Time-loop formalism for irreversible quantum problems: Steady-state transport in junctions with asymmetric dynamics

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Nonunitary quantum mechanics has been used in the past to study irreversibility, dissipation, and decay in a variety of physical systems. In this work, we employ a general scheme to deal with systems governed by non-Hermitian Hamiltonians. We argue that the Schwinger-Keldysh formalism gives a natural description for those problems. To elucidate the method, we study a simple model inspired by mesoscopic physics—an asymmetric junction. The system is governed by a non-Hermitian Hamiltonian, which captures essential aspects of irreversibility.

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Non-Hermitian formulations of quantum-mechanical problems have attracted substantial interest in almost all areas of physics. In most cases, nonunitary approaches are utilized to describe irreversible processes—such as decay and dissipation—in open quantum systems. This kind of problems has been addressed since the early days of quantum mechanics when the complex eigenvalue method was pioneered to describe the α decay of nuclei.[1,2] Since then, nonunitary approaches have been applied to theories of K and B meson decay,[3,4] scattering and absorption of particles by nuclei,[5] nuclear reactions,[6,7] multiphoton ionization of atoms,[8,9] optical resonators,[10] and free-electron lasers.[11] Growth models have been investigated by mapping a master equation into a Shrödinger equation with a non-Hermitian Hamiltonian.[12] In the last decade, non-Hermitian theories were also applied to condensed-matter systems with localization-delocalization transitions. Pinning/depinning of flux lines from columnar defects was studied[13] in type-II superconductors, and the effects of a single columnar defect on fluctuating flux lines was considered by mapping to a non-Hermitian Luttinger liquid model and using the density-matrix renormalization group (DMRG).[14] Generalized DMRG has been applied also to a one-dimensional reaction-diffusion model with nonunitary time evolution[15] and a non-Hermitian spin-1/2 Heisenberg chain.[16] The closing of the Mott gap has been investigated in the non-Hermitian Hubbard model[17] and evaporatively cooled Bose-Einstein condensates (BECs) have been studied by a nonunitary quantum dynamics approach.[18] All of the above studies use a variety of case-specific methods and are mainly concerned with either time-independent or transient behaviors. In addition, usually a particular class of non-Hermitian problems is discussed, a case when the energy eigenstates have only negative imaginary parts (thus describing only decay or dissipation). In this paper we present a framework that we apply to a steady-state formulation of an irreversible system.

To define our approach we start with the Schwinger-Keldysh (SK) formalism,[19,20] which turns out to be very natural in the non-Hermitian case. In the SK formulation, the evolution of a system is described on a time loop (Keldysh contour, K) with "forward" ("−") and "backward" ("+") directions (see Fig. 1), thus defining two distinct branches for time evolution. Special care should be taken to define proper evolution operators for each direction. One could argue that the time evolution operator is the same along the full path, as in the Hermitian case, $\hat{U}_K(t,t_0)=\hat{U}_+\hat{U}_-=T_K e^{-i\int_{t_0}^{t}dt'\hat{H}(t')}$ (where T_K is the time-ordering operator along the Keldysh contour), which preserves the normalization along the contour, $\hat{U}_K(t_0^+,t_0^-)=\mathbb{1}$. This would mean that the time evolution would be governed by $\hat{H}$ on both branches. Even though this choice ensures that the backward evolution is the algebraic inverse of the forward one and it may seem a good choice, we should emphasize that it does not describe the physical process faithfully. Physically, in the backward branch, the system should *rewind* its forward evolution and therefore $\hat{H}^{\dagger}$ should be the operator that dictates the dynamics. Then the backward time evolution operator is given by $\hat{U}_+(t_0,t)=\hat{U}_-^{\dagger}(t,t_0)$ $=\widetilde{T}e^{i\int_{t_0}^{t}dt'\hat{H}^{\dagger}(t')}\neq\hat{U}_-^{-1}(t,t_0)$, which is automatically antitime ordered (with $\widetilde{T}$ representing the antitime-ordering operator).[32] Of course, one recovers the familiar result in the Hermitian case. We see that a double-time approach is essential and rather natural for non-Hermitian problems. Thus, the + branch is governed by the Hermitian conjugate theory and the time-ordered Green's function (G^{--}) is mapped into the antitime-ordered one (G^{++}) by Hermitian conjugation, which is all natural and unambiguous in a time-loop formalism. This makes an extended SK method an appealing choice.[33]

