coherent probability propagators [Eq. (A28)] and their incoherent counterparts obtained from Eq. (24) are also reflected in the current and mean-squared displacement. As we move to the incoherent regime due to strong dissipation we observe $S(t)\propto t$ [in the long-time limit, Eq. (32)], whereas $S(t)\propto t^2$ in the asymptotic limit of the weak-dissipative regime [Eq. (C6)]. Thus, the marked differences in the mean-squared displacement as depicted by Eq. (C6) and Eq. (32) reflect the strong differences between the coherent and the incoherent motion. On the other hand, the Bloch kind of oscillation can be observed in the temporal behavior of the current in the weak-dissipative regime. But the increase in dissipation strength and temperature destroys this Bloch oscillation. This can also be regarded as the display of a clear transition from the coherent-to-incoherent regime due to the increase in dissipation strength and the temperature.

The results presented here for the weak dissipation are expected to be of relevance in applications to quantum devices where the objective is to preserve quantum coherence to the extent possible by minimizing the dissipative influence of the surroundings. A nanowire, such as a quantum dot or a qubit, can, therefore, serve as a paradigm for the contemporary challenging issues of quantum information theory. A combination of the strong-dissipation results with those of weak dissipation, therefore, provides a complete scenario of coherentto-decoherent transition of the tunneling phenomenon in a quantum wire, that is, expected to be of much relevance to the topical interest in nanodevices.

APPENDIX A: CALCULATION OF $P_m^{(2)}(t)$: WEAK DISSIPATION

In this Appendix we display all the calculation details to obtain $P_m^{(2)}(t)$. First we will show explicit calculations of I_1–I_4,

$$
\begin{aligned}
I_1 &= \langle k|\hat{G}_1|k'\rangle = \xi^*(\tau)\langle k|\hat{N}\hat{U}^\dagger(\tau)\hat{N}\hat{U}^\dagger(t'-\tau)\hat{\rho}(0)\hat{U}(t')|k'\rangle \\
&= \xi^*(\tau)\langle k|\hat{N}\exp\left[-i\int_0^\tau d\tau'\hat{V}'_+(\tau')\right]\hat{N} \\
&\quad\times\exp\left[-i\int_\tau^{t'} dt''\hat{V}'_+(t'')\right]\hat{\rho}(0)\exp\left[-i\int_0^{t'} dt''\hat{V}'_+(t'')\right]|k'\rangle \\
&= \frac{\xi^*(\tau)}{(2\pi)^3}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\sum_{m'',m'''}m''m'''e^{-i[(k-k'')m''+(k''-k''')m''']} \\
&\quad\times\exp\left\{-i[\int_0^\tau d\tau' V_+^{\prime k''k'''}(\tau')+\int_0^{t'}dt''V_+^{\prime k'''k'}(t'')]\right\}, \\
I_1 &= -\frac{\xi^*(\tau)}{(2\pi)}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\delta(k-k'')\delta(k''-k''') \\
&\quad\times\frac{d}{dk'''}\exp\left\{i\frac{\Delta}{F_0 d}[\cos k'''[u(t')-u(\tau)]-\sin k'''[v(t')-v(\tau)]]\right\} \\
&\quad\times\frac{d}{dk''}\exp\left\{i\frac{\Delta}{F_0 d}[u(\tau)\cos, k''-v(\tau)\sin k''+v(t')\sin k'-u(t')\cos k']\right\},
\end{aligned}
\tag{A1}
$$

where we have used the fact that $\exp(-i\int_0^t dt'V_+^{\prime(k,k')}(t'))=\exp(i\frac{\Delta}{F_0}[u(t)(\cos k-\cos k')-v(t)(\sin k-\sin k')])$. After performing the derivative with respect to k''' and k'' and performing the integrations we obtain

$$
\begin{aligned}
I_1 &= \frac{\xi^*(\tau)}{2\pi}\left(\frac{\Delta}{F_0 d}\right)^2\exp\left(i\frac{\Delta}{F_0 d}[u(t')(\cos k-\cos k')-v(t')(\sin k-\sin k')]\right) \\
&\quad\times[z_1(t',\tau)\sin^2 k+z_2(t',\tau)\cos^2 k+z_3(t',\tau)\sin k\cos k],
\end{aligned}
\tag{A2}
$$

where $z_1(t',\tau)=u(\tau)[u(t')-u(\tau)]$, $z_2(t',\tau)=v(\tau)[v(t')-v(\tau)]$, and $z_3(t',\tau)=[u(t')-u(\tau)+u(2\tau)-u(\tau+t')]$. In a similar fashion we can calculate the other three terms I_2–I_4 which are explicitly given below in this Appendix through Eqs. (A8)–(A10), respectively. The combined results of $I1-I2-I3+I4$ is shown in Eq. (A11) which consists of seven terms. We derive all the seven terms explicitly in this Appendix. Let us proceed further to derive I_2–I_4,

$$
I_2=\frac{\xi^*(\tau)}{(2\pi)^3}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\sum_{m'',m'''}m''m'''e^{-i[(k-k'')m''+(k'''-k')m''']}\exp\left\{-i\left[\int_0^\tau d\tau'V_+^{\prime(k,k'')}(\tau')+\int_0^{t'}dt''V_+^{\prime(k'',k''')}(t'')\right]\right\},
\tag{A3}
$$

$$
I_3=\frac{\xi(\tau)}{(2\pi)^3}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\sum_{m'',m'''}m''m'''e^{-i[(k-k'')m''+(k'''-k')m''']}\exp\left\{-i\left[\int_0^\tau d\tau'V_+^{\prime(k''',k')}(\tau')+\int_0^{t'}dt''V_+^{\prime(k'',k''')}(t'')\right]\right\},
\tag{A4}
$$

$$
I_4=\frac{\xi(\tau)}{(2\pi)^3}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\sum_{m'',m'''}m''m'''e^{-i[(k''-k''')m''+(k'''-k')m''']}\exp\left\{-i\left[\int_0^\tau d\tau'V_+^{\prime(k'',k''')}(\tau')+\int_0^{t'}dt''V_+^{\prime(k,k'')}(t'')\right]\right\}.
\tag{A5}
$$

