Exact Diagonalization Notes

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1 Hamiltonians:

$H = t\sum_{i=i}^{N-1}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + c_{i+1\sigma}^{\dagger}c_{i\sigma}) + \sum_{i=i}^{N}\epsilon_i c_{i\sigma}^{\dagger}c_{i\sigma} + \sum_{i=i}^{N}U_i c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}$

a) Anderson model: $\epsilon_i = \epsilon\delta_{i,1}$ and $U_i = U\delta_{i,1}$. Only the first site has Coulomb repulsion and atomic energy.

b) Hubbard model: $\epsilon_i = \epsilon$ and $U_i = U$.

The basis state represntation is chosen in the convention $c_{1\uparrow}^{\dagger}...c_{N\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}...c_{N\downarrow}^{\dagger}|0>$, such that the hopping term for the nearest neighbor is always positive. In the code, the basis is represented as 0 (empty), -1 (spin down), 1 (spin up), and 2 (double occupied), so the basis looks like $|0, 1, -1, 2>$. The basises is build based on two symmetries: the total charge (N) and the total spin S_Z. The quantum number is represnted as Q and S_Z, each Q and S_Z has subspace r . Normally the highly symmetric state has the largest subspace, e.g. for $N = 4$, $Q = 0$ and $S_Z = 0$ has $r = 1...400$ 400 basises. Noted that in the note, the real S_Z need to be devided by 2, because the code's S_Z is set to integer for the convinience of building basis. Similarily, the real total charge Q need to be added by a total size of the chain N, since it runs from $-N \leq Q \leq N$ for the convinience of building basis.

The full exact diagonalization is performed in each subspace (block diagonal for each Q and S_Z), and the energies is recorded in "energiesXXXXX.dat".

2 Zero Temperature Spectral Function and Green's function:

Here we discuss the implementation of zero temperature Lehmann representation for spectral function. For simplicity, we calculate the spectral function at the first site with spin up, $A_{1\uparrow}(\omega)$.

$A_{1\uparrow}(\omega) = \sum_{Q,S_Z,r} |_{diag} < 0,0,0|c_{1\uparrow}|Q, S_Z, r >_{diag} |^2\delta(\omega - E_{0,0,0} + E_{Q,S_Z,r}) +$

$\sum_{Q,S_Z,r} |_{diag} < 0,0,0|c_{1\uparrow}^{\dagger}|Q, S_Z, r >_{diag} |^2\delta(\omega - E_{Q,S_Z,r} + E_{0,0,0})$

Since we know that onlt the state $Q = 1, S_Z = 1$ or $Q = -1, S_Z = -1$, for $c_{1\uparrow}$ and $c_{1\uparrow}^{\dagger}$ respectly, can survive for the bracket, we only need to focus on their

subspace r. Noted that the subscript diag means the $|Q, S_Z, r >_{diag}$ is the eigenvector for the energy $E_{Q,S_Z,r}$. Here we focus on the ${}_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag}$ term, the other term can be calculated similarily.

The ${}_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag}$ is not easy to calculate, because each eigenstate $|Q, S_Z, r >_{diag}$ is the mix state of the original basis $|Q, S_Z, r >_{old}$, where $|Q, S_Z, r >_{old}$ is the primitive basis, e.g. $|0, 1, -1, 2 >$ for $Q = 0, S_Z = 0$. However, the ${}_{old} < 0,0,0|c_{1\uparrow}|1,1,r >_{old}$ is easy to calculate. So we can do a basis transformation:

${}_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag} = \sum_{r'}\sum_{r''} {}_{diag} < 0,0,0|0,0,r' >_{old} {}_{old} < 0,0,r'|c_{1\uparrow}|1,1,r'' >_{old}$
${}_{old} < 1,1,r''|1,1,r >_{diag}$

The term ${}_{diag} < 0,0,0|0,0,r' >_{old}$ and ${}_{old} < 1,1,r''|1,1,r >_{diag}$ are the orthonormal transformation matrices, which is stored in the code variable "states". Thus, the braket can be easily evaluate using the simple matrix multiplication. We first evaluate the matrix ${}_{old} < 0,0,r'|c_{1\uparrow}|1,1,r'' >_{old}$ by simple index look up, then multiply it by transform matrix.

${}_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag(1\times M)} = U^T_{0,0(1\times L)} \cdot {}_{old} < 0,0,r'|c_{1\uparrow}|1,1,r'' >_{old(L\times M)}$
$\cdot U_{1,1(M\times M)}$

The dimension for $U^T_{0,0}$ is $1 \times L$, where L is the size of subspace $Q = 0, S_Z = 0$. The dimension for $U_{1,1}$ is $M \times M$, where M is the size of subspace $Q = 1, S_Z = 1$. After obtained ${}_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag}$, the square of it is called spectral weight, which is printed out in "spectralWeightsXXXXX.dat". Pluging in the energies $E_{1,1,r}$ and the corresponding spectralweight $|_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag}|^2$ into $A_{1\uparrow}(\omega)$ we obtain the electron part of the spectral function. The hole part $|_{diag} < 0,0,0|c_{1\uparrow}| - 1,-1,r >_{diag}|^2$ can be calculated similarily. We can check that:

$\sum_r (|_{diag} < 0,0,0|c_{1\uparrow}|-1,-1,r >_{diag}|^2 + |_{diag} < 0,0,0|c_{1\uparrow}|1,1,r >_{diag}|^2) = 1$

the total spectralweight is 1. Finally, the spectralfunction is outputed as "spectralFunctionXXXXX.dat". The Green's function can be evaluated by the Kramer-Kronig relation:

$G_{1\uparrow}(\omega) = \int_{-\infty}^{\infty} d\omega' \frac{A(\omega')}{\omega - \omega'}$

and the output is "greenFunctionXXXXX.dat".

