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A real-frequency solver for the Anderson impurity model based on bath optimization and cluster perturbation theory

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ABSTRACT

Recently solvers for the Anderson impurity model (AIM) working directly on the real-frequency axis have gained much interest. A simple and yet frequently used impurity solver is exact diagonalization (ED), which is based on a discretization of the AIM bath degrees of freedom. Usually, the bath parameters cannot be obtained directly on the real-frequency axis, but have to be determined by a fit procedure on the Matsubara axis. In this work we present an approach where the bath degrees of freedom are first discretized directly on the real-frequency axis using a large number of bath sites (≈50). Then, the bath is optimized by unitary transformations such that it separates into two parts that are weakly coupled. One part contains the impurity site and its interacting Green's functions can be determined with ED. The other (larger) part is a non-interacting system containing all the remaining bath sites. Finally, the Green's function of the full AIM is calculated via coupling these two parts with cluster perturbation theory.

1. Introduction

The single-orbital Anderson impurity model (AIM) [1] can be represented exactly by an interacting site coupled to a bath of infinitely many non-interacting sites. In approaches based on exact diagonalization (ED), the number of sites in the interacting system is restricted, and thus the bath needs to be truncated [2–4]. This is a delicate step, because no unique procedure exists. Different ways are used, e.g., fits on the Matsubara axis or continuous fraction expansions [3,5,6].

Various methods improving on ED have been presented in recent years, e.g., the variational exact diagonalization [7], the distributional exact diagonalization [8] and methods based on a restriction of the basis states [9–13]. Another way of going beyond ED is the use of cluster perturbation theory (CPT) [14–16], i.e. the more advanced variational cluster approximation (VCA) [17–19], as a solver for the AIM [20,21].

From now on, we assume a single-orbital AIM coupled to a finite but large bath of $L-1$ non-interacting sites. The basic idea of using CPT as an impurity solver is to separate the L-site AIM into a cluster of size L_C, which includes the impurity site and L_C-1 bath sites, and a non-interacting system consisting of the remaining bath sites. In general, the non-interacting Green's function is specified by the Hamiltonian H^0, that is a matrix in orbital space of size $L\times L$. For illustration purposes (see the sketch in Fig. 1), we denote the upper left $L_C\times L_C$ block in H^0 as the interacting cluster, subsequently H_C^0. The remaining, lower $(L-L_C)\times(L-L_C)$ block describes the remainder of the bath, subsequently H_R^0. Additionally, there are two off-diagonal blocks T connecting H_C^0 and H_R^0. The onsite Hubbard interaction $H_U=Un_{I,\uparrow}n_{I,\downarrow}$, where I labels the impurity site, is now added to the cluster Hamiltonian, $H_C=H_C^0+H_U$. There are no interactions in the bath degrees of freedom, hence H_R^0 remains unchanged.

In CPT both Hamiltonians (H_C and H_R^0) are solved exactly for their single-particle Green's functions $G_C(\omega)$ and $G_R(\omega)$. To obtain $G_C(\omega)$ we use the Lanczos procedure at zero temperature [22,23]. Note that $G_R(\omega)=G_R^0(\omega)$, as the remainder of the bath is a non-interacting system. Subsequently, the two systems are joined to yield the single-particle Green's function of the full system $G(\omega)$ via the CPT relation [15]

$$G^{-1}(\omega)=\begin{pmatrix} G_C(\omega) & 0 \\ 0 & G_R(\omega)\end{pmatrix}^{-1}-V, \tag{1}$$

where V is a $L\times L$ coupling matrix consisting only of the T blocks. Eq. (1) is exact in the case of a non-interacting system ($U=0$). In the interacting case, the CPT relation is no longer exact, but a result of perturbation theory in V. CPT approximates the self-energy of the full system by the self-energy of the interacting cluster.

In general, the non-interacting bath can always be transformed to a tridiagonal representation via a Lanczos tridiagonalization, yielding a chain representation of the AIM. This representation straight forwardly

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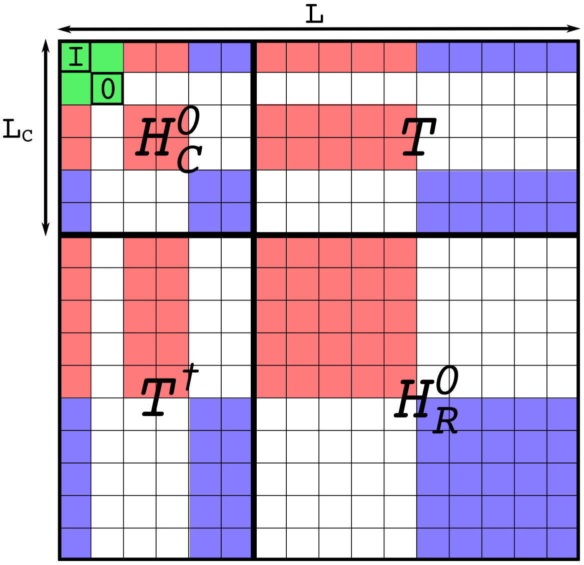

Fig. 1. Splitting of the Hamiltonian H^0 into an interacting cluster H_C^0 of $L_C = 6$ sites, the remaining reservoir H_R^0 and the coupling of those two system T. In the specific example of a particle-hole symmetric system the unitary updates are performed in the space of negative energies (red) and equivalently in the space of positive energies (blue). No non-zero matrix elements are generated in the white blocks by the two-dimensional rotation matrices used in this work. The diagonal blocks from top to bottom represent: (1) the impurity, (2) the zero mode inside the cluster, (3) two negative modes inside the cluster, (4) two positive modes inside the cluster, (5) the remaining negative modes in the reservoir and (6) the remaining positive modes in the reservoir.

allows to define the separation of the interacting cluster and the remainder of the bath. However, the situation is not so clear in other representations. Consider for example the case of a star geometry, where all bath sites couple directly to the impurity site. Incorporating just a random set of these star sites into the interacting cluster will lead to a poor discretization of the bath, and hence a poor self-energy.

