Classical mapping for Hubbard operators: Application to the double-Anderson model

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A classical Cartesian mapping for Hubbard operators is developed to describe the nonequilibrium transport of an open quantum system with many electrons. The mapping of the Hubbard operators representing the many-body Hamiltonian is derived by using analogies from classical mappings of boson creation and annihilation operators vis-à-vis a coherent state representation. The approach provides qualitative results for a double quantum dot array (double Anderson impurity model) coupled to fermionic leads for a range of bias voltages, Coulomb couplings, and hopping terms. While the width and height of the conduction peaks show deviations from the master equation approach considered to be accurate in the limit of weak system-leads couplings and high temperatures, the Hubbard mapping captures all transport channels involving transition between many electron states, some of which are not captured by approximate nonequilibrium Green function closures.

I. INTRODUCTION

The development of numerical techniques to study the dynamics of open quantum systems driven out-of-equilibrium is central to our understanding of nonequilibrium transport phenomena in correlated systems. There exist a variety of techniques to obtain the numerically exact (converged) description of the transient dynamics and the approach to steady-state, for example, by means of time-dependent numerical renormalization-group techniques, many-body wave function approaches, diagrammatic techniques to real-time path-integral formulation, or reduced dynamic methods combined with a numerically exact impurity solver. These numerical approaches work well for simple model systems such as the Anderson impurity model or the (extended)-Holstein model, but less so in describing the nonequilibrium dynamics of correlated systems with many electronic states.

The treatment of systems with many electrons has thus followed a different path, mainly adopting approximate methods rather than resorting to numerically exact, brute-force techniques. Several different schemes have been developed. The most crude technique is based on a master equation (ME) approach and its recent generalizations, valid for weak system-lead couplings and high temperatures. The most popular is the nonequilibrium Green function (NEGF) formalism. In principle, NEGF formalism is exact, but in practice relies on approximations to obtain the self-energy, most commonly are based on a many-body perturbation expansion of some sort. Moreover, the description of two-time correlations necessary for nonequilibrium dynamics is rather challenging to implement. Another powerful tool, which in principle is also exact, is the time-dependent density functional theory (TD-DFT), which naturally describes nonequilibrium dynamics, but may often suffer in accuracy due to the approximation introduced to obtain the exchange/correlation functional and the single-particle character of the DFT methodology. As a result it often fails to predict important conduction channels.

Recently, we have developed an alternative to these fully quantum mechanical approaches, based on mapping the many-body Hamiltonian to a classical one, where the dynamics follow Hamilton’s equations of motion. The Miller-White mapping adopted by Swenson et al. provides a semi-quantitative description for the non-interacting resonant level model, but falls short in describing the effect of a gate voltage and does not capture the Franck-Condon and Coulomb blockades. To overcome these shortcomings, a new mapping procedure based on representing the product of creation and annihilation operators by quaternions. The new mapping allows us to express the fermionic creation and annihilation operators separately rather than mapping pairs of creation and annihilation operators separately rather than mapping pairs of creation and annihilation operators by quaternions. The accuracy of the neue “Hubbard” mapping is tested for a double quantum dot (QD) array coupled to two macroscopic leads, i.e., an extended Hubbard model also known as the double Anderson model. Since the model...
II. MODEL AND MAPPING

A. Double Anderson model

The model Hamiltonian for the double Anderson model describes a system of two coupled quantum dots (QDs) connected to two macroscopic leads. The entire setup has the following general form:

\[ \hat{H} = \hat{H}_B + \hat{H}_S + \hat{H}_I, \]

(1)

where \( \hat{H}_B \) describes the macroscopic leads (left and right contacts), \( \hat{H}_S \) describes the system of interest, and \( \hat{H}_I \) is the interaction Hamiltonian between the system and the leads. The leads (left \((L)\) and right \((R)\)) are modeled by ideal electron gases, and are assumed to be each at its own equilibrium, characterized by chemical potentials \( \mu_L \) and \( \mu_R \), where the difference \( \frac{1}{2}(\mu_L - \mu_R) = V_{ad} \) is the applied voltage bias across the junction. The leads’ Hamiltonian is given by

\[ \hat{H}_B = \sum_{\sigma,k \in \{L,R\}} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}, \]

(2)

where \( c_{k\sigma}^\dagger \) (\( c_{k\sigma} \)) creates (annihilates) an electron with energy \( \epsilon_{k\sigma} \) and spin \( \sigma \in \{\uparrow, \downarrow\} \) in the left/right lead. The double QD system is described by an extended Hubbard model:

\[ \hat{H}_S = \sum_{\sigma,m \in \{\alpha, \beta\}} \epsilon_{m\sigma} n_{m\sigma} + U \sum_m n_{m\uparrow} n_{m\downarrow} + V \sum_{\sigma,\sigma'} n_{\alpha\sigma} n_{\beta\sigma'} + h \sum_{\sigma} (\delta_{\alpha\sigma} \delta_{\beta\sigma} + h.c.), \]

