Decoherence in a double-dot Aharonov-Bohm interferometer: Numerical renormalization group study

Björn Kubala,[1,2] David Roosen,[3] Michael Sindel,[4] Walter Hofstetter,[3] and Florian Marquardt[1,5]
[1]*Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany*
[2]*Institut für Theoretische Physik, Universität Ulm, Albert Einstein-Allee 11, 89069 Ulm, Germany*
[3]*Institut für Theoretische Physik, Goethe Universität, 60438 Frankfurt am Main, Germany*
[4]*Physics Department, ASC, and CeNs, Ludwig-Maximilians-Universität, 80333 Munich, Germany*
[5]*Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1, Bau 24, 91058 Erlangen, Germany*
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Coherence in electronic interferometers is typically believed to be restored fully in the limit of small voltages, frequencies, and temperatures. However, it is crucial to check this essentially perturbative argument by nonperturbative methods. Here we use the numerical renormalization group to study ac transport and decoherence in an experimentally realizable model interferometer, a parallel double quantum dot coupled to a phonon mode. The model allows us to clearly distinguish renormalization effects from decoherence. We discuss finite-frequency transport and confirm the restoration of coherence in the dc limit.

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I. INTRODUCTION

Quantum coherence and its degradation by interaction with the environment are crucial ingredients in electronic transport through nanostructures. Generically, perturbation theory suggests that coherence is fully restored in the limit of small applied bias voltage, ac frequency, and temperature. In this limit, the particles do not have enough energy to leave behind a trace in the environment. However, it is highly desirable to check whether such a statement remains valid beyond perturbation theory. In this work we propose to employ the numerical renormalization group (NRG) [1] to study this question. This method can readily be applied to transport through interacting localized electronic levels such as quantum dots and molecules. Investigating decoherence in such systems offers the advantages of (some degree of) experimental control of the type and strength of decoherence mechanisms and, on the theoretical side, of a wealth of powerful, advanced methods.

In discussing the effects of coupling a system to an environment true decoherence has to be carefully distinguished from a mere renormalization of the system's characteristics due to the coupling [2]. Electron-phonon coupling, for example, affects transport in several ways: Incoherent processes, in which phonons are absorbed or emitted, may increase or decrease the total transport through a single site [3] and coherent contributions to transport will also be renormalized. Considering an interferometer, the most obvious way to study decoherence in electronic transport, it thus turns out to be advantageous not to consider the overall change in the amplitude of the current or conductance as a measure of decoherence. Instead, we want to focus on the special case of destructive interference, i.e., the case of half a quantum of magnetic flux for an Aharonov-Bohm interferometer (ABI) (see Fig. 1). The advantage [4] is that in an interferometer with perfectly symmetric arms renormalization processes will not lift the destructive interference and any finite current is a true sign of decoherence.

In this work we consider a double-dot Aharonov-Bohm interferometer (see Fig. 1), where electrons on the dots couple to a single optical phonon mode, representing the environment. This interferometer scenario can be experimentally realized in tunneling transport through two quantum dots placed between two electron reservoirs [5] and possibly in molecular electronics for quasidegenerate molecular levels of different parity [6]. On the one hand, one can then consider specifically engineered phononic environments, for instance, for quantum dots defined within freestanding nanobeams [7] or a quantum dot coupling to a cantilever [8]; on the other hand, the simple single-mode scenario can easily be generalized to model multiple phonon modes in standard heterostructures or molecular electronics [9]. (Moreover, some results of this study are also expected to carry over to quantum dots coupled to a generic two-level system.) We focus on the linear ac conductance, which is readily accessible by the NRG method and is of great general [10,11] and current [12,13] interest. The nonperturbative NRG results will be complemented by nonequilibrium Green's functions (NEGFs) [14] methods.

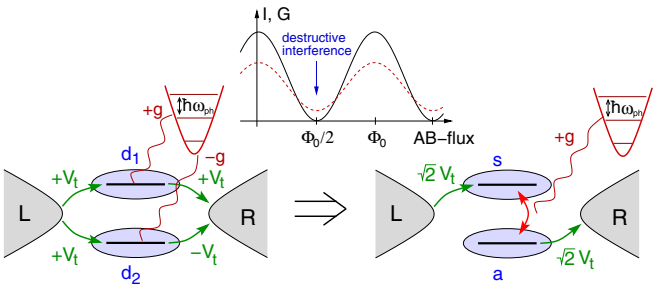

FIG. 1. (Color online) Double-dot Aharonov-Bohm interferometer. Decoherence suppresses the amplitude of AB oscillations (dashed line). At destructive interference, $\phi_{AB} = \Phi_0/2$, only incoherent transport processes contribute in a symmetric setup. Mapping the Hamiltonian to (anti)symmetric combinations of the dot levels allows for a transparent exploitation of this cancellation of coherent transport.

