Fermion-parity duality and energy relaxation in interacting open systems

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We study the transient heat current out of a confined electron system into a weakly coupled electrode in response to a voltage switch. We show that the decay of the Coulomb interaction energy for this repulsive system exhibits signatures of electron-electron *attraction*, and is governed by an interaction-independent rate. This can only be understood from a general duality that relates the nonunitary evolution of a quantum system to that of a dual model with inverted energies. Deriving from the fermion-parity superselection postulate, this duality applies to a large class of open systems.

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Energy decay due to heat currents is of key importance in the continued downscaling of electronic devices [1]. The quantum [2-6] and interaction effects [7-9] that arise on the nanoscale give rise to new possibilities [10-13] and motivate both fundamental [14] and application oriented [3,4,8,13,15] studies on quantum heat engines, possibly realized in, e.g., cold atoms, trapped ions, or quantum dots. The successful control and exploitation of heat in nanodevices requires both a fundamental understanding and the practical ability to detect and manipulate *few-electron* heat currents. Under stationary conditions, progress has been achieved using various approaches [16–18], including heat transfer through molecular-scale devices [19] with electrostatic gating [20]. However, any device is eventually adjusted by some external agent that provokes a time-dependent response. In the context of electronic heat currents, this raises a very basic question that, despite recent promising theoretical [21-27] and experimental [28-30] studies, has not been answered so far: how does a small electron system, typically governed by a strong level quantization and Coulomb interaction, dissipate in time its stored energy into a coupled electronic bath?

The essence of time-dependent transport in such systems is already captured by the simple model sketched in Figs. 1(a) and 1(b). Here, an instant energy shift of a single electronic orbital in a quantum dot leads to a time-dependent charge current $I_N(t)$ [31,32] and heat current $I_O(t)$ into a tunnel-coupled electrode. In the weak-coupling regime, expressions for these currents can be calculated straightforwardly, and in the case of the transient charge current $I_N(t)$ also allow for an intuitive physical understanding [33]. This is, however, not the case for the heat current $I_Q(t) = a_c e^{-\gamma_c t} + a_p e^{-\gamma_p t}$. Compared to the charge current $I_N(t) \propto e^{-\gamma_c t}$, the heat current contains a second decay mode. The mere presence of this mode can be expected: it originates from the dissipation of the Coulomb energy. However, what is quite remarkable is that its rate γ_n turns out to be completely independent of the interaction strength U[34-37]—despite entering the heat current only as a consequence of the interaction. Even more surprisingly, as indicated by the blue dashed line in Fig. 1(e), both excitation amplitudes, a_c and a_p , show an abrupt change at an energy typically associated with electron-electron attraction [38], even though we are dealing with a system governed by *repulsive* interaction. As we will show, both surprising effects have a fundamental origin and they can occur in a broad class of systems.

The difficulty in explaining the counterintuitive observations in the heat current ultimately stems from the nonunitarity of the dynamics of open quantum systems. In closed systems, the hermiticity of the Hamiltonian implies that its left and right eigenvectors are simply adjoint to each other. Thanks to this property, the amplitude with which an energy eigenstate enters the full time evolution of the system is simply given by the overlap between this eigenstate and the initially prepared state.



FIG. 1. (a), (b) Quantum dot with charging energy U subject to a gate-voltage switch. The instant level shift from ϵ_0 to ϵ causes two electrons to be sequentially expelled. (c) Inverted stationary state for the *dual* model obtained from the final state (b) by inverting all energies, as prescribed by Eq. (4). (d), (e) Amplitude of the charge mode, a_c , and of the parity mode, a_p , in the time-dependent heat current $I_Q(t) = a_c e^{-\gamma_c t} + a_p e^{-\gamma_p t}$, plotted versus the initial (ϵ_0) and final (ϵ) level position for $T = 0.1U \gg \Gamma$. The black crosses mark the switch in (a) and (b), and the circles a switch to $\epsilon = \mu$.

For dissipative open systems, a similar and equally insightful relation for the amplitudes of the decay modes is not known. Yet, such a relation would be extremely valuable, not only for the understanding of the transient heat current in Fig. 1, but also for a broad class of other dynamical problems, ranging from qubit dynamics to molecular electron transfer.

In this Rapid Communication, we identify a duality relation between decay modes and amplitudes. This duality applies to *all open* fermionic systems that can be modeled by a Hamiltonian $H^{\text{tot}} = H + H^{\text{R}} + H^{\text{T}}$ with an arbitrary local Hamiltonian H and (a) effectively noninteracting, wide-band fermionic reservoirs H^{R} , with a coupling H^{T} that is (b) bilinear in the fermion fields and (c) energy independent, but otherwise arbitrarily strong. Under these very general assumptions, the duality emerges mainly as a consequence of the fermion-parity superselection postulate of quantum mechanics [39–42], by which states with even and odd fermion number cannot be superposed. Applied to the system shown in Fig. 1, it explains in full detail the poorly understood heat decay.