(3)

where \( n_{\alpha\sigma} = d_{\alpha\sigma}^\dagger d_{\alpha\sigma} \) is the number operator of the electron occupying dot \( i \in \{\alpha, \beta\} \) with spin \( \sigma \) and energy \( \epsilon_{\alpha\sigma} \), the repulsion energy between two electrons on the same dot (intra-dot repulsion) is denoted by \( U \) while \( V \) is the repulsion energy between two electrons on different sites (inter-dot repulsion), and \( h \) is the coupling strength for electron hopping between the two sites. The tunneling Hamiltonian has a tight binding form:

\[ \hat{H}_I = \sum_{\sigma, k \in \{L,R\}} (t_{k\sigma} d_{\sigma}^\dagger + h.c.) \]

\[ + \sum_{\sigma, k \in \{L,R\}} (t_{k\sigma}^* d_{\sigma}^\dagger d_{\sigma} + h.c.). \]

(4)

The index \( m \) runs over the site index \( \{\alpha, \beta\} \). The parameter \( t_{k\sigma}^\dagger \) represents the coupling strength (hybridization) between the system and the leads, and are determined from the spectral density:

\[ J_{L/R}(\epsilon) = \frac{\Gamma_{L/R}}{(1 + e^{\epsilon - \mu_{L/R}/\beta})(1 + e^{\epsilon - (\mu_{L/R} + U)/\beta})}, \]

(5)

where \( \Gamma_L = \Gamma_R = \frac{1}{2} \Gamma, \ A = 5\Gamma, \) and \( B = 20\Gamma. \) With these definitions, \( t_{k\sigma}^* = t_{k\sigma} \varepsilon_{k\sigma} \). We use 400 modes to represent each lead with \( \delta \epsilon = 0.075\Gamma \). This was sufficient to converge the results up to a time \( t_{\text{max}} = 10\hbar/\Gamma \) for which a steady-state was observed.

B. Hubbard operators

The double-Anderson model can host up to 4 electrons in different 16 many-body states. In the occupation number (ON) vector representation these are denoted by \( |n_{\alpha\uparrow} n_{\alpha\downarrow} n_{\beta\uparrow} n_{\beta\downarrow}\rangle \). In what follows, we represent these states in Fock space as \(|\{0\}, \{1\}, \ldots, \{15\}\rangle \), where \( |0\rangle \) refers to the state \(|0000\rangle \) (empty system), \(|1\rangle - |4\rangle \) refer to the one-electron states, \(|5\rangle - |10\rangle \) refer to the two-electron states, \(|11\rangle - |14\rangle \) refer to the three-electron states and \(|15\rangle \) refers to the fully occupied system (i.e., \(|11111\rangle \)). We now define the Hubbard operator as

\[ X_{p,q} = |p\rangle \langle q| = D_p^\dagger D_q, \]

(6)

in which \( X_{p,q} \) describes the transition from the many-body state \(|q\rangle\) to \(|p\rangle\); \( D_p^\dagger(D_q) \) create (annihilate) the many-body state \(|p\rangle(|q\rangle\). The electron creation and annihilation operators can be expressed in terms of the Hubbard operators (see the Appendix for more details). For example: The creation operator of the spin down electron on dot \( \alpha \) is given by

\[ d_{\alpha\downarrow} = X_{2,0} - X_{5,1} + X_{6,3} + X_{8,4} + X_{14,7} - X_{11,9} + X_{12,0} - X_{15,13} = D_{1,0}^\dagger D_0 - D_{2,1}^\dagger D_1 + D_{6,3}^\dagger D_3 + D_{8,4}^\dagger D_4 \]

\[ + D_{14,7}^\dagger D_7 - D_{11,9}^\dagger D_9 - D_{12,0}^\dagger D_{10} - D_{15,13}^\dagger D_{13}, \]

(7)

where we used the multiplication rule:

\[ X_{p,q} X_{r,t}^\dagger = \delta_{qr} X_{p,t}. \]

(8)

The Hubbard operator \( X_{p,q} \) has either a bosonic character or fermionic character depending on the difference between the number of electrons in states \(|q\rangle\) and \(|p\rangle\). If the difference is even then the operator has bosonic character, otherwise it has a fermionic character. This also reflects on the character of the many-body states creation/annihilation operators, \( D_q^\dagger(D_q) \), since they can be expressed in term of Hubbard operators, as \( D_q = X_{q,0}^\dagger X_{q,0} \). The Hubbard operators will obey the following commutation/anti-commutation relation depending on their character (bosonic/fermionic, respectively):

\[ [X_{p,q}, X_{r,t}^\dagger] = \delta_{qr} X_{p,t} \mp \delta_{p,t} X_{r,q}^\dagger, \]

(9)

where \( \mp \) stands for commutation/anti-commutation, respectively.
C. Reformulating $\hat{H}_0$ and $\hat{H}_i$ in terms of Hubbard operators

The system’s Hamiltonian in terms of the Hubbard operators is given by

$$\hat{H}_i = \sum_{i=0}^{15} \sum_{\sigma} \left( r^\dagger_{\sigma} \right)_{i,j} \cdot r^\dagger_{\kappa} c_{\kappa} D^\dagger_i D_j$$

with $r_{i,j} \in \{ \pm 1, 0 \}$. The non-zero elements of the symmetric matrix $(r_{i,j} = r_{j,i})$ are

$$r_{1,3} = r_{2,4} = r_{5,10} = r_{7,10} = 1,$n$$

$$r_{5,6} = r_{6,7} = r_{11,13} = r_{12,14} = -1,$n$$

and the energies of the many-body states are summarized in Table I.

