Strong-to-weak-coupling duality in the nonequilibrium interacting resonant-level model

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A strong-to-weak-coupling duality is established for the nonequilibrium interacting resonant-level model, describing tunneling through a single spinless level, capacitively coupled to two leads by a contact interaction. For large capacitive coupling, $U$, and in the presence of a finite voltage bias, the model maps onto an equivalent model with a small capacitive coupling $pU^2 \sim 1/\rho U$. Here $\rho$ is the conduction-electron density of states. This duality is generic to all high-energy cutoff schemes, however its details may vary from one regularization scheme to another. In particular, it has the status of an exact mapping within Abelian bosonization, applicable to all repulsive interactions whether weak, intermediate or strong. On a lattice the mapping is restricted to large $U$, and is controlled by the small parameter $1/\rho U$. Explicit expressions are given for the low-energy scale, differential conductance, and occupancy of the level in the limit where $U$ is large.

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I. INTRODUCTION

The remarkable progress in nanofabrication techniques has focused considerable experimental and theoretical interest on quantum impurity systems out of thermal equilibrium. Typically the impurity is realized by a small nanostructure, e.g., a semiconductor quantum dot or an individual molecule, which is attached to two leads. Application of a voltage bias between the leads causes steady-state current to flow through the device. Being strongly correlated, such systems cannot be studied perturbatively over the full range of parameters, e.g., temperature or voltage bias, which calls for the development of nonperturbative techniques capable of treating the nonequilibrium steady state.

In contrast to the plethora of methods available for tackling quantum impurities in thermal equilibrium, only limited progress has been made out of equilibrium. The difficulty lies in the need to work directly with open systems, subject to appropriate boundary conditions imposed by the bias. The latter boundary conditions can be incorporated either at the level of the many-particle wave function through solution of a suitable Lippmann-Schwinger equation (the time-independent formulation), or by adopting a two-operator description as in the Keldysh approach (the time-dependent formulation). Unfortunately, most of the powerful approaches that are available in equilibrium are presently inadequate for treating open systems. In particular, leading numerical methods such as Wilson’s numerical renormalization group or the density-matrix renormalization group are presently confined to closed finite-size systems.

Recently, a step forward was taken by Mehta and Andrei who generalized the Bethe ansatz approach to allow the description of nonequilibrium systems in a steady state. In the traditional thermodynamic Bethe ansatz (TBA), one typically works with closed systems, namely, finite-size systems subject to periodic boundary conditions. The limit $L \to \infty$, $L$ being the size of the system, is taken only at the end of the construction. This approach, while yielding all the thermodynamic quantities, does not allow for the description of the nonequilibrium steady state that develops in a biased two-lead system, where particles cross the impurity and dissipate their energy asymptotically in the leads. A description of such processes requires different asymptotic behaviors in the past and in the future, represented by $x \to \pm \infty$ in the time-independent formulation. Thus, in the scattering Bethe ansatz (SBA) approach one works directly with open systems, where the limit $L \to \infty$ is implemented from the outset. The many-particle scattering states defined on the open system satisfy the Lippmann-Schwinger equation with asymptotic boundary conditions of free biased leads at $x \to -\infty$.

As a first demonstration of the approach, Mehta and Andrei applied it to the interacting resonant-level model (IRLM) describing tunneling through a single spinless level with capacitive coupling to the leads. The exact SBA solution revealed several surprising features, including a nonmonotonic dependence of the current on the capacitive coupling $U$, and an apparent duality between $U = 0$ and $U \to \infty$. These results have stimulated considerable interest in the nonequilibrium IRLM, providing complementary points of view and benchmarks for comparison.

In this paper we provide such a benchmark, by establishing a strong-to-weak-coupling duality for the nonequilibrium IRLM. In equilibrium, duality means that one can map the effective low-energy Hamiltonians for large and small $U$. Out of equilibrium the mapping must also preserve the boundary conditions imposed by the bias, which sets a far more stringent constraint on the mapping. In the following we show that duality between strong and weak coupling is a generic feature of the nonequilibrium IRLM, independent of the cutoff scheme.
used. However, its details may vary from one regularization scheme to another. This is an important point to bear in mind whenever comparing different computational schemes. Indeed, within Abelian bosonization we find an exact mapping between $U$ and $U' = 4/(\pi^2 \rho U)$, where $\rho$ is the conduction-electron density of states per lattice site. Thus, $U = 0$ and $U \to \infty$ are equivalent within bosonization, in agreement with the SBA. A similar duality between $\rho U \gg 1$ and $\rho U' \sim 1/\rho U \ll 1$ is found on a lattice, however the mapping is only approximate, and is accompanied by a significant reduction of the associated low-energy scale according to $T_0(\rho U \gg 1) \sim T_0(U = 0)/(\rho U)^2$. Explicit analytical expressions are given in the limit $\rho U \gg 1$ for the low-energy scale, $T_0$, the differential conductance, and occupation of the level, $n_d$.

