DMRG evaluation of the Kubo formula – Conductance of strongly interacting quantum systems

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Abstract. – In this paper we present a novel approach combining linear response theory (Kubo) for the conductance and the Density Matrix Renormalization Group (DMRG). The system considered is one-dimensional and consists of non-interacting tight binding leads coupled to an interacting nanostructure via weak links. Electrons are treated as spinless fermions and two different correlation functions are used to evaluate the conductance.

Exact diagonalization calculations in the non-interacting limit serve as a benchmark for our combined Kubo and DMRG approach in this limit. Including both weak and strong interaction we present DMRG results for an extended nanostructure consisting of seven sites. For the strongly interacting structure a simple explanation of the position of the resonances is given in terms of hard-core particles moving freely on a lattice of reduced size.

Introduction. – During the past decade improved experimental techniques have made production of and measurements on one-dimensional systems possible [1], and hence led to an increasing theoretical interest in these systems. Since its formulation in 1992 [2] the Density Matrix Renormalization Group method (DMRG) has been established as a very powerful, quasi-exact method for numerical calculations of properties of (quasi) one-dimensional systems.

In this paper we present a new approach for calculating linear response conductance for one-dimensional interacting nanostructures coupled to non-interacting tight binding leads. The method combines Kubo expressions for the conductance with numerical DMRG calculations and is valid for arbitrary interaction strength. It facilitates a unified description of strong and weak interactions and provides conductance directly from a transport calculation, without relying on relations between equilibrium and transport properties.

We employ current-density and current-current correlation functions to calculate the conductance and in the non-interacting case compare to exact diagonalization calculations.

In the strongly interacting limit a simple interpretation of the position of the resonances is given in terms of freely moving hard-core particles on a reduced size lattice [10], and quantitative comparison with numerical DMRG results shows good agreement.

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where the current is given by

\[ \hat{A} \]

lead operators, the procedure. The number operator is taken as a symmetric combination of the left and right unbiased structure, since we apply it to the quasi-exact ground state given by the DMRG and henceforth neglected in all numerical calculations.

\[ M \]

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\[ \gamma \]

The parameter controls the smoothing of the interaction on the dot over the contact links as discussed in [3], and \( U_g \) is a gate voltage on the structure. In this work we set \( t = t_{\text{Dot}} = 1 \).

\[ M \]

Model. – We are interested in studying the effect of correlations on transport within a microscopic model of an interacting one-dimensional nanostructure coupled to two non-interacting tight binding leads, as shown in Fig. 1. Electrons are treated as spinless and only nearest neighbor interaction is considered. The corresponding Hamiltonian is

\[ \begin{align*}
\hat{H}_0 &= \hat{H}_{\text{NS}} + \hat{H}_{L} + \hat{H}_{C}, \\
\hat{H}_{\text{NS}} &= \sum_{j=n_1}^{n_2-1} U_g \hat{c}_j^\dagger \hat{c}_j + \sum_{j=n_1+1}^{n_2-1} \left( -t_{\text{Dot}} (\hat{c}_{j-1}^\dagger \hat{c}_j + \hat{c}_j \hat{c}_{j-1}) + V \hat{c}_j^\dagger \hat{c}_j \hat{c}_{j-1} \right), \\
\hat{H}_L &= -t \sum_{i=2}^{n_1} (\hat{c}_i^\dagger \hat{c}_{i-1} + \hat{c}_{i-1} \hat{c}_i) - t \sum_{i=n_2+1}^{M} (\hat{c}_i^\dagger \hat{c}_{i-1} + \hat{c}_{i-1} \hat{c}_i), \\
\hat{H}_C &= -t_L (\hat{c}_{n_1}^\dagger \hat{c}_{n_1-1} + \hat{c}_{n_1-1} \hat{c}_{n_1}) - t_R (\hat{c}_{n_2}^\dagger \hat{c}_{n_2-1} + \hat{c}_{n_2-1} \hat{c}_{n_2}) + \gamma V (\hat{c}_{n_1}^\dagger \hat{c}_{n_1-1} \hat{c}_{n_1-1} + \hat{c}_{n_2}^\dagger \hat{c}_{n_2-1} \hat{c}_{n_2-1}).
\end{align*} \]