To illustrate the formalism, we shall study a simple model of a single-mode asymmetric tunneling junction (see inset of Fig. 2), which captures essential aspects of irreversibility. A similar model has been studied in connection with spin-valve devices.[21] We shall study the steady-state transport of the

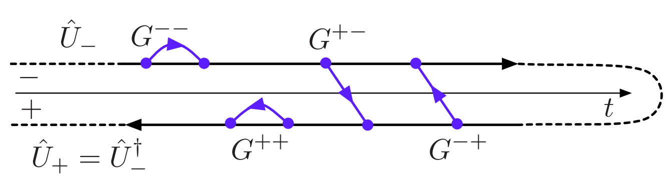

FIG. 1. (Color online) Sketch of the Keldysh contour. The arrows show the direction of the time evolution. Here G^{--} is the time-ordered Green's function, G^{++} is the antitime-ordered Green's function, G^{+-} is the "greater" Green's function, and G^{-+} is the "lesser" Green's function.

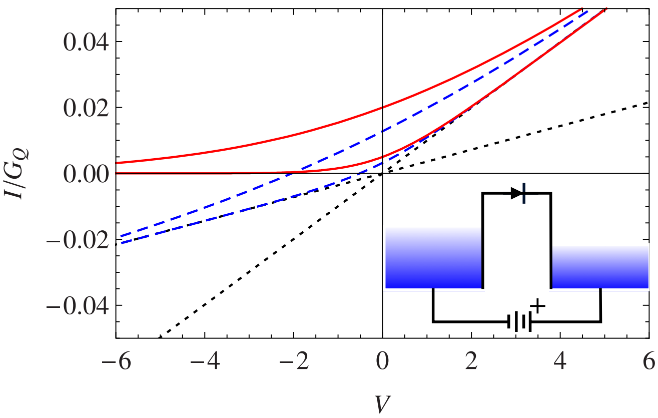

FIG. 2. (Color online) Current, I, as a function of voltage, V, for different temperatures (in arbitrary units). The current is shown for $t_R = t_L = 0.05$ and $t_R = t_L = 0.03$ (SJ case, dotted lines), for $t_R = 0.05$ and $t_L = 0.03$ (dashed lines), and for $t_R = 0.05$ and $t_L = 0$ (solid lines). The temperature increases from bottom to top and G_Q indicates the quantum of conductance. Inset: Sketch of the tunneling setup.

system. The Hamiltonian of the model is given by $\hat{H} = \hat{H}_0 + \hat{H}_t$, where

$$\hat{H}_0 = \sum_{r=R,L} \hat{H}_{0,r} = -iv \sum_{r=R,L} \int dx \hat{\psi}_r^\dagger(x) \partial_x \hat{\psi}_r(x) \tag{1}$$

describes noninteracting left (L) and right (R) leads in a one-dimensional formulation.[22] $\hat{\psi}_r^\dagger(x)$ $[\hat{\psi}_r(x)]$ represent electron creation [annihilation] operators in the corresponding lead and v is the Fermi velocity, which is taken to be the same for both leads.

The irreversible nature of the problem is given by

$$\hat{H}_t = 2v \sum_{r \neq r'} t_r \hat{\psi}_r^\dagger(x=0) \hat{\psi}_{r'}(x=0), \tag{2}$$

which describes the tunneling with rates $t_L \neq t_R^*$ in the asymmetric junction (AJ) case.[34] (In this paper, $k_B = \hbar = e = 1$.)