II. MODEL

Our system is described by the Hamiltonian $\hat{H} = \hat{H}_{\rm imp} + \sum_{\alpha=L/R}(\hat{H}_{{\rm res},\alpha} + \hat{H}_{T,\alpha})$ with the lead Hamiltonian $\hat{H}_{{\rm res},\alpha} = \sum_k \epsilon_{k\alpha}\hat{c}^\dagger_{k\alpha}\hat{c}_{k\alpha}$ and spinless electrons on two degenerate dot levels $n = 1,2$ coupling to a single phonon mode

$$\hat{H}_{\rm imp} = \sum_{n=1,2} \varepsilon \hat{d}^\dagger_n \hat{d}_n + \hbar\omega_{\rm ph}\hat{b}^\dagger\hat{b} + g(\hat{b}+\hat{b}^\dagger)(\hat{d}^\dagger_1\hat{d}_1 - \hat{d}^\dagger_2\hat{d}_2), \tag{1}$$

where the level energy ϵ is taken with respect to the Fermi level of the leads. Assuming an electron-phonon coupling of equal magnitude but different signs for the two dots, the phonons effectively act as a kind of "which-path" detector decohering the electrons.

In a symmetric, destructive interferometer, i.e., for a tunneling Hamiltonian $\hat{H}_{T,\alpha} = \sum_{k,\,n=1,2} V_{\alpha,n}\hat{c}^\dagger_{k\alpha}\hat{d}_n$ + c.c., where $V_{L/R,\,1} = V_{L,\,2} = -V_{R,\,2} = V_t$, it is decoherence alone that allows for transport, overcoming the destructive interference. This is seen by mapping the Hamiltonian onto a new basis $\hat{a}/\hat{s} = (\hat{d}_1 \mp \hat{d}_2)/\sqrt{2}$ of (anti)symmetric combinations of the original dot levels. The impurity Hamiltonian then reads

$$\hat{H}_{\rm imp} = \varepsilon(\hat{s}^\dagger\hat{s} + \hat{a}^\dagger\hat{a}) + g(\hat{b}+\hat{b}^\dagger)(\hat{s}^\dagger\hat{a} + \hat{a}^\dagger\hat{s}), \tag{2}$$

with the (anti)symmetric level coupling to the left (right) lead only with tunneling matrix elements $V_{L,\,s} = V_{R,\,a} = \sqrt{2}V_t$ and $V_{R,\,s} = V_{L,\,a} = 0$ (see Fig. 1). It decouples into separated left and right parts for $g = 0$, whereas transport across the interferometer becomes possible due to a tunneling term between the two new levels, which is coupled to the phonon mode. The appearance of such a term is generically linked to the path-detecting (and thus decohering) nature of the asymmetric electron-phonon coupling chosen in Eq. (1); a symmetric coupling cannot yield transport of electrons across the interferometer [15]. While it is obvious from Eq. (2) that the noninteracting contribution vanishes, we will later show that destructive interference also cancels renormalized processes, reflected in the vanishing of certain classes of diagrams after performing the mapping. This particularly advantageous feature of only observing (in calculation and experiment) incoherent transport processes offered by the setup considered here was not present in other theoretical studies of various interference effects in related setups [16] or in studies of electron-phonon interaction for a single dot [17–20].

III. TECHNIQUES

We will present two approaches to study this system. First, we employ the NEGF theory, where, based on the exact noninteracting result [21], the electron-phonon interaction is perturbatively included using Keldysh diagrams. Particularly tailored to treat nonequilibrium situations, which can easily be realized in quantum-dot systems by an applied dc bias, the NEGF or Keldysh method [14] has been widely used as a physically transparent tool to investigate the electron-phonon interaction in such systems, often, as here, in a perturbative manner [17–19] or employing extensions of the polaron approach [18,20], which allows tackling strong electron-phonon coupling for weakly tunnel-coupled systems. In this work we focus on the linear ac conductance $\mathcal{G}_{\alpha\beta}$, giving the finite-frequency current $I_\alpha(\omega_{\rm ac}) = \mathcal{G}_{\alpha\beta}(\omega_{\rm ac})\,V_\beta(\omega_{\rm ac})$ flowing out of lead α in response to a small ac-excitation voltage V_β of frequency $\omega_{\rm ac}$ applied to lead β [22]. It is connected to a (retarded) current-current correlator $\mathcal{G}_{\alpha\beta}(\omega_{\rm ac}) = [K_{\alpha\beta}(\omega_{\rm ac}) - K_{\alpha\beta}(0)]/i\omega_{\rm ac}$, where