The parameter \( \gamma V \) controls the smoothing of the interaction on the dot over the contact links as discussed in [3], and \( U_g \) is a gate voltage on the structure. In this work we set \( t = t_{\text{Dot}} = 1 \).

\[ \begin{align*}
\hat{K} &= \hat{H}_0 + \delta \hat{H}, \\
\langle \tilde{J}_n(t) \rangle &= \tilde{J} - i \int_{-\infty}^{t} dt' \langle \psi_0 | [\tilde{J}_n(t), \delta \hat{H}(t')] | \psi_0 \rangle, \\
\tilde{J}_n(t) &= -it_n [\hat{c}_n^\dagger(t) \hat{c}_{n-1}^\dagger(t) - \hat{c}_{n-1}^\dagger(t) \hat{c}_n(t)],
\end{align*} \]

where \( \hat{H}_0 \) is the Hamiltonian in eq. [1] the applied voltage perturbation is \( \delta \hat{H}(t) = V_{\text{SD}}(t) \hat{N} \), \( \hat{A}(t) = e^{i\hat{H}_0 t} \hat{A} e^{-i\hat{H}_0 t} \) denotes the interaction picture time evolution of the operator \( \hat{A} \), and \( | \psi_0 \rangle \) denotes the ground state. Note that in this approach \( \hat{A}(t) \) contains all correlations of the unbiased structure, since we apply it to the quasi-exact ground state given by the DMRG procedure. The number operator is taken as a symmetric combination of the left and right lead operators, \( \hat{N} = \frac{1}{2}(\hat{N}_L - \hat{N}_R) \), and \( \hat{J} \) is the equilibrium current included for completeness and henceforth neglected in all numerical calculations.

Kubo Expressions. – Using linear response in applied source-drain voltage, \( V_{\text{SD}}(t) \), the current is given by

\[ \begin{align*}
\langle \tilde{J}_n(t) \rangle &= \tilde{J} - i \int_{-\infty}^{t} dt' \langle \psi_0 | [\tilde{J}_n(t), \delta \hat{H}(t')] | \psi_0 \rangle, \\
\tilde{J}_n(t) &= -it_n [\hat{c}_n^\dagger(t) \hat{c}_{n-1}^\dagger(t) - \hat{c}_{n-1}^\dagger(t) \hat{c}_n(t)],
\end{align*} \]

The Kubo conductance in the DC limit, \( g = \frac{e^2}{h} \langle \tilde{J} \rangle / V_{\text{SD}} \), can be expressed in terms of two

Fig. 1 – One-dimensional interacting nanostructure with \( M \) sites, coupled to non-interacting tight binding leads. The total system size is denoted \( M \), the number of lead sites is \( M_L \). The interdot and interlead hopping elements are \( t_{\text{Dot}} \) and \( t \) respectively, while the contact between the nanostructure and leads are via \( t_L \) and \( t_R \).
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\[ g_{j,N} = \frac{\epsilon^2}{\hbar} \langle \psi_0 | \hat{J}_n | \hat{N} | \psi_0 \rangle, \quad (8) \]

\[ g_{J,\bar{J}} = \frac{\epsilon^2}{\hbar} \langle \psi_0 | \hat{J}_n | \hat{N} | \psi_0 \rangle, \quad (9) \]

where the positions \( n_1 \) and \( n_2 \) are defined in Fig. 1. Analogous Kubo expressions were used by Louis and Gros in [4], where Quantum Monte Carlo calculations for the density-density correlator were performed.

**Damped Boundary Conditions.** – To improve the finite size scaling and to facilitate the use of sufficiently short leads we use exponentially damped boundary conditions, decreasing the hopping elements towards the end of the leads exponentially as shown for the right lead in eq. (10)

\[ [-t, \cdots, -t, -t, -t, \cdots, -t] \rightarrow \left[ -t, \cdots, -t, -td, -td^2, \cdots, -td^{MD-1}, -td^{MD} \right], \quad (10) \]

where \( d < 1 \). The improvement of the finite size scaling relies on two properties of the DBC’s:

1. They allow for use of a smaller \( \eta \) and
2. Serve as a particle bath for the nanostructure.

The first property is caused by the introduction of exponentially small energies in the system thus reducing the finite size level splitting at the Fermi energy at half filling. The second property can be understood from the fact that the energy cost of adding or removing a particle from the damped region is of the order of the exponentially small hopping element. (2)

The DBC’s introduce two more parameters in the model, the number of damped bonds \( M_D \) and the damping factor \( d \), and these must take values such that physical quantities do not depend sensitively on the particular choice.

