Recursive computation of matrix elements in the numerical renormalization group

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ABSTRACT

The numerical renormalization group is an efficient method to diagonalize model Hamiltonians describing correlated orbitals coupled to conduction states. While only the resulting eigenvalues are needed to calculate the thermodynamical properties for such models, matrix elements of Fermi operators must be evaluated before excitation and transport properties can be computed. The traditional procedure to calculate matrix elements is typically as expensive as the diagonalization of the model Hamiltonian. Here, we present a substantially faster alternative that demands much less memory, yields equally accurate matrix elements and is easier to code.

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1. Introduction

The numerical renormalization-group (NRG) method was developed in the mid 1970s, to compute the thermodynamical properties of dilute magnetic alloys [1,2]. Generalizations followed. The procedure was extended to calculate excitation [3–7] and transport properties [8], spatial correlations [9,10], and nonequilibrium properties [11–14]. Besides being versatile, the method is reliable, because it depends on strictly controllable approximations. Recent applications include the diagonalization of various impurity-model Hamiltonians and the computation of their physical properties [15].

The NRG procedure is efficient. With special techniques outside the scope of this paper, 10 s of CPU time in a standard desktop computer diagonalize spin-degenerate single-impurity Hamiltonians with sufficient accuracy to determine the temperature-dependent magnetic susceptibility with less than 1% error at any temperature. This performance notwithstanding, gains in efficiency are prized, because both time and memory requirements grow exponentially with the number of impurities and with the degeneracy of the electronic states.

While thermodynamical properties, such as the impurity-added contribution to the susceptibility, can be obtained directly from the eigenvalues of the model Hamiltonian, the computation of excitation and transport properties calls for the evaluation of matrix elements between the eigenstates. A straightforward procedure determining such matrix elements has long been known [4]; unfortunately, its computational cost is relatively high. Even when it is applied to simple Hamiltonians the computation of matrix elements takes as much time and memory as diagonalizing the model Hamiltonian. In more complex problems it can magnify the computational effort over an order of magnitude.

Here we present a simple, cost-effective recursive procedure that yields accurate results for the matrix elements of the fermionic operators defining the quantum basis upon which the NRG procedure projects the model Hamiltonian. As we will show, the computational time is small in comparison with the diagonalization time, and memory requirements are insignificant. The new procedure is also easier to code than the traditional one.

To define the notions and expressions upon which the recursive approach is constructed, our presentation will cursorily recapitulate the transformations constituting the NRG approach. We will then describe the recursive computation of matrix elements. Finally, to monitor the efficiency and accuracy of the new method in a specific setting, we will evaluate the temperature-dependent conductances of two elementary nanostructured devices, two functions that have already been extensively studied [8,15–17]; we have chosen them as examples because their solutions exhibit benchmarks against which we can check the accuracy of the recursive procedure.

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2. Numerical renormalization-group method

Excellent descriptions of the NRG approach being available and even practical aspects having been described [2,15], we need not dwell on its conceptual basis. We will briefly recapitulate the procedure and refer readers interested in additional detail to Appendix A, which implements the numerical diagonalization, and Appendix B, which explains how physical properties are computed from the resulting eigenvalues and eigenstates.

2.1. Model Hamiltonian

To be specific, we will consider the Anderson model constituted by a spin-degenerate impurity level c_d coupled to a non-interacting conduction band with N levels c_k. The impurity is described by the Hamiltonian

$$H_d = \epsilon_d c_d^\dagger c_d + U n_{d\uparrow} n_{d\downarrow}, \tag{1}$$

where ϵ_d denotes the impurity energy and U the Coulomb repulsion in the doubly occupied level. In the first term on the right-hand side we have left out both the spin indices and the sum over spins, a practice that we will apply to quadratic terms throughout this paper.

The conduction band is defined by the diagonal Hamiltonian [18]

$$H_{cb} = \int_{-D}^{D} \epsilon_k c_k^\dagger c_k \, d\epsilon_k, \tag{2}$$

where the energies ϵ_k, measured from the Fermi level, define a structureless half-filled band extending from $\epsilon_k = -D$ to $\epsilon_k = D$, with density of states $\rho = N/2D$.

In the simplest form of the model, the impurity is coupled to a Wannier state centered at the impurity position. The coupling Hamiltonian is, then,

$$H_{coupl} = \sqrt{2}V \, (c_d^\dagger f_0 + H.c.), \tag{3}$$

where, sticking to NRG tradition, we have introduced the short-hand

$$f_0 \equiv \frac{1}{\sqrt{2D}} \int_{-D}^{D} c_k \, d\epsilon_k, \tag{4}$$

to denote the normalized Fermi operator that annihilates an electron at the Wannier orbital directly coupled to the impurity.