$$K_{\alpha\beta}(\omega_{\rm ac}) = -\frac{i}{\hbar}\int_0^\infty dt\, e^{i\omega_{\rm ac}t}\langle\big[\hat{I}_\alpha(t), \hat{I}_\beta(0)\big]\rangle. \tag{3}$$

To calculate this correlator, and hence the ac conductance, we use a recently developed Meir-Wingreen-type formula for the linear ac conductance [23], which allows straightforward diagrammatic calculations perturbatively including electron-phonon interaction, complementing previous works building on a fully time-dependent Green's function formalism [24] (see, e.g., Ref. [25], treating electron-electron interactions) and rate-equation approaches [26].

While the perturbative NEGF approach is only valid for weak electron-phonon interactions, our second approach, the NRG method, developed by Wilson [1], is especially tailored for strongly interacting systems. Throughout the past two decades numerous enhancements of the numerical renormalization group method have been introduced, improving the accuracy of correlation functions [27–30] and offering the possibility to study quantum impurity systems coupled to a bosonic bath [31]. Here we present the NRG calculation of ac conductance in a quantum-dot system with an additional bosonic degree of freedom (cf. NRG studies on ac conductance with an electron-electron interaction, for instance, in the Kondo regime [32], and investigations of electron-phonon coupling effects on linear dc conductance, spectral density, and spin and charge susceptibilities [33,34]). For a quantum impurity system with a fermionic bath and an additional bosonic mode coupled to the impurity directly, the numerical renormalization group can be applied in a similar fashion as in the pure fermionic case without the bosonic mode. The mapping to the Wilson chain is not affected by the additional bosonic mode [30,33] since the bosons only enter in the very first step of the iterative diagonalization procedure. We implemented a NRG algorithm using the reduced density matrix [28] as well as the complete basis of the underlying Fock space. Furthermore, we performed a z trick averaging [35] over 32 slightly different discretizations of the conduction band to improve on the logarithmic resolution of energy (and thereby also frequency) around the Fermi energy inherent to the NRG. In that manner, reliable numerical results up to frequencies of some 10% of the bandwidth could be achieved with reasonably small numerical errors and artifacts.

IV. RESULTS AND INTERPRETATION

To investigate the effects of *weak electron-phonon coupling* on ac transport, we employ the NEGF, considering contributions to the ac conductance from diagrams with up to a single phonon line, which gives contributions up to $O(g^2)$. Using the mapping to (anti)symmetric dot levels in a diagrammatic representation for the ac conductance automatically exploits the main characteristic of transport in the symmetric destructive ABI, namely, the complete cancellation of coherent transport processes due to destructive interference. For instance, considering the ac conductance

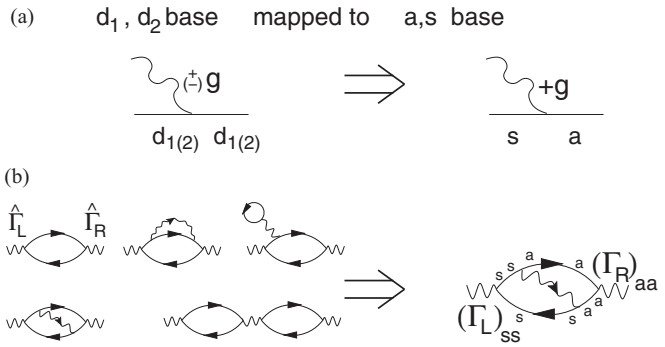

FIG. 2. Mapping the Hamiltonian to (anti)symmetric combinations of the dot levels: (a) the mapped electron-phonon interaction vertex restricts (b) the number and type of diagrams in a perturbative calculation of ac conductance, reflecting the destructive interference of all coherent contributions. (Solid lines denote the electron Green's functions and wiggly lines stand for phonon propagators.)