Mode-amplitude duality for open systems. An open quantum system is most naturally described in terms of its reduced density matrix $\rho(t)$, whose equation of motion is $\partial_t \rho(t) = -i[H, \rho(t)] + \int_0^t dt' \mathcal{W}(t - t') \rho(t') \text{ (with } \hbar = k_{\rm B} =$ e = 1). The kernel W takes into account the coupling to the external reservoirs [43–46] that causes $\rho(t)$ to decay. Introducing the Laplace transform of \mathcal{W} , $W(\omega) = \int_0^\infty dt \, e^{i\omega t} \mathcal{W}(t)$, the decay dynamics can be expressed in terms of the frequency(ω)dependent right eigenvectors of $W(\omega)$, the *decay modes*. The decay amplitude for each mode is determined by the overlap between the initial state ρ_0 and the left eigenvector of $W(\omega)$ for the same eigenvalue, the *amplitude covector*. Since W is non-Hermitian, left and right eigenvectors are not simply each others' adjoint. However, under the very general assumptions stated above, we can prove that the vectors are still linked by the duality relation

$$W(\omega; H, H^{\mathrm{T}}, \{\mu\})^{\dagger} = -\Gamma + \mathcal{P}W(\bar{\omega}; \bar{H}, \bar{H}^{\mathrm{T}}, \{\bar{\mu}\})\mathcal{P}.$$
 (1)

The physical consequences of Eq. (1) arise from the three operations it involves: (i) a constant shift by Γ —the lumped sum of constant couplings characterizing H^{T} ; (ii) the fundamental transformation \mathcal{P} , which multiplies an operator by the fermion-parity operator $(-1)^N := e^{i\pi N}$ with local fermion-number operator N; and (iii) a parameter substitution in the original model, which constructs a dual model with inverted local energies $\bar{H} := -H$, a dual coupling $\bar{H}^{T} := i H^{T}$ to reservoirs with dual chemical potentials $\bar{\mu} := -\mu$ at dual frequency $\bar{\omega} := i\Gamma - \omega^*$, but with same Hamiltonian $H^{\rm R}$ and temperature T. The duality Eq. (1) therefore links in a nontrivial way the left eigenvectors of W to those of W^{\dagger} , which are in turn the right eigenvectors of W for the dual model. The physics behind the derivation of Eq. (1) is summarized at the end of this paper, and the proof is given in [47]. In the following, we apply the duality to the transient dynamics of the system depicted in Figs. 1(a) and 1(b), and show that it provides the key insight to interpret the remarkable features of the heat current.

Transient dynamics. The system of interest is a spindegenerate single-level quantum dot with Hamiltonian $H = \epsilon N + U N_{\uparrow} N_{\downarrow}$, where ϵ is the tunable level position and U the local interaction (see Fig. 1). Here, $N = N_{\uparrow} + N_{\downarrow}$

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is the occupation operator, with $N_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$ and d_{σ} the field operators of the dot electrons ($\sigma = \uparrow, \downarrow$). The dot is tunnel coupled by $H^{T} = \sum_{k,\sigma} \tau_{k,\sigma} c_{k\sigma}^{\dagger} d_{\sigma} + H.c.$ to a single noninteracting electrode $H^{R} = \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k\sigma}^{\dagger} c_{k\sigma}$. Here, $c_{k\sigma}$ is the field operator for reservoir electrons with spin σ , orbital index k, and energy $\epsilon_{k,\sigma}$, while $\tau_{k,\sigma}$ is the tunnel amplitude. The grand-canonical reservoir state is $\rho^{R} = e^{-(H^{R} - \mu N^{R})/T} / \operatorname{Tr}_{R} e^{-(H^{R} - \mu N^{R})/T}$, where $N^{R} = \sum_{k,\sigma} c_{k\sigma}^{\dagger} c_{k\sigma}$. In the wide-band limit, the tunnel coupling is characterized by $\Gamma_{\sigma} = 2\pi \sum_{k} \delta(\omega - \epsilon_{k}) |\tau_{k,\sigma}|^{2}$, assumed ω independent, with total strength $\Gamma := \sum_{\sigma} \Gamma_{\sigma}$ and $\Gamma_{\uparrow} = \Gamma_{\downarrow} = \Gamma/2$ in our spin-independent case.

