Exact diagonalization of the Anderson impurity model

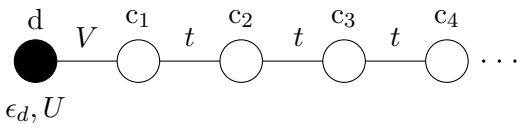
Emmanuel Bogacz

Exact diagonalization (ED) is a numerical method to find the eigenvalues and eigenvectors of a Hamiltonian, as well as computing expectation values and correlators. The Hamiltonian is diagonalized entirely, which is computationally expensive, as the Hamiltonian matrix scales exponentially with the number of sites in the system. In the Anderson impurity model (AIM), the size of the matrix to diagonalize scales as 4^n (which is the size of the Hilbert space), where n is the number of fermionic sites. This matrix can be block diagonalized, which can make the computation more efficient, but is still limited to small number of site.

1 Model and basis representation

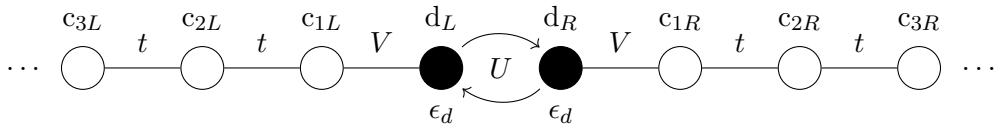
The AIM Hamiltonian is as follows, with pictorial representation below:

$$\begin{aligned} \mathrm{H}_{AIM} = \epsilon_d \sum_{\sigma\in\{\uparrow,\downarrow\}} \mathrm{d}^\dagger_\sigma \mathrm{d}_\sigma + U\, \mathrm{d}^\dagger_\uparrow \mathrm{d}_\uparrow \mathrm{d}^\dagger_\downarrow \mathrm{d}_\downarrow + V \sum_\sigma \left(\mathrm{d}^\dagger_\sigma \mathrm{c}_{1\sigma} + H.c.\right) \\ +\ t \sum_{\sigma,i=1}^{N-1} \left(\mathrm{c}^\dagger_{i\sigma} \mathrm{c}_{i+1,\sigma} + H.c.\right) \end{aligned} \tag{1}$$



where N is here the number of non-interacting bath sites, which are represented with a clear circle. This representation is spin-full and has interactions between the two spin species, in which the impurity is denoted with a filled black disc. Its Hilbert space is $\{0,\uparrow,\downarrow,\uparrow\downarrow\}^{\otimes(N+1)}$ and has dimensionality $4^{(N+1)}$. An alternative representation is possible, dubbed the 'unfolded' representation, where labels 'L=left' and 'R=right' are swapped for $\uparrow$ and $\downarrow$ spin species. The Hamiltonian is as follows:

$$\begin{aligned} \mathrm{H}_{AIM} = \epsilon_d \sum_{\alpha\in\{L,R\}} \mathrm{d}^\dagger_\alpha \mathrm{d}_\alpha + U\, \mathrm{d}^\dagger_L \mathrm{d}_L \mathrm{d}^\dagger_R \mathrm{d}_R + V \sum_\alpha \left(\mathrm{d}^\dagger_\alpha \mathrm{c}_{1\alpha} + H.c.\right) \\ +\ t \sum_{\alpha,i=1}^{N-1} \left(\mathrm{c}^\dagger_{i\alpha} \mathrm{c}_{i+1,\alpha} + H.c.\right) \end{aligned} \tag{2}$$



In this unfolded representation, up spins live on the left hand side of the system, and down spins live on the right hand side. This representation is therefore spinless, and the interactions are accounted for as a capacitive coupling between the left and right impurities. The dimensionality

of the Hilbert space remains the same: $2^{2(N+1)} = 4^{(N+1)}$. The computational basis is therefore binary: $\{0,1\}^{\otimes 2(N+1)}$, where 1 indicates an electron and 0 no electron; which helps saving memory. We therefore have the basis states $|b_1, b_2, \dots b_{2(N+1)}\rangle$, where b_i is a binary number, for $i \in [1, 2(N+1)]$ Using conserved quantum numbers charge Q and spin S_z, we can arrange the basis states by block. We define $Q = \sum_{i=1}^{2(N+1)} b_i - (N+1)$, relative to half filling ($Q := 0$), where $N+1$ labels the left-impurity. We also use $2S_z = \sum_{i=1}^{N+1} b_i - \sum_{i=N+2}^{2(N+1)} b_i$, which is the double of the difference between number of spin ups and spin downs. Basis states are then labeled by an integer q_i, denoting a unique combination of (Q, S_z). The Hamiltonian can be setup as a block diagonal matrix

$$H = diag(H_{q_1}, \dots, H_{q_{max}}) \tag{3}$$

each block can thus be diagonalized separately.
The advantage of this 'unfolded' basis, other than memory efficiency, is that there are no negative signs to be accounted for in the tunnelling term of the Hamiltonian. The proof is as follows, we look at the term $t_i \, \mathrm{c}^\dagger_{i+1,\alpha} \, \mathrm{c}_{i\alpha}$, for two basis states $|\phi\rangle$ and $|\tilde{\phi}\rangle$. The tunnelling element t_i is t between bath sites, V between a bath site and the left/right impurity, and 0 between the two impurity sites.