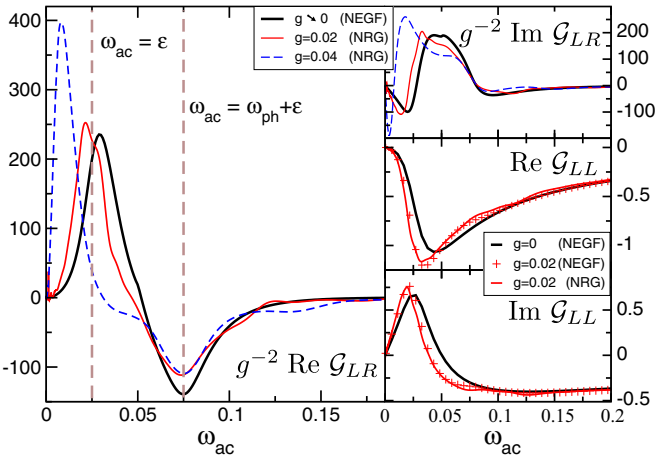

FIG. 3. (Color online) Plot of the ac conductance through the destructive ABI. In the limit of weak electron-phonon coupling the NRG and perturbative calculations match. For stronger electron-phonon coupling $g/\omega_{\rm ph} \approx 1$, additional side peaks at $\omega_{\rm ac} = \epsilon + n\omega_{\rm ph}$ ($n \in \mathbb{N}$) appear and the first resonance is shifted to lower frequency. Here $\mathcal{G}_{LR}(\omega_{\rm ac} = 0) \equiv 0$ is found also for strong electron-phonon coupling. The parameters are $\omega_{\rm ph} = 0.05$, $\epsilon = 0.025$, $\Gamma = 2\pi(\rho_L + \rho_R)|V_t|^2 = 0.02$ in units of the bandwidth, and conductances in units of e^2/h and we consider the zero-temperature limit and no dc bias.

$\mathcal{G}_{LR}(\omega_{\rm ac})$, there are a zeroth-order and several second-order diagrams constructible from the original electron-phonon interaction vertex (Fig. 2), while no zeroth-order and only a single second-order diagram can be constructed from the mapped electron-phonon coupling vertex and the mapped lead-dot couplings. The nonexistence of those diagrams reflects the notion that in the destructive ABI the coherent zeroth-order contribution, as well as contributions where transport is merely renormalized, will interfere destructively and thus vanish. There are, however, diagrammatic contributions for the diagonal conductances $\mathcal{G}_{LL/RR}(\omega_{\rm ac})$, describing electrons tunneling back and forth between the (anti)symmetric level and the (left) right lead, as the chemical potential of the lead is varied with frequency $\omega_{\rm ac}$. The noninteracting result thus found (see the lower right panel of Fig. 3), which is also accessible by simpler techniques [11,24], reproduces for small frequencies the universal behavior of a mesoscopic RC circuit with a quantized charge relaxation resistance [10,11]. The second-order contribution to $\mathcal{G}_{LL}$ constitutes a small correction to the noninteracting result, which yields additional features at $\omega_{\rm ac} = \epsilon + \omega_{\rm ph}$. Turning to the conductance across the interferometer $\mathcal{G}_{LR}$, we find, as argued above, no zeroth order and only a single, topologically distinct diagram in second order, namely, an electronic loop with a crossing phonon line [see Fig. 2(b)]. One can now easily use Keldysh diagrammatic rules to find the corresponding integral expression for the ac conductance in terms of the electronic Green's functions and the bare phononic propagators $D^{R/A}_{E'} = (E' - \omega_{\rm ph} \pm i\eta)^{-1} - (E' + \omega_{\rm ph} \pm i\eta)^{-1}$. Interestingly, there are contributions from the δ peak at the phonon energy $\omega_{\rm ph}$ as well as from the principal-value part. For the dissipative real part of the conductance $\mathrm{Re}\,\mathcal{G}_{LR}$ (see the left panel of Fig. 3), we find that contributions from the latter yield a resonant peak at $\omega_{\rm ac} = \epsilon$. Around $\omega_{\rm ac} = \epsilon + \omega_{\rm ph}$, where the excitation frequency is in resonance with the dot level position after the excitation of a phonon, there is a smaller negative peak, stemming from the δ contributions. Corresponding features at the same frequencies are found for the imaginary part $\mathrm{Im}\,\mathcal{G}_{LR}$.