The interaction Hamiltonian in terms of the Hubbard operators is given by

$$\hat{H}_i = \sum_{i,j=0}^{15} \sum_{\sigma,k} \left( r^\dagger_{\sigma} \right)_{i,j} \cdot r^\dagger_{\kappa} c_{\kappa} D^\dagger_i D_j$$

where the terms $(r^\dagger_{\sigma})_{i,j}$ are the prefactors of the Hubbard operators in the expansion of the electron creation/annihilation operators (see the Appendix for more details). For example,

$$d_{\beta} = D^\dagger_i D_3 - D^\dagger_i D_0 - D^\dagger_i D_6 + D^\dagger_i D_7$$

$$+ D^\dagger_{11} D_{11} - D^\dagger_{14} D_{14} - D^\dagger_{10} D_{13} + D^\dagger_{12} D_{15},$$

Thus, the non-zero elements of $(r^\dagger_{\beta})_{i,j}$ are

$$(r^\dagger_{\beta})_{0,3} = (r^\dagger_{\beta})_{4,7} = (r^\dagger_{\beta})_{5,11} = (r^\dagger_{\beta})_{12,15} = 1,$n$$

$$(r^\dagger_{\beta})_{1,9} = (r^\dagger_{\beta})_{2,6} = (r^\dagger_{\beta})_{8,14} = (r^\dagger_{\beta})_{10,13} = -1.$n$$

D. Classical mapping for the Hubbard operators

The main goal of the present work is to establish a simple mapping for the Hubbard representation of the Hamiltonian of a quantum dot coupled to fermionic leads. One possible route is based on the Cartesian mapping of Li and Miller, which provides a recipe to map products of even number of fermionic operators. Here, however, the interactions Hamiltonian contains odd number of terms (cf. Eq. (19)). Therefore, we define a new Cartesian mapping of the electron creation and annihilation operators:

$$c_{\kappa} \rightarrow \frac{1}{2} \{(x_{\kappa \sigma} + p_{\kappa \sigma}) - \sqrt{-1}(y_{\kappa \sigma} - p_{\kappa \sigma})\},$$

$$c^\dagger_{\kappa} \rightarrow \frac{1}{2} \{(x_{\kappa \sigma} + p_{\kappa \sigma}) + \sqrt{-1}(y_{\kappa \sigma} - p_{\kappa \sigma})\},$$

where $r_{\kappa \sigma} = \{x_{\kappa \sigma}, y_{\kappa \sigma}\}$ and $p_{\kappa \sigma} = \{p_{\kappa \sigma}, p_{\kappa \sigma}\}$ are position and conjugate momentum vectors in 2-dimensions. Similarly, we define the same mapping for the many-body states creation and annihilation operators:

$$D^\dagger_q \rightarrow \frac{1}{2} \{(X_q + P_{Y,q}) - \sqrt{-1}(Y_q - P_{X,q})\},$$