Furthermore, simplification of I_2–I_4 can be performed as follows:

$$
\begin{aligned}
I_2 &= \frac{\xi^*(\tau)}{(2\pi)^2}e^{i(\Delta/F_0 d)[u(\tau)\cos k-v(\tau)\sin k]}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\delta(k-k'')\frac{d}{dk''}e^{i(\Delta/F_0)\{\cos k''[u(t')-u(\tau)]-\sin k''[v(t')-v(\tau)]\}} \\
&\quad\times\delta(k'-k''')\frac{d}{dk'''}e^{i(\Delta/F_0 d)[-u(t')\cos k'''+v(t')\sin k''']},
\end{aligned}
\tag{A6}
$$

$$
\begin{aligned}
I_3 &= \frac{\xi^*(\tau)}{(2\pi)^2}e^{i(\Delta/F_0 d)[v(\tau)\sin k'7-u(\tau)\cos k']}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\delta(k-k'')\frac{d}{dk''}e^{i(\Delta/F_0)[\cos k''u(t')-\sin k''v(t')]} \\
&\quad\times\delta(k'-k''')\frac{d}{dk'''}e^{i(\Delta/F_0 d)\{[u(\tau)-u(t')]\cos k'''+[v(t')-v(\tau)]\sin k'''\}},
\end{aligned}
\tag{A7}
$$

$$
\begin{aligned}
I_4 &= -\frac{\xi^*(\tau)}{(2\pi)^2}e^{i(\Delta/F_0 d)u(t')\cos k-v(t')\sin k}\int_{-\pi}^{\pi}dk''\int_{-\pi}^{\pi}dk'''\delta(k-k'')\frac{d}{dk''}e^{i(\Delta/F_0)\{\cos k''[u(\tau)-u(t')]+\sin k''[v(t')-v(\tau)]\}} \\
&\quad\times\delta(k'-k''')\frac{d}{dk'''}e^{i(\Delta/F_0 d)[v(\tau)\sin k'''-u(\tau)\cos k''']}.
\end{aligned}
\tag{A8}
$$

After taking the derivative and performing the integrations we obtain

$$I_2 = \frac{\xi^*(\tau)}{2\pi}\left(\frac{\Delta}{F_0 d}\right)^2 e^{i(\Delta/F_0)[u(t')(\cos k-\cos k')-v(t')(\sin k-\sin k')]}[z_4(t',\tau)\sin k\, \sin k' + z_5(t',\tau)\cos k\, \cos k' + z_6(t',\tau)\sin k\, \cos k' + z_7(t',\tau)\cos k\, \sin k'], \quad (A9)$$

where $z_4(t',\tau) = u(t')[u(t') - u(\tau)]$, $z_5(t',\tau) = v(t')[v(t') - v(\tau)]$, $z_6(t',\tau) = v(t')[u(t') - u(\tau)]$, and $z_7(t',\tau) = u(t')[v(t') - v(\tau)]$,

$$I_3 = \frac{\xi(\tau)}{2\pi}\left(\frac{\Delta}{F_0 d}\right)^2 e^{i(\Delta/F_0)[u(t')(\cos k-\cos k')-v(t')(\sin k-\sin k')]} \times [z_4(t',\tau)\sin k\, \sin k' + z_5(t',\tau)\cos k\, \cos k' - z_6(t',\tau)\sin k\, \cos k' - z_7(t',\tau)\cos k\, \sin k'], \quad (A10)$$

$$I_4 = -\xi(\tau)2\pi\left(\frac{\Delta}{F_0 d}\right)^2 e^{i(\Delta/F_0)[u(t')(\cos k-\cos k')-v(t')(\sin k-\sin k')]} \times [z_3(t',\tau)\sin k' \cos k' - z_1(t',\tau)\sin^2 k' - z_2(t',\tau)\cos^2 k'], \quad (A11)$$

Now, we are in a position to write $I = I_1 - I_2 - I_3 + I_4$,

$$I = \left(\frac{\Delta}{F_0 d}\right)^2 e^{i(\Delta/F_0 d)[u(t')(\cos k-\cos k')-v(t')(\sin k-\sin k')]} \times (z_1(t',\tau)[\xi^*(\tau)\sin^2 k + \xi(\tau)\sin^2 k'] + z_2(t',\tau)[\xi^*(\tau)\cos^2 k + \xi(\tau)\cos^2 k'] + [\xi^*(\tau)\sin k\, \cos k - \xi(\tau)\sin k' \cos k']z_3(t',\tau) - [\xi^*(\tau)+\xi(\tau)] \times [z_4(t',\tau)\sin k\, \sin k' + z_5(t',\tau)\cos k\, \cos k'] - [\xi^*(\tau)-\xi(\tau)][z_6(t',\tau)\sin k\, \cos k' + z_7(t',\tau)\cos k\, \sin k']). \quad (A12)$$

Denoting all the terms inside the big third bracket of Eq. (A10) as $Z(t',\tau,k,k')$, we can rewrite the second-order term of the probability propagator as follows:

$$P_m^{(2)}(t) = -\left(\frac{\Delta}{F_0 d}\right)^2 \frac{1}{(2\pi)^2}\int_0^t dt' \int_0^{t'} d\tau \int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dk' e^{i(k-k')m} \times e^{i(\Delta/F_0)\{[u(t-t')+u(t')](\cos k-\cos k')+[v(t-t')-v(t')](\sin k-\sin k')\}} Z(t',\tau,k,k'). \quad (A13)$$

After utilizing the following Bessel identities:

$$e^{\pm iu(t)\sin k} = \sum_{n=-\infty}^{\infty} J_n[u(t)]e^{\pm ink}, \quad (A14)$$

$$e^{\pm iv(t)\cos k} = \sum_{n=-\infty}^{\infty} J_n[v(t)]e^{\pm ink}e^{\pm in\pi/2}, \quad (A15)$$

in Eq. (A13) we can write

$$P_m^{(2)}(t) = -\left(\frac{\Delta}{F_0 d}\right)^2 \sum_{n_1}\sum_{n_2}\sum_{n_3}\sum_{n_4}\int_0^t dt' \int_0^{t'} d\tau \int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dk' J_{n_1} \times [\tilde{u}(t,t')]J_{n_2}[\tilde{v}(t,t')]J_{n_3}[\tilde{u}(t,t')]J_{n_4}[\tilde{v}(t,t')]e^{i(m+n_1+n_2)k}e^{-i(m+n_3+n_4)k'}e^{i(n_1-n_3)\pi/2}Z(t',\tau,k,k'), \quad (A16)$$

where $\tilde{u}(t,t') = u(t-t') + u(t')$, $\tilde{v}(t,t') = v(t-t') - v(t')$. Now, using Euler's formula $\sin k = \frac{e^{ik}-e^{-ik}}{2i}$, $\cos k = \frac{e^{ik}+e^{-ik}}{2}$, we obtain the first term of $P_m^{(2)}(t)$ with the first term of $Z(t',\tau,k,k')$,

$$P_{m,1}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \sum_{n_1}\sum_{n_2}\sum_{n_3}\sum_{n_4}\int_0^t dt' \int_0^{t'} d\tau\, J_{n_1}(\tilde{u})J_{n_2}(\tilde{v})J_{n_3}(\tilde{u})J_{n_4}(\tilde{v})e^{i(n_1-n_3)(\pi/2)}z_1(t',\tau) \times \left[\xi^*(\tau)\frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, e^{i(m+n_1+n_2)k}(2-e^{2ik}-e^{-2ik})\frac{1}{2\pi}\int_{-\pi}^{\pi} dk' e^{-i(m+n_3+n_4)k'} + \xi(\tau)\frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, e^{i(m+n_1+n_2)k}\frac{1}{2\pi}\int_{-\pi}^{\pi} dk' e^{-i(m+n_3+n_4)k'}(2-e^{2ik'}-e^{-2ik'})\right]. \quad (A17)$$