The outline of the paper is as follows. In Sec. II we introduce the nonequilibrium IRLM, and specify our formulation of the finite bias. Using Abelian bosonization, an exact mapping between $U$ and $U' = 4/(\pi^2 \rho U)$ is derived in Sec. IIII followed by treatment of a general lattice cutoff in Sec. IV. Explicit analytic expressions are obtained in turn in Sec. V for the low-energy scale, differential conductance, and occupancy of the level, in the limit where $U$ is large. Finally, we present our conclusions in Sec. VI.

II. NONEQUILIBRIUM INTERACTING RESONANT-LEVEL MODEL

As already indicated above, there are several possible ways to formulate quantum impurity systems out of equilibrium. Here we adopt a two-operator formalism, consisting of the Hamiltonian of the unbiased system, $\mathcal{H}$, and the nonequilibrium operator, $Y_0$, which specifies the bias. This choice of operators arises naturally when starting from a coupled system in thermal equilibrium, and switching on the bias at some remote time $t_0$. Thus, the system is described at time $t_0$ by the density operator $\rho_0 = e^{-\beta \mathcal{H}}/\text{Tr}[e^{-\beta \mathcal{H}}]$, and evolves henceforth in time according to the Hamiltonian of the biased system, $\mathcal{H}_b = \mathcal{H} + Y_0$. Steady state is reached if the limit $t_0 \to -\infty$ exists, as can be shown in this case.\textsuperscript{26}

An equivalent, more common formulation of steady state starts from two decoupled leads, each in thermal equilibrium with its own chemical potential. Tunneling is then switched on at time $t_0$, which drives the system to a new steady state. Both formulations illustrated above give identical results.\textsuperscript{2} However, we shall focus on the former one, as it affords a more concise presentation. In the SBA approach, applied directly in the steady-state limit, the second formulation was adopted with $\rho_{\text{initia l}} = e^{-\beta (Y_0 - Y_0')}/\text{Tr}[e^{-\beta (Y_0 - Y_0')}]$. Here $\mathcal{H}_0$ describes the biased system with the leads decoupled.

With the former formulation in mind, the nonequilibrium IRLM is defined in the continuum limit by the Hamiltonian

$$\mathcal{H} = i\hbar v_F \sum_{j=1,2} \int_{-\infty}^{\infty} \psi_j^\dagger(x) \partial_x \psi_j(x) dx + \epsilon_d d^1 d + \sum_{j=1,2} \sqrt{a} t_j \left\{ \psi_j^\dagger(0)d + \text{H.c.} \right\} + U a \left( d^1 d - \frac{1}{2} \right) \sum_{j=1,2} \psi_j^\dagger(0) \psi_j(0):$$

and nonequilibrium operator

$$Y_0 = \frac{eV}{2} \int_{-\infty}^{\infty} \left[ \psi_1^\dagger(x) \psi_1(x) - \psi_2^\dagger(x) \psi_2(x) \right] dx.$$

Here, the left-moving fields $\psi_j^\dagger(x)$ with $j = 1, 2$ describe free conduction electrons in lead $j$; $d^1$ creates an electron on the level; $a$ is a short-distance cutoff corresponding to a lattice spacing; $t_j$ is the tunneling matrix element between the level and lead $j$; $U$ is the capacitive coupling (contact interaction) between the level and the leads; and $V$ is the applied voltage bias. Note that we allow for different tunneling matrix elements to each of the leads, but the capacitive coupling is taken to be equal. As for the fields $\psi_j^\dagger(x)$, these obey canonical anticommutation relations

$$\{ \psi_i(x), \psi_j^\dagger(y) \} = \delta_{ij} \delta(x - y),$$

subject to the regularization $\delta(0) = 1/a$. Hence, the conversion between a Wilson-type tight-binding representation and the continuum limit is specified by the relation $c_{j,0}^\dagger = \sqrt{a} \psi_j^\dagger(0)$, where $c_{j,0}^\dagger$ creates a localized electron (zeroth Wilson shell) on lead $j$. As for the symbol $: \psi_j^\dagger \psi_j :$, it stands for normal ordering with respect to the unperturbed Fermi seas of the two leads.