$$D_q \rightarrow \frac{1}{2} \{(X_q + P_{Y,q}) + \sqrt{-1}(Y_q - P_{X,q})\}.$$
where
\[
N_q = \frac{1}{4}((X_q + P_{Y,q})^2 + (Y_q + P_{X,q})^2 - \lambda)
\]  
(18)
is the many-body state occupation. In the above equations, \( \lambda \) is the Langer correction which is treated as a parameter (see more details below). The interaction Hamiltonian in Eq. (12) is mapped to
\[
H_I = \frac{1}{4} \sum_{i,j=0}^{15} \sum_{\sigma,k\in L} \left( r^\sigma_{i,j} \cdot r^\sigma_{k\alpha} \right) F(k\sigma, i, j)
\]  
(19)
where
\[
F(k\sigma, i, j) = X_i X_j x_{k\sigma} + X_i X_j p_{x,k\sigma} + X_i Y_j y_{k\sigma}
\]  
\[= X_i Y_j p_{x,k\sigma} - X_i P_{x,j} y_{k\sigma} + X_i P_{x,j} p_{x,k\sigma}
\]  
\[+ Y_i X_j p_{x,k\sigma} + Y_i Y_j y_{k\sigma} + Y_i Y_j p_{y,k\sigma}
\]  
\[- Y_i P_{x,j} x_{k\sigma} - Y_i P_{x,j} y_{k\sigma} - Y_i P_{x,j} p_{x,k\sigma} + Y_i P_{x,j} y_{k\sigma} p_{x,k\sigma}
\]  
\[+ P_{x,i} P_{x,j} y_{k\sigma} - P_{x,i} P_{x,j} p_{x,k\sigma} + P_{x,i} P_{x,j} y_{k\sigma}
\]  
\[+ P_{x,i} X_j y_{k\sigma} + P_{x,i} Y_j y_{k\sigma} - P_{x,i} Y_j p_{y,k\sigma} + P_{x,i} Y_j y_{k}\sigma
\]  
\[+ P_{x,i} Y_j p_{y,k\sigma} - P_{x,i} P_{x,j} y_{k\sigma} + P_{x,i} P_{y,j} p_{x,k\sigma}
\]  
\[+ P_{x,i} P_{y,j} y_{k\sigma} + P_{x,i} P_{y,j} p_{y,k\sigma}.
\]  
(20)
Finally, the leads Hamiltonian in Cartesian mapped coordinates is given by
\[
\hat{H}_R = \sum_{\sigma,k\in[L,R]} \xi_{k\sigma} n_{k\sigma},
\]  
(21)
where
\[n_{k\sigma} = \frac{1}{4}((x_{k\sigma} + p_{x,k\sigma})^2 + (y_{k\sigma} + p_{y,k\sigma})^2 - \lambda).
\]
We assume that the dynamics of the all Cartesian variables (system and leads) follow from Hamilton equations of motions. Within this classical approximation, one can show that the Hubbard mapping of the double-Anderson model (and all other models discussed in this work) preserves the normalization \( \sum N_i = 1 \) of the many-body states, an additional restriction to physical subspace.50 This sum rule is violated, for example, if the Cartesian mapping is used for the \( D_q / D'_q \) operators (see further discussion in Subsection III B).

E. Initial conditions

We adopt the procedure outlined in Refs. 39 and 41 to obtain the initial conditions for \( n_{k\sigma} \), \( p_{x,k\sigma} \), \( Y_{q,k\sigma} \), and \( P_{q,k\sigma} \) which recovers the correct statistical behavior (at \( t = 0 \)). We enforce quantum statistics on the initial conditions for each DoF by setting the initial occupation of the leads, \( n_{k\sigma} \), to either 0 or 1 such that its expectation value, averaged over the set of initial conditions, satisfies the Fermi-Dirac distribution:
\[
n_{k\sigma} = \begin{cases} 
0 & \xi > f(\xi_{k\sigma} - \mu_{L/R}) \\
1 & \xi \leq f(\xi_{k\sigma} - \mu_{L/R})
\end{cases},
\]  
(22)
where \( \xi \) is a random number in the interval \([0...1]\), \( f(\xi) = (\exp(\beta \xi) + 1)^{-1} \) is the Fermi-Dirac distribution and \( \beta = (K_B T)^{-1} \) is the inverse of the temperature. For the system, we set \( N_0 = 1 \) and \( N_{q,k\sigma} = 0 \) consistent with an empty system. Once the populations are chosen, we set the values for the phase-space variables according to
\[
x_{k\sigma} = \frac{1}{2} \sqrt{4n_{k\sigma} + \lambda \cos(\theta_{k\sigma})},
\]  
\[
p_{x,k\sigma} = -\frac{1}{2} \sqrt{4n_{k\sigma} + \lambda \sin(\theta_{k\sigma})},
\]  
\[
y_{k\sigma} = \frac{1}{2} \sqrt{4n_{k\sigma} + \lambda \cos(\theta_{k\sigma})},
\]  
\[
p_{y,k\sigma} = \frac{1}{2} \sqrt{4n_{k\sigma} + \lambda \cos(\theta_{k\sigma})},
\]  
and
\[
X_q = \frac{1}{2} \sqrt{4N_q + \lambda \cos(\Theta_q)},
\]  
\[
P_{X,q} = -\frac{1}{2} \sqrt{4N_q + \lambda \sin(\Theta_q)},
\]  
\[
Y_q = \frac{1}{2} \sqrt{4N_q + \lambda \sin(\Theta_q)},
\]  
\[
P_{Y,q} = \frac{1}{2} \sqrt{4N_q + \lambda \cos(\Theta_q)},
\]  
where \( \theta_{k\sigma} \) and \( \Theta_q \) are random variables in the interval \([0...2\pi]\). We note that the above choice of initial conditions is not unique and other choices that satisfy the relations \((X_q + P_{X,q}) = \sqrt{4N_q + \lambda \cos(\Theta_q)} \) and \((Y_q - P_{X,q}) = \sqrt{4N_q + \lambda \sin(\Theta_q)} \) (and similarly for \( n_{k\sigma} \), \( \xi_{k\sigma} \), \( p_{x,k\sigma} \), and \( p_{y,k\sigma} \)) yield similar results. However, the above form seems to converge better than other choices tested and thus, is the procedure adopted for the present work.