Investigating *strong electron-phonon coupling*, comparisons of NRG calculations to the perturbative results are shown in Fig. 3. For weak electron-phonon coupling, there is good qualitative and also quantitative agreement between the NRG and the perturbative results: In the limit $g \searrow 0$, we reach the noninteracting results for $\mathcal{G}_{LL}$ (thick black lines in the two lower right panel of Fig. 3), while for $\mathcal{G}_{LR}$ we recover the perturbative $O(g^2)$ result derived above. The left panel of Fig. 3 also demonstrates the main effects of stronger electron-phonon coupling on $\mathrm{Re}\,\mathcal{G}_{LR}$. Most importantly, one finds additional resonances at sidebands of the level energy $\omega_{\rm ac} = \epsilon + n\omega_{\rm ph}$ ($n \in \mathbb{N}$), which stem from processes involving several phonons. Furthermore, we observe a shift of the first resonance from $\omega_{\rm ac} \approx \epsilon$ to smaller frequencies reminiscent of a polaron shift.

In the following, we want to highlight two particular remarkable features of our results at low frequency. The first, observable already in the weak-coupling limit, is the fact that ac transport is already possible for excitation frequencies smaller than the phonon energy $\omega_{\rm ac} < \omega_{\rm ph}$. Let us first emphasize that this is in striking contrast to the case of finite-bias dc transport, where in the weak-coupling limit there is a sharp threshold for incoherent transport processes becoming possible only for $eV_{\rm dc} \geqslant \omega_{\rm ph}$. Using the mapping to (anti)symmetric dot states, the dc current through a destructive ABI can be shown to contain only incoherent contributions. These contributions are characterized by the explicit appearance (cf. Eq. 66 in Ref. [17]) of self-energies $\Sigma^{\gtrless,\,\rm ph}$ due to emission or absorption of phonons. In lowest order in the electron-phonon coupling (and for zero temperature) transport takes place through two transport channels at $\omega = \epsilon, \epsilon + \omega_{\rm ph}$ within a transport window $\mu_L > \omega > \mu_R + \omega_{\rm ph}$. In particular, the resulting I-V curve has a sharp gap at low bias $eV_{\rm dc} < \omega_{\rm ph}$ as any incoherent transport process necessarily involves the emission of a phonon whose energy has to be provided by the applied bias. The naive expectation that in ac

transport the frequency of the infinitesimal ac-excitation voltage providing energy for emission of phonons acts in a similar manner does not hold. In fact, subthreshold ac transport apparently is possible without the real emission of phonons. Considering the Hamiltonian of the destructive ABI in the mapped base, we see that virtual tunneling back and forth processes between symmetric and antisymmetric levels with emission and absorption of phonons will yield an effective charge-charge interaction between the two sites. Such an interaction then leads to finite ac conductance, but vanishing dc conductance, just like the electrostatic interaction in a plate capacitance.

While both of these arguments explain the vanishing of conductance in the dc limit in lowest order in the electron-phonon coupling, note as a second, most important, feature of the results in Fig. 3 that our NRG results indicate that this holds for strong coupling also. Indeed, while in a lowest-order process phonons can only be excited exactly at their bare frequency ω_{ph}, considering higher orders, one may naturally ask about the effects of the broadening of the phonon propagator due to coupling to the electrons. Some (though not all) higher-order effects can thus be captured by calculating the electronic self-energies with a phonon propagator dressed with electronic polarization bubbles. In the dc case, one finds that electrons can indeed absorb an energy up to eV from the phononic bath broadened by coupling to the electrons, instead of needing to emit ω_{ph} as in lowest order. Nonetheless, the weight of such contributions is small, leading to a current dependence $I \propto (eV)^3$ for small bias voltage for the considered higher-order contributions in the electron-phonon coupling and consequently a vanishing linear conductance at zero frequency. This agrees with the dc limit of our NRG results for the ac conductance, which indicates as discussed that all higher-order contributions to the linear zero-temperature conductance vanish. We thus confirm the naive perturbative argument that there are no incoherent transport processes at vanishing frequency, temperature, and transport voltage.

V. CONCLUSION

We have studied decoherence and the effects of electron-phonon coupling on ac transport in a double-dot interferometer. A diagrammatic calculation reveals that renormalization processes can be clearly distinguished from decoherence for the case of destructive interference and it explains low-frequency transport as a consequence of phonon-mediated charge-charge interactions in a mapped system. Numerical renormalization group calculations for stronger coupling show characteristic features due to multiphonon processes. With increasing coupling, the phonon mode broadens and effectively yields a continuous environment spectrum. Nevertheless, the nonperturbative NRG result confirms that coherence is fully restored in the zero-frequency limit of the linear conductance at zero temperature.

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