Energy conductance across a mesoscopic junction in a nonequilibrium spin-boson model under the influence of telegraph noise

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A spin-boson model in the presence of a telegraph noise (TN) source is employed to calculate the energy conductance between a tunnel junction and two bosonic baths. A polaron-transformed coupling term with the bosonic baths allows for treating quantum damping to arbitrary orders of strength. However, the polaron transformation yields a dressed tunneling frequency which is assumed small and treated perturbatively as is familiar in the noninteracting blip approximation in the context of the nonequilibrium spin-boson model. While the coupling with the bosonic baths leads to decoherence in an otherwise coherent tunneling process, the TN induces a different kind of fluctuation, that is, in the asymmetry of the underlying two-level system. It is the interplay of these two different relaxation effects, one triggered by the two quantum (bosonic) baths and the other through a classical bath (creating a TN), that is investigated here in detail. The TN that mimics the classical, fluctuating environment makes a nontrivial contribution to the self-energy that helps compute the imaginary part of the spin susceptibility which, in turn, determines the energy transfer across the junction. The range of validity of the TN is clarified at the outset and its efficacy in tuning the environmental influence is pointed out. The present paper complements an earlier similar study—albeit for fermionic baths—and provides additional input in terms of the TN to a previous investigation of energy transfer between a nanojunction and bosonic reservoirs without, however, the noisy environment.

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I. INTRODUCTION

A mesoscopic junction is a nanodevice that may comprise a pair of quantum dots or a qubit which, when in contact with quantum reservoirs through leads, can exchange particles and energy. Such a device can store quantum information through coherent processes involving the quantum phase. The undertaken investigation is expected therefore to have some relevance in the currently pursued topic of transport phenomena in mesoscopic junctions. While quantum dissipation due to the coupling with reservoirs can lead to decoherence, a more undesirable element is the omnipresence of an environment which for most purposes is classical and noisy. An understanding of the effect of such an environment is crucial for effective control of the consequent incoherence inflicted on the mesoscopic device.

Fabrication of nanoscale conductors such as molecular junctions has been achieved in chemical laboratories [1,2]. From the perspective of experiments, multiple techniques have been developed to measure energy transfer at a microscopic level such as the time-domain thermo-reflectance method [3], scanning thermal microscopy [4], and laser Raman scattering thermometry [5,6].

On the theoretical side, we have recently investigated the influence of telegraphic noise (TN) on heat currents in an electronic junction that is connected via leads to two fermionic reservoirs [7], henceforth referred to as paper I; see also [8]. The TN is an elementary fluctuator that randomly jumps between two states [9,10], the possible sources for which are discussed in [11–14]. The TN can be easily generalized to more than two states and even a continuum of states, as in the so-called Kubo-Anderson process, and in the limit of rapid jumps can mimic a Gaussian process [9]. Paper I is a critique of the TN as to whether the latter is a good model for the environment of a mesoscopic system. We address this criticism anew and in detail, given the widespread use of the TN (see also [15–20]) In contrast to I, however, the quantum reservoirs and baths are taken to be bosonic systems (and not fermionic). The choice of a bosonic bath has the advantage that with a proper tuning of the underlying spectral density it can represent either a phonon reservoir or an electron reservoir (comprising electron-hole excitations near the Fermi surface), hence covering a whole range of systems of experimental interest. The junction is thus couched within the much-studied nonequilibrium spin-boson (NESB) model. The latter is a two-state system, endowed with a diagonal energy term and an off-diagonal term, that is coupled with a bath which is characterized by bosonic excitations [21]. The NESB model is therefore an apt depiction of dissipative tunneling in a two-state quantum system that can describe a Josephson junction or macroscopic quantum tunneling in a squid [22], a point defect such as hydrogen tunneling between two inequivalent sites in a metal [23,24], and myriad other systems in chemical physics [25]. The NESB contraption along with the familiar Ohmic dissipation model has earlier been adapted to mesoscopic physics in the context of energy transfer—with dissipative coupling of arbitrary strength [26], hereafter cited

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as paper II. While we focus on the same model here, we incorporate the additional presence of the environment as described by a TN and analyze in detail the interplay of the latter with quantum dissipation triggered by the bosonic baths. In doing this, we find it much more straightforward to employ the well-known resolvent operator method of chemical physics [27]. The latter, with an additional polaron transformation [28] of the interaction term (with the bosonic baths), and a concomitant dressed tunneling energy that is assumed to be effectively small can deal with a wide range of dissipative coupling from weak to strong and is known to yield results for the resolvent [29,30] that are equivalent to the Green's function technique of Keldysh, adopted in II.

The TN is incorporated within a stochastic model of the total Hamiltonian that contains fluctuating terms arising from a bath whose temperature is assumed at the outset to be much larger than those of the bosonic leads. The resultant theory, like in I, rests on a generalization of the Blume model for the theory of spectral line shapes that assumes the underlying stochastic process to be stationary and Markovian, of which TN is just a special case [31]. The principal concern raised in I about the limitation of the TN for describing the mesoscopic environment pertains to the persistence of energy transfer from the fluctuator to the quantum baths even when the fluctuator's effective temperature is equal to (or smaller than) the temperatures of the quantum baths. We state here that the classical stochastic heat bath is by design at a temperature much higher than the temperature for the quantum reservoirs for which Bose (or Fermi) statistics is relevant. Thus, one should not push the TN beyond the realm of its validity to temperatures lower than the reservoir temperature. We recognize therefore that we are dealing here with a nonequilibrium process in which there is a one-way heat transfer from the fluctuator to the molecular junction, and we pursue the efficacy of the TN in modulating the quantum dissipation by tuning the mean rate of jumps of the TN from slow to the rapid regime, for which results are presented.

In order to delve into the origin of the TN, we imagine that our fully quantum system plus the bosonic baths (i.e., the leads) are embedded in yet another (much larger) phononic reservoir, henceforth referred to as a heat bath in order to distinguish it from the quantum baths of H_B. The larger bath is envisaged to be at an elevated temperature T ($\gg T_L$, T_R), and therefore the underlying bosonic (phononic) character is expected to give way to a classical heat bath just as Bose-Einstein (or for that matter, Fermi-Dirac) statistics reduces to Boltzmann statistics at appropriately high temperatures [32]. The aforesaid limit of how a TN emerges from this microscopic Hamiltonian can be achieved in the so-called stationary Markov approximation in which phenomena on timescales $\sim\hbar/k_BT$ can be ignored as well as all frequency dependence of dissipation and rate coefficients in an underlying rate theory description of the master equation of a reduced density operator [30].

Given this motivation, the paper is organized as follows. The full stochastic Hamiltonian of the system and the justification for taking the stochastic route are provided in Sec. II, in terms of a microscopic approach, following [19], which facilitates the computation of the energy transfer and energy conductance, which boils down to the calculation of the imaginary part of the spin susceptibility for the underlying NESB model. In Sec. III we perform the polaron transformation and rewrite the susceptibility in terms of the Laplace transform of an underlying correlation function in which the original coupling terms (with the two quantum baths) occur in exponentiated forms such that coupling to arbitrary orders can be accounted for. The price one pays, however, is that the tunneling term is effectively treated perturbatively. The resolvent technique for the evaluation of the correlation function is spelled out in Sec. IV, with algebraic details relegated to the Appendix. Section V is devoted to the analysis of the derived results that dovetail the effect of the noisy environment to the influence of the bosonic baths on the molecular junction. In particular, we reestablish the observation in I that the spin susceptibility exhibits two peaks located at the two possible frequencies that the TN fluctuates between, which eventually merge into a single peak centered around zero frequency as the relaxation rate of the TN is enhanced. Many of our analytical results including the graphical illustrations are worked out for the symmetric (on the average) case ($\epsilon = 0$) under the so-called dilute bounce gas approximation that assumes the effective part of the tunneling Hamiltonian to be small (see chapters 8.2–8.4 in [30]). It is fair to mention here that the problem of energy transfer in a mesoscopic junction in contact with leads has been earlier studied in depth, using the Green's function method and numerical techniques, by several investigators, such as in [33–36], to cite a few. What is unique here is to investigate the further influence of a noisy environment and employ as an example a TN to additionally manipulate the process. Finally, Sec. VI contains summary remarks and the main conclusions of the paper.