III. RESULTS AND DISCUSSION

A. Resonant level model

In order to assess the accuracy of the Hubbard mapping, we first apply it to the resonant level model (Landauer model). In this case (of non-interacting electrons), it can be shown that the Hubbard mapping is exact and the results do not depend on the choice of the Langer correction parameter, \( \lambda \), despite the fact that \( \lambda \) enters the initial sampling of phase-space coordinates (cf., Eqs. (23) and (24)). In Fig. 1, the time dependent current for different values of the source-drain voltage \((V_{sd})\), gate voltage \((V_g)\), and different temperatures is presented. As clearly evident, the agreement with the exact quantum mechanical results39 is excellent for all parameters and temperatures studied, as it should be. In fact, the quality of the Hubbard mapping approximation is identical in this respect to the Cartesian mapping of fermions.41,44 Furthermore, we find that indeed, the results are independent of the choice of \( \lambda \) (not shown).
B. Anderson impurity model

The resonant level model is a necessary test of the new Hubbard mapping approach but not a sufficient one. Since the Hubbard mapping aims at systems with electron-electron and also hopping interactions, a more subtle assessment is required. The simplest model that accounts for electron-electron correlations is the single-site Anderson impurity model, for which the system Hamiltonian is given by

\[ H_s = \sum_\sigma \varepsilon_\sigma n_\sigma + U n_\uparrow n_\downarrow, \]

where \( n_\sigma = c_\sigma^\dagger c_\sigma \) is the fermionic particle number operator. The interaction Hamiltonian is given by

\[ \hat{H}_I = \sum_{\sigma, k} \frac{\lambda}{k} (\varepsilon_\sigma c_{k, \sigma}^\dagger d_{k, \sigma} + \text{h.c.}), \]

and the bath Hamiltonian is

\[ \hat{H}_b = \sum_{\sigma, k} \frac{\varepsilon_{\sigma, k}}{k} c_{k, \sigma}^\dagger c_{k, \sigma}. \]

Here, the single QD is coupled to both reservoirs and the system can accommodate only 2 electrons in 4 many-particle states.

Following the derivation outlined above, the fermionic creation \((d_\sigma^\dagger)\) and annihilation \((d_\sigma)\) operators are given in terms of the many-body states creation \((D_{\sigma}^\dagger)\) and annihilation \((D_{\sigma})\) operators, as

\[
\begin{align*}
{d_\uparrow} &= D_{\uparrow}^\dagger D_{0}^\dagger + D_{\downarrow}^\dagger D_{2}, \\
{d_\downarrow} &= D_{\uparrow} D_{1}^\dagger + D_{\downarrow} D_{3}, \\
{d_{\uparrow}} &= D_{\uparrow}^\dagger D_{0} - D_{\downarrow}^\dagger D_{1}, \\
{d_{\downarrow}} &= D_{\uparrow} D_{2}^\dagger - D_{\downarrow} D_{3},
\end{align*}
\]

where \( |0\rangle = |0, 0\rangle, |1\rangle = |\uparrow, 0\rangle, |2\rangle = |0, \downarrow\rangle, \) and \( |3\rangle = |\uparrow, \downarrow\rangle. \)

The system and interaction Hamiltonians are described by

\[
H_s = \varepsilon_\uparrow D_{\uparrow}^\dagger D_{\uparrow} + \varepsilon_\downarrow D_{\downarrow}^\dagger D_{\downarrow} + (\varepsilon_\uparrow + \varepsilon_\downarrow + U) D_{\uparrow} D_{\downarrow}
\]

and

\[
H_I = \sum_k t_k^\dagger \left( c_{k, \uparrow}^\dagger D_{\uparrow}^\dagger D_{0} + D_{\downarrow}^\dagger D_{0} D_{\uparrow}^\dagger + c_{k, \downarrow}^\dagger D_{\downarrow}^\dagger D_{2} + D_{\uparrow} D_{2} D_{\downarrow}^\dagger \right)
\]

\[
+ \sum_k t_k^\dagger \left( c_{k, \uparrow}^\dagger D_{\uparrow}^\dagger D_{2} + D_{\downarrow}^\dagger D_{0} D_{\downarrow}^\dagger - c_{k, \downarrow}^\dagger D_{\downarrow}^\dagger D_{3} + D_{\uparrow} D_{3} D_{\downarrow}^\dagger \right),
\]

respectively. We note in passing, that for a single-site Anderson impurity model, the Hubbard Hamiltonian (cf., Eq. (26)) is equivalent to the slave-boson Hamiltonian.\(^{61,62}\) The latter sets out by defining directly the \(D_q\) and \(D_q^\dagger\) operators rather than the Hubbard operators, \(X^{\uparrow\downarrow}\), and thus, it is straightforward to define the statistics of the \(D_q/D_q^\dagger\) operators in this case.