The Anderson Hamiltonian is defined by the equality

$$H_A = H_{cb} + H_{coupl} + H_d. \tag{5}$$

Numerical treatment of H_A calls for projection on a basis with a manageable number of states. The definition of this basis, the projection of the right-hand side of Eq. (5) upon it, and the iterative diagonalization of the projected Hamiltonian are distinguishing features of the NRG construction, which will be recapitulated in Section 3.

3. NRG procedure

3.1. Discretization of the conduction band

The (continuous) conduction-band Hamiltonian (2) is scale invariant. Given a dimensionless parameter $\Lambda > 1$ and any conduction-band energy ϵ_k, the energy $\epsilon_{k'} = \epsilon_k/\Lambda$ will also belong to the band. That invariance will inevitably be broken by any discretization of the conduction band. Nonetheless, a mesh that preserves scaling in a restricted sense can be constructed. To this end, given the discretization parameter $\Lambda > 1$, the following two logarithmic sequences of intervals are marked on the conduction band:

$$\mathit{l}_{m\pm} = \{\epsilon_k \mid D\Lambda^{-m} > \pm\epsilon_k > D\Lambda^{-m-1}\} \quad (m = 0, 1, \ldots). \tag{6}$$

For each interval, a normalized Fermi operator $a_{m\pm}$ is defined as the combination of the conduction-band operators c_k within the interval that is most localized around the origin, i.e., the impurity site. The model Hamiltonian is then projected on the basis of the $a_{m\pm}$. Since the impurity is coupled to a Wannier state centered at the origin, this definition of the $a_{m\pm}$ insures that the coupling H_{coupl} be unaffected by the discretization. This makes the diagonalization procedure uniformly accurate, i.e., equally accurate for large or small couplings V and impurity energies ϵ_d and U.

3.2. Lanczos transformation

The basis of the operators $a_{m\pm}$ is infinite, albeit discrete. The projection of the model Hamiltonian on that basis is an infinite diagonal series. It would be easy to drop the terms associated with the smallest energies, but this simple-minded truncation would eliminate operators $a_{m\pm}$ that are directly coupled to the impurity and hence introduce uncontrollable deviations. Before any truncation, therefore, the conduction band is Lanczos transformed, i.e., a new infinite basis $\{f_n\}$ ($n = 0, 1, \ldots$) is defined by the requirements that (i) the first element in the basis be the operator in Eq. (4), which defines the coupling (3) to the impurity; and (ii) the conduction-band Hamiltonian has the tridiagonal form

$$H_{cb} = \sum_{n=0}^{\infty} t_n(f_n^\dagger f_{n+1} + H.c.). \tag{7}$$

The coefficients t_n in the summand having been analytically shown to decay exponentially with n [1], the series on the right-hand side of Eq. (7) can now be truncated at $n = N$, with N chosen to make t_N small in comparison with a typical energy scale of interest, such as the thermal energy $k_B T$ or an excitation energy $\mathcal{E}$. When the truncated conduction-band Hamiltonian is substituted for the conduction-band Hamiltonian on the right-hand side of Eq. (5), and the result is divided by the scaled bandwidth

$$\mathcal{D}_N = D \frac{1 - \Lambda^{-1}}{\log \Lambda} \Lambda^{-(N-1)/2}, \tag{8}$$

the following scaled, truncated Hamiltonian results:

$$H_A^N = \frac{1}{\mathcal{D}_N} \left(\sum_{n=0}^{N-1} t_n(f_n^\dagger f_{n+1} + H.c.) \right.$$
$$\left. + \sqrt{2}V(c_d^\dagger f_0 + H.c.) + H_d \right). \tag{9}$$

As discussed in Appendix A.3, the Hamiltonian H_A^N is formally important because it defines a renormalization-group transformation. As discussed in Appendix A.4 it is also convenient for numerical treatment, since it can be iteratively diagonalized. The diagonalization yields eigenvalues classified by charge and spin, which determine the thermodynamical properties, and eigenvectors, from which excitation and transport properties can be computed.

3.3. Computation of the electrical conductance

As an illustration, we will compute in Section 5 the conductance through semiconductor nanostructures coupled to electron gases. Of special interest are the two alternative experimental setups described in Appendix B.3: the single-electron transistor (SET),