II. BASIC FORMALISM

A. Model Hamiltonian and the underlying basis of stochasticity

The Hamiltonian is given by

$$H = H_s(t) + H_I + H_B, \tag{2.1}$$

$$H_s(t) = \tfrac{1}{2}[\varepsilon + \delta f(t)]\sigma_z + \tfrac{1}{2}\Delta\sigma_x, \tag{2.2}$$

where $f(t)$ jumps randomly between two values $+1$ and -1 and Δ is the tunneling between the two levels split by the energy $[\varepsilon \pm \delta]$. The system Hamiltonian H_s may be taken to describe a two-site quantum dot (a qubit) with the static energy ε specifying the difference between the site energies, which are further modulated by a fluctuating term $\delta f(t)$, while Δ is the hopping energy between the sites [13]. Thus, even if the stochastic process $f(t)$ averages out to zero, the bias ε remains, the importance of which on energy conductance on a nanoscale was emphasized in II. The dot is regarded as a tunnel junction juxtaposed between two bosonic baths, left (L) and right (R), at temperatures T_L and T_R, respectively, jointly described by a bath Hamiltonian H_B, while H_I subsumes the two interaction terms:

$$H_B = \Sigma_{v=L,R} H_B^v = \Sigma_{j,v=L,R}\omega_{j,v} b_{j,v}^\dagger b_{j,v}, \tag{2.3}$$

$$H_I = \sigma_z \Sigma_{j,v=L,R} g_{j,v}(b_{j,v}^\dagger + b_{j,v}), \tag{2.4}$$

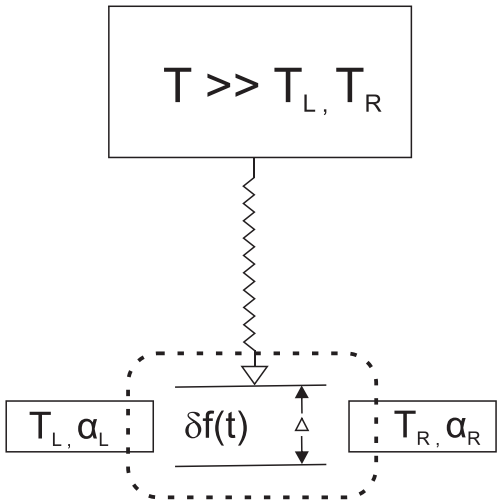

FIG. 1. Schematic of the two-state junction coupled with left (L) and right (R) bosonic reservoirs characterized by coupling constants α_L and α_R and temperatures T_L and T_B, which are eventually taken equal for energy conductance calculation. The stochastic modulation arising from a heat bath-driven TN is also indicated, in which the bath temperature T is stipulated to be much larger than T_L and T_R.

with $b^{\dagger}_{j,\nu}$ ($b_{j,\nu}$) the creation (annihilation) operator of the jth mode in the νth bosonic bath and $g_{j,\nu}$ the system-bath coupling strength. (At the outset we set $\hbar = 1$ and $k_B = 1$.) If the TN is absent, $f(t) = 0$, and the Hamiltonian is time-independent: it reduces to the one studied in II. Further, if tunneling $\Delta = 0$, the leads are decoupled from the junction and the problem reduces to one of a pure jump process governed by a TN. In order to schematically appreciate the meaning of the Hamiltonian H we put forward in Fig. 1 a sketch of the junction, in contact with two bosonic leads and further modulated by a TN induced by a stochastic heat bath.

The underlying stochastic process—assumed stationary and Markovian—is characterized by W, the transition probability matrix which, for a TN, can be written as [37]

$$W = \gamma(T - I), \tag{2.5a}$$

where the element of the T matrix between the stochastic variables a and b that run over the values $+1$ and -1 is given by

$$(a|T|b) = P_b, \tag{2.5b}$$

γ being the rate of jump from one stochastic state to the other and P_b the *a priori* probability of the occupation of the state $|b)$. (Note that we denote here the stochastic state $|a)$, $|b)$, etc., with round brackets in contrast to angular bra-ket for quantum states, as described in [31]).

In order to see how the above stochastic picture emerges from a more microscopic consideration, we follow [19] and modify the system part of the Hamiltonian in Eq. (2.2) as

$$H_s = \delta[\tau_z - < \tau_z >]\sigma_z + \Delta\sigma_x + (E_o/2)\tau_z + \tau_x \Sigma_k G_k (B^{\dagger}_k + B_k) + \Sigma_k \Omega_k B^{\dagger}_k B_k. \tag{2.6}$$

Here the τ operators refer to yet another two-state pseudospin that is envisaged to encode the dichotomic TN. Note that all the attributes of this heat bath are written in capital letters to unambiguously distinguish them from the corresponding quantities of the quantum baths described by H_B. This enlarged system Hamiltonian has to be combined with H_I and H_B to constitute a full Hamiltonian, which, it must be noted, is now explicitly time-independent, as in the Schrödinger picture of quantum mechanics.

We now clarify how the model in Eq. (2.6) can lead to a TN. The Hamiltonian in Eq. (2.6) describes the environment of a quantum junction. The last three terms can, for instance, account for phonon-assisted jumps of a point defect in an asymmetric (parametrized by the asymmetry energy E_o) double well, for which the two minima are mapped into the eigenstates $\tau_z = 1$ and $\tau_z = -1$ of the pseudospin Pauli operator τ_z [29,30]. The jumps of strength governed by the coupling constant G are triggered by the pseudospin τ_x, which is off-diagonal in the $\tau_z$representation, facilitated by the phonon operators B_k and $B^{\dagger}_k$, which are further modulated by the free boson (last) term. The underlying physics is as follows: τ_x flips τ_z between $+1$ and -1, thereby shifting the defect from one well to the other. It is such incoherent jumps that are represented in our model [see Eq. (2.2)] by a TN. The passage to a TN is aided by several approximations: the neglect of the system parameters δ and Δ and the energy E_o in the time evolution, a Markov assumption via the neglect of the frequency dependence in the self-energy, and above all, perception of the heat bath as classical. Operationally, this implies that the fluctuations in the heat bath variables live on much shorter timescales than the timescale set by E_o^{-1}. The energy E_o, however, enters into reckoning in the detailed balance of transitions between the levels split by E_o via appropriate Boltzmann factors:

$$P_+(T) = \frac{\exp(\frac{E_o}{2k_BT})}{2\cosh(E_o/2k_BT)}, \qquad P_-(T) = 1 - P_+(T). \tag{2.7}$$

We will assume at the outset, and in consonance with the remarks concerning the nature of the stochastic bath, that $k_BT \gg E_o$ so that

$$P_-(T) = P_+(T) = 1/2. \tag{2.8}$$

B. Spectral function and the energy current and conductance in terms of spin correlation

The influence of the quantum baths is contained in the spectral density function

$$I_\nu(\omega) = 2\pi \Sigma_{j\varepsilon\nu} g^2_{j,\nu} \delta(\omega - \omega_{j,\nu}). \tag{2.9}$$

Assuming Ohmic dissipation with an exponential cutoff ω_c for each bath the spectral function is

$$I_\nu(\omega) = \pi\alpha_\nu\omega \exp\left(-\frac{\omega}{\omega_c}\right). \tag{2.10}$$

We shall employ the following definition of the energy current from the νth bosonic bath to the system, consistent with quantum thermodynamics [38]:

$$J_\nu = -\frac{\partial}{\partial t}\langle H^\nu_B\rangle, \tag{2.11}$$

where the time derivative has to be computed from the Heisenberg equation of motion involving the total Hamiltonian. The calculation of J_ν is facilitated by the fact that the time derivative of the averaged total Hamiltonian is zero, from conservation of energy.