**Numerical Calculations.** – Before actual numerical calculations can be performed the parameters of the model, \( M_D \), \( d \), and \( \eta \), must be determined. This is done using exact diagonalization calculations for the non-interacting systems, specifically the resonant value at \( U_g = 0 \). (3) For fixed \( M_D \) we do indeed find a range of \( d \) values that produce essentially identical physical results, indicating the range of validity of the DBC’s. Additionally we find that the actual value of \( M_D \) is not significant (for reasonably large values) as long as the corresponding value of \( d \) is tuned such that the damping at the edge reaches values of the same order of magnitude. The leads used are sufficiently long to keep the damped region separated from the nanostructure, thus allowing Friedel oscillations at the structure edge to decay before reaching the damped region.

The magnitude of the parameter \( \eta \) is bounded by physical arguments; from below by the fact that it should be larger than the finite size level splitting to allow transport, and from above by the fact that Modified BC’s in connection with DMRG were introduced by Vekic and White in [5] using soft boundary conditions to reduce finite size effects. Note that exponential damping corresponds to the hopping Hamiltonian in the Numerical Renormalization Group, which models the logarithmic discretization.

(1) Modified BC’s in connection with DMRG were introduced by Vekic and White in [5] using soft boundary conditions to reduce finite size effects. Note that exponential damping corresponds to the hopping Hamiltonian in the Numerical Renormalization Group, which models the logarithmic discretization.

(2) In principle properties (1) and (2) of the DBC’s could be obtained by using longer non-damped leads. However these leads would have to be exponentially long making such a direct approach impossible.

(3) Considering structures consisting of an odd number of sites has the advantage that the central resonance (by symmetry) remains at \( U_g = 0 \) for half filled leads. Due to the bath property of the DBC’s it is safe to assume that half filling is maintained in the parts of the leads that are close to the nanostructure. In contrast the strongly damped regions act like particle baths and therefore cannot maintain half filling for non-zero external potential.
above by the broadening of physical results by any finite \( \eta \), and should thus be much smaller than the width of the resonances we wish to resolve. It is important to note, that \( \eta \) is an inherent property of any transport calculation and can only be avoided if one finds a way to obtain transport properties from equilibrium properties.

The conductances in eqs. 8 and 9 are given in terms of ground state correlators and hence DMRG is directly applicable. To evaluate the correlators we use the correction vector DMRG [6–8] in the zero frequency limit. Calculating, e.g., the correlator in eq. 9 is done by formulating the linear problems,

\[
\frac{1}{\hat{H}_0 - E_0 + i\eta} \hat{J}_{n_j} |\psi_0\rangle = |\phi_{j}\rangle \quad \Rightarrow \quad \hat{J}_{n_j} |\psi_0\rangle = [\hat{H}_0 - E_0 + i\eta] |\phi_{j}\rangle,
\]

which can be solved for \( |\phi_{j}\rangle \) by a linear solver. Having solved for the correction vector \( |\phi_{j}\rangle \) the conductance is found as the vector overlap,

\[
|\phi_{j}\rangle = |\phi_{j}^{R}\rangle + i|\phi_{j}^{I}\rangle, \quad g_{JJ} = -\frac{8\pi e^2}{\hbar} \langle \phi_{1}^{I} | \phi_{2}^{R} \rangle.
\]

In our DMRG calculations we target apart from the ground state also the real and imaginary parts of the two correction vectors, \( |\phi_{1}\rangle \) and \( |\phi_{2}\rangle \), as well as the states \( \hat{N} |\psi_0\rangle \) and \( \hat{J}_{n_{1,2}} |\psi_0\rangle \) to ensure that the DMRG basis is suitable for describing the conductance accurately [7, 8].