Employing Kronecker δ formula $\frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, e^{ik(r-n)} = \delta_{r,n}$, one can obtain

$$P_{m,1}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \sum_{n_1}\sum_{n_2}\sum_{n_3}\sum_{n_4}\int_0^t dt' \int_0^{t'} d\tau J_{n_1}(\tilde{u})J_{n_2}(\tilde{v})J_{n_3}(\tilde{u})J_{n_4}(\tilde{v})e^{i(n_1-n_3)(\pi/2)}z_1(t',\tau)$$
$$\times [\xi^*(\tau)(\delta_{(m+n_1+n_2),0} - \delta_{(m+2+n_1+n_2),0} - \delta_{(m-2+n_1+n_2),0})\delta_{(m+n_3+n_4),0}$$
$$+ \xi(\tau)(\delta_{(m+n_3+n_4),0} - \delta_{(m+2+n_3+n_4),0} - \delta_{(m-2+n_3+n_4),0})\delta_{(m+n_1+n_2),0}]. \tag{A18}$$

It can be further simplified as

$$P_{m,1}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \sum_{n_1}\sum_{n_3}\int_0^t dt' \int_0^{t'} d\tau\, e^{i(n_1-n_3)(\pi/2)}z_1(t',\tau)\big(\xi^*(\tau)\big\{J_{n_3}(\tilde{u})J_{-(m+n_3)}(\tilde{v})\big[J_{n_1}(\tilde{u})J_{-(m+n_1)}(\tilde{v})$$
$$- J_{n_1}(\tilde{u})J_{-(m+2+n_1)}(\tilde{v}) - J_{n_1}(\tilde{u})J_{-(m-2+n_1)}(\tilde{v})\big]\big\}$$
$$+\xi(\tau)\big\{J_{n_1}(\tilde{u})J_{-(m+n_1)}(\tilde{v})\big[J_{n_3}(\tilde{u})J_{-(m+n_3)}(\tilde{v}) - J_{n_3}(\tilde{u})J_{-(m+2+n_3)}(\tilde{v}) - J_{n_3}(\tilde{u})J_{-(m-2+n_3)}(\tilde{v})\big]\big\}\big). \tag{A19}$$

Applying Graf's addition theorem,

$$\sum_{n=-\infty}^{\infty} e^{in\theta}J_{n+\nu}[u(t)]J_n[v(t)] = \left(\frac{u(t)-v(t)e^{-i\theta}}{u(t)-v(t)e^{i\theta}}\right)^{\nu/2} J_\nu[\sqrt{u^2(t)+v^2(t)-2u(t)v(t)\cos\theta}], \tag{A20}$$

we obtain

$$P_{m,1}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau z_1(t',\tau)[\xi^*(\tau)+\xi(\tau)]$$
$$\times \big\{2J_m^2[W(t',\tau)] - J_m[(W(t',\tau)]J_{m+2}[W(t',\tau)] - J_m[W(t',\tau)]J_{m-2}[W(t',\tau)]\big\}, \tag{A21}$$

where $W(t',\tau) = \sqrt{\frac{\Delta}{F_0}\tilde{u}^2(t',\tau) + \tilde{v}^2(t',\tau)}$. In a similar fashion we can obtain other terms of $P_m^{(2)}(t)$ and they are given as follows:

The second term of $P_m^{(2)}(t)$ is as follows:

$$P_{m,2}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_2(t',\tau)[\xi^*(\tau)+\xi(\tau)]$$
$$\times \big\{2J_m^2]W(t',\tau)] + J_m[W(t',\tau)]J_{m+2}[U(t',\tau)] + J_m[W(t',\tau)]J_{m-2}[W(t',\tau)]\big\}. \tag{A22}$$

The third term is given as

$$P_{m,3}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_3(t',\tau)\frac{2[\xi^*(\tau)-\xi(\tau)]}{i}(J_m[W(t',\tau)]\{J_{m+2}[W(t',\tau)] - J_{m-2}[W(t',\tau)]\}). \tag{A23}$$

The fourth term is given as

$$P_{m,4}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_4(t',\tau)[\xi^*(\tau)+\xi(\tau)]\big\{J_{m+1}^2[W(t',\tau)] + J_{m-1}^2[W(t',\tau)] - 2J_{m-1}(W)J_{m+1}(W)\big\}. \tag{A24}$$

The fifth term is given as

$$P_{m,5}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_5(t',\tau)[\xi^*(\tau)+\xi(\tau)]\big\{J_{m+1}^2[W(t',\tau)] + J_{m-1}^2[W(t',\tau)] + 2J_{m-1}(W)J_{m+1}(W)\big\} \tag{A25}$$

The sixth term is given as

$$P_{m,6}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_6(t',\tau)\frac{[\xi^*(\tau)-\xi(\tau)]}{i}\big\{J_{m+1}^2[W(t',\tau)] - J_{m-1}^2[W(t',\tau)]\big\}. \tag{A26}$$

The seventh term is given as

$$P_{m,7}^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau\, z_7(t',\tau)\frac{[\xi^*(\tau)-\xi(\tau)]}{i}\big\{J_{m+1}^2[W(t',\tau)] - J_{m-1}^2[W(t',\tau)]\big\}. \tag{A27}$$