Within the time-independent scenario of Eq. (2.6) (before transiting to the stochastic picture) we can express the energy current (from the left bath to the junction) in a Landauer type of formula as shown in [26]:

$$J_L = \frac{\alpha\xi}{4}\int_0^\infty d\omega\omega^2 \exp(-\omega/\omega_c)[n_L(\omega) - n_R(\omega)]\chi_z''(\omega), \tag{2.12}$$

where

$$\alpha = \alpha_L + \alpha_R, \quad \xi = \frac{4\alpha_L\alpha_R}{\alpha^2} \tag{2.13}$$

and $n_\nu(\omega)$ is the Bose-Einstein factor. The corresponding term for the right bath is simply obtained from the energy conservation: $J_L + J_R = 0$. As expected, the energy transfer is related to the power absorbed, which, in response theory is given by the imaginary part of the susceptibility $\chi_{zz}''(\omega)$, that in turn is given in the NESB model by $\tilde{C}$(s). Very similar expressions for the energy transfer, as in Eq. (2.12), are arrived at in I though, as is obvious, the Bose-Einstein factors are replaced there by the Fermi-Dirac distributions [33]. As shown in II the energy conductance K can also be calculated from Eq. (2.12), in the linear response limit:

$$K = (\alpha\xi/4)\int_0^\infty d\omega[(\omega/2T_B)/\sinh(\omega/2T_B)]^2\omega \times \exp(-\omega/\omega_c)\chi_Z''(\omega)|_{T_L=T_R=T_B}. \tag{2.14}$$

Thus, both the energy current and the energy conductance are given by the imaginary part of the susceptibility, which is turn is determined by the spin-spin correlation function (see the Appendix). The latter will be the focus of our attention in the next section.

III. POLARON TRANSFORMATION ON THE CORRELATION FUNCTION

At this stage we point out a major departure in the methodology of our treatment from that in II (and I), as is indicated in the Introduction. In II the susceptibility is calculated using the nonequilibrium Green's function (NEGF) technique (Keldysh) along with a Majorana fermion representation of the underlying Dyson series. We, on the other hand, employ a standard resolvent operator method, well known in chemical physics (see [30], for instance) using a polaron transformation on the coupling with the baths (see below), which is referred to in II as the PT-NEGF, and derive equivalent results. In addition, of course, our main objective, as stressed earlier, is to examine the influence of a TN as an additional energy input, not considered in II.

As shown in Appendix A 1, the susceptibility, in linear response theory, is given in terms of the Laplace transform of the time-dependent correlation function of the operator σ_z, the central quantity of our present interest [9]:

$$\tilde{C}(s) = \int_0^\infty dt e^{-st} C(t), \tag{3.1}$$

where $C(t)$ is defined by

$$C(t) = < \sigma_z(0)\sigma_z(t) >, \tag{3.2}$$

and the Laplace transform variable s is complex, which follows the usual convention that its imaginary part is $-\omega$ and its real part is taken to be zero at the end of computing the integral in Eq. (3.1) in order to ensure its convergence. The angular brackets indicate statistical average over an equilibrium ensemble governed by the time-independent total Hamiltonian, as explained in the discussion following Eq. (2.6).

As stated earlier our aim is to employ a polaron transformation which yields results valid over a range of system-bath coupling strengths, especially in the so-called nonadiabatic limit $\frac{\Delta}{\omega_c} \ll 1$ (cf. II). This is achieved with the aid of the unitary transformation

$$S = \exp(i\sigma_z\Omega/2), \tag{3.3a}$$

where

$$\Omega = 2i\Sigma_{j,\nu} g_{j,\nu}(b_{j,\nu}^\dagger - b_{j,\nu})/\omega_{j,\nu}, \tag{3.3b}$$

under which the total Hamiltonian transforms into

$$H_T = S^\dagger H S = \tilde{H}_0 + \tilde{H}_I, \tilde{H}_0 = \tilde{H}_s + \tilde{H}_B, \tag{3.4}$$

$$\tilde{H}_s = \delta(\tau_z - < \tau_z >)\sigma_z + \left(\frac{E_o}{2}\right)\tau_z + \tau_x\Sigma_k G_k(B_k^\dagger + B_k) + \Sigma_k\omega_k B_k^\dagger B_k, \tag{3.5}$$

$$\tilde{H}_B = \Sigma_{j,\nu=L,R}\omega_{j,\nu} b_{j,\nu}^\dagger b_{j,\nu}, \tag{3.6}$$

and

$$\tilde{H}_I = \Delta[\sigma_+ \exp(-i\Omega) + \sigma_- \exp(i\Omega)]/4 = \Delta(\sigma_+ A_L^- A_R^- + \text{H.c.})/4,$$
$$A_\nu^- = \exp[2\Sigma_j g_{j,\nu}(b_{j,\nu}^\dagger - b_{j,\nu})/\omega_{j,\nu}]. \tag{3.7}$$

Clearly, the new interaction Hamiltonian contains the old coupling constants g_j to all orders. Further, the correlation function $C(t)$ transforms to

$$C(t) = < \sigma_z(0)[\exp(iH_T t)\sigma_z(0)\exp(-iH_T t)] >, \tag{3.8}$$

where H_T is given by Eq. (3.4). The latter lives in the product Hilbert space: $(\sigma \otimes \tau)$ of the σ and τ Hilbert spaces. The σ space, on the other hand, embraces the Hilbert spaces of the two baths (the leads) while the τ space encompasses the Hilbert space of the larger heat bath. The expectation value $< \cdot >$ in Eq. (3.8) specifies the statistical mechanical average of the entire product space.

Of specific interest, however, is the dynamical variable σ_z in computing the susceptibility all other degrees of freedom would have to be averaged over. In carrying out this procedure in a systematic order, we do the usual thing, namely, first eliminate the system that is most strongly coupled. That in the pecking order, in terms of the scenario we have laid out, is clearly the large heat bath that is linked with the τ spins. As elaborated upon in Sec. 1.7 of [30], we may perform this task via a master equation for a reduced density operator in which the degrees of freedom of the larger heat bath are traced out. The validity and limitation of this approach have been

discussed in detail in [30]: how a classical Markovian description of the heat bath ensues when phenomena on timescales $\sim\hbar/k_B$ T are ignored as well as all frequency dependences in the dissipation and rate coefficients in an underlying rate theory treatment of the reduced density operator, as was already emphasized in the introductory section of this paper and at the end of the discussion before Eq. (2.7).

The outcome is a reappraisal of the heat bath as a stochastic bath and the quantum operator τ_z as a classical stochastic process $f(t)$ which, for a two-state spin variable like τ_z, is a Markovian TN. We are thus led to the explicitly time-dependent Hamiltonian of Eq. (2.1). The earlier product Hilbert space of σ and τ is now abstracted into a product space of σ and the two-state TN. From this point onwards we can appropriate the Blume model into our description of decoherence inflicted by the environment of a mesoscopic system, and that was precisely the approach adopted in I.

IV. RESOLVENT METHOD FOR CORRELATION FUNCTION

In the light of the stratagem outlined above the Laplace transform of the spin-correlation function $C(t)$ in Eq. (2.8) can be rewritten as

$$\tilde{C}(s) = \Sigma_{\mu\nu}\mu\nu(\mu\mu|\{\ll [\tilde{U}(s)]_{av} \gg\}|\nu\nu), \tag{4.1}$$

where the double angular brackets $<< \cdot \gg$ have been employed here to distinguish from the single angular brackets in Eq. (3.2). Recall that earlier in Eq. (3.2) we needed to perform an average over an ensemble governed by a time-independent Hamiltonian. But now the latter has a piece that is stochastic and hence the full average factors into a quantum statistical average over the variables of the leads only denoted by $<< \cdot \gg$, while the rest of the heat bath is subsumed into a stochastic average denoted by $(\cdot)_{av}$. Note once again that "states" of Liouville (super) operators are denoted by round brackets with two entries in contrast to the angular brackets with one entry, used for ordinary operators. The quantity $U(t)$, in an extension of the Blume analysis, is a super-operator given by

$$U(t) = \exp_T[i\int_0^t dt\frac{1}{2}[\varepsilon + \delta f(t')]\sigma_z^\times + it(\tilde{H_I^\times} + \tilde{H_B^\times})], \tag{4.2}$$

where the suffix T underneath "exp" implies a suitable time ordering, the superscript $\times$ denotes a Liouville operator associated with the corresponding Hamiltonian (for a review of the properties of Liouville operators, see [9]), and $\tilde{H}_I$ and H_B are given, respectively, by Eq. (3.7) and Eq. (3.6).