We consider the regime of high temperature and weak coupling to the electrode $\Gamma \ll T$, and the response to a sudden shift of the level position $\epsilon_0 \rightarrow \epsilon$ at t = 0, due to, e.g., a switch of the gate voltage. Immediately after the level shift, the dot state equals the initial state ρ_0 before the shift. At later times t > 0, the density operator $\rho(t)$ of the dot obeys the Born-Markov master equation

$$\partial_t | \rho(t) \rangle \approx W | \rho(t) \rangle, \qquad W := \lim_{\omega \to i0} W(\omega), \qquad (2)$$

where $W = \sum_{ij} W_{ij}|i\rangle(j|$ for i, j = 0, 1, 2. Here and below, we write an operator x as $|x\rangle := x$, and its covector acting on an argument • as $(x|\bullet := \operatorname{Tr} x^{\dagger} \bullet [48]$. The basis vectors denote unit-trace physical-state operators¹ with 0, 1, and 2 electrons: $|0\rangle := |0\rangle\langle 0|, |1\rangle := \frac{1}{2}\sum_{\sigma} |\sigma\rangle\langle \sigma|, |2\rangle := |2\rangle\langle 2|$. The coefficients W_{ij} , given in [47], represent the golden-rule transition rates between the different electronic states (see, e.g., [34]).

For t > 0, a standard way of solving Eq. (2) proceeds by expanding $\rho(t)$ in the right eigenvectors of *W*—the decay modes—and obtaining their coefficients from the corresponding left eigenvectors—the amplitude covectors:

$$|\rho(t)\rangle = e^{Wt}|\rho_0\rangle$$
(3)
= |z)(z'|\rho_0) + e^{-\gamma_p t}|p)(p'|\rho_0) + e^{-\gamma_c t}|c)(c'|\rho_0).

We denote the eigenvalues of W by $-\gamma_x$, where γ_x is a positive decay rate for x = c, p. Since the system reaches a unique stationary state $\lim_{t\to\infty} |\rho(t)\rangle = |z\rangle$, one eigenvalue of W is 0.

To explicitly calculate the rates and vectors in Eq. (3), one can now straightforwardly determine the left and right eigenvectors of the 3×3 matrix representing W. However, this does not give any systematic, *physical* insight into how the excitation amplitudes and rates of the decay modes are related. As we illustrate in the following, the duality, Eq. (1), does provide such insight. In the Born-Markov approximation, we expand Eq. (1) to linear order in Γ , and take the limit $\omega, i\Gamma \rightarrow i0$ in the frequency arguments. This yields² $W^{\dagger} = -\Gamma - \mathcal{PIWIP}$, where \mathcal{I} denotes the parameter substitution that constructs the dual model: $\mu \rightarrow -\mu, \epsilon \rightarrow -\epsilon$ and, importantly, $U \rightarrow -U$. For a known mode $|x\rangle = x$ with decay rate γ_x , application of this relation to $\mathcal{PI}|x\rangle$ determines

¹The empty state is $|0\rangle$, whereas $|\sigma\rangle := d_{\sigma}^{\dagger}|0\rangle$ and $|2\rangle := d_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}|0\rangle$. ²Since $W \propto \Gamma \propto (H^{T})^{2}$, the dual coupling $H^{T} \rightarrow i H^{T}$ effectively inverts the sign of W.

an amplitude covector $(y') \bullet$ with

$$y' = (-1)^N \mathcal{I} x$$
 and rate $\gamma_y = \Gamma - \mathcal{I} \gamma_x$. (4)

The key result, Eq. (4), *cross-links* left and right eigenvectors with different rates. For our model, it allows one to physically relate all the rates and vectors in Eq. (3). First, the zero eigenvector of *W* is simply the trace-normalized stationary equilibrium state $|z| = e^{-(H-\mu N)/T}/\mathcal{Z}$ of the quantum dot with $\mathcal{Z}(\epsilon, U, \mu) = \text{Tr } e^{-(H-\mu N)/T}$. Its amplitude in Eq. (3) is $(z'|\rho_0) = 1$, since probability conservation [Tr $\rho(t) = 1$] for all times *t* requires that the left eigenvector associated with the zero eigenvalue is (z'| = (1|. The mere existence of this left zero eigenvector implies by duality (4) that there is a maximal [47] rate $\gamma_p = \Gamma$ which depends only on the bare tunnel coupling, and whose mode is given by the fermion-parity operator:

$$|p\rangle = |(-1)^N) \text{ with } \gamma_p = \Gamma.$$
(5)