Collecting all the terms we can write

$$P_m^{(2)}(t) = -\left(\frac{\Delta}{2F_0 d}\right)^2 \int_0^t dt' \int_0^{t'} d\tau([\xi^*(\tau)+\xi(\tau)]\big\{z_1(t',\tau)\big(2J_m^2 - J_mJ_{m+2} - J_mJ_{m-2}\big) + z_2(t',\tau)\big(2J_m^2 + J_mJ_{m+2}$$
$$+J_mJ_{m-2}\big) + z_4(t',\tau)\big(J_{m+1}^2 + J_{m-1}^2 - 2J_{m-1}J_{m+1}\big)$$

$$+z_5(t',\tau)\big(J_{m+1}^2+J_{m-1}^2+2J_{m-1}J_{m+1}\big)\Big\}+\frac{[\xi^*(\tau)-\xi(\tau)]}{i}\Big\{2z_3(t',\tau)(J_mJ_{m+2}-J_mJ_{m-2}) \\ +[z_6(t',\tau)+z_7(t',\tau)]\big(J_{m+1}^2-J_{m-1}^2\big)\Big\}\Big), \tag{A28}$$

where we omit the argument $W(t',\tau)$ of Bessel functions for ease of representation and the other relevant quantities are given below

$$z_1(t',\tau)=u(\tau)[u(t')-u(\tau)],\quad z_2(t',\tau)=v(\tau)[v(t')-v(\tau)], \\ z_3(t',\tau)=[u(t')-u(\tau)+u(2\tau)-u(t'+\tau)],\quad z_4(t',\tau)=u(t')[u(t')-u(\tau)], \\ z_5(t',\tau)=v(t')[v(t')-v(\tau)],\quad z_6(t',\tau)=v(t')[u(t')-u(\tau)], \\ z_7(t',\tau)=u(t')[v(t')-v(\tau)].\quad W(t',\tau)=\frac{\Delta}{F_0d}\sqrt{\tilde{u}^2(t',\tau)+\tilde{v}^2(t',\tau)}, \tag{A29}$$

with $\tilde{u}(t',\tau)=u(t'-\tau)+u(t')$ and $\tilde{v}(t',\tau)=v(t'-\tau)-v(t')$.

APPENDIX B: NEW CLASS OF SUM RULES FOR PRODUCTS OF BESSEL FUNCTIONS

Following Ref. [61], we can evaluate sums of the form $B_{k,s}=\sum_{n=-\infty}^{\infty}n^kJ_n(x)J_{n-s}(x)$ for integer values of $k\geqslant 0$ and s. They have found a recursion relation of $C_{k,s}=i^kB_{k,s}$ as follows:

$$C_{k+1,n}=inC_{k,n}+i\frac{y}{2}[C_{k,n+1}+C_{k,n-1}], \tag{B1}$$

with $C_{0,n}=\delta_{n,0}$. Using this recursion relation one can obtain following sum rules which we have used to find mean-squared displacement Eq. (23):

$$\sum_{=-\infty}^{\infty}m^2\big(2J_m^2-J_mJ_{m+2}-J_mJ_{m-2}\big)=\frac{x^2}{2},\quad \sum_{m=-\infty}^{\infty}m^2\big(2J_m^2+J_mJ_{m+2}+J_mJ_{m-2}\big)=\frac{3x^2}{2}, \\ \sum_{m=-\infty}^{\infty}m^2\big(J_{m+1}^2+J_{m-1}^2-2J_{m-1}J_{m+1}\big)=\frac{x^2}{2}+1,\quad \sum_{m=-\infty}^{\infty}m^2\big(J_{m+1}^2+J_{m-1}^2+2J_{m-1}J_{m+1}\big)=\frac{3x^2}{2}+1, \\ \sum_{m=-\infty}^{\infty}m^2(J_mJ_{m+2}-J_mJ_{m-2})=0,\quad \sum_{m=-\infty}^{\infty}m^2\big(J_{m+1}^2-J_{m-1}^2\big)=0. \tag{B2}$$

For the derivation of mean displacement Eq. (17) we can show that

$$\sum_{m=-\infty}^{\infty}m\big[J_{m+1}^2-J_{m-1}^2\big]=\sum_{m=-\infty}^{\infty}m[J_{m+1}(J_{m+1}+J_{m-1})-J_{m-1}(J_{m+1}+J_{m-1})]=\sum_{m=-\infty}^{\infty}\frac{2m^2}{x}[J_mJ_{m+1}-J_mJ_{m-1}]=1. \tag{B3}$$

The other sums vanish for the mean displacement using the above recursion relation Eq. (B1).

APPENDIX C: EXPLICIT EXPRESSIONS OF $\langle\hat{N}(t)\rangle$ AND $S(t)$

In this Appendix we derive explicit expressions of mean displacement $\langle\hat{N}(t)\rangle$ and mean-squared displacement $S(t)$ at low temperatures as well as at high temperatures. We express all the expressions in dimensionless form using the time variable as $x=\omega_ct$, and dimensionless parameters $a=\frac{F_0d}{\omega_c}$, $\frac{\gamma}{\omega_c}$, and $\beta\omega_c$. Let us first consider the low-temperature limit $k_BT\ll\omega_c$. In this limit the mean displacement can be obtained from Eq. (17) by completing double integrations,

$$\langle\hat{N}(x)\rangle=2\frac{\gamma}{\omega_c}\left(\frac{\Delta}{2F_0d}\right)\Bigg[-\frac{\cos(ax)}{a}+\frac{i}{4}\cosh(a)[\mathrm{Si}(z)-\mathrm{Si}(z^*)+\sin(z)-\sin(z^*)-z\,\mathrm{Ci}(z)+z^*\mathrm{Ci}(z^*)] \\ +\sinh(a)[\mathrm{Ci}(z^*)+\mathrm{Ci}(z)+\cos(z)+z\,\mathrm{Si}(z)+\cos(z^*)+z^*\mathrm{Si}(z^*)] \\ +\frac{\cosh(a)}{a^2}\ln[(ax)^2+a^2]+i\sinh(2a)[\mathrm{Si}(2z)-\mathrm{Si}(2z^*)]+\cosh(2a)[\mathrm{Ci}(2z)+\mathrm{Ci}(2z^*)]+\frac{i}{10}\sinh(a)[E_1(z)-E_1(z^*)]\Bigg], \tag{C1}$$

where Si and Cui are sine integral and cosine integral, respectively, ith arguments $z = a(x+i)$, $z^* = a(x-i)$. Thus, the current at low temperatures can be written as

$$I(x) = 2q\gamma\left(\frac{\Delta}{2F_0 d}\right)\Bigg[\sin(ax) + a\sinh(a)\left\{\frac{\cos(z)}{z} + \frac{\cos(z^*)}{z^*} + \mathrm{Si}(z^*) + \mathrm{Si}(z)\right\} + \frac{i}{4}a\cosh(a)\left\{\frac{\sin(z)}{z} - \frac{\sin(z^*)}{z^*} + \mathrm{Ci}(z^*) - \mathrm{Ci}(z)\right\} + \frac{a}{2}\cosh(2a)\left\{\frac{\cos(2z)}{z} + \frac{\cos(2z^*)}{z^*}\right\} + i\frac{a}{2}\sinh(2a)\left\{\frac{\sin(2z)}{z} - \frac{\sin(2z^*)}{z^*}\right\} + 2\frac{\cosh(a)}{a}\frac{ax}{(ax)^2 + a^2} + \frac{i}{10}\sinh(a)\left\{\frac{e^{-z}}{z} - \frac{e^{-z*}}{z*}\right\}\Bigg]. \tag{C2}$$