It should be mentioned that the damped boundary conditions make the convergence rate in numerical calculations much slower. In addition any finite external gate voltage, \( U_g \), changes the particle number in the structure and the excess particles come from the bath property of the DBC’s. We therefore face the problem that the damping should be sufficiently strong to provide a reasonable particle bath but at the same time a strong damping decreases the coupling of the highly damped region to the rest of the system. To remedy the slow convergence in the DMRG calculations we turn on the damping in steps and perform several finite system DMRG sweeps for each such damping step. In other words, we perform a complete finite lattice calculation employing typically 11 sweeps and then initiate the scaling sweeps. This allows DMRG to gradually optimize the basis to include the damping in the leads and provides a more gradual decoupling of the damped regions from the rest of the system, thus improving the convergence rate at the cost of more DMRG iterations.

Nevertheless the resolvent equations, eq. 11, are still ill-conditioned and standard solvers like the Conjugate Gradient Method do not converge. We use instead a preconditioned Davidson type solver similar to Ramasesha [9] modified with a Gauss-Seidel enhanced block diagonal preconditioner. The DMRG calculations presented in Fig. 2 were done using up to \( m = 1200 \) states. In our DMRG implementation we do not fix the number of states per block to be \( m \) but rather fix the dimension of the target space to be at least \( m^2 \). In the calculations presented this corresponds to an increase of block states of typically 15% - 30%.

**Results.** — Here we present DMRG and (in the non-interacting limit) exact diagonalization calculations for a single resonant level, Fig. 2(a), and a nanostructure consisting of seven sites coupled symmetrically to two non-interacting leads. For the extended structure we present results in the non interacting limit, Fig. 2(b) and for weak and strong interaction, Fig. 2(c) and 2(d).

The spinless single resonant level is generically non-interacting and serves as a testing ground for the approach. The exact result for the conductance in the symmetrically coupled case can be shown to be a Lorentzian of full width \( 4t'^2 \) at half maximum, where \( t' = t_L = t_R \).
In Fig. 2(a) we show exact diagonalization and DMRG calculations for the single resonant level and the two sets are virtually indistinguishable. This verifies that the truncation error introduced by the DMRG is negligible. Furthermore we have plotted the exact Lorentzian result, and the agreement between the three curves is very good, demonstrating the accuracy of our combined Kubo and DMRG approach.

There is a systematic difference between the current-current and the current-density correlators, specifically close to resonances the current-density correlator generally gives better results. This is due to the additional energy dependent broadening given by $\hat{H}_0 - E_0$ in the current-current correlator. The opposite is true in the tails where the current-current correlator is more reliable since it is less sensitive to changes of the particle number.

In numerical calculations the parameter $\eta$ is always finite making the expected form of
the conductance peaks that of an area normalized Lorentzian \((L_A)\) of half-width \(\eta\) convoluted with the “bare” physical result. Assuming as a first approximation that the latter is a height normalized Lorentzian \((L_H)\) of width \(\Gamma\), the expression for the expected numerical results is of the general form

\[
(L_A * L_H)(x) = \frac{\Gamma}{2} \frac{\eta + \Gamma/2}{(x - x_0)^2 + (\eta + \Gamma/2)^2}.
\]

To leading order in \(\eta\) the conductance at the resonant level is then given by \(g_{\text{res}} \approx 1 - 2\eta/\Gamma\), which demonstrates that one needs small \(\eta\) to reach the unitary limit, \(g_{\text{res}} = 1\). However \(\eta\) is known from the input and \(\Gamma\) can be extracted from the results. Thus a conductance value on resonance of \(1 - 2\eta/\Gamma\) is explained entirely by the broadening by the finite leads and therefore suggests that infinite leads in this case would yield the unitary limit. Our calculations indicate, that the peak width is only slightly affected by the interaction on the nanostructure, as long as the nanostructure remains in the Luttinger liquid regime. However, once the structure is driven into the charge density wave regime the peak width decreases rapidly. A more detailed study of the resonance shapes is considered future work.