$$\langle\phi| t_i \, \mathrm{c}^\dagger_{i+1,\alpha} \, \mathrm{c}_{i\alpha} \, |\tilde{\phi}\rangle = t_i \langle b_1 \dots b_{i-1} 0_i 1_{i+1} b_{i+2} \dots b_{2(N+1)}| \, \mathrm{c}^\dagger_{i+1} \, \mathrm{c}_i \, |b_1 \dots b_{i-1} 1_i 0_{i+1} b_{i+2} \dots b_{2(N+1)}\rangle \tag{4}$$

$$= t_i \langle 0| \prod_{j=2(N+1), b_j \neq 0}^{i-1} \mathrm{c}_j \cdot \mathrm{c}_{i+1} \cdot \prod_{k=i+2, b_k \neq 0}^{1} \mathrm{c}_k \, | \, \mathrm{c}^\dagger_{i+1} \, \mathrm{c}_i \, | \prod_{l=1, b_l \neq 0}^{i-1} \mathrm{c}^\dagger_l \cdot \mathrm{c}^\dagger_i \cdot \prod_{m=i+2, b_m \neq 0}^{2(N+1)} \mathrm{c}^\dagger_m \, |0\rangle \tag{5}$$

We label the products from left to right as products 1 to 4, which contain J, K, K and J terms/operators respectively. We anticommute through the operator $\mathrm{c}^\dagger_{i+1}$ to retrieve normal ordering, to the right of $\mathrm{c}^\dagger_i$. This operation costs a factor of $(-1)^{K+2} = (-1)^K$. Similarly, we bring the operator c_i to the right of right of c_{i+1}, which yields a factor of $(-1)^K$. We have now a normal ordered inner product which evaluates to 1, with a prefactor of $t_i(-1)^{2K} = t_i$.

2 Observables

In order to compute observables, it is useful to define the relationship between basis states and eigenstates. An eigenstate $|\psi_i\rangle$ is related to the basis states $\{|\phi_k\rangle\}_{k=1}^{2(N+1)}$ by the eigenvector matrix U, such as

$$|\psi_i\rangle = \sum_k U_{ki} |\phi_k\rangle \tag{6}$$

For example, computing the up spin impurity at zero temperature, we thus compute the occupation number of the left impurity d_L in the ground state $|gs\rangle$.

$$\begin{aligned} \langle gs| \, \mathrm{n}_{d_L} \, |gs\rangle_{T=0} &= \sum_{ij} U^\dagger_{j0} U_{i0} \langle \phi_j| \, \mathrm{n}_{d_L} \, |\phi_i\rangle \\ &= \sum_i U^\dagger_{i0} U_{i0} \langle \phi_i| \, \mathrm{n}_{d_L} \, |\phi_i\rangle \\ &= \sum_i U^\dagger_{i0} U_{i0} \; b^{\phi_i}_{d_L} \end{aligned} \tag{7}$$

At finite temperature, the (left-) impurity occupation number is given by:

$$\langle \mathrm{n}_{d_L} \rangle_T = \frac{1}{Z} \sum_i \langle \psi_i| \, \mathrm{n}_{d_L} \, |\psi_i\rangle e^{-\beta E_i} \tag{8}$$

where

$$\begin{aligned}\langle\psi_i|\,\mathrm{n}_{d_L}\,|\psi_l\rangle &= \sum_{jk} U_{ji}U_{lk}\langle\phi_j|\,\mathrm{n}_{d_L}\,|\phi_k\rangle \\ &= \sum_{k} U_{ki}U_{lk}b^{\phi_k}_{d_L}\end{aligned} \tag{9}$$

We can also compute the local Green's function of the impurity at zero-temperature using the Lehmann representation [1]. The greater GF for the up-spin is computed as

$$G^{>}_{d_L}(z) = \sum_n \frac{|\langle\psi_n|\,\mathrm{d}^\dagger_L\,|gs\rangle|^2}{z-(E_n-E_{gs})} \tag{10}$$

where $z=\omega+\imath 0^+$, n belongs to the sector $(Q_{gs}+1, S_{z_{gs}}+1)$, which is the only sector to connect to the ground state via $\mathrm{d}^\dagger_L$, which has quantum numbers $(Q_{gs}, S_{z_{gs}})$. The numerator can be computed by using 6. Similarly, the lesser GF can be computed as:

$$G^{<}_{d_L}(z) = \sum_{n'} \frac{|\langle\psi_{n'}|\,\mathrm{d}_L\,|gs\rangle|^2}{z+(E_{n'}-E_{gs})} \tag{11}$$

where n' belongs to the sector $(Q_{gs}-1, S_{z_{gs}}-1)$, which is the only sector to connect to the ground state via d_L, which has quantum numbers $(Q_{gs}, S_{z_{gs}})$. The retarded GF $G^R_d(z) = G^{>}_d(z) - G^{<}_d(z)$ is then used to retrieve the spectral function $A(\omega) = -\Im G^R_d(z)/\pi$.
For finite temperature calculations, the GF expression can be generalized as in [1]. Here are the expressions for greater and lesser GF, for general eigenstates $|\psi_n\rangle$ and $|\psi_{n'}\rangle$:

$$G^{>}_{d_L}(z) = \frac{1}{Z}\sum_{nn'} e^{-\beta E_n}\frac{|\langle\psi_n|\,\mathrm{d}_L\,|\psi_{n'}\rangle|^2}{z-(E_{n'}-E_n)} \tag{12}$$

$$G^{<}_{d_L}(z) = -\frac{1}{Z}\sum_{nn'} e^{-\beta E_n}\frac{|\langle\psi_n|\,\mathrm{d}^\dagger_L\,|\psi_{n'}\rangle|^2}{z+E_{n'}-E_n} \tag{13}$$

Again we retrieve $G^R_d(z) = G^{>}_d(z) - G^{<}_d(z)$.

References

[1] Henrik Bruus and Karsten Flensberg. *Many-body quantum theory in condensed matter physics: an introduction*. OUP Oxford, 2004.