Any unitary transformation on the non-interacting bath degrees of freedom leaves the physics of the interacting AIM invariant. However, such a transformation will influence the self-energy of the interacting cluster significantly, since it changes the cluster Hamiltonian H_C. Additionally, such transformations will also alter the off-diagonal block T, rendering the resulting perturbation in some cases larger than in others. There exist an infinite number of representations which all describe the non-interacting bath exactly and which are related via unitary transformations. However, the CPT method itself suggests which baths might be the best: Those which "minimize" the off-diagonal perturbative elements in T. The key idea of this work is to use unitary transformations to find those bath representations with minimal couplings between the cluster and the remainder of the bath.

In the following, we outline a way to construct CPT-favorable bath representations in Section 2, and present results for a $L = 64$ AIM with a semi-circular particle-hole symmetric bath in Section 3.

2. Method

The general form of the non-interacting Hamiltonian for an L-site AIM is

$$H_0 = \epsilon_I c_I^\dagger c_I + \sum_{i=1}^{L-1} (t_{iI} c_i^\dagger c_I + \text{h. c.}) + \sum_{i,j=1}^{L-1} t_{ij} c_i^\dagger c_j \tag{2}$$

where the impurity is denoted by the index I and the $L - 1$ bath sites by i and j. We omit the spin indices. To obtain H_0 for an L-site system one can use a star representation, where each bath site couples only to the impurity site. Then, the parameters of H_0 can be determined by a discretization of the non-interacting bath DOS into equally spaced intervals. Each interval is represented by a delta peak, where the energy positions of the delta peaks correspond to the on-site energies and the hopping parameters are obtained from the spectral weights in the intervals. Of course, the higher the number of bath sites the better the result of this discretization.

Under a unitary transformation R, performed in the bath only, with $c_i = \sum_\alpha R_{i\alpha} d_\alpha$ and $c_i^\dagger = \sum_\alpha d_\alpha^\dagger R_{\alpha i}^*$, where $RR^\dagger = \mathbb{1}$, the transformed Hamiltonian reads

$$H'_0 = \epsilon_I c_I^\dagger c_I + \sum_{\alpha=1}^{L-1} (h_{\alpha I} d_\alpha^\dagger c_I + \text{h. c.}) + \sum_{\alpha,\beta=1}^{L-1} h_{\alpha\beta} d_\alpha^\dagger d_\beta. \tag{3}$$

The parameters of the Hamiltonian transform like $h_{\alpha I} = \sum_i R_{\alpha i}^* t_{iI}$ and $h_{\alpha\beta} = \sum_{i,j} R_{\alpha i}^* t_{ij} R_{j\beta}$. Such a transformation leaves the impurity state I and consequently ϵ_I invariant.

We define an "energy" of a certain bath representation via the 2-norm of the off-diagonal blocks T

$$E = \frac{1}{N_T} \sum_{i,j} |T_{ij}|^2, \tag{4}$$

where the number of elements in T is $N_T = L_C \cdot (L - L_C)$. Transformations on the bath degrees of freedom included in the interacting cluster do not influence the resulting self-energy. The same is true for transformations performed only in the remainder of the bath. This imposes a constraint on the energy E, namely, it has to be invariant with respect to such transformations, which is indeed fulfilled by the 2-norm.

The aim is now to find an optimal bath representation for CPT by minimizing the energy E. Since the configuration space of T_{ij} is high dimensional, we use a Monte Carlo procedure. Initially, we perform global updates in all dimensions with random rotation matrices to obtain a randomized starting representation of H_0. Then, we move through the space of possible H_0 by proposing random local updates R. In general, any unitary update would be allowed, but here we restrict ourselves to two-dimensional rotation matrices for the local updates

$$R = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & 0 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & \dots & \cos(\phi) & 0 & \dots & -\sin(\phi) & \dots & 0 \\ 0 & 0 & \dots & 0 & 1 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & \dots & \sin(\phi) & 0 & \dots & \cos(\phi) & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

A local update matrix $R(i, j, \phi)$ is drawn by choosing two random integers $i, j \in [1, L - 1]$ representing the plane of rotation and one rotation angle $\phi \in [0, 2\pi[$. A new representation with energy E' is accepted with probability $p = \min(1, e^{-\gamma(E'-E)})$. We use simulated annealing to obtain low-energy CPT bath representations by increasing the parameter γ.

Although bath rotations leave the particle-hole symmetry invariant on the L-site H_0, they destroy it on the L_C-site cluster. Therefore, as shown in Fig. 1, we split the bath sites into an equal amount of positive (blue elements) and negative energy (red elements) sites and one zero mode (green 0). Updates are performed simultaneously on the positive and negative modes which leaves the whole bath, the bath in the cluster as well as the remaining bath particle-hole invariant. To avoid a Kramers-degenerate ground state, clusters with an even number of sites L_C are chosen. This implies that one bath site (the zero mode) is exactly located at zero energy. Zero mode updates cannot be achieved by two-dimensional rotations without breaking the particle-hole symmetry of the cluster, but would rather require special unitary transformations involving at least three bath sites. For the proof of concept presented here, we refrain from updating the zero mode, i.e. the green elements in Fig. 1 do not change. Hence, the zero mode coupling is determined by the initial discretization of the system. Although this restricts the space of trial bath representations, we leave the zero mode updates for future works.