III. ABELIAN BOSONIZATION

We first treat the nonequilibrium problem defined in Eqs. (1) and (2) using Abelian bosonization. In the standard fashion, two bosonic fields $\Phi_j(x)$ are introduced, one boson field for each left-moving fermion field. The fermion fields are written as

$$\psi_j(x) = \frac{e^{i\Phi_j(x)}}{\sqrt{2\pi a}} e^{-i\Phi_j(x)},$$

where the $\Phi$'s obey

$$[\Phi_j(x), \Phi_j(y)] = -i\delta_{ij} \pi \text{sign}(x - y).$$

The ultraviolet momentum cutoff $\alpha^{-1} = \pi/a$ is related to the conduction-electron bandwidth $D$ and the density of states per lattice site $\rho$ through $D = \hbar v_F/\alpha$ and $\rho = 1/(2D) = \alpha/(2\hbar v_F)$, respectively. The operator $e^{i\Phi}$ in Eq. (4) is a phase-factor operator, which comes to ensure
that the different fermions anticommute. Our explicit choice for $\hat{\varphi}$ reads

$$\hat{\varphi} = \frac{\pi}{2} \left( \hat{N}_1 - \hat{N}_2 + 2d^d d \right),$$

(6)

where $\hat{N}_j$ is the total number operator for electrons in lead $j$. Alternatively, one can replace the phase-factor operator appearing in Eq. (3) with a Majorana fermion.

In terms of the boson fields, the Hamiltonian $\mathcal{H}$ and nonequilibrium operator $Y_0$ take the forms

$$\mathcal{H} = \frac{\hbar v_F}{4\pi} \sum_{j=1,2} \int_{-\infty}^{\infty} (\nabla \Phi_j(x))^2 dx + \epsilon_d d^d d$$

$$+ \frac{t_j}{\sqrt{2}} \left\{ e^{i\phi_j(0)} e^{-i\hat{\varphi}d} + \text{H.c.} \right\}$$

$$+ \delta \frac{\alpha}{\pi^{2} \rho} \left( d^d d - \frac{1}{2} \right) \sum_{j=1,2} \nabla \Phi_j(0)$$

(7)

and

$$Y_0 = \frac{eV}{4\pi} \int_{-\infty}^{\infty} \left[ \nabla \Phi_1(x) - \nabla \Phi_2(x) \right],$$

(8)

where

$$\delta = \arctan \left( \frac{\rho U}{2} \right)$$

(9)

is the phase shift associated with $U$. This bosonized form of the $U$ interaction term stems from the cutoff scheme used in bosonization. It follows from the requirement that the exact scattering phase shift be reproduced in the limit $t_1, t_2 \to 0$. Importantly, $\delta$ is bounded in magnitude by $\pi/2$. Although the bosonic Hamiltonian of Eq. 7 does support larger values of $|\delta|$, this parameter must not exceed $\pi/2$ in order for Eq. (2) to possess a fermionic counterpart of the form specified in Eq. (1).

We proceed by converting to new charge and flavor fields, $\Phi_c$ and $\Phi_f$, corresponding to even and odd combinations of $\Phi_1$ and $\Phi_2$:

$$\Phi_c(x) = \frac{1}{\sqrt{2}} [\Phi_1(x) + \Phi_2(x)],$$

(10)

$$\Phi_f(x) = \frac{1}{\sqrt{2}} [\Phi_1(x) - \Phi_2(x)].$$

(11)

In this manner, Eqs. (1) and (8) are rewritten as

$$\mathcal{H} = \frac{\hbar v_F}{4\pi} \sum_{\nu=c,f} \int_{-\infty}^{\infty} (\nabla \phi_{\nu}(x))^2 dx + \epsilon_d d^d d$$

$$+ \frac{t_1}{\sqrt{2}} \left\{ e^{\frac{i}{2} \phi_c(0) + \phi_f(0)} e^{-i\hat{\varphi}d} + \text{H.c.} \right\}$$

$$+ \frac{t_2}{\sqrt{2}} \left\{ e^{\frac{i}{2} \phi_c(0) - \phi_f(0)} e^{-i\hat{\varphi}d} + \text{H.c.} \right\}$$

$$+ \delta \frac{\alpha}{\pi^{2} \rho} \left( d^d d - \frac{1}{2} \right) \nabla \phi_c(0)$$

(12)

and

$$Y_0 = \frac{eV}{2\sqrt{2}\pi} \int_{-\infty}^{\infty} \nabla \phi_f(x).$$

(13)

Note that the phase operator $\hat{\varphi}$ of Eq. (6) involves only the flavor field $\Phi_f$, and therefore commutes with $\Phi_c$.