Let us derive a local theory that captures the essential physics of the junction. After integrating out the leads exactly for $x \neq 0$ in a path-integral formulation (dropping the coordinate dependence of the electron creation and annihilation operators), the local action reads[22,23]

$$\mathcal{A} = \int_{-\infty}^{\infty} \bar{\Psi}(t) \mathbf{G}^{-1}(t-t') \Psi(t') dt dt', \tag{3}$$

where $\Psi = (\psi_L^- \ \ \psi_R^- \ \ \psi_L^+ \ \ \psi_R^+)^T$. We have doubled the basis of the problem, which is customary in the SK formulation, and assigned extra indices − and + to the fields according to the particular branch of the Keldysh contour they belong to. In Eq. (3), we explicitly imposed the steady-state constraint by specifying the time dependence of the inverse Green's function $\mathbf{G}^{-1}$. In the steady state, the Green's function depends only on the time difference, $t-t'$, and not on the "center-of-mass" time $(t+t')/2$. Thus, the Fourier transform (with respect to the time difference) is given by

$$\frac{\mathbf{G}^{-1}(\omega)}{-2vi} = \begin{pmatrix} -s_L & -it_L & s_L - 1 & 0 \\ -it_R & -s_R & 0 & s_R - 1 \\ s_L + 1 & 0 & -s_L & it_R^* \\ 0 & s_R + 1 & it_L^* & -s_R \end{pmatrix}, \tag{4}$$

where $s_r = \tanh\frac{\omega - \mu_r}{2T_r}$. Here, we assumed that the leads are in equilibrium at their respective chemical potentials (μ_L and μ_R) and temperatures (T_L and T_R).

Using Green's functions, we can calculate the transport properties of a generic AJ. By comparing to the symmetric junction (SJ) case, one sees the effects due to the nonunitary nature of the tunneling dynamics.

Current—We first describe a current flowing across the junction. We expect that there should be an asymmetry between positive and negative voltage bias. We define the current operator in the usual way by $\hat{I} = \frac{1}{2}\partial_t \Delta\hat{N}$, where $\Delta\hat{N} = \hat{N}_R - \hat{N}_L$, and $\hat{N}_L$ and $\hat{N}_R$ are the particle number operators for the left and right leads, respectively. While the current operator is defined by the above formula, for an AJ the definition needs to be supplemented by specifying on which branch $\Delta\hat{N}$ resides. On the − branch, the current operator is given by $\hat{I}^- = \frac{1}{2}\partial_t \Delta\hat{N}^- = \frac{i}{2}[\hat{H}, \Delta\hat{N}^-]$, since $\hat{H}$ governs the time evolution on this branch. This prompts us to use the time-ordered ("−−" component) Green's functions for calculations. The current is thus given by (cf. Ref. 24)

$$I^- = 2v \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [t_L G_{RL}^{--}(\omega) - t_R G_{LR}^{--}(\omega)]. \tag{5}$$

Of course, we get the same final results if we do calculations on the + branch. In this case, the current operator reads $\hat{I}^+ = \frac{1}{2}\partial_t \Delta\hat{N}^+ = \frac{i}{2}[\hat{H}^\dagger, \Delta\hat{N}^+]$, in analogy with the − branch. Here $\hat{H}^\dagger$ defines the time evolution and we should use the antitime-ordered ("++" component) Green's functions. Now the current has the same form as in Eq. (5) but with time-ordered Green's functions replaced by antitime-ordered ones and $t_{L/R} \to t_{R/L}^*$. Direct calculations indeed show that $I^- = I^+ = I$.

In the SJ limit, calculations can be done analytically and the current is given by $I = GV$, where $G = \frac{2|t|^2}{\pi(1+|t|^2)^2}$ (Ref. 25) and $V = \mu_L - \mu_R$. The well-known symmetry of the conductance in the SJ case, $|t| \to 1/|t|$, is generalized to $t_{R/L} \to 1/t_{L/R}^*$ for the AJ one. The results for the current in the weak tunneling limit are shown on Fig. 2, where we see the anticipated asymmetric behavior for unequal tunneling strengths. For large voltages the behavior is similar to the SJ case with the corresponding tunneling rate ($t = t_R, t_L$ for positive or negative bias, respectively). In the extreme limit when $t_L = 0$, we see a clear diodelike behavior. The results also show temperature dependence (that disappears in the SJ limit), in particular, the current is nonzero for zero voltage due to finite temperature effects ($I_0 \propto T$). For intermediate and large tunneling strengths, the current is significantly different from the SJ value even for large voltages. This can be seen on Fig. 3, which shows the conductance as a function of tunneling rate.