We may indeed view the time-evolution operator $U(t)$ as the starting point of the central theme behind our detailed calculation of the spin-correlation function, as presented below. In the Blume model the Laplace transform of the time-evolution super-operator can be expressed as [31]

$$\tilde{U}(s) = [s - i(\epsilon/2)\sigma_z^\times - W - i(\delta/2)F\sigma_z^\times - i(H_I^\times + H_B^\times)]^{-1}, \tag{4.3}$$

where

$$(a|F|b) = a\delta_{ab}. \tag{4.4}$$

It is pertinent to mention here that the stationary Markov description of the larger bath, yielding a time-independent rate matrix W at the outset, has led to a simplified (compared to I) treatment of the Laplace transform and the averaging procedure over TN, as a whole.

Our task now in the pecking order, outlined in Sec. III, is to perform the stochastic average. The special nature of the TN then gives rise to the following random phase approximation-like structure of many-body theory for the average [37]:

$$[\tilde{U}(s)]_{av} = [U_o(s+\gamma)]_{av}/\{1 - \gamma[U_o(s+\gamma)]_{av}\}, \tag{4.5}$$

where

$$2[U_o(s+\gamma)]_{av} = \left[s + \gamma - \frac{i}{2}(\varepsilon+\delta)\sigma_z^\times - i\tilde{H}_I^\times - iH_B^\times\right]^{-1} + \left[s+\gamma - \frac{i}{2}(\varepsilon-\delta)\sigma_z^\times - i\tilde{H}_I^\times - iH_B^\times\right]^{-1}. \tag{4.6}$$

Expression (IV.5) clearly matches Eq. (4.3) in the static limit ($\gamma = 0$). On the other hand, when $\delta = 0$ (no TN),

$$[\tilde{U}(s)]_{av} = \tilde{U}(s) = \left[s - i\frac{\varepsilon}{2}\sigma_z^\times - i\tilde{H}_I^\times - iH_B^\times\right]^{-1}, \tag{4.7}$$

the starting point of the propagator (in the Laplace-transformed space) in [29,30] and indeed also in II.

V. RESULTS AND ANALYSIS

While the detailed treatment of Eq. (4.5) and further averaging over the quantum baths are dealt with in the Appendix, we quote here the final result from Eqs. (A8) and (A9):

$$\ll [\tilde{U}(s)]_{av} \gg = \{s + \ll \tilde{H}_I^\times[s - iH_B^\times + (\delta\sigma_z^\times)^2/(s+\gamma - iH_B^\times)]^{-1}H_I^\times \gg\}^{-1}. \tag{5.1}$$

In arriving at Eq. (5.1) we have ignored ε from further consideration—without loss of generality—in order to simplify the algebra. Because the super-operators occurring in the resolvent in Eq. (5.1), within the square brackets $[\cdot]$, all commute with each other, they can be treated as C numbers. Hence, we may suggestively regroup the equation as

$$\ll [\tilde{U}(s)]_{av} \gg = [s + \Sigma_+(s) + \Sigma_-(s)]^{-1}, \quad \Sigma_\pm(s) = \ll H_I^\times(Q_\pm H_I^\times \gg, \tag{5.2}$$

being the so-called self-energy, where

$$Q_+(s) = \frac{\{1/2 + (\gamma/2)/[\gamma^2 - (2\delta\sigma_z^\times)^2]^{1/2}\}}{\{(s+\gamma/2 - iH_B^\times) - (1/2)[\gamma^2 - (2\delta\sigma_z^\times)^2]^{1/2}\}}, \tag{5.3}$$

$$Q_-(s) = \frac{\{1/2 - (\gamma/2)/[\gamma^2 - (2\delta\sigma_z^\times)^2]^{1/2}\}}{\{(s+\gamma/2 - iH_B^\times) + (1/2)[\gamma^2 - (2\delta\sigma_z^\times)^2]^{1/2}\}}. \tag{5.4}$$

This stratagem helps evaluate the Laplace-transformed quantities in Eq. (5.1) back in the time domain, as detailed below.

Evidently, for $\gamma = 0$ (no relaxation)

$$Q_{\pm}(s) = (1/2)/(s - iH_B^{\times} \mp i\delta\sigma_z^{\times}), \tag{5.5}$$

which suggests a superposition of contributions due to two static frequencies $+\delta$ and $-\delta$, weighted by the factor one-half. On the other hand, in the case of rapid relaxation($\gamma \gg \delta$), $Q_-(s)$ is vanishingly small, whereas

$$Q_+(s) \approx 1/[s - iH_B^{\times} + (\delta\sigma_z^{\times})^2/4\gamma], \tag{5.6}$$

the motionally averaged result that indicates a single pole at $s = 0$. This transition from a two-pole to a single-pole structure as the relaxation rate γ is increased has been discussed in detail, pictorially as well in I.

We now turn our attention to the final calculation of the self-energy in Eq. (5.2) (the intermediate steps for which are assigned to Appendix A 3), the relevant matrix elements of which are quoted from Eq. (A25):

$$\begin{aligned}(++|\Sigma_+(s)|++) &= (--|\Sigma_+(s)|--)\\ &= -(--|\Sigma_+(s)|++) = -(++|\Sigma_+(s)|--) \equiv Z_+(s)\\ &= 1/4\Delta^2(1+\gamma/\eta)\int_0^{\infty} dt e^{-st}\exp[-t(\gamma-\eta)/2][\phi(t)+\phi'(t)].\end{aligned} \tag{5.7}$$

The corresponding matrix elements of $\Sigma_-(s)$ are derived from Eq. (5.7) by replacing η by $-\eta$, which, when added to the matrix elements of $\Sigma_+(s)$, yield the matrix elements of the total self-energy $\Sigma(s)$. Here $\phi'(t)$ is obtained by replacing t in the argument by $-t$. Further, η is quoted once again defined in Eq. (A3):

$$\eta \equiv (\gamma^2 - 16\delta^2)^{1/2}. \tag{5.8}$$

The (product) correlation function is given by Eq. (8.27) of [30] [also compare with Eq. (39) of [26]],

$$\phi(t) = \exp[i\alpha\pi\,\mathrm{sgn}(t)]\{\pi T_B/[\omega_c \sinh(\pi T_B|t|)]\}^{2\alpha}, \tag{5.9}$$

where α is defined in Eq. (2.13). In writing Eq. (5.9) we have assumed that the two quantum baths are at the same temperature T_B (i.e., $T_L = T_R = T_B$), which is taken to be much smaller than the cutoff frequency ω_c (in appropriate units). As expected, in the limit of zero relaxation ($\gamma = 0$, i.e., no TN), Eq. (5.7) matches the self-energy in Eq. (8.50) of [30]. The Laplace transform of $\phi(t)$ [cf. Eq. (8.53) of [30]] is

$$\begin{aligned}\tilde{\phi}(s) = \frac{1}{\omega_c}&\exp(i\alpha\pi)(2\pi T_B/\omega_c)^{2\alpha-1}\\ &\times \frac{\Gamma(1-2\alpha)\Gamma(\alpha + s/2\pi T_B)}{\Gamma(1-\alpha+s/2\pi T_B)},\end{aligned} \tag{5.10}$$

$\Gamma(\cdot)$ being the Gamma function. Equations (5.9) and (5.10) are in complete agreement with Eqs. (39) and (44) of II, respectively, though in the latter a very different method, *viz.*, the nonequilibrium Green's function treatment of Keldysh, is employed.

Recall from Eq. (4.1) that the correlation function is given by

$$\begin{aligned}\tilde{C}(s) = &[(++|\ll[\tilde{U}(s)]_{av}\gg|++)\\ &+(--|\ll[\tilde{U}(s)]_{av}\gg|--)]\\ &-[(++|\ll[(\tilde{U}(s)]_{av}\gg|--)\\ &+(--|\ll[\tilde{U}(s)]_{av}\gg|++)],\end{aligned} \tag{5.11}$$

where the computation of $\ll[\tilde{U}(s)]_{av}\gg$ requires the inversion of a 2×2 matrix in accordance with Eq. (5.2). The latter can be written as

$$\begin{aligned}\ll[\tilde{U}(s)]_{av}\gg &= \begin{pmatrix} s+Z_+(s) & -Z_+(s)\\ -Z_-(s) & s+Z_-(s)\end{pmatrix}^{-1}\\ &= [s(s+2Z(s)]^{-1}.\begin{pmatrix} s+Z_-(s) & Z_+(s)\\ Z_-(s) & s+Z_+(s)\end{pmatrix},\end{aligned} \tag{5.12}$$

where [cf. Eq. (5.7)]

$$Z(s) = Z_+(s) + Z_-(s), \tag{5.13}$$

$Z_+(s)$ being given by Eq. (5.7) and $Z_-(s)$ is obtained by replacing η by $-\eta$.