At this point two successive transformations are carried out. First the canonical transformation $\mathcal{H}' = U \mathcal{H} U^\dagger$, $Y_0' = U Y_0 U^\dagger$ with $U = \exp \left[i\sqrt{2} \Phi_f(0) \left(d^d d - \frac{1}{2}\right)\right]$ is performed, to be followed by $\Phi_c(x) \to -\Phi_c(x)$. The latter operation is just a bosonic version of the particle-hole transformation $\psi_1(x) \to \psi_2(x)$, $\psi_2(x) \to \psi_1(x)$. The nonequilibrium operator $Y_0'$ is left unchanged by this sequence of steps, and remains given by Eq. (13). The Hamiltonian $\mathcal{H}'$, on the other hand, acquires one small but important modification as compared to Eq. (12): the parameter $\delta$ is replaced with $\delta' = \frac{\pi}{2} - \delta$. As long as $|\delta'| \leq \pi/2$, i.e., $U \geq 1$, one can revert the series of steps leading to Eqs. (12) and (13), to recast $\mathcal{H}'$ and $Y_0'$ in fermionic forms. The end result of these manipulations is just the original pair of operators that appear in Eqs. (1) and (2), with the renormalized interaction strength

$$U \to U' = \frac{4}{\pi^{2} \rho^{2} \rho^2 U}. $$

(14)

All other model parameters, the voltage bias included, are unaffected by the mapping. This proves an exact strong-to-weak-coupling duality of the nonequilibrium IRML in the framework of bosonization.

Proceeding to observables, the duality transformation leaves unchanged the operators describing both the occupation of the level, $\hat{n}_d = d^d d$, and the current outgoing from lead $j$, $\hat{I}_j = i(\epsilon/h) \sqrt{\alpha} t_j [d^d \psi_j(0) - \psi_j(0) d]$. Hence the associated averages, $n_d = \langle \hat{n}_d \rangle$ and $I = \langle \hat{I}_j \rangle$, obey the identities

$$n_d(T, V; \epsilon_d, t_1, t_2, U) = n_d(T, V; \epsilon_d, t_1, t_2, U'),$$

(15)

$$I(T, V; \epsilon_d, t_1, t_2, U) = I'(T, V; \epsilon_d, t_1, t_2, U').$$

(16)

In particular, since $U \to \infty$ maps onto $U = 0$, occupancy of the level and the steady-state current are identical for $U \to \infty$ to those of the noninteracting level. This result is in agreement with that of the SBA including the associated low-energy scale being equal to $\Gamma = \Gamma_1 + \Gamma_2$. Here $\Gamma_j = \pi \rho t_j^2$ is half the tunneling rate to lead $j$. We emphasize, however, that our mapping extends the equivalence of $U \to \infty$ and $U = 0$ to all moments of the current, implying identical full counting statistics.

The detailed agreement with the SBA suggests that an analogous duality is present in the latter approach, in the form of $\pi \rho U_{\text{SBA}} \to 1/(\pi \rho U_{\text{SBA}})$. Here the notation $U_{\text{SBA}}$ comes to emphasize that the coupling $U$ is defined within the SBA cutoff scheme. The structure of the duality is reflected in the expression for the low-energy scale $T_0$, which is given for $\pi \rho U_{\text{SBA}} \leq 1$ by

$$T_0^{\text{SBA}}(\pi \rho U \leq 1) = D \left( \frac{\Gamma}{\gamma} \right) \pi / [\pi + \zeta(\pi U^2)].$$