Furthermore, we obtain the mean-squared displacement $S(t)$ at low temperatures which is defined as $S(t) = d^2[\langle\hat{N}^2(t)\rangle - \langle\hat{N}(t)\rangle^2]$. We can write it in terms of dimensionless variable $x = \omega_c t$ or $z = a(x+i)$, $(z^* = a(x-i)$ and dimensionless parameters $a = \frac{F_0 d}{\omega_c}$, $\frac{\gamma}{\omega_c}$, and $\beta\omega_c$. Thus, we have

$$\langle\hat{N}^2(x)\rangle = \left(\frac{\Delta}{2F_0 d}\right)^2\left(\frac{\gamma}{\omega_c}\right)^2\Bigg[\sinh(2a)(\cos[2a(x+i)] + \cos[2a(x-i)] + 2a(x+i)\mathrm{Si}[2a(x+i)] + 2a(x-i)\mathrm{Si}[2a(x-i)]) + \frac{i}{2}[\sinh(2a) + \cosh(2a)]\{\sin[2a(x-i)] - \sin[2a(x+i)] + 2a(x+i)\mathrm{Ci}[2a(x+i)] - 2a(x-i)\mathrm{Ci}[2a(x-i)]\}\Bigg]. \tag{C3}$$

Let us now move to the high-temperature expressions. First we express mean displacement in terms of dimensionless variable $x = \omega_c t$ and other dimensionless parameters as mentioned above,

$$\langle N(x)\rangle = 4\pi\left(\frac{\Delta}{2F_0 d}\right)\frac{\gamma}{\omega_c}\frac{1}{\beta\omega_c}\left[\frac{ax}{1+a^2} - \frac{ae^{-x}}{1+a^2}\left(\cos(ax) + \frac{\sin(ax)}{a}\right) - \frac{ae^{-x}}{(1+a^2)^2}[a\sin(ax) - \cos(ax) + e^x]\right]. \tag{C4}$$

Furthermore, we can obtain the expression of current as follows:

$$I(x) = \frac{\pi q\gamma}{\beta\omega_c}\left(\frac{\Delta}{2F_0 d}\right)\left[\frac{ae^{-x}}{1+a^2}[a\sin(ax) - \cos(ax)] + \frac{a}{1+a^2} - \frac{e^{-x}a}{[1+a^2]}\cos(ax) + \frac{e^{-x}a}{[1+a^2]}\left(\cos(ax) + \frac{\sin(ax)}{a}\right)\right]. \tag{C5}$$

Finally, the $\langle\hat{N}^2(x)\rangle$ can be written as follows:

$$\langle\hat{N}^2(x)\rangle = \left(\frac{\Delta}{2F_0 d}\right)^2\frac{\gamma}{\omega_c}\frac{4\pi}{\beta\omega_c}\left[\frac{\sin(2ax)}{2a} - \frac{e^{-x}}{1+(2a)^2}\{2a\sin(2ax) - \cos(2ax) + e^x\} - \frac{\sin(ax)}{a} + \frac{e^{-x}}{1+(a)^2}\{a\sin(ax) - \cos(ax) + e^x\}\right] + \frac{1}{[1+a^2]^2}\{(a^2-1) - e^{-x}[2a\sin(ax) + (a^2-1)\cos(ax)] - 1\} + \frac{1}{[1+a^2][1+(2a)^2]}\{(1-2a^2) + e^{-x}[3a\sin(2ax) + (2a^2-1)\cos(2ax)]\} + \frac{1}{[1+a^2]}\left\{(x^2+1) - \left(\cos(ax) + \frac{\sin(ax)}{a}\right)\right\}. \tag{C6}$$

APPENDIX D: STRONG DISSIPATION: METHOD

In this Appendix our investigation will be based on the Liouville space formalism [62] and apply it to study the transport dynamics for our tight-binding system coupled with a Bosonic bath. A Liouville space $\mathcal{L}$ is the Cartesian product of several Hilbert spaces. The description of open quantum systems usually involved spaces consisting of the Hilbert space H_s of a closed system, the heat-bath Hamiltonian H_B, and the interaction Hamiltonian H_{sB}, i.e., $\mathcal{L} \equiv H_s \otimes H_B \otimes H_{sB}$. This actually raises the description from the quantum states $\psi(t)$ to the density matrices $\hat{\rho}(t)$. When we transform from the original Hilbert space to its derived Liouville space, the quantum dynamics cannot be described by the Schrödinger equation but by the von Neumann equation. Thus, our starting point is the Liouville–von Neumann equation for the overall density operator [63] $\hat{\rho}(t)$,

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -i[\hat{H}(t), \hat{\rho}(t)], \tag{D1}$$

where the Hamiltonian H, delineating the system H_S, the bath H_B and their coupling H_{SB}, is as given earlier [63].

1. Polaron transformation

We now introduce a unitary polaronic transformation under which Eq. (D1) yields

$$\frac{\partial \hat{\rho}'(t)}{\partial t} = -i[\hat{H}'(t), \hat{\rho}'(t)], \tag{D2}$$

where

$$\hat{\rho}'(t) = \hat{S}\hat{\rho}(t)\hat{S}^{-1}, \quad \hat{S} = \exp\left[it\hat{N}\left\{dF_0 - \sum_l \frac{g_l}{\omega_l}(\hat{b}_l - \hat{b}_l^\dagger)\right\}\right], \tag{D3}$$

$$\hat{\rho}'(t) = \hat{S}\hat{\rho}(t)\hat{S}^{-1}, \quad \hat{S} = \exp\left[it\hat{N}\left\{dF_0 - \sum_l \frac{g_l}{\omega_l}(\hat{b}_l - \hat{b}_l^\dagger)\right\}\right], \tag{D4}$$

$$\hat{H}'(t) = -\frac{\Delta}{2}[\hat{K}\hat{B}_+ \exp(-idF_0t) + \text{H.c.}] - \chi\hat{N}^2 + H_B, \quad \chi = \sum_l \frac{g_l^2}{\omega_l}, \tag{D5}$$

and

$$\hat{B}_\pm = \exp\left[\pm\sum_l \frac{g_l}{\omega_l}(\hat{b}_l - \hat{b}_l^\dagger)\right]. \tag{D6}$$