From Eq. (5.11),

$$\tilde{C}(s) = 2/[s + 2Z(s)], \tag{5.14}$$

which, from Eq. (5.11), takes the particularly simple structure

$$\begin{aligned}\tilde{C}(s) = 2/\{s + \Delta^2[&(1+\gamma/\eta)F(s+\gamma/2-\eta/2)\\ &+(1-\gamma/\eta)F(s+\gamma/2+\eta/2)]\}.\end{aligned} \tag{5.15}$$

Here

$$\begin{aligned}\tilde{F(s)} = (1/\omega_c)(2\pi T_B/\omega_c)^{1/2}&\cos(\pi\alpha)\\ &\frac{\Gamma(1-2\alpha)\Gamma(\alpha+s/2\pi T_B)}{\Gamma(1-\alpha+s/2\pi T_B)}.\end{aligned} \tag{5.16}$$

This surprisingly-simple looking expression in (5.15) has rich physics content. When the TN is a very slow process,

$$\tilde{C(s)} \approx 2/\{s + \Delta^2[F(s+2i\delta) + F(s-2i\delta)]\}, \tag{5.17}$$

implying the occurrence of a two-peak structure at 2δ and -2δ, discussed in depth in I. On the other hand, when the TN is extremely rapid,

$$\tilde{C(s)} \approx 2/[s + \Delta^2 F(s + 4\delta^2/\gamma)], \tag{5.18}$$

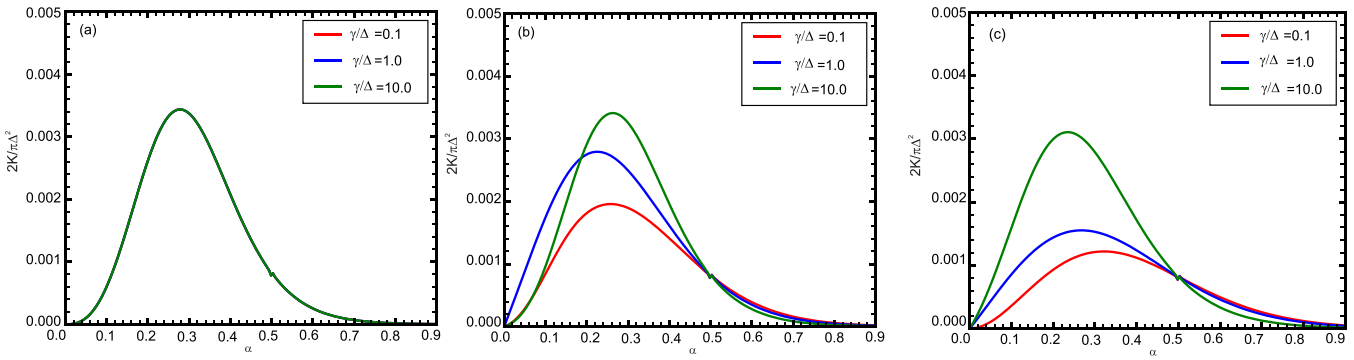

FIG. 2. (a) The energy conductance plotted against the reservoir-induced coupling constant α for $\delta/\Delta = 0$ and for three different values of the jump rate γ/Δ (= 0.1, 1.0, and 10.0) of the TN. Evidently when the site energy is zero the TN has no effect and all three jump rates yield the same curve, leading to the case considered in II. There is a discernible kink at the special value of $\alpha = 0.5$, called the Toulouse limit of the spin-boson model [21] at which $\cos(\pi\alpha)$ and the argument of the gamma function $\Gamma(1-2\alpha)$ change sign. (b) The same as in (a) but now for $\delta/\Delta = 0.5$. Interestingly, when $\gamma/\Delta = 10.0$, rapid relaxation makes the presence of δ nonnoticeable (the so-called motionally averaged limit of the TN) and the graph merges with (a). (c) The same as in (a) and (b) but now for $\delta/\Delta = 1.\ 0$. The phenomenon of motional averaging is visible here as well.

signifying a pole at $s = 0$ and a line shape that has a width, approximately given by $\Delta^2 F(4\delta^2/\gamma)$. In between there is a smooth transition from the result of II to a motionally averaged result, fully displaying the interplay of incoherent quantum tunneling across the mesoscopic junction but further decohered by the TN. Finally, if $\delta = 0$ (no telegraph noise), $\gamma = \eta$, and we recover from Eq. (5.14) the zero-bias case of II:

$$\tilde{C}(s) \approx 2/[s + \Delta^2 F(s)]. \tag{5.19}$$

Final expression for the energy conductance and graphical results

We now collate all the derived steps, in both the text and the Appendix, and collect them together in one place, in arriving at the final result for the energy conductance K, which is more straightforward to compute than the energy current, yet is illustrative of the competition between the reservoir-induced quantum noise and the classical TN arising from the larger heat bath. For computational and graphical purposes, it is convenient to rescale the conductance K and all other parameters (of dimension of frequency or energy) on the right-hand side of Eq. (5.15) by dividing by the tunneling energy Δ. Denoting all the rescaled quantities by a prime on the corresponding symbols we can easily show from Eq. (2.14) that

$$K' = (\alpha/4\pi)\int_0^\infty d\omega'[(\omega'/2T_B')\mathrm{cosech}(\omega'/2T_B')]^2 \omega' \exp(-\omega'/\omega_c')\mathrm{Re}C'(-i\omega'),$$
$$K' = K/\Delta^2, \quad \omega' = \omega/\Delta, \quad T_B' = T_B/\Delta, \quad \omega_c' = \omega_c/\Delta. \tag{5.20}$$

The rescaling of the physical quantities as in the above allows us to discuss the results in terms of dimensionless quantities. Thus, a value 30 for ω_c' implies that the cutoff frequency for bath excitations is taken to be as large as 30 times the bare tunneling frequency, ensuring the nonadiabatic limit (see II).

The Laplace transform of the correlation function, on the other hand, is given by Eq. (5.15),

$$C'(-i\omega') = 2/[-i\omega' + (1+\gamma'/\eta')F'(-i\omega' + \gamma'/2 - \eta'/2) + (1-\gamma'/\eta')F'(-i\omega' + \gamma'/2 + \eta'/2)], \tag{5.21}$$

where [cf. Eq. (5.8)]

$$\eta' \equiv (\gamma'^2 - 16\delta'^2)^{1/2}, \quad \gamma' = \gamma/\Delta, \delta' = \delta/\Delta, \tag{5.22}$$

and $F'(s)$ [cf. Eq. (5.16)]:

$$F'(-i\omega') = (1/\omega_c')(2\pi T_B'/\omega_c')^{2\alpha-1}\cos(\pi\alpha)\Gamma(1-2\alpha) \Gamma(\alpha - i\omega'/2\pi T_B')/\Gamma(1-\alpha-i\omega'/2\pi T_B'). \tag{5.23}$$

As mentioned earlier we have assumed here that $\alpha_L = \alpha_R = \alpha/2$ and $\mathrm{T}_L = \mathrm{T}_R = T_B$.

In presenting the plots for the energy conductance K' as in Eq. (5.20) we use $2K/\pi\Delta^2$ as the y axis with the x axis being given by the (dimensionless) parameter α which arises out of the coupling with the quantum leads and hence is a measure of decoherence. On top of that we have γ/Δ that characterizes dissipation induced by the TN of the heat bath, and hence each panel of Fig. 2 is plotted for three different values of $\gamma/\Delta =$ 0.1, 1.0, and 10.0. Each figure has three graphs, one each for the fluctuating on-site energy $\delta/\Delta = 0$, 0.5, and 1. The other quantum bath parameters: the common temperature T_B/Δ has been taken as $1/2\pi$ and the cutoff frequency ω_c/Δ has been set equal to 30.0. When $\delta/\Delta = 0$ [Fig. 2(a)], the TN is absent, and hence naturally, all the graphs for different values of γ/Δ merge into one and we recover the case studied in II. It is also interesting to note that for $\gamma/\Delta = 10.0$ the graph tends to coincide with Fig. 2(a) even for finite values of δ/Δ [cf. Figs. 2(b) and 2(c)] as we reach the "motionally averaged" limit of the TN. Figure 2(a) (for $\delta/\Delta = 0$) and Fig. 2(b) for the jump rate $\gamma/\Delta = 10.0$ can be directly compared with Fig. 6 in II.