(17)
with
\[ \zeta(x) = 2 \arctan(x). \] (18)
Assuming the SBA duality then yields
\[ T^\text{SBA}_0(\pi \rho U \geq 1) = D \left( \frac{\Gamma}{D} \right)^{\pi/(\pi + \zeta(1/\pi \rho U))}, \] (19)
which has the asymptotic form
\[ T^\text{SBA}_0(\pi \rho U \gg 1) \approx D \left( \frac{\Gamma}{D} \right)^{-2/(\pi^2 \rho U)}. \] (20)
This form will be examined later in Sec. \[ \text{V} \]
Thus, the property of duality, Eq. (14), provides a simple perspective on the nonmonotonic $U$ dependence of the low-energy scale $T_0$, discussed in Ref. [3]. Starting from $U = 0$ and $T_0 = \Gamma$, the low-energy scale increases as a function of small $U/\rho$ before dropping back to its noninteracting value as $U \to \infty$. It must therefore decrease as a function of large $U$, attaining a maximum at some intermediate coupling $U_{\text{max}}^\Gamma$. Assuming a single extremum, the maximal $T_0$ must occur at the self-dual point $U' = U$, corresponding to $U_{\text{max}} = 2/(\pi \rho)$ in bosonization and $U_{\text{max}} = 1/(\pi \rho)$ in the SBA. Indeed, the estimate $U_{\text{max}}^\Gamma = 2/(\pi \rho)$ is explicitly found in the Anderson-Yuval approach.\[ \text{I} \] Although the precise value of $U_{\text{max}}$ may vary from one realization scheme to another, the general estimate $\rho U_{\text{max}} \sim 1$ should apply to all cutoff schemes, in agreement with the weak-coupling scheme used. Generally speaking, all regularizations are expected to share the same qualitative physics. However, details, such as the parametric dependence of $T_0(U)$, may vary from one realization scheme to another. It is quite remarkable in that respect that bosonization and the SBA coincide for $U \to \infty$, as both approaches employ seemingly unrelated cutoffs. Focusing on the large-$U$ limit, we proceed to analyze the strong-to-weak-coupling duality for a general lattice cutoff. Here by lattice cutoff we mean an arbitrary conduction-electron dispersion $\epsilon_k$ with a large but finite bandwidth, $D$.

Consider a general lattice model for the conduction electrons in the leads. Using a Wilson-type construction,\[ \text{I} \] any lattice model can be cast as a semi-infinite tight-binding chain with the impurity coupled to the open end:
\[ \mathcal{H} = \sum_{j=1,2} \sum_{n=0}^{\infty} \left[ \epsilon_n c_{j,n}^\dagger c_{j,n} + \xi_n \left\{ c_{j,(n+1)}^\dagger c_{j,n} + \text{H.c.} \right\} \right]. \]

\[ + \epsilon_d d^\dagger d + \sum_{j=1,2} t_j \left\{ c_{j,0}^\dagger d + \text{H.c.} \right\} \]
\[ + U \left( d^\dagger d - \frac{1}{2} \right) \sum_{j=1,2} \left( c_{j,0}^\dagger c_{j,0} - \frac{1}{2} \right). \] (21)

Here $c_{j,n}^\dagger$ creates an electron in the $n$th Wilson shell of lead $j$. The nonequilibrium operator is given accordingly by
\[ Y_0 = \frac{eV}{2} \sum_{n=0}^{\infty} \left[ c_{1,n}^\dagger c_{1,n} - c_{2,n}^\dagger c_{2,n} \right]. \] (22)

Different lattice models are distinguished by the tight-binding parameters $\epsilon_n$ and $\xi_n$, which are uniquely determined by the underlying band structure and the microscopic details of the coupling to the level. For instance, the case where $\epsilon_n$ is zero for all $n$ corresponds to particle-hole symmetric bands. The bandwidth $D$ is determined in this case by the largest hopping matrix element $\xi_n$ along the chain. For convenience, we restrict attention hereafter to $\epsilon_n = 0$, taking the leads to have identical forms. As commented on below, both assumptions can be relaxed without altering the main physical result.

Focusing on $U \gg D, t_j, |\epsilon_d|$, we carry out a systematic expansion in $1/U$. For large $U$, it is favorable energetically to first satisfy the large capacitive coupling between the level $d^\dagger$ and the two local lead electrons $c_{j,0}^\dagger$ with $j = 1, 2$. Diagonalization of the local problem with $t_1$ and $t_2$ set to zero reveals two low-lying states: $c_{1,0}^\dagger c_{2,0}^\dagger |0\rangle$ with energy $-U/2$, and $d^\dagger |0\rangle$ with energy $-U/2 + \epsilon_d$. The six remaining states are each removed in energy by $U/2 \pm \epsilon_d$ or more, as detailed in Table \[ \text{I} \].

Defining the operator
\[ \hat{D} = c_{1,0}^\dagger c_{2,0}^\dagger d, \] (23)
it is easy to verify that (i) $\hat{D} \hat{D}^\dagger$ projects onto the state $d^\dagger |0\rangle$; (ii) $\hat{D} \hat{D}^\dagger$ projects onto the state $c_{1,0}^\dagger c_{2,0}^\dagger |0\rangle$; and (iii) $\hat{D}^2 = (\hat{D}^\dagger)^2 = 0$. In addition, $\hat{D}$ and $\hat{D}^\dagger$ anti-commute with all electronic operators further down the chain, namely, $c_{j,n}$ with $n \geq 1$. Thus, $\hat{D}$ acts as a conventional fermion annihilation operator within the truncated Hilbert space where only the two lowest lying local states are kept.