3 Examples:

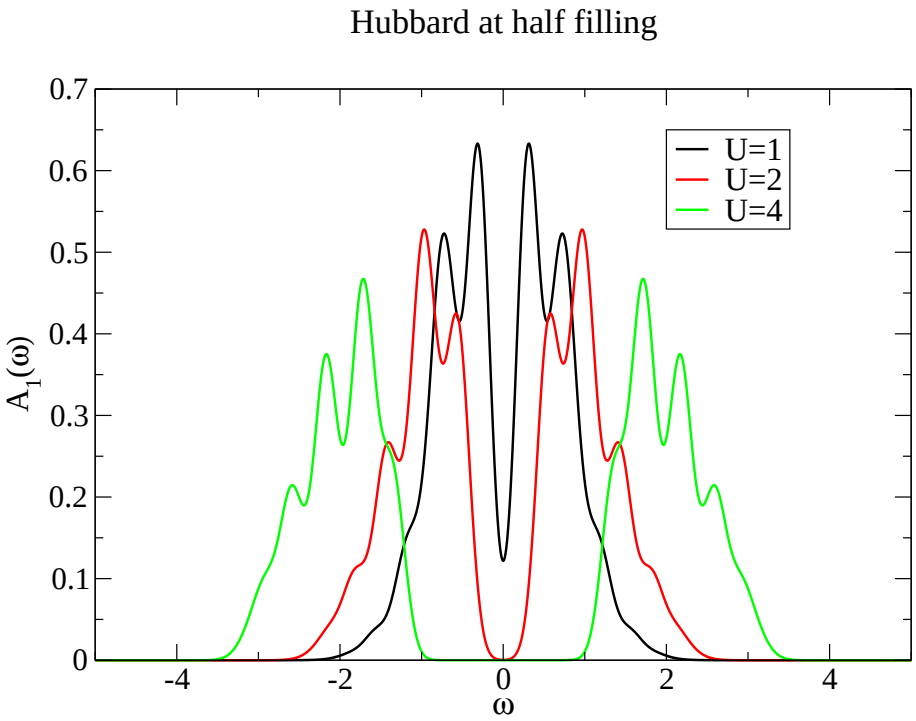

Figure 1: $\mu = -U/2$, $t = -0.5$, and broadening is 0.2.

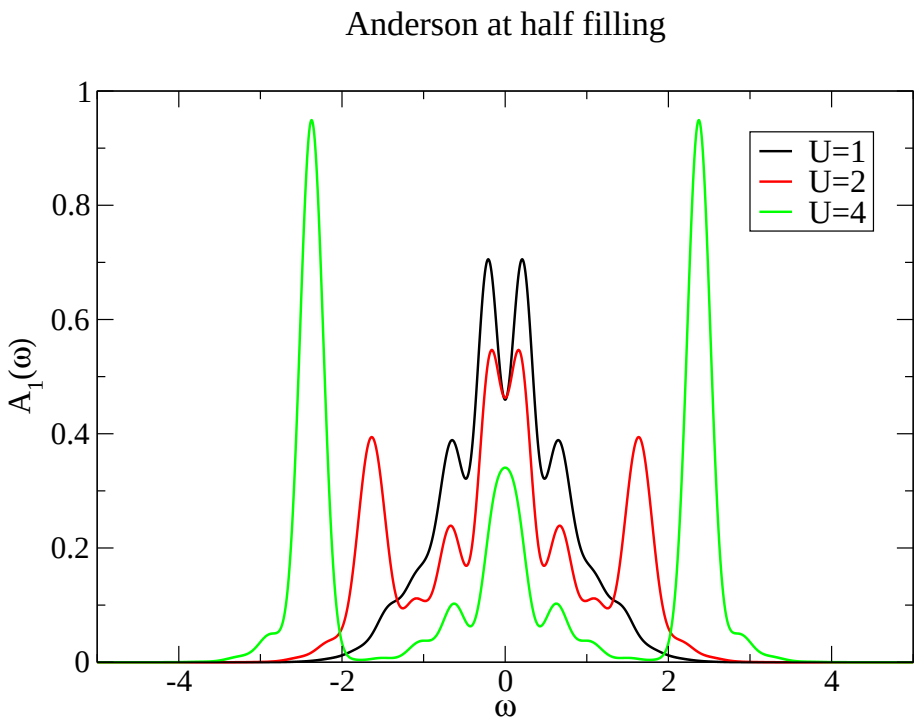

Figure 2: $\mu = -U/2$, $t = -0.5$, and broadening is 0.2.