While the presence of quantum noise as characterized by the parameter α is essential for energy conductance (and for energy current for that matter), the graphs show that for small values of α (the weakly decoherent regime) the conductance increases, reaches a maximum, and then decreases, implying

incoherence. The turnover point depends of course on the strength of the classical damping parameter γ: the smaller γ is, the flatter and broader is the energy conductance as the telegraph process tends to give equal weight to the site energies $+\delta$ and $-\delta$.

VI. SUMMARY REMARKS

The popularly employed spin-boson model in the domain of dissipative quantum mechanics is appropriated here in the context of energy transfer in a molecular junction in contact with leads that juxtapose with two bosonic reservoirs kept at a common temperature. A polaron transformation within a resolvent operator treatment of the underlying propagator enables us to elucidate on a wide range of coupling to the reservoirs—from weak to strong damping. The additionally important feature is to ascertain how this mesoscopic phenomenon can be manipulated by tuneable—in terms of the relaxation rate—telegraphic noise (TN). When TN is absent, we recover the previous results of Liu *et al.* (II), while in the absence of the leads we make contact with the two-state jump model, widely used in the theory of spectral line shapes. The present theoretical results can construe a useful supplement to the literature on nonequilibrium statistical mechanics in the regime of nanoscale physics.

The physical significance of our theoretical results is summarized in Fig. 2 in which the energy conductance K is plotted versus the leads-induced decoherence parameter α for three distinct values of the fluctuating (because of the TN) site energy δ, all suitably rescaled as described in the figure caption. There are three different sketches in each figure corresponding to different values of the dissipation parameter γ induced by the TN. This figure then encapsulates the competitive presence of both decoherence (due to the bosonic reservoirs) and incoherence (because of the TN arising from the stochastic bath). The two dissipative parameters α and γ make their presence felt in two distinct manners. The parameter α characterizes the decoherence induced by the quantum baths. When $\alpha = 0$, the coupling with the baths is absent, tunneling is quantum-coherent, and the conductance K vanishes (Fig. 2). Since conductance (inverse of resistance) requires the presence of dissipative effects, some amount of α is essential for nonzero K. However, as α exceeds a certain value tunneling gets suppressed and K starts decreasing (see Fig. 2 and also Fig. 6 of II). On the other hand, the introduction of γ, parametrizing the jump rate of an external telegraph noise, brings a qualitatively different effect on the conductance. When γ is small or the jumps between the asymmetry parameter $+\delta$ and $-\delta$ and vice versa are infrequent, the two-level system exists in an ensemble of asymmetric double wells in which the energy difference between the left well and the right well can be both positive and negative. This implies two poles (i.e., resonance) in the underlying correlation function, analyzed in detail in I. Consequently, this is indicated here by the parameter η' of Eq. (5.8), which becomes imaginary. In such a situation tunneling remains weakly decoherent for small values of α. The same scenario recurs as the jump rate γ becomes large, η' in Eq. (5.8) becomes real, and eventually we reach the motional narrowed limit (*viz.*, the graphs for $\gamma = 10.0$ in Fig. 2). Tunneling is once again weakly decoherent for small values of α. This is why the green ($\gamma' = 10.0$) and red ($\gamma' = 0.1$) graphs coincide for small values of the quantum coupling parameter: $\alpha < 0.1$. However, for an intermediate value of $\gamma' = 1.0$ (blue graph) and especially for the chosen value of δ' as in Fig. 2(b), η' remains imaginary while γ' is sizable leading to a broad distribution (intermediate between a two-pole structure and a single motional-narrowed peak) as is familiar in the theory of spectral line shapes [9]. This is also evident in the context of the correlation function in Eq. (5.17) and (5.18). Understandably, the aforesaid effect is less pronounced for a larger value of $\delta' = 1.0$ as in Fig. 2(c) because the resonance effect is more dominant now than for $\delta' = 0.5$ of Fig. 2(b). The presented results clearly demonstrate the influence of an external noisy environment on the energy transfer characteristics of a nanojunction in contact with leads.

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APPENDIX

1. Energy conductance in terms of spin correlation function

Using the golden rule of perturbation theory, the absorptive part of the susceptibility is given by [cf. Eq. (I.65) and (I.72) of [15]]

$$\chi_z''(\omega) = \Sigma_{if}\rho_i < f|\sigma_z|i >< i|\sigma_z|f > \delta(\omega_{fi} - \omega), \quad \text{(A1)}$$

where ρ_i is the density operator in equilibrium for the ith many-body quantum state $|i>$ and the δ function takes into account energy (or frequency) conservation in the absorption process in which the frequency ω from an external source is absorbed between the final state frequency ω_f and the initial state frequency ω_i. The δ function has the further representation

$$\begin{aligned}\delta(\omega_{fi} - \omega) &= 1/\pi \lim_{\Gamma\to 0}\Gamma/[\Gamma^2 + (\omega_{fi} - \omega)^2] \\ &= 1/\pi \lim_{\Gamma\to 0}\mathrm{Re}\int_0^\infty dt\, \exp[-t(\Gamma + i\omega + i\omega_{fi})].\end{aligned} \quad \text{(A2)}$$

Substituting in Eq. (A1),

$$\begin{aligned}\chi_z''(\omega) &= 1/\pi \lim_{\Gamma\to 0}\mathrm{Re}\int_0^\infty dt\, \exp[-t(\Gamma + i\omega)]\Sigma_{if}\rho_i \\ &\quad \times < f|\sigma_z|i >< i|\exp(i\omega_I t)\sigma_z \exp(-i\omega_f t)|f > \\ &= 1/\pi \lim_{\Gamma\to 0}\mathrm{Re}\int_0^\infty dt\, \exp[-t(\Gamma + i\omega)] \\ &\quad \times < \sigma_z(0)\sigma_z(t) >,\end{aligned} \quad \text{(A3)}$$

where we have employed the Heisenberg time evolution in writing $\sigma_z(t)$ (recalling that the Planck constant $\hbar$ is unity) and rewritten the summations over i and f with the weight ρ_i as a statistical mechanical expectation value denoted by the

angular brackets $< \cdot >$. Finally, we can write

$$\chi_z''(\omega) = 1/\pi \lim_{\Gamma\to 0} \mathrm{Re}\tilde{C}(s), \tag{A4}$$

where the Laplace transform of the correlation function has been introduced in the main text [cf. Eq. (3.1)].

2. Averaged time-development operator

We may define

$$G_{\pm}(s+\gamma) = [s+\gamma - i/2(\varepsilon \pm \delta)\sigma_z^{\times} - \tilde{H_I^{\times}} - iH_B^{\times}]^{-1}, \tag{A5}$$

so that

$$[U_o(s+\gamma)]_{av} = [G_+(s+\gamma) + G_-(s+\gamma)]/2. \tag{A6}$$

Having carried out the stochastic average our stated aim is to now perform a statistical average over the quantum states of the bath (leads) Hamiltonian. To this end we would like to treat the effective tunneling contained in $\tilde{H_I^{\times}}$ perturbatively, up to second order as in [29,30]. Thus,

$$\begin{aligned}[U_o(s+\gamma)]_{av}^{-1} = R^{-1}(s+\gamma) + \tfrac{1}{2}R^{-1}(s+\gamma)\big\{ &- i[P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)] \\ &+ P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)H_I^{\times}P_-(s+\gamma) \\ &- \tfrac{1}{2}[P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)]R^{-1}(s+\gamma) \\ &\times [P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)]\big\}R^{-1}(s+\gamma).\end{aligned}$$

where

$$\begin{aligned}P_{\pm}(s+\gamma) &= [s+\gamma - i/2(\varepsilon \pm \delta)\sigma_z^{\times} - iH_B^{\times}]^{-1}, \\ R(s+\gamma) &= [P_+(s+\gamma) + P_-(s+\gamma)]/2.\end{aligned} \tag{A7}$$