To eliminate the locally excited states, we perform a canonical transformation akin to the Schrieffer-Wolff transformation\[ \text{I} \] for the Anderson model: $\mathcal{H}' = e^{\hat{S}} \mathcal{H} e^{-\hat{S}}$. Here the anti-hermitian operator $S$ is chosen such that the excited and low-lying sectors are decoupled within $\mathcal{H}'$ to linear orders in $t_1$, $t_2$, and $\xi_0$. The explicit form of the operator $S$ is quite cumbersome, and will not be specified here. Instead, we proceed directly to the end result. Projecting $\mathcal{H}'$ onto the low-energy subspace and settling with linear order in $1/U$, the effective low-energy Hamiltonian reads
\[ \mathcal{H}' = \sum_{j=1,2} \sum_{n=1}^{\infty} \xi_n \left[ c_{j,(n+1)}^\dagger c_{j,n} + \text{H.c.} \right] \]
TABLE I: Eigenstates and eigenenergies of the local problem, defined by the Hamiltonian terms $\epsilon_d$ and $U$ in Eq. (21) (i.e., the couplings $t_1$, $t_2$, and $\xi_0$ are all set to zero). Here $|0\rangle$ denotes the empty state with no particles available. For large $U$, the local spectrum consists of two low-lying states: $c_{1,0}^\dagger c_{2,0}|0\rangle$ with energy $-U/2$, and $d^\dagger|0\rangle$ with energy $-U/2 + \epsilon_d$. The six remaining states involve an excitation energy of $U/2 \pm \epsilon_d$ or more.

| Eigenstate           | Eigenenergy        |
|----------------------|--------------------|
| $|0\rangle$          | $U/2$              |
| $d^\dagger|0\rangle$ | $-U/2 + \epsilon_d$ |
| $c_{1,0}^\dagger|0\rangle$ | 0                  |
| $c_{2,0}^\dagger|0\rangle$ | 0                  |
| $d^\dagger c_{1,0}^\dagger|0\rangle$ | $\epsilon_d$       |
| $d^\dagger c_{2,0}^\dagger|0\rangle$ | $-U/2$             |
| $d^\dagger c_{1,0}^\dagger d^\dagger c_{2,0}^\dagger|0\rangle$ | $U/2 + \epsilon_d$ |

Eqs. (25) and (26), respectively. The same differences carry over to the main observables of interest, namely, the occupancy of the level and the current outgoing from lead $j$. Explicitly, the corresponding operators transform according to

$$\hat{n}_d' = e^S \hat{n}_d e^{-S} = \hat{D}^\dagger \hat{D},$$

(28)

$$\hat{I}_j' = e^S \hat{I}_j e^{-S} = i(e/h) t_j' \left[ \hat{D} \hat{c}_{j,1} - \hat{c}_{j,1} \hat{D} \right],$$

(29)

where we have again settled with linear order in $1/U$ and with projection onto the low-energy sector. Thus, the nonequilibrium IRLM defined by Eqs. (21) and (22) has been mapped for large $U$ onto a weakly interacting version of the same model. This includes the physical content of the operators $\hat{I}_j'$ and $\hat{n}_d'$ describing the current and occupancy of the level.

Evidently, the nonequilibrium IRLM possess a strong-to-weak-coupling duality also when placed on a lattice. However, in contrast to bosonization, mapping of large to small $U$ is only approximate, being controlled by the small parameter $\xi_0/U \ll 1$, and involves a significant reduction of the effective tunneling matrix elements according to Eq. (24). On the other hand, the renormalized interaction strength of Eq. (26) is in good qualitative agreement with the predictions of bosonization, which follows from the fact that $\xi_0 \sim 1/\pi \rho$ for conventional lattice models.

Our discussion thus far has focused on identical leads with $\epsilon_n = 0$ along the chain. We conclude this section by briefly commenting on the case where either the $\epsilon_n$’s are not identically zero in Eq. (21) (marking departure from particle-hole symmetry), or if the leads have different underlying band structures [i.e., $\epsilon_n \rightarrow \epsilon_{j,n}$ and $\xi_0 \rightarrow \xi_{j,n}$ in Eq. (21)]. In the most general case, Eqs. (25) and (26) are replaced with

$$t_j' = 4 \frac{t_j \xi_0}{U}$$

(30)

and

$$U' \rightarrow U' = 4 \frac{(\xi_{j,0})^2}{U},$$

(31)

while $\epsilon_d$ acquires the additional shift $\epsilon_d \rightarrow \epsilon_d - \epsilon_{1,0} - \epsilon_{2,0}$. Here $\bar{j} = 3 - j$ is the lead index opposite to $j$. Hence, the capacitive coupling $U'$ becomes lead dependent when the leads have different structures. Another crucial point pertains to the particle-hole transformation of Eq. (27), which maps each lead onto a particle-hole reflected image of its partner. Consequently, the structure of each lead is generally altered by the mapping. These modifications, however, do not change the main physical result, namely, that the nonequilibrium IRLM with large $U$ is mapped onto a weakly interacting variant of the same model.
V. PHYSICAL PROPERTIES FOR LARGE $U$