As we are only interested in the reduced density operator, obtained upon tracing over the bath variables, it is natural to implement a further unitary transformation effected by the bath Hamiltonian H_B. Thus,

$$\hat{\rho}''(t) = \exp(i\hat{H}_Bt)\hat{\rho}'(t)\exp(-i\hat{H}_Bt), \quad \frac{\partial \hat{\rho}''(t)}{\partial t} = -i[\hat{H}''(t), \hat{\rho}''(t)]. \tag{D7}$$

At this stage, we can drop the all superscripts of Eq. (D7) and write the effective Liouville equation of the polaron transformed density matrix as follows:

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -i[\hat{H}(t), \hat{\rho}(t)], \quad \hat{H}(t) = \hat{H}_s + \hat{V}(t), \quad \hat{H}_s = \chi\hat{N}^2, \quad \hat{V}_p(t) = -\frac{\Delta}{2}[\hat{K}\hat{B}_+(t)\exp(-iF_0dt) + \text{H.c.}]. \tag{D8}$$

2. Cumulant expansion and solution

As discussed in Ref. [9] [p. no. 25; Eq. (I.A.26)], upon averaging over bath degrees of freedom and considering up to second order in the cumulant, we can obtain the solution for the reduced density operator of the system,

$$\hat{\rho}_s(t) = \exp_T\left[-iH_s^\times t - \int_0^t dt' \int_0^{t'} dt'' \langle\langle \hat{V}_p^\times(t')\hat{V}_p^\times(t'')\rangle\rangle\right]\rho_s\hat{(}0), \tag{D9}$$

where superscript $\times$ denotes a Liouville operator and $\exp_T$ denotes time ordering later times to the left. Following Ref. [9] [Eq. (I.A.37)], one can obtain

$$\frac{d\hat{\rho}_s(t)}{dt} = -\hat{H}_s^{\ \times}\hat{\rho}_s(t) - \int_0^t dt'[\ll \hat{V}_p^\times(t)\hat{V}_p^\times(t') > \hat{\rho}_s(t')] \tag{D10}$$

Furthermore, we obtain

$$\begin{aligned}\frac{d\hat{\rho}_s(t)}{dt} = {} & -\hat{H}_s^{\ \times}\hat{\rho}_s(t) - \int_0^t d\tau\, \phi(t-\tau)[(e^{-iF_0d(t-\tau)}\hat{K}\hat{K}^\dagger + \text{H.c.})\hat{\rho}_s(\tau) - (e^{-iF_0d(t-\tau)}\hat{K}^\dagger\hat{\rho}_s(\tau)\hat{K} + \text{H.c.})] \\ & + \int_0^t d\tau\, \phi'(t-\tau)[-\hat{\rho}_s(\tau)(e^{-iF_0d(t-\tau)}\hat{K}\hat{K}^\dagger + \text{H.c.}) + (e^{+iF_0d(t-\tau)}\hat{K}^\dagger\hat{\rho}_s(\tau)\hat{K} + \text{H.c.})],\end{aligned} \tag{D11}$$

where, the bath correlation function $\phi(t)$ is given by

$$\phi(t) = \frac{\Delta^2}{4}\exp\left\{-\sum_l \frac{g_l^2}{\omega_l^2}\left[\coth\left(\frac{\beta\hbar\omega_l}{2}\right)[1-\cos(\omega_lt)] - i\,\sin(\omega_lt)\right]\right\}, \tag{D12}$$

and $\phi'(t) = \phi(-t)$. Finally, we obtain the time-evolution equation of the reduced density matrix as follows:

$$\frac{d\hat{\rho}_s(t)}{dt} = -\hat{H}_s^{\times}\hat{\rho}_s(t) - 2\int_0^t d\tau\,\mathrm{Re}[\phi(\tau)]\cos(F_0 d\tau)[2\hat{\rho}_s(t-\tau) - \{\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K} + \hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]\} - 2\int_0^t d\tau\,\mathrm{Im}[\phi(\tau)]\sin(F_0 d\tau)[\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K} - \hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]. \tag{D13}$$

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3. Explicit expressions: Current and MSD

a. High temperature: $T \gg \omega_c$

The long-time behavior is already discussed in detail in Sec. V. Furthermore, we can also study the temporal behavior of the current at short times, i.e. for $\omega_c t \ll 1$. In this limit we have

$$\sin[A_1(t)] = \sin\{\mathrm{Im}[\ln\,\phi(t)]\} \simeq \sin(\pi\gamma\omega_c t), \quad \exp[-A_2(t)] = \exp\{\mathrm{Re}[\ln\,\phi(t)]\} \simeq \exp\left[-\frac{\gamma\omega_c^2 t^2}{2}\right]. \tag{D14}$$

Henceforth, the particle current at short times is given as follows:

$$\begin{aligned} I(t) &= q\,d\Delta^2\int_0^t d\tau\;\sin(F_0 d\tau)\sin(\pi\gamma\omega_c\tau)\exp\left(-\gamma\omega_c^2\tau^2/2\right) \\ &= q\,d\Delta^2\frac{-i\sqrt{\pi}}{8\sqrt{c}}\left\{e^{-[(a-b_1)^2/4c_1]}\left[\mathrm{erfi}\left(\frac{a-b_1+2ic_1t}{2\sqrt{c_1}}\right) + \mathrm{erfi}\left(\frac{-a+b_1+2ic_1t}{2\sqrt{c_1}}\right)\right]\right. \\ &\quad \left. + e^{-[(a+b_1)^2/4c_1]}\left[\mathrm{erfi}\left(\frac{a+b_1-2ic_1t}{2\sqrt{c_1}}\right) - \mathrm{erfi}\left(\frac{a+b_1+2ic_1t}{2\sqrt{c_1}}\right)\right]\right\}, \end{aligned} \tag{D15}$$

where we have used $a = \frac{F_0 d}{\omega_c},\ b_1 = \pi\gamma\omega_c$, and $c_1 = \gamma\omega_c^2/2$.

b. Low temperature: $T \ll \omega_c$

In the low-temperature regime along with the long-time limit $\omega_c t \gg 1$, one can find

$$A_1(t) = \mathrm{Im}[\ln\,\phi(t)] = 2\gamma\ \tan^{-1}(\omega_c t) \simeq \pi\gamma\ \mathrm{sgn}(t), \quad A_2(t) = \mathrm{Re}[\ln\,\phi(t)] \simeq 2\gamma\ \ln[\omega_c\tilde{\tau}\ \sinh(t/\tilde{\tau})]. \tag{D16}$$