The mapping to classical phase-space variable follows the rules outlined above for the double-Anderson model. The mapped system and interaction Hamiltonians for the Anderson impurity model are given by

\[
H_s = \varepsilon_\uparrow N_1 + \varepsilon_\downarrow N_2 + (\varepsilon_\uparrow + \varepsilon_\downarrow + U) N_3
\]

and

\[
H_I = \sum_k t_k^\dagger \left( F(k, \uparrow, 0, 1) + F(k, \uparrow, 2, 3) \right)
\]

\[
+ \sum_k t_k^\dagger \left( F(k, \downarrow, 0, 2) - F(k, \downarrow, 1, 3) \right),
\]

respectively, where \(N_q\) and \(F\) are given by Eqs. (18) and (20). The mapped bath Hamiltonian is identical to that given by Eq. (21) for the double Anderson model.

In Fig. 2 we compare the Hubbard mapping results for the Anderson model with the NEGF equation-of-motion approach,\(^{50,51,63}\) which is considered accurate in the Coulomb-blockade regime studied. The upper panel of Fig. 2 shows the depends of the steady-state current on the Langer parameter, \(\lambda\). As clearly evident, the results are quite sensitive to the value of \(\lambda\). We find that the best agreement is achieved for \(\lambda = 3/2\), which described properly the “S-shaped” curve of the current versus voltage Coulomb-blockade characteristics. This value for \(\lambda\) is close to \(\lambda = 2(\sqrt{3} - 1) \approx 1.464\) derived by Cotton and Miller for the Meyer-Miller mapping.\(^{64}\)
The lower panel of Fig. 2 compares the Hubbard mapping results with the NEGF approach for different values of $U$. Also shown are results based on the Cartesian mapping of fermions of Ref. 41 and "mixed" mapping for which the statistics of the operators $D_0/D_0^\dagger$ were imposed. For the single-site Anderson impurity model $D_0$ and $D_1$ are bosons and $D_2$ are fermions and thus, we assume the Meyer-Miller\textsuperscript{45} mapping for the bosons and the Hubbard mapping for the fermions of both the system and the leads. The Cartesian mapping slightly out-performs the Hubbard mapping (which is rather good) for the Anderson impurity model for all values of $U$. However, for the double-Anderson model this is not the case, as further shown below. Comparing the results of the mixed mapping to the Hubbard mapping approach, it is clear that the latter performs much better in describing the Coulomb-blockade effect. Furthermore, the mixed mapping approach is insensitive to the value of $\lambda$ and thus, the Langer parameter cannot be used to improve its performance.

We further note that when operator statistics is considered, one can replace the Hubbard mapping with the Cartesian mapping of fermions\textsuperscript{41} since the interaction Hamiltonian contains only even number of products of fermionic operators (this is true for both the single- and double-site Anderson models). We find that the Cartesian mapping combined with the Meyer-Miller mapping of bosons violates the normalization sum rule $\sum_i N_i = 1$ and thus can lead to unphysical situations. Moreover, it imposes a different sum rule for which $\sum_{\alpha} (N_1 + N_2 + \sum_{\alpha} N_\alpha) = 0$, implying that the total population of the fermionic mapped DoF is conserved, imposing another unphysical constraint.

C. Double Anderson model

In Fig. 3 we plot the differential conductance as a function of the bias voltage for the double-Anderson model for various typical model parameters. The results obtained from the Hubbard and Cartesian mappings are compared to those calculated using the many-particle ME approach\textsuperscript{18,65} and the equation-of-motion approach to NEGF (closure "2" of Ref. 51). For the weak coupling, high temperature regime, the ME approach is fairly accurate\textsuperscript{66} and thus, is used as a measure of the quality of our mapping approximations. The NEGF results are also provided in order to compare our results with an approach often used in nonequilibrium transport problems. The specific implementation of the NEGF approach is described in detail in Ref. 51, where 4 different closures have been studied for the double-Anderson model. Closure 2 provided the most accurate description of the differential conductance with respect to the other closures studied, and is the one presented in Fig. 3.

For the symmetric case ($\epsilon_{d_\uparrow} = \epsilon_{d_\downarrow} = \epsilon_{b_\uparrow} = \epsilon_{b_\downarrow}$), the Cartesian mapping that was successful in describing the Coulomb blockade in the single-site Anderson impurity model, fails to capture some of the peaks in the conductance. It recovers successfully conductance peaks associated with transitions between an empty system and one-electron states, but fails to capture transitions between one-electron and two-electron states.\textsuperscript{51} This failure has also been reported for many of the NEGF closures.\textsuperscript{51} On the other hand the Hubbard mapping describes the position of all peaks nearly quantitatively, while it deviates from the ME results with respect to the width and amplitude of the conductance peaks.

For the asymmetric case ($\epsilon_{d_\uparrow} = \epsilon_{d_\downarrow} \neq \epsilon_{b_\uparrow} = \epsilon_{b_\downarrow}$), the overall performance of the classical Hubbard approach is similar to the symmetric case and out performs the NEGF and the Cartesian mapping for both $V = 0$ and $V = 0.8U$. Importantly, it captures the peak associated with the transition from a two-electron to a three-electron state and also does not predict negative differential conductance that appears in the NEGF calculations but not in the ME approach.