Focusing on the limit where $U$ is large, we next exploit the duality between strong and weak coupling to derive explicit analytic expressions for the main physical quantities of interest. These include the low-energy scale $T_0$, the differential conductance, $G$, and the occupancy of the level, $n_d$.

The scale $T_0$ is extracted from the equilibrium Hamiltonian $\mathcal{H}$, with the voltage bias set to zero. Starting from the dual Hamiltonian $\mathcal{H}'$, the latter can easily be brought to the canonical form considered in Ref. 3 by converting to the “bonding” and “anti-bonding” combinations

$$\psi_b(x) = \frac{t_1}{t'} \psi_1(x) + \frac{t_2}{t'} \psi_2(x),$$

$$\psi_a(x) = \frac{t_2}{t'} \psi_1(x) - \frac{t_1}{t'} \psi_2(x).$$

Here

$$t' = \sqrt{t_1^2 + t_2^2}$$

is the tunneling matrix element between the level and the “bonding” band. No tunneling takes place between the level and the “anti-bonding” electrons, only capacitive coupling is left. Equations (32)–(34) pertain to the level and the “anti-bonding” electrons, only capacitive coupling is left. Equations (32)–(34) pertain to the dual Hamiltonian obtained within bosonization. A similar construction applies to the lattice version of $\mathcal{H}'$, in which case Eq. (34) is replaced with

$$t' = \frac{4\xi_0}{U} \sqrt{t_1^2 + t_2^2}$$

[see Eq. (25)]. Note that the conversion to “bonding” and “anti-bonding” modes is a standard transformation in equilibrium. However, it loses its usefulness when a finite bias is applied as the two modes couple within $Y_0$.

In the notations of Borda et al., the converted Hamiltonian corresponds to $N = 2$, $\xi_0 = t'$, and $U = U'$. Hence, one can read off the low-energy scale from the renormalization-group equations derived by these authors, which give

$$T_0(\rho U \gg 1) = D \left( \frac{\Gamma'}{D} \right)^{1-2\rho U'},$$

with

$$\Gamma' = \begin{cases} 1 & \text{Bosonization} \\ \frac{4\xi_0}{U} & \text{Lattice cutoff} \end{cases}.$$  (37)

Here $U'$ is specified by Eqs. (14) and (20) for the cutoff schemes used in bosonization and on a lattice, respectively. In writing Eqs. (36) and (37) for a lattice cutoff, we have implicitly assumed that the effective bandwidth $D$ and density of states $\rho$ are left unchanged upon converting from $\epsilon_{j,0}$ to $\epsilon_{j,1}$.

In case of bosonization, Eq. (36) takes the explicit form

$$T_0(\rho U \gg 1) = D \left( \frac{\Gamma'}{D} \right)^{1-2\rho U'},$$

consistent with Eq. (21) upon the simple substitution $1/U_{SBA} \rightarrow 4/U_{bosonization}$. This relation between the couplings defined within the different cutoff schemes also showed up in the form of the assumed duality in the SBA: $\pi\rho U_{SBA} \rightarrow 1/(\pi\rho U_{SBA})$ as compared to $\pi\rho U \rightarrow 4/(\pi\rho U)$ in bosonization. It is, however, easy to check that this simple relation between the coupling constants defined within the two schemes holds only at strong coupling, and does not extend to weak coupling. (The relation, in general, is nonanalytic, and may include singular points.) Note that both the SBA and bosonization expressions for $T_0$ approach $\Gamma$ as $U \rightarrow \infty$. Indeed, fixing $\Gamma$ and increasing $U$, Eq. (36) reduces asymptotically to $\Gamma'$, which equals $\Gamma$ in case of bosonization. In contrast, $T_0(U)/T_0(0)$ equals $(4\xi_0/U)^2$ for sufficiently large $U$ in case of a lattice cutoff. The latter result agrees well with numerical renormalization-group calculations, where $\xi_0$ is given by the hopping matrix element between the zeroth and first Wilson shells.

