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Exercise Sheet No. 5
"Computational Condensed Matter Theory"

13 Wilson's Numerical Renormalization Group method (NRG)

The Single Impurity Anderson Model (SIAM) describes a localised impurity in an otherwise non-interacting electronic conduction band. The Hamiltonian of this system is given by

$$H_{\text{SIAM}} = \sum_\sigma \varepsilon^d_\sigma \hat{n}^d_\sigma + U\hat{n}^d_\uparrow \hat{n}^d_\downarrow + \sum_\sigma V_\sigma \left(\hat{c}^\dagger_{0,\sigma}\hat{d}_\sigma + \text{h.c.}\right) - t \sum_{<i,j>,\sigma} \left(\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}\right),$$
$$\text{with} \quad \hat{n}^d_\sigma = \hat{d}^\dagger_\sigma \hat{d}_\sigma.$$

As shown in the lecture the Hamiltonian can be mapped onto a semi-infinite tight-binding chain. Due to the logarithmic discretisation of the conduction band, the hopping elements of the Hamiltonian become site dependend and decrease with distance as

$$H_M = \varepsilon^d \sum_\sigma \hat{n}^d_\sigma + U\hat{n}^d_\uparrow \hat{n}_\downarrow + t_1 \left(c^\dagger_{1,\sigma} d_\sigma + d^\dagger_\sigma c_{1,\sigma}\right) - t \sum_{\ell=2}^{M} \sum_\sigma \Lambda^{\frac{2-\ell}{2}} \left(c^\dagger_{\ell-1,\sigma} c_{\ell,\sigma} + c^\dagger_{\ell,\sigma} c_{\ell-1,\sigma}\right). \tag{1}$$

which in the limit $M \to \infty$ recovers the the full Hamiltonian.
The central aspect of the renormalization algorithm is, that the Hamiltonians H_M obeye the recursion relation

$$H_{M+1} = H_M - t\Lambda^{-\frac{M-1}{2}} \sum_\sigma \left(c^\dagger_{M,\sigma} c_{M+1,\sigma} + c^\dagger_{M+1,\sigma} c_{M,\sigma}\right). \tag{2}$$

In the formulas above, $c^\dagger_{l,\sigma}, c_{l,\sigma}$ denote fermionic creation and annihilation operators acting on site l of a one-dimensional chain, $d^\dagger_\sigma, d_\sigma$ are fermionic creation and annihilation operators acting on the single impurity site. The state of a single site of the chain as well as the impurity are characterized by four dimensional state vectors $|\alpha\rangle = (|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |2\rangle)^T$ denoting empty, single or double occupied sites.

The low-energy spectrum of the Hamiltonian H_M (Eq. 1) can be exploited applying an iteration scheme in which at every step the system is enlarged by adding a new site l and after diagonalization only the quarter of states with the lowest energy are kept.

In order to avoid the problem of exponentially small energies and to pave the ground for fixpoints one actually applies the method to the rescaled Hamiltonian

$$\tilde{H}_1 = H_1 \qquad \tilde{H}_M \;=\; \Lambda^{\frac{M-2}{2}} H_M \text{ for } M \geq 2 \tag{3}$$

$$\tilde{H}_{M+1} = \Lambda^{1/2} \tilde{H}_M - t \sum_\sigma \left(c^\dagger_{M,\sigma} c_{M+1,\sigma} + c^\dagger_{M+1,\sigma} c_{M,\sigma} \right) . \tag{4}$$

a) Solve H_1

Write the Hamiltonian H_1 (Eq. 1) for $M = 1$ as matrix in the basis $|\alpha\rangle_d \otimes |\alpha\rangle_1$. Diagonalize this 16×16 matrix and project the Hamiltonian to its eigenbasis $|\lambda\rangle_1$. The energies should be relative to the groundstate, thus subtract the lowest eigenvalue $\lambda_1 \mathbb{1}$.

b) Transform $\hat{c}_{1,\uparrow}$ and $\hat{c}_{1,\downarrow}$

Write the annihilation operators $\hat{c}_{1,\uparrow}$ and $\hat{c}_{1,\downarrow}$ in the basis $|\alpha\rangle_d \otimes |\alpha\rangle_1$ and, using the result of a), transform them into the new basis $|\lambda\rangle_1$.

c) Iteration step $\tilde{H}_M \to \tilde{H}_{M+1}$

Build an iteration step $\tilde{H}_M \to \tilde{H}_{M+1}$ as given by the recursion relation (Eq. 4):
Assume you have an Hamiltonian $\tilde{H}_M$ in its eigenbasis $|\lambda\rangle_M$ and $\hat{c}_{\sigma,M}$ given in the same basis. Enlarge the system by a site $\ell = M + 1$ which results in a larger basis $|\tilde{\lambda}\rangle_{M+1} = |\lambda\rangle_M \otimes |\alpha\rangle$. Construct the Hamiltonian $\tilde{H}_M$ and the operators $\hat{c}_{\sigma,M}$, $\hat{c}^\dagger_{\sigma,M+1}$ in this new basis and calculate $\tilde{H}_{M+1}$.

d) Projection in energy space

Diagonalize $\tilde{H}_{M+1}$ and select the N_C lowest eigenvalues $\lambda = \lambda_1 \ldots \lambda_{N_C}$ and the corresponding eigenvectors $|\lambda\rangle_{M+1} = |\lambda_1\rangle \ldots |\lambda_{N_C}\rangle$. Construct a projection to the subspace spanned by these eigenvectors $|\lambda\rangle_{M+1}$. Project $\tilde{H}_{M+1}$ and $\hat{c}_{\sigma,M+1}$ on $|\lambda\rangle_{M+1}$ and as in a) subtract the groundstate energy $E_G = \lambda_1$ from $\tilde{H}_{M+1}$.

e) Many particle spectrum

Choose as parameters the values $\Lambda = 0.5$, $U = t$, $\varepsilon^d = -U/2$, $t_1 = 0.2t$ and $N_C = 100$. Starting with H_1 and repeatedly applying steps c) and d) calculate the spectrum of $\tilde{H}_M - E_G$, for M=1..50. Plot the 20 lowest values as function of M. The energies vary between even and odd number of sites, thus plot odd and even M in two seperate graphs. Interpret your results.