IV. CONCLUDING REMARKS

We have presented a new classical Cartesian mapping, denoted the “Hubbard” mapping, for the quantum many-body creation and annihilation operators which allows the calculation of nonequilibrium properties in extended Hubbard models. As a first step one rewrites a general second-quantized many-electron Hamiltonian in the language of the Hubbard operators, and then maps the resulting Hamiltonian to a classical Hamiltonian, where the dynamics follow Hamilton’s equations of motion. As opposed to the Cartesian mapping of Li and Miller,\textsuperscript{44} which provides a recipe to map products of even number of fermionic operators, the present mapping can deal with an odd number of many-body creation/annihilation operators and thus copes with situations where 3 operators terms are present in the Hamiltonian, which is the case considered here.

FIG. 3. Plots of the differential conductance versus the bias voltage for the double-Anderson model. Left panels: Results for the symmetric bridge, $\epsilon_{d_\uparrow} = \epsilon_{d_\downarrow} = \epsilon_{b_\uparrow} = \epsilon_{b_\downarrow} = 0.35U$. Upper left: $V = 0$ and $h = 0.3U$. Lower left: $V = 0.3U$ and $h = 0.7U$. Right panels: Results for the asymmetric bridge, $\epsilon_{d_\uparrow} = \epsilon_{d_\downarrow} = 0.15U$ and $\epsilon_{b_\uparrow} = \epsilon_{b_\downarrow} = 0.2U$. Upper right: $V = 0$ and $h = 0.3U$. Lower right: $V = 0.8U$ and $h = 0.7U$. In all simulations $\Gamma_{0L} = \Gamma_{0R} = \Gamma_{1L} = \Gamma_{1R} = 0.015U$ and $\beta = 40/U$. The zero-, one-, two-, and three-electron states are denoted |0>, |I>, |II>, and |III> respectively. The notation |I> → |II> means that the peak belongs to a transition from one of the one-electron states to one of the two-electron states. The ground state for the upper-left panel is the zero electron state, and for all the other panels the ground state is a single electron state.
The Hubbard mapping approach ignores the quantum statistics (fermionic or bosonic) of the many-body creation/annihilation operators and treats all operators on the same footing. In fact, when bosonic and fermionic statistics are imposed (the “mixed” mapping), we find that the mixed mapping fails to recover the Coulomb-blockade effect in the single-site Anderson impurity model. Perhaps, this can be traced to the fact that the mixed mapping is insensitive to the value of the Langer parameter (\( \lambda \)) and thus, \( \lambda \) cannot be used to improve the performance. In this respect the results obtained from the Hubbard mapping are sensitive to \( \lambda \); the best results were obtained for \( \lambda = \frac{1}{3} \).

The Hubbard mapping approach provides excellent agreement (similar to the quaternion mapping \(^{1}\)) for the time dependent current for the resonant level model in comparison to exact quantum mechanical calculations for a wide range of model parameters, including different temperatures, gate voltages and bias voltages. While the quaternion mapping performs better in describing the Coulomb-blockade effect in the single-site Anderson impurity model, the Hubbard mapping shows significant improvements for the more evolved double Anderson models, which includes electron-electron and hopping interactions. The results obtained from the Hubbard and Cartesian mappings are compared to those calculated using the many-particle ME approach and the equation-of-motion approach to NEGF. For the weak coupling, high temperature regime, the ME approach is consider to be accurate and thus, is used as a measure of the quality of our mapping. While the Cartesian mapping and the NEGF approaches fail to capture all the conductance peaks predicted by the ME approach, the Hubbard mapping reproduces the position of all peaks nearly quantitatively, which deviates from the ME results with respect to the width and amplitude of the conductance peaks.

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**APPENDIX: ELECTRON OPERATORS EXPRESSED BY THE HUBBARD OPERATORS**

To express the electron creation and annihilation operators in terms of the Hubbard operators, it is beneficial to calculate the operation of the electronic operator on the many-body states. For example, let us compute the effect of \( d_{\alpha \uparrow}^{\dagger} \) on the many-body states \(| 0 \rangle \) to \(| 15 \rangle \):

\[
d_{\alpha \uparrow}^{\dagger} |0000\rangle = d_{\alpha \uparrow}^{\dagger} |0 \rangle = |0100\rangle = |2\rangle \rightarrow D_{2}^{\dagger} D_{0},
\]

\[
d_{\alpha \uparrow}^{\dagger} |1000\rangle = d_{\alpha \uparrow}^{\dagger} |1 \rangle = -|1100\rangle = -|5\rangle \rightarrow -D_{5}^{\dagger} D_{1},
\]

\[
d_{\alpha \uparrow}^{\dagger} |0010\rangle = d_{\alpha \uparrow}^{\dagger} |3 \rangle = |0110\rangle = |6\rangle \rightarrow D_{6}^{\dagger} D_{3},
\]

\[
d_{\alpha \uparrow}^{\dagger} |0001\rangle = d_{\alpha \uparrow}^{\dagger} |4 \rangle = |0101\rangle = |8\rangle \rightarrow D_{8}^{\dagger} D_{4},
\]