Since $U'$ is a marginal operator that drops to zero as $U \rightarrow \infty$, the nonequilibrium IRLM reduces asymptotically to a noninteracting level (albeit with a strongly renormalized hybridization width in case of a lattice cutoff). The effect of $U'$ is controlled by the dimensionless parameter $\rho U' \ln(D/\Gamma')$. When made sufficiently small, the differential conductance and occupancy of the level assume standard noninteracting forms:

$$G = \frac{G_0}{2} \left[ \frac{T_0^2}{(\epsilon_d + eV/2)^2 + T_0^2} + \frac{T_0^2}{(\epsilon_d - eV/2)^2 + T_0^2} \right]$$  (39)

and

$$n_d(T, V) = \frac{1}{2} - \frac{1}{\pi} \frac{\Gamma_L}{\Gamma} \arctan \left( \frac{\epsilon_d - eV/2}{T_0} \right) - \frac{1}{\pi} \frac{\Gamma_R}{\Gamma} \arctan \left( \frac{\epsilon_d + eV/2}{T_0} \right),$$  (40)

with

$$G_0 = \frac{e^2}{4\hbar} \frac{4\Gamma_L\Gamma_R}{(\Gamma_L + \Gamma_R)^2}.\quad (41)$$

Here we have settled for brevity with zero temperature. The extension to finite temperature is straightforward. Note that the peak conductance, $G_0$, is independent of the cutoff scheme, and is identical to its value when $U = 0$. This follows from the fact that $t_R'/t_L'$ is equal to $t_R/t_L$ in Eq. (25). This result for $G_0$ is in fact more general. It extends to all values of $U$, as can be seen from a phase-shift analysis.
VI. CONCLUSIONS

The description of quantum impurities out of equilibrium remains an outstanding theoretical challenge, with an urgent need for benchmark results. In this paper we provided such a result, by showing that the nonequilibrium IRLM with strong capacitive coupling is equivalent to a weakly coupled version of the same model. When expressed in terms of the proper low-energy scale, the differential conductance and occupancy of the level reduce for large $U$ to standard noninteracting forms. This result is universal, independent of the cutoff scheme used. Different cutoffs are distinguished by the parametric form of $T_0$, which is nonuniversal. In this respect there appears to be a qualitative difference between lattice cutoffs with a finite bandwidth, and continuum-limit cutoffs of the type used in bosonization and the SBA, where the high-energy cutoff is sent to infinity. Within the latter schemes, $T_0(U=0)=\Gamma$, as $U \to \infty$. By contrast, $T_0$ decays to zero as $T_0(U) \sim T_0(U=0)/(\rho U)^2$ when placed on a lattice. This difference must be kept in mind whenever comparing different computational schemes. On the other hand, the peak conductance is independent of the cutoff scheme used, being equal to its $U=0$ value.

We further wish to emphasize that the strong-to-weak-coupling duality reported in this paper is a distinct property of the IRLM with two screening channels, or leads. The IRLM with a single screening channel has long been known to map onto the anisotropic Kondo model. The limit $U \to \infty$ corresponds in this mapping to $J_z \to \infty$ ($J_z$ being the longitudinal Kondo coupling), while $\epsilon_d$ translates to a local magnetic field. From the mapping one clearly sees that the single-channel IRLM with $\epsilon_d = 0$ flows to the same low-energy fixed point whether $U$ is small or large. Namely, all values of $U$ are physically equivalent at energies much smaller than $T_0(U)$. However, unlike the two-channel case, large and small $U$ are inequivalent at energies comparable to and exceeding $T_0(U)$. Indeed, repeating the strong-coupling expansion of Sec. [9] for the case of a single screening channel one readily finds two low-lying local states: $d^\uparrow|0\rangle$ and $d^\downarrow|0\rangle$. As these states are occupied by a single electron each, charge fluctuations are strongly suppressed between the local complex and truncated chain at energies far below $U$. As a result, formation of a scattering center is driven entirely by local dynamics when $U$ is large, in contrast to the case where $U$ is small.

A far more dramatic effect is found when the number of screening channels exceeds three. Here $U = 0$ and $U \to \infty$ flow to different low-energy fixed points, one ($U=0$) corresponding to a strongly hybridized level, and the other ($U \to \infty$) to a free impurity. The strong-coupling and free-impurity phases of the model are separated in this case by a finite-$U$ Kosterlitz-Thouless transition line, analogous to the ferromagnetic-antiferromagnetic transition line of the anisotropic Kondo model. A detailed analysis of the IRLM with multiple screening channels will be published elsewhere.

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The impurity comprises in this case of the level $d^\dagger$, plus the two local lead degrees of freedom to which it is coupled (i.e., $c^\dagger_{j\alpha}$ with $j = 1, 2$).

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