Recognizing that [cf. Eq. (4.5)],

$$[U(s)]_{av} = \{[U_o(s+\gamma)]_{av}^{-1} - \gamma\}^{-1}, \tag{A8}$$

we subtract γ, and rewrite

$$\begin{aligned}[U_o(s+\gamma)]^{-1} - \gamma = Q^{-1}(s)(1 + \tfrac{1}{2}Q(s)R^{-1}(s+\gamma)\{&-i[P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times} + P_-(s+\gamma)] \\ &+ P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)H_I^{\times}P_-(s+\gamma) \\ &- \tfrac{1}{2}[P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)]R^{-1}(s+\gamma) \\ &\times [P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)]\}R^{-1}(s+\gamma)),\end{aligned}$$

where

$$\begin{aligned}Q^{-1}(s) = R^{-1}(s+\gamma) - \gamma = s - i\varepsilon/2\sigma_z^{\times} - iH_B^{\times} \\ + (\delta/2\sigma_z^{\times})^2/(s+\gamma - i\varepsilon/2\sigma_z^{\times} - H_B^{\times}).\end{aligned} \tag{A9}$$

Note that $P(s)$, $Q(s)$, and $R(s)$ only involve commuting super-operators $\sigma_z^{\times}$ and $H_B^{\times}$, and hence, do not require any specific ordering in writing them out.

Taking a further inverse and ignoring terms linear in $H_I^{\times}$ because they would eventually average out to zero (over the quantum baths),

$$\begin{aligned}[U(s)]_{av} = \{[U_o(s+\gamma)]_{av}^{-1} - \gamma\}^{-1} = Q(s) - \frac{1}{2}Q(s)R^{-1}(s+\gamma)[P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) \\ + P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)]R^{-1}(s+\gamma)Q(s) + \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) \\ \times R^{-1}(s+\gamma)P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)R^{-1}(s+\gamma)R^{-1}(s+\gamma)Q(s) + \frac{1}{4}Q(s)R^{-1}(s+\gamma)H_I^{\times}P_-(s+\gamma) \\ \times R^{-1}(s+\gamma)P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)R^{-1}(s+\gamma)Q(s) + \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_+(s+\gamma)H_I^{\times}P_+(s+\gamma) \\ \times R^{-1}(s+\gamma)P_-(s+\gamma)H_I^{\times}P_-(s+\gamma)R^{-1}(s+\gamma)Q(s) + \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_-(s+\gamma)H_I^{\times}P_-(s+\gamma) \\ \times R^{-1}(s+\gamma)P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)R^{-1}(s+\gamma)Q(s) - \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_+(s+\gamma)H_I^{\times}P_+(s+\gamma)R^{-1}(s+\gamma)Q(s)\end{aligned}$$

$$\times R^{-1}(s+\gamma)P_+(s+\gamma)H_I^\times P_+(s+\gamma)P_+(s+\gamma)R^{-1}(s+\gamma)Q(s) - \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_-(s+\gamma)H_I^\times P_-(s+\gamma)$$
$$\times R^{-1}(s+\gamma)Q(s)R^{-1}(s+\gamma)P_-(s+\gamma)H_I^\times P_-(s+\gamma)R^{-1}(s+\gamma)Q(s) - \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_+(s+\gamma)H_I^\times P_+(s+\gamma)$$
$$\times R^{-1}(s+\gamma)Q(s)R^{-1}(s+\gamma)P_-(s+\gamma)H_I^\times P_-(s+\gamma)R^{-1}(s+\gamma)Q(s) - \frac{1}{4}Q(s)R^{-1}(s+\gamma)P_-(s+\gamma)H_I^\times P_-(s+\gamma)$$
$$\times R^{-1}(s+\gamma)Q(s)R^{-1}(s+\gamma)P_+(s+\gamma)H_I^\times P_+(s+\gamma)R^{-1}(s+\gamma)Q(s). \quad \text{(A10)}$$

In order to establish the veracity of the rather long algebraic expression in (A10) we may carry out the customary check on two special cases.

(1) The first is somewhat trivial, namely, the limit of zero tunneling when $H_I^\times$ vanishes, consequently making $H_B^\times$ ineffective. In that case, barring the first term on the right of Eq. (A6), all other terms go to zero, and we are left with [cf. Eqs. (A8) and (A9)]

$$[U(s)]_{av} = Q(s) = \{s - i\varepsilon/2\sigma_z^\times + (\delta/2\sigma_z^\times)^2/ [s+\gamma - i\varepsilon/2\sigma_z^\times]\}^{-1}, \quad \text{(A11)}$$

a standard result that finds a place in the line shape expressions under the TN [see, for instance, Eq. (VIII. 30) or Eq. (VIII. 51) of [9]].

(2) The second limiting case of no TN ($\delta = 0$) is a bit more involved. Now [cf. Eq. (A7) and Eq. (A9)],

$$P_\pm(s+\gamma) = (s+\gamma - i\varepsilon/2\sigma_z^\times - iH_B^\times)^{-1} = R(s+\gamma),$$
$$Q(s) = (s - i\varepsilon/2\sigma_z^\times - iH_B^\times)^{-1}. \quad \text{(A12)}$$

The second through sixth terms on the right of Eq. (A10) together cancel out, whereas the last four terms are all identical, thus yielding

$$[\tilde{U}(s)]_{av} = Q(s)[1 - H_I^\times Q(s)H_I^\times Q(s)]. \quad \text{(A13)}$$

We note from Eq. (4.1) that the problem at hand involves a further averaging in Eq. (A3) over the diagonal states of the quantum baths, indicated there by double angular brackets. Now, the super-operator $Q(s)$ on its own on either side of $H_I^\times$, when averaged as such, would be left devoid of $H_B^\times$ (see Appendix A 1 of [30]), hence

$$\ll [\tilde{U}(s)]_{av} \gg = Q_o(s)[1 - << H_I^\times Q(s)H_I^\times >> Q_o(s)],$$
$$Q_o(s) = (s - i\varepsilon/2\sigma_z^\times)^{-1}, \quad \text{(A14)}$$

which can be further rearranged to yield

$$\ll [\tilde{U}(s)]_{av} \gg = [Q_o^{-1}(s) + << H_I^\times Q(s)H_I^\times >>]^{-1}$$
$$= [s - i\varepsilon/2\sigma_z^\times + \Sigma(s)]^{-1}, \quad \text{(A15)}$$

where $\Sigma(s)$ is the so-called self-energy defined by

$$\Sigma(s) = \ll H_I^\times Q(s)H_I^\times \gg . \quad \text{(A16)}$$

The Laplace transform of the time-development operator, as given in Eq. (A5) is identical to that for dissipative tunneling in an asymmetric double well under the so-called dilute bounce gas approximation or NIBA [see Eq. (8.49) of [30]]. As it turns out, this result is also completely equivalent to the corresponding PT-NEGF expression, derived for the imaginary part of the pseudospin susceptibility in II for what that paper calls the0 biased case, as is further discussed in the text.

Having confirmed that the algebraic expression in Eq. (A10) does reduce to the expected results in the separate instances of TN and dissipative tunneling in a two-state system we now turn our attention to the core issue at hand, namely, to assess the interplay of a mesoscopic tunnel junction leaking energy and particle currents to two leads modeled as bosonic baths. Because the TN, at least in the slow-relaxation limit ($\gamma \ll \delta$), does create two distinct "biases" $+\delta$ and $-\delta$ we may ignore ε in further considerations, in order to simplify the algebra.