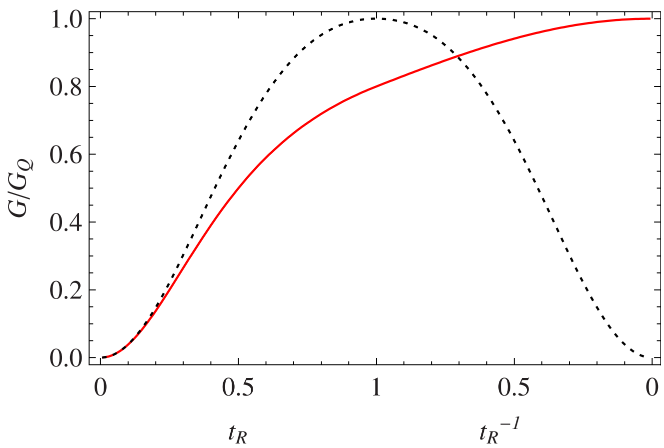

FIG. 3. (Color online) Large-voltage conductance as a function of tunneling strength (t_R) for a SJ, $t=t_R$ (dotted line), and in the extreme AJ case, $t_L=0$ (solid line).

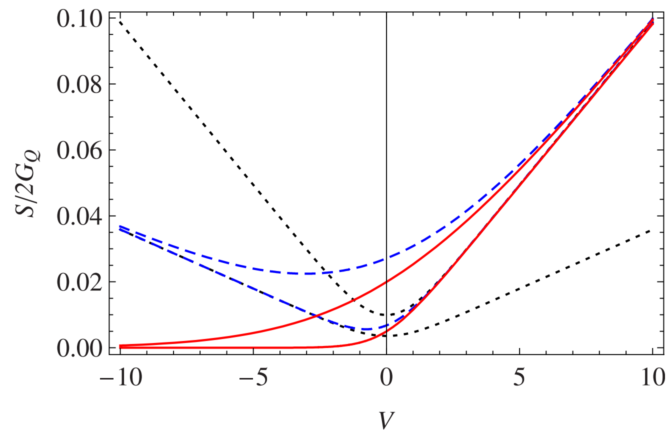

FIG. 4. (Color online) Current noise power, $S(\omega=0)$, as a function of voltage, V, for different temperatures (in arbitrary units). The line styles and parameters are the same as in Fig. 2.

The behavior of the conductance can be understood in terms of a perturbative expansion. For weak tunneling ($t,t_R \ll 1$), the expansions for the symmetric and asymmetric cases are identical (i.e., the leading orders coincide). While for intermediate tunneling ($t,t_R \sim 1$), many processes that are allowed for the SJ are not allowed for the extreme asymmetric one; hence the reduction of the conductance. For large tunneling strengths ($t,t_R \gg 1$), the conductance decreases in the SJ case due to a resonance developing at the junction. In the AJ case, this resonance is suppressed and, therefore, the conductance increases and saturates at the quantum of conductance in the limiting case ($t_R \to \infty$).

Noise—Now we turn to the noise, which is a ω-dependent response.[25,26] Bearing in mind the SK formalism, we define the current-current correlation function as

$$S(t,t') = \sum_{\eta \neq \eta'} \langle T_K :\hat{I}^{\eta}(t)::\hat{I}^{\eta'}(t'):\rangle, \tag{6}$$

where :: denotes normal ordering and is equivalent to the standard definition given in the literature.[25]

From the definitions of the current operators on the corresponding branches, using Wick's theorem[27] and Fourier transforming, we get the current noise power

$$\frac{S(\omega)}{4v^2} = \sum_{r\neq r'} t_r t_r^{*}[(G_{rr}^{+-} \circ G_{r'r'}^{-+}) + (G_{r'r'}^{-+} \circ G_{rr}^{+-})] - \sum_{r\neq r'} t_r t_{r'}^{*}[(G_{r'r}^{+-} \circ G_{r'r}^{-+}) + (G_{r'r}^{-+} \circ G_{r'r}^{+-})],$$

where the correlation product $(G_1 \circ G_2)(\omega)$ is defined as usual.[26] In the SJ limit, we get the well established result[25]

$$S(\omega=0) = 8\pi G^2 T + 2G(1-2\pi G)V \coth\frac{V}{2T}. \tag{7}$$

The dependence of $S(\omega=0)$ on bias voltage and temperature for weak tunneling is shown in Fig. 4. The results show similar asymmetric behavior as for the current. For large voltages, the behavior of the noise power is similar to that of the SJ with the corresponding tunneling rate (in exact analogy with the behavior of the current). In the limiting case with $t_L=0$, we see the suppression of the noise for negative voltage bias, which is consistent with the diodelike behavior and is due to the reduction of the current in this regime (see Fig. 2). In the shot-noise limit ($V \gg T$), the Fano factor $F \equiv S(\omega=0)/(2I)=1$ for weak tunneling, as in the SJ case.