The position of the resonances can be described by the addition spectrum,

\[
U_{N_D - 1 \rightarrow N_D} = E_{0}^{N_D - 1} - E_{0}^{N_D},
\]

where \(E_{0}^{N_D}\) is the energy of the isolated nanostructure occupied by \(N_D\) particles. In the large interaction limit the kinetic energy of the particles can be approximated by freely moving fermions on an effective lattice of size \(M_S = M_S - N_D\). In this approximation one describes the interacting fermions by effective hard-core particles of the size of the interaction range, compare \([10, 11]\). Thus eq. 15 can be expressed as

\[
U_{N_D - 1 \rightarrow N_D} = V + 2t \left( \sum_{n=1}^{N_D} \cos \left( \frac{\pi n}{M_S - N_D} \right) - \sum_{n=1}^{N_D-1} \cos \left( \frac{\pi n}{M_S - (N_D-1)} \right) \right),
\]

where \(N_D\) should be small enough that the nanostructure is still in a delocalized state.

In an effective charging model the additional splitting of the levels due to the interaction is linear in the charging interaction \(V\). By contrast, in our microscopic model the interaction leads to an overall offset for the non-central peaks, while their mutual splitting is governed by the kinetic energy, \(\sim t\).

In tab. I we show a comparison of resonance positions as predicted by the reduced lattice (RL) model in eq. 16, as predicted by exact diagonalization (ED) of the isolated nanostructure, and resonances found in our DMRG calculations for interaction strengths \(V = 5, 20, 30\). The position of the outermost resonance from \(0 \rightarrow 1\) particle fits fairly well for both predictions, while the next ones deviate somewhat. The RL prediction for the transition \(2 \rightarrow 3\) is not expected to be accurate since \(N_D = 3\) is a localized charge density wave like state. All exact diagonalization predictions are correct to lowest order in \(t/V\) as expected.

**Conclusion.** – In this work we have presented a new approach for linear conductance calculations of interacting one-dimensional nanostructures, combining linear response for conductance and DMRG. We have benchmarked this new approach against exact diagonalization calculations in the non-interacting case and found excellent agreement, which serves as a real test for the real space DMRG. For the resonant level we also compared our results to the exact Lorentzian result, and found excellent agreement.

For the interacting case we have presented conductance curves for a seven site nanostructure in both the Luttinger Liquid \((V = 1)\) and the charge density wave \((V = 5)\) regimes,
Table I – Table of peak positions for the $M_s = 7$ site structure with interaction $V = 5, 20, 30$, as predicted by the reduced lattice (RL) model, by exact diagonalization (ED) of the isolated nanostructure, and as found from the conductance peaks in our DMRG calculations. The RL prediction for $N_D = 3$ is not expected to be accurate since the nanostructure is in a localized charge density wave like state. Except for the RL prediction for $V = 5$, $N_D = 3$, all predictions are correct to linear order in $t/V$.

| $N_D$ | 1 | 2 | 3 | 1 | 2 | 3 | 1 | 2 | 3 |
|-------|---|---|---|---|---|---|---|---|---|
| $U_{N_D-1}^{N_D}$ RL | 6.73 | 5.50 | 2.76 | 21.73 | 20.50 | 17.76 | 31.73 | 30.50 | 27.76 |
| $U_{N_D-1}^{N_D}$ ED | 6.77 | 5.88 | 3.85 | 21.75 | 20.63 | 18.03 | 31.74 | 30.59 | 27.94 |
| $U_{N_D-1}^{N_D}$ DMRG | 6.76 | 5.79 | 3.66 | 21.74 | 20.59 | 17.97 | 31.74 | 30.60 | 27.95 |

thus demonstrating the versatility of our approach. We find the largest conductance when the particle number in the structure fluctuates, in agreement with physical intuition.

In the large interaction limit we have shown that a simple picture based on effective hard-core particles moving freely on a reduced size lattice describes the position of the resonances quite well. However, the peak width is strongly decreased by strong interaction.

We expect that further finetuning of the method and numerical parameters will lead to significantly more precise results facilitating calculations for more complicated structures and allow to quantitatively describe resonance peaks for strongly interacting and extended structures.

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