Recall that the central quantity of interest $\ll [\tilde{U}(s)]_{av} \gg$ is just a 4×4 matrix in the Liouville operator space of $\sigma_z^\times$ and that the special nature of the spin-correlation function is such that only the left, upper block of the matrix labeled by $|++), |--), |+-)$, and $|-+)$, respectively, is relevant, as is made clear in Eq. (4.1). Within that subspace the operators like $\sigma_z^\times$ and $(\sigma_z^\times)^2$, taken separately, make no contribution. Therefore, ignoring also $H_B^\times$ in terms on either side of the right-hand side of Eq. (A10) (as argued earlier) the matrix of $\ll [U(s)]_{av} \gg$ within the upper left block can be simplified as

$$\ll [\tilde{U}(s)]_{av} \gg = \frac{1}{s} - \frac{1}{2}(1/s)^2 \ll H_I^\times [P_+(s+\gamma) + P_-(s+\gamma)]H_I^\times \gg + \frac{1}{4}(1/s)^2 \ll H_I^\times R^{-1}(s+\gamma) [P_+(s+\gamma) + P_-(s+\gamma)]^2 H_I^\times \gg + \frac{1}{4}(1/s)^2 \ll H_I^\times Q(s)R^{-2}(s+\gamma)[P_+(s+\gamma) + P_-(s+\gamma)]^2 H_I^\times \gg, \quad \text{(A17)}$$

This expression is drastically reduced by noting that [cf. Eq. (A7)] the P's sum to $2R$, and therefore, the second line on the right of Eq. (A7) vanishes, leaving

$$\ll [\tilde{U}(s)]_{av} \gg = 1/s - (1/s)^2 \ll H_I^\times Q(s) H_I^\times \gg \approx [s + \ll H_I^\times Q(s)H_I^\times \gg]^{-1}, \quad \text{(A18)}$$

where $Q(s)$ is now given by Eq. (A1). The self-energy [cf. Eq. (A16)] then is

$$\Sigma(s) = \ll H_I^\times \{s - iH_B^\times + (\delta/2\sigma_z^\times)^2/ [(s+\gamma) - iH_B^\times]\}^{-1} H_I^\times \gg . \quad \text{(A19)}$$

This is one of the principal results of our paper signifying the combined effects of TN and dissipative tunneling.

3. Computation of self-energy

Our first focus is on the positive branch of the self-energy $\Sigma_+(s)$. Given that we are interested in only the left upper block of the 4×4 matrix elements of $\Sigma_+(s)$, we may write

$$\begin{aligned}(\mu\mu|\Sigma_+(s)|\nu\nu) = \Sigma_{\mu'\nu'}\Sigma_{i_B,i_{B'}}\Sigma_{j_B,j_{B'}} &< i_B|\rho_B|i_B > \\ &\times (\mu i_B \mu i_B|H_I^{\times}|\mu' j_B \nu' j_{B'}) \\ &\times [\mu' j_B \nu' j_{B'}|Q_+(s)|\mu' j_B \nu' j_{B'}] \\ &(\mu' j_B \nu' j_{B'}|H_I^{\times}|\nu i_{B'} \nu i_{B'}),\end{aligned} \tag{A20}$$

where ρ_B is the density operator for the quantum bath comprising the two leads, which, in the present instance, is governed by the Bose-Einstein statistics.

The next steps involve expanding Eq. (A20) by writing out the matrix elements of the Liouvillian $H_I^{\times}$ and following the lines of argument as in the Appendix of chapter VII of [30]. We find

$$\begin{aligned}&(\mu\mu|\Sigma_+(s)|\nu\nu) \\ &= \Sigma_{i_B} < i_B|\rho_B|i_B > (\delta_{\mu\nu}\Sigma_{\mu',j_B} \\ &\times \{< \mu i_B|H_I|\mu' j_B >< \mu' j_B|H_I|\mu i_B > \\ &\times (\mu' j_B \mu i_B|Q_+(s)|\mu' j_B \mu i_B) + < \mu i_B|H_I|\mu' j_B > \\ &\times < \mu' j_B|H_I|\mu i_B > (\mu i_B \mu' j_B|Q_+(s)|\mu i_B \mu' j_B)\} \\ &- \Sigma_{i_{B'}} < \mu i_B|H_I|\nu i_{B'} >< \nu i_{B'}|H_I|\mu i_B > \\ &\times \{(\mu i_B \nu i_{B'}|Q_+(s)|\mu i_B \nu i_{B'}) + (\nu i_{B'} \mu i_B|Q_+(s)|\nu i_{B'} \mu i_B)\}).\end{aligned} \tag{A21}$$

From this we directly go to the four relevant matrix elements, upon employing the expression for $Q_+(s)$ in Eq. (5.5):

$$\begin{aligned}&(++|\Sigma_+(s)|++) \\ &= -(++|\Sigma_+(s)|--) = 1/4\Delta^2 \\ &\times (1+\gamma/\eta)\int_0^\infty dt e^{-st}\exp[-t(\gamma-\eta/2)] \\ &\times [<< A_L^-(0)A_R^-(0)A_L^+(t)A_R^+(t) \gg \\ &+ << A_L^-(t)A_R^-(t)A_L^+(0)A_R^+(0) \gg], \\ \\ &(--|\Sigma_+(s)|--) \\ &= -(--|\Sigma_+(s)|++) = 1/4\Delta^2 \\ &\times (1+\gamma/\eta)\int_0^\infty dt e^{-st}\exp[-t(\gamma-\eta/2)] \\ &\times [<< A_L^+(0)A_R^+(0)A_L^-(t)A_R^-(t) \gg \\ &+ << A_L^+(t)A_R^+(t)A_L^-(0)A_R^-(0) \gg],\end{aligned} \tag{A22}$$

where we have used the Heisenberg time evolution of the operators $A_{L,R}^{\pm}$ occurring in the interaction Hamiltonian H_I in Eq. (3.7) and have defined

$$\eta \equiv (1-\gamma^2/4\delta^2)^{1/2}. \tag{A23}$$

The corresponding matrix elements of $\Sigma_-(s)$ are simply obtained by replacing the η by $-\eta$.

Because the L and R baths are statistically independent, the correlation functions, indicated by double angular brackets in Eq. (A5) factor, thus

$$\begin{aligned}&\ll A_L^-(0)A_R^-(0)A_L^+(t)A_R^+(t) \gg \\ &=\ll A_L^-(0)A_L^+(t) \gg \ll A_R^-(0)A_R^+(t) \gg \equiv \phi(t).\end{aligned}$$

In addition,

$$\begin{aligned}&\ll A_L^+(0)A_R^+(0)A_L^-(t)A_R^-(t) \gg \\ &=\ll A_L^+(0)A_L^-(t) \gg = \ll A_R^+(0)A_R^-(t) \gg \equiv \phi(t).\end{aligned}$$

Furthermore,

$$\begin{aligned}&\ll A_L^-(t)A_R^-(t)A_L^+(0)A_R^+(0) \gg \\ &=\ll A_L^-(t)A_L^+(0) \gg \ll A_R^-(t)A_R^+(0) \gg = \phi(-t).\end{aligned} \tag{A24}$$

Substituting in Eq. (A2),

$$\begin{aligned}&(++|\Sigma_+(s)|++) \\ &= (--|\Sigma_+(s)|--) \\ &= -(--|\Sigma_+(s)|++) = -(++|\Sigma_+(s)|--) = \frac{1}{4}\Delta^2 \\ &\times (1+\gamma/\eta)\int_0^\infty dt e^{-st}\exp[-t(\gamma-\eta)/2][\phi(t)+\phi(-t)].\end{aligned} \tag{A25}$$

The (product) correlation function is given by Eq. (8.27) of [30] [also compare with Eq. (39) of II],

$$\phi(t) = \exp[i\alpha\pi\,\mathrm{sgn}(t)]\{\pi T_B/[\omega_c \sinh(\pi T_B|t|]\}^{2\alpha}, \tag{A26}$$

where α is defined in Eq. (II.13). In writing Eq. (A9) we have assumed that the two quantum baths are at the same temperature T_B (i.e., $T_L = T_R = T_B$), which is taken to be much smaller than the cutoff frequency ω_c (in appropriate units). As expected, in the limit of zero relaxation ($\gamma = 0$, i.e., no TN), Eq. (A5) matches the self-energy in Eq. (8.50) of [30]. The Laplace transform of $\phi(t)$ [cf. Eq. (8.53) of [30]] is

$$\begin{aligned}\tilde{\phi}(s) = \frac{1}{\omega_c}\exp(i\alpha\pi)(2\pi T_B/\omega_c)^{2\alpha-1}[\Gamma(1-2\alpha) \\ \times \Gamma(\alpha + s/(2\pi T_B)]/[\Gamma(1-\alpha+s/(2\pi T_B)],\end{aligned} \tag{A27}$$

$\Gamma(\cdot)$ being the Gamma function. Equations (A6) and (A7) are in complete agreement with Eqs. (39) and (44) of II, respectively, though in the latter a very different method, *viz.*, the nonequilibrium Green's function treatment of Keldysh, was employed.

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