Heat current—Now we shall turn to the thermal conductivity, calculate the heat current, I_Q, and check the Wiedemann-Franz law. To define the heat current, we use the first law of thermodynamics to write

$$đ\Delta Q = d\Delta E + \mu_L dN_L - \mu_R dN_R, \tag{8}$$

where $\Delta Q = Q_R - Q_L$ and $\Delta E = \langle \hat{H}_{0,R} - \hat{H}_{0,L}\rangle$. By using the usual definitions for the currents, choosing a particular branch (−) on the Keldysh contour, and defining the average chemical potential $\bar{\mu}=(\mu_L+\mu_R)/2$, we get $I_Q^- = I_E^- - \bar{\mu} I^-$. Using the equations of motion for the electron creation and annihilation operators, and performing some algebra, the heat current reads

$$I_Q^- = 2v \int \frac{d\omega}{2\pi}(\omega - \bar{\mu})[t_L G_{RL}^{--}(\omega) - t_R G_{LR}^{--}(\omega)]. \tag{9}$$

Our calculations on the backward branch yield $I_Q^+ = I_Q^- = I_Q$, in exact analogy with the result for the electric current. In the SJ case, we obtain the well-known result[28] $I_Q = K\Delta T$ with $K = \frac{2\pi \bar{T}|t|^2}{3(1+|t|^2)^2}$, where $\Delta T = T_L - T_R$ and $\bar{T}=(T_R+T_L)/2$. The Wiedemann-Franz law holds and is given by $K/(G\bar{T}) = \pi^2/3 \equiv L_0$, the Lorentz number.

In general, if bias voltages and temperature gradients are applied, the electric and heat currents are given by

$$I = L_{11}V + L_{12}\Delta T + I_0,$$

$$I_Q = L_{21}V + L_{22}\Delta T. \tag{10}$$

For the SJ case, $L_{11}=G$, $L_{22}=K$, and $L_{12}=L_{21}=0$, so no thermoelectric effects are observed. For the AJ case, expanding the result to linear order in V and ΔT, we see that still $L_{12} = L_{21}=0$. (Notice that thermoelectric effects are observed in this case but not at the linear order.) In terms of the transport coefficients, the Lorentz number is defined as $L_{22}/(L_{11}\bar{T})$. Our calculations show deviations from the Wiedemann-Franz law. This behavior is due to the same effects as in the case of the conductance and the presence of the nonzero I_0 for the AJ case; $L_0 \simeq \pi^2/3$ for small tunneling strengths, but it increases as the strength increases.

We have presented a minimal extension of the Schwinger-Keldysh formalism to systems with non-Hermitian Hamiltonians and have shown that it is a natural choice for such applications. As an example, we have studied a simple model of an asymmetric tunneling junction where irreversibility is explicitly encoded into the Hamiltonian; hence making it non-Hermitian. We have calculated the steady-state transport properties of the junction and seen that the behavior of the observables goes along with our physical expectations for the model. The approach is not limited to systems with steady states and can be used to address general nonequilibrium situations. We intend to apply it, for instance, to study the formation and evaporation dynamics of interacting BECs, where a steady state is not achieved, and explore regimes (e.g., the unitary limit) that are not accessible with present methods.

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[32] The described ambiguity in the definition of the evolution operator stems form the convention arbitrariness of the time-independent density matrix for non-Hermitian problems (Refs. 14 and 29). Our identification singles out a particular choice, which describes the correct time evolution within the SK formalism.
[33] We would like to point out another formalism with a doubled time basis that has been applied to transients in irreversible quantum dynamics (Ref. 30), in which the doubling of the states is related to the time-reversal invariance properties and the state-space doubling described by Wigner (Ref. 31).
[34] The asymmetry described here refers to the non-Hermitian dynamics of the junction.