Thus, the particle current at low temperatures can be written as

$$\begin{aligned} I(t) &= \frac{2^{b-1}c^{1+b}}{b^2+(ac)^2}e^{\omega_c t(1/c-ia)}(e^{\omega_c t/c} - e^{-\omega_c t/c})^{1-b}\left[(ac-ib)F_1^2\left(1, \frac{2-b-iac}{2}; \frac{2+b+iac}{2}; e^{(2\omega_c t/c)}\right)\right. \\ &\quad \left. + e^{2ia\omega_c t}(ac+ib)F_1^2\left(1, \frac{2-b+iac}{2}; \frac{2+b+iac}{2}; e^{(2\omega_c t/c)}\right)\right], \end{aligned} \tag{D17}$$

where we use $a = \frac{F_0 d}{\omega_c},\ b = 2\gamma,\ c = \frac{\omega_c\beta}{\pi}$, and $F_1^2(a, b; c; x)$ is the hypergeometric function. On the other hand, the zero-temperature case can be analyzed as follows. Considering zero temperature and long time, i.e., $\omega_c t \gg 1$; we have

$$A_1(t) = \mathrm{Im}[\ln\,\phi(t)] \simeq \pi\gamma\ \mathrm{sgn}(t), \quad A_2(t) = \mathrm{Re}[\ln\,\phi(t)] \simeq 2\gamma\ \ln(\omega_c t). \tag{D18}$$

Thus, the particle current is given by

$$I = q\,d\Delta_{\mathrm{eff}}^2\int_0^t d\tau\frac{\sin(F_0 d\tau)}{(\omega_c\tau)^{2\gamma}} = \frac{e\Delta_{\mathrm{eff}}^2(F_0 dt)^2}{2(1-\gamma)(\omega_c t)^{2\gamma}}F_2^1\left(1-\gamma, 3/2; 2-\gamma, -\frac{(F_0 dt)^2}{4}\right) \tag{D19}$$

On the other hand, the particle current at short times ($\omega_c t \ll 1$) and at zero temperature for $\gamma = 1/2$ is given by

$$\begin{aligned} I(t) &= e\,d\Delta^2\int_0^t dt'\frac{\sin(F_0 dt')\sin(\omega_c t')}{[1+(\omega_c t')^2]} \\ &= \frac{e\,d\Delta^2}{4\omega_c}\left[i\,\cosh\left(\frac{F_0 d-\omega_c}{\omega_c}\right)\left\{\mathrm{Ci}\left[(F_0 d-\omega_c)\left(t+\frac{i}{\omega_c}\right)\right] - \mathrm{Ci}\left[(F_0 d-\omega_c)\left(t-\frac{i}{\omega_c}\right)\right]\right\}\right. \\ &\quad \left. + \sinh\left(\frac{F_0 d-\omega_c}{\omega_c}\right)\left\{\mathrm{Si}\left[(F_0 d-\omega_c)\left(-t+\frac{i}{\omega_c}\right)\right] - \mathrm{Si}\left[(F_0 d-\omega_c)\left(t+\frac{i}{\omega_c}\right)\right]\right\}\right] \end{aligned}$$

$$-\frac{1}{4\omega_c}\left[i\cosh\left(\frac{F_0d+\omega_c}{\omega_c}\right)\left\{\mathrm{Ci}\left[(F_0d+\omega_c\left(t+\frac{i}{\omega_c}\right)\right]-\mathrm{Ci}\left[(F_0d+\omega_c)\left(t-\frac{i}{\omega_c}\right)\right]\right\}\right.$$
$$\left.+\sinh\left(\frac{F_0d+\omega_c}{\omega_c}\right)\left\{\mathrm{Si}\left[(F_0d+\omega_c)\left(-t+\frac{i}{\omega_c}\right)\right]-\mathrm{Si}\left[(F_0d+\omega_c)\left(t+\frac{i}{\omega_c}\right)\right]\right\}\right]. \tag{D20}$$

4. Mean-squared displacement

In this subsection we will discuss the temporal behavior of mean-squared displacement. Particularly, we are interested on the particle diffusion coefficient which is defined as

$$D=\frac{1}{2}\lim_{t\to\infty}\frac{d\langle\Delta\hat{N}^2\rangle}{dt}=\frac{1}{2}\lim_{t\to\infty}\left[\frac{d\langle\hat{N}^2(t)\rangle}{dt}-\frac{d\langle\hat{N}(t)\rangle^2}{dt}\right]. \tag{D21}$$

Let us proceed further to calculate the mean-squared displacement. For this purpose we need to calculate $\mathrm{Tr}_s[(\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K})\hat{N}^2]$ and $\mathrm{Tr}_s\{[\hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]\hat{N}^2\}$. We know that

$$\hat{K}\hat{N}^2=\hat{N}\hat{K}\hat{N}+\hat{K}\hat{N}=\hat{N}(\hat{N}\hat{K}+\hat{K})+(\hat{N}\hat{K}+\hat{K}),$$
$$\hat{K}^\dagger\hat{N}^2=\hat{N}\hat{K}^\dagger\hat{N}-\hat{K}^\dagger\hat{N}=\hat{N}(\hat{N}\hat{K}^\dagger-\hat{K}^\dagger)-(\hat{N}\hat{K}^\dagger-\hat{K}^\dagger). \tag{D22}$$

Henceforth, we can write

$$\mathrm{Tr}_s\{[\hat{K}^\dagger\hat{\rho}_s(t-\tau)\hat{K}]\hat{N}^2\}=\langle\hat{N}^2(t-\tau)\rangle+2\langle\hat{N}(t-\tau)\rangle+1,$$
$$\mathrm{Tr}_s\{[\hat{K}\hat{\rho}_s(t-\tau)\hat{K}^\dagger]\hat{N}^2\}=\langle\hat{N}^2(t-\tau)\rangle-2\langle\hat{N}(t-\tau)\rangle+1, \tag{D23}$$

Finally, we obtain the equation which governs the temporal behavior of $<\hat{N}^2(t)$,

$$\frac{d\langle\hat{N}^2(t)\rangle}{dt}=\Delta^2\int_0^t d\tau\{\mathrm{Re}[\phi(\tau)]\cos(F_0d\tau)\}\mathrm{Tr}_s[\hat{\rho}_s(t-\tau)]-2\Delta^2\int_0^t d\tau\{\mathrm{Im}[\phi(\tau)]\sin(F_0d\tau)\}[\hat{N}(t-\tau)]. \tag{D24}$$

a. High temperature

Let us consider $\psi(t)=\langle\hat{N}^2(t)\rangle,\ \beta(t)=\langle\hat{N}(t)\rangle$, and their Laplace transform as $\tilde{\psi}(z)$ and $\tilde{\beta}(z)$, respectively. Considering long-time limit, i.e., $\omega_c t\gg 1$ we have already obtained bath correlations $A_1(t)$ and $A_2(t)$ in Eq. (D16). Utilizing them in Eq. (D24) and taking the Laplace transform of the same we obtain

$$z\tilde{\psi}(z)=\psi(0)+\Delta^2_{\mathrm{eff}}\frac{(z+2\gamma\pi/\beta)}{z[(z+2\gamma\pi/\beta)^2+(F_0d)^2]}-2\Delta^2_{\mathrm{eff}}\frac{F_0d}{[(z+2\gamma\pi/\beta)^2+(F_0d)^2]}\tilde{\beta}(z). \tag{D25}$$