Analogously, the parity amplitude covector is found by applying Eq. (4) to the stationary mode $|z\rangle$, giving

$$(p'| = ((-1)^N z_i| \text{ with } \gamma_p = \Gamma.$$
(6)

It contains $z_i = \mathcal{I}z = z(-\epsilon, -U, -\mu)$, the stationary state of the dual quantum-dot model with attractive interaction obtained by the parameter substitution \mathcal{I} , i.e., by inverting the energies as illustrated in Fig. 1(c). Therefore, we call $|z_i\rangle$ the *inverted stationary state*. Finally, the charge-decay rate is self-dual, $\gamma_c = \Gamma - \mathcal{I}\gamma_c = \frac{1}{2}\Gamma\{f^+(\epsilon) + f^-(\epsilon + U)\}$ [33] with $f^{\pm}(\epsilon) = (e^{\pm(\epsilon-\mu)/T} + 1)^{-1}$. Its amplitude and mode (see [47]) are thus also connected by the fermion-parity and the dual model: $(c'| = 2[\mathcal{PII}c)]^{\dagger}$.

The existence of a decay mode with a rate Γ that surprisingly only depends on the bare coupling was pointed out in previous works [33–37]. However, it was not understood where the independence from all physical attributes except the "interface" property Γ stems from. The duality (4) sheds an entirely new light onto this problem. It shows that the constant decay rate Γ is fixed by the fundamental requirement of probability conservation, via the duality based on the fermion-parity superselection principle. Moreover, the duality relates the complete decay dynamics to the *stationary state* $|z_i\rangle$ of the attractive dual model, as seen most explicitly in $(p'| = ((-1)^N z_i)$. It is this relation to the dual model which dictates the amplitudes in the heat decay.

Heat decay. We now apply the results derived above to study the transient heat current out of the dot after a sudden switch of the level position $\epsilon_0 \rightarrow \epsilon$. In the Born-Markov limit, we can evaluate this heat current [47] as $I_Q(t) = -\partial_t(H - \mu N | \rho(t))$, with $\rho(t)$ given in Eq. (3), and all its ingredients obtained by the duality, Eq. (4). This way, one not only finds the announced double-exponential form of the heat current, $I_Q(t) = a_c e^{-\gamma_c t} + a_p e^{-\gamma_p t}$. Importantly, the amplitudes

$$a_{c} = \left[\epsilon - \mu + \frac{1}{2}(2 - N_{i})U\right](N_{0} - N_{z})\gamma_{c},$$
(7)

$$a_p = U \Big[\frac{1}{2} (N_{\rm i} - 1)(N_0 - 1) + \frac{1}{4} (p_{\rm i} + p_0) \Big] \gamma_p, \qquad (8)$$

can now also be expressed entirely in terms of quantities with a clear physical meaning: assuming that the dot is initially in the stationary state $|\rho_0\rangle = |z(\epsilon_0)\rangle$ with initial level position ϵ_0 , the

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occupation number of the dot $N_0 = (N | \rho_0)$ and the parity $p_0 =$ $((-1)^N | \rho_0)$ in the initial state carry all dependence on ϵ_0 , as expected. However, the dependence on the final level position ϵ enters not only through the stationary occupation $N_z =$ (N|z), but also through the occupation $N_i = (N|z_i)$ and parity $p_i = ((-1)^N | z_i)$ of the inverted stationary state, governed by attractive interactions. To illustrate the consequence of this dependence, we plot the amplitudes a_c, a_p in Figs. 1(d) and 1(e) for a level switch $\epsilon_0 \rightarrow \epsilon$. Most prominently, both a_c and a_p exhibit a very sharp, large change when tuning the final level through $\epsilon - \mu = -U/2$. As revealed by Eqs. (7) and (8), the reason for this jump is that all terms in the heat current which relate to the Coulomb energy dissipation, i.e., the parity amplitude a_p and the correction $\propto U$ in a_c , are governed by the dual stationary occupation number N_i . An attractive interaction, which here enters through the dual model, is well known [38] to force N_i to jump directly from 0 to 2 at $\epsilon - \mu = -U/2$, avoiding $N_i = 1$ and keeping an even parity $p_i = +1$. By contrast, a sweep of the *initial level* $\epsilon_0 - \mu$ causes the initial charge to traverse $N_0 = 0, 1, 2$, and the parity to alternate, $p_0 = 1, -1, 1$. This yields sharp changes of a_p and a_c at the expected energies for a repulsive system, the two Coulomb resonances $\epsilon_0 - \mu = 0$ or -U. We stress that while the end result for $I_O(t)$ also follows from a straightforward calculation of left and right eigenvectors of W, it does not lead to an equally concise, physically motivated form of a_p and a_c . Most importantly, the peculiar ϵ dependence of these amplitudes is only revealed by the duality.