\[
d_{\alpha \uparrow}^{\dagger} |0011\rangle = d_{\alpha \uparrow}^{\dagger} |7 \rangle = |0111\rangle = |14\rangle \rightarrow D_{14}^{\dagger} D_{7},
\]

\[
d_{\alpha \uparrow}^{\dagger} |1010\rangle = d_{\alpha \uparrow}^{\dagger} |9 \rangle = -|1110\rangle = -|11\rangle \rightarrow -D_{11}^{\dagger} D_{9},
\]

\[
d_{\alpha \uparrow}^{\dagger} |1001\rangle = d_{\alpha \uparrow}^{\dagger} |10 \rangle = -|1101\rangle = -|12\rangle \rightarrow -D_{12}^{\dagger} D_{10},
\]

\[
d_{\alpha \uparrow}^{\dagger} |1011\rangle = d_{\alpha \uparrow}^{\dagger} |13 \rangle = -|1111\rangle = -|15\rangle \rightarrow -D_{15}^{\dagger} D_{13}.
\]

The operation of \( d_{\alpha \uparrow}^{\dagger} \) on any of the other many-body states equals 0. Thus,

\[
d_{\alpha \uparrow}^{\dagger} = D_{2}^{\dagger} D_{0} - D_{3}^{\dagger} D_{1} + D_{6}^{\dagger} D_{3} + D_{8}^{\dagger} D_{4} + D_{14}^{\dagger} D_{7} - D_{12}^{\dagger} D_{10} - D_{15}^{\dagger} D_{13}.
\]

With these simple rules, the full list of the electron operators in terms of the Hubbard operators is given by

\[
d_{\alpha \uparrow} = D_{2}^{\dagger} D_{0} + D_{3}^{\dagger} D_{2} + D_{6}^{\dagger} D_{3} + D_{10}^{\dagger} D_{4} + D_{13}^{\dagger} D_{7} + D_{12}^{\dagger} D_{8} + D_{14}^{\dagger} D_{14},
\]

\[
d_{\alpha \downarrow} = D_{2}^{\dagger} D_{1} + D_{3}^{\dagger} D_{5} + D_{6}^{\dagger} D_{9} + D_{10}^{\dagger} D_{11} + D_{13}^{\dagger} D_{13} + D_{12}^{\dagger} D_{12} + D_{14}^{\dagger} D_{15},
\]

\[
d_{\alpha \uparrow} = D_{2}^{\dagger} D_{0} - D_{3}^{\dagger} D_{1} + D_{6}^{\dagger} D_{3} + D_{8}^{\dagger} D_{4} + D_{14}^{\dagger} D_{7} - D_{11}^{\dagger} D_{9} - D_{12}^{\dagger} D_{10} - D_{15}^{\dagger} D_{13},
\]

\[
d_{\alpha \downarrow} = D_{2}^{\dagger} D_{2} - D_{3}^{\dagger} D_{5} + D_{6}^{\dagger} D_{8} + D_{14}^{\dagger} D_{14} - D_{11}^{\dagger} D_{11} - D_{10}^{\dagger} D_{12} - D_{15}^{\dagger} D_{15},
\]

\[
d_{\beta \uparrow} = D_{2}^{\dagger} D_{0} - D_{3}^{\dagger} D_{1} - D_{6}^{\dagger} D_{2} + D_{11}^{\dagger} D_{5} - D_{14}^{\dagger} D_{8} - D_{13}^{\dagger} D_{10} + D_{15}^{\dagger} D_{12},
\]

\[
d_{\beta \downarrow} = D_{2}^{\dagger} D_{3} - D_{3}^{\dagger} D_{9} - D_{2}^{\dagger} D_{6} + D_{3}^{\dagger} D_{7} + D_{14}^{\dagger} D_{11} - D_{10}^{\dagger} D_{13} + D_{12}^{\dagger} D_{15},
\]

\[
d_{\gamma \uparrow} = D_{2}^{\dagger} D_{0} - D_{10}^{\dagger} D_{1} - D_{2}^{\dagger} D_{2} - D_{3}^{\dagger} D_{3} + D_{12}^{\dagger} D_{5} + D_{14}^{\dagger} D_{6} + D_{13}^{\dagger} D_{9} - D_{11}^{\dagger} D_{11},
\]

\[
d_{\gamma \downarrow} = D_{2}^{\dagger} D_{4} - D_{10}^{\dagger} D_{9} - D_{2}^{\dagger} D_{8} - D_{3}^{\dagger} D_{7} + D_{3}^{\dagger} D_{12} + D_{4}^{\dagger} D_{14} + D_{3}^{\dagger} D_{13} - D_{15}^{\dagger} D_{15}.
\]

\(^{1}\text{S. R. White, Phys. Rev. Lett. 69, 2863 (1992).}\)

\(^{2}\text{F. Schmitteckert, Phys. Rev. B 70, 121302 (2004).}\)