Taking the Laplace transform of Eq. (26) one can show that

$$\tilde{\beta}(z)=-\frac{\Delta^2_{\mathrm{eff}}F_0d}{z^2[(z+2\gamma\pi/\beta)^2+(F_0d)^2]}, \tag{D26}$$

where we consider the initial condition $\beta(0)=0$. Now, we can rearrange Eq. (D25) as follows:

$$\frac{1}{2}[\lim_{z\to0}z^2\tilde{\psi}(z)-2\lim_{z\to0}z^2\tilde{\beta}(z)\lim_{z\to0}z\tilde{\beta}(z)]=2\Delta'^2_{\mathrm{eff}}\frac{2\gamma\pi/\beta}{[(2\gamma\pi/\beta)^2+(F_0d)^2]}, \tag{D27}$$

where $\Delta'^2_{\mathrm{eff}}=\Delta^2\cos(\pi\gamma)$. The left-hand side of Eq. (D27) is nothing but diffusion coefficient $D=\frac{1}{2}\lim_{t\to\infty}[\frac{d\langle\hat{N}^2\rangle}{dt}-2\frac{d\langle\hat{N}\rangle}{dt}\langle\hat{N}(t)\rangle]$. Taking the inverse Laplace transform of Eq. (D26) we may derive temporal behavior of $\langle\hat{N}(t)\rangle$,

$$\frac{\langle\hat{N}(t)\rangle}{\Delta^2_{\mathrm{eff}}}=a\left[\frac{2\lambda}{(a^2+\lambda^2)^2}-\frac{t}{(a^2+\lambda^2)}+\frac{(a^2-\lambda^2)\sin(at)-2a\lambda\cos(at)}{a(a^2+\lambda^2)^2}\right], \tag{D28}$$

where, we use $\lambda=2\gamma\pi/\beta$ and $a=\frac{F_0d}{\omega_c}$. On the other hand, we derive the temporal behavior of $\langle\hat{N}^2(t)\rangle$ by taking the inverse Laplace transform of Eq. (D25),

$$\langle\hat{N}^2(t)\rangle=\Delta'^2_{\mathrm{eff}}\left[\frac{\lambda t}{(a^2+\lambda^2)}+\frac{(a^2-\lambda^2)}{(a^2+\lambda^2)^2}+\frac{e^{-\lambda t}\{(\lambda^2-a^2)\cos(at)-2a\lambda\sin(at)\}}{(a^2+\lambda^2)^2}\right]$$
$$+2\Delta^4_{\mathrm{eff}}\left[\frac{a^2t^2}{2(a^2+\lambda^2)^2}-\frac{8a\lambda^2t}{(a^2+\lambda^2)^3}+\frac{2a^2(5\lambda^2-a^2)}{(a^2+b_2^2)^4}\right.$$

$$+\frac{2ae^{-b_2t}\left[3b_2\left(a^2-b_2^2\right)\sin(at)+a\left(a^2-5b_2^2\right)\cos(at)\right]}{\left(a^2+b_2^2\right)^4}$$
$$+\frac{e^{-\lambda t}[\sin(at)\{a^4t-\lambda^3+3\lambda a^2-3\lambda^2a^2t\}+\cos(at)\{\lambda^3at+3\lambda a^3t\}]}{2\lambda^3(a^2+\lambda^2)^3}\Bigg]. \tag{D29}$$

Utilizing Eqs. (D28) and (D29) one can easily show that $D=\lim_{t\to\infty}\frac{\langle\hat{N}^2(t)\rangle-\langle\hat{N}(t)\rangle^2}{2t}$ matches with Eq. (D27). Furthermore, we can show that mean-squared displacement at short times behaves as follows:

$$S(t)=\langle\hat{N}^2(t)\rangle-\langle\hat{N}(t)\rangle^2\sim\frac{\Delta_{\rm eff}^{\prime 2}\lambda t}{(a^2+\lambda^2)}. \tag{D30}$$

b. Low temperature

In this subsection, we discuss diffusion and mean-squared displacement at low temperatures, i.e., for $T\ll\omega_c$. In this regime we have

$$A_1(t)={\rm Im}[\ln\phi(t)]=2K\,\tan^{-1}(\omega_ct),\quad A_2(t)={\rm Re}[\ln\phi(t)]=2K\,\ln\left[\frac{\omega_c\beta}{\pi}\sinh\left(\frac{\pi\omega_ct}{\omega_c\beta}\right)\right]. \tag{D31}$$

Considering $\omega_ct\gg 1$ and $\gamma=1/2$ we obtain

$$D=\lim_{t\to\infty}\left[\frac{d\langle\hat{N}^2(t)\rangle}{dt}-\frac{d\langle\hat{N}(t)\rangle^2}{dt}\right]=\frac{(\pi\Delta)^2}{(\omega_c\beta)^2}\int_0^\infty dt'\frac{\cos(F_0dt')}{t'\sinh(\pi t'/\beta)}=\frac{(\pi\Delta)^2}{(\omega_c\beta)^2}\ln\left[{\rm sech}\left(\frac{F_0d\beta}{2}\right)\right]. \tag{D32}$$

Furthermore, we can discuss the case of zero temperature at long-times $\omega_ct\gg 1$. The diffusion coefficient is given by

$$D=\frac{d^2\Delta_{\rm eff}^{\prime 2}}{\omega_c^{2K}}\int_\epsilon^\infty dt'\frac{\cos(F_0dt')}{t'^{2K}}$$
$$=(i)^{2K+1}\frac{2d^2\Delta_{\rm eff}^{\prime 2}(F_0d)^{2K-1}}{\omega_c^{2K}}\{\Gamma[(1-2K),iF_0d\epsilon]-(-1)^{2K}\Gamma[(2K-1),-iF_0d\epsilon]\}, \tag{D33}$$

where ϵ is a very small number close to zero. Furthermore, we can write the mean-squared displacement as follows:

$$S(t)=2Dt, \tag{D34}$$

where D is already mentioned in Eq. (D33).

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