Another notable feature of Figs. 1(d) and 1(e) is that the parity mode dominates $I_Q(t)$ whenever it is excited: in the red areas in Fig. 1(e), its amplitude assumes the constant, maximal value $a_p = \Gamma U$, whereas $|a_c| \lesssim \frac{1}{2} \Gamma U$ [47] in Fig. 1(d). This offers an interesting possibility of experimentally accessing the decay dynamics of the parity mode. Measuring γ_p is a nontrivial task, since the parity mode $|(-1)^N|$ does not enter single-particle observables like the average charge current, which indeed decays at a single rate: $I_N(t) = -\partial_t(N|\rho(t)) =$ $(N_0 - N_z) \gamma_c e^{-\gamma_c t}$. Methods to detect γ_p have been proposed in Refs. [34,37], by coupling the dot to a quantum point contact or a sensor quantum dot. Figures 1(d) and 1(e) show that the heat current provides a very natural and more direct way to gain this information. In fact, $I_O(t)$ can be obtained using a pump-probe scheme by extending well-established techniques of mesoscopic charge detection [49,50]. By measuring the rise of the stationary electrode temperature as a function of the delay time, one can extract the full time-resolved heat current. Simultaneous measurement of the charge current then allows one to demonstrate-without fitting-the predicted constancy of the rate $\gamma_p = \Gamma$ as well as the attractive-interaction signature of a_p , as sketched in [47].

An important insight for this kind of experiment is provided again by the duality and is illustrated in Figs. 1(a)–1(c). For $U \gg T$, the amplitude $a_p \approx (z_i | \rho_0) U\Gamma$ essentially equals the overlap of the initial state with the inverted stationary state. To infer which switch excites the parity mode, one can thus proceed as follows: given the targeted final level position ϵ , one calculates the stationary state of the attractive dual system, $|z_i(\epsilon)\rangle$, and chooses the initial level position ϵ_0 such that the initially prepared state $|\rho_0\rangle = |z(\epsilon_0)\rangle$ has the same occupation as $|z_i(\epsilon)\rangle$.

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In such measurements of the heat current, one can *resolve* in time that two sequentially tunneling electrons carry equal charge but different energy. (Only for U = 0, the heat current is simply "tightly coupled" to the particle current [13], $I_Q \propto I_N$ since $a_p = 0$.) For example, for an initially doubly occupied dot and a switch expelling both electrons—the situation at the cross in Figs. 1(d) and 1(e)—the heat current simplifies to $I_Q(t) \approx (\epsilon - \mu)I_N(t) + U\Gamma e^{-\gamma_p t}$. While the excess orbital energy $\epsilon - \mu$ is carried by each of the two electrons tunneling out, the charging energy U is dissipated already with the *first* electron. Notably, when switching ϵ to one of the two Coulomb resonances—e.g., at the open circle in Figs. 1(d) and 1(e)—the heat current is even *entirely* due to the tunneling of the first particle, taking place on the shortest, temperature-independent time scale Γ^{-1} .

General duality. We conclude by discussing the main physical principles behind the general duality relation, Eq. (1). The derivation of Eq. (1) is technical but straightforward³ if one uses the insights established in [35,36]. The main point is that in the wide-band limit, the best reference solution for a perturbative calculation of the dynamics is *not* the

uncoupled solution $(H^{T} = 0)$, but rather the exact solution of the coupled system in the limit of infinite temperature $T \to \infty$. With respect to this solution, the propagator $\Pi(t)$ for the density matrix of the system, $\rho(t) = \Pi(t)\rho_0$, needs to be expanded in terms of only part of the coupling, as a consequence of the fermion-parity superselection principle [35,36]. What is crucial for the result, Eq. (1), is that the adjoints of the operators occurring in this simpler expansion can always be expressed in parity operations [47]. This allows one to derive order by order the time-propagator duality $\Pi(t; H, H^{\mathrm{T}}, \{\mu\})^{\dagger} = e^{-\Gamma t} \mathcal{P} \Pi(t; \bar{H}, \bar{H}^{\mathrm{T}}, \{\bar{\mu}\}) \mathcal{P}$. This is equivalent to Eq. (1) and holds under the general conditions stated in the introduction, i.e., it applies also to nontrivial low-temperature, strong-coupling, nonequilibrium regimes of complex multilevel fermionic systems. In the commonly used expansion about the uncoupled system $(H^{T} = 0)$, the duality remains completely elusive. Extending the duality beyond the wide-band limit is challenging but seems possible using [35,36].

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