Intensive Week Course:

Numerical methods for many-particle systems

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`http://www.thp.uni-koeln.de/~mitchell/intensive.html`

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Problem sheet III Wednesday, 07.03.2012

In this computer practical session, we consider non-trivial interacting systems for which no exact analytic solution exists. Specifically we will perform the exact numerical diagonalization of a small Hubbard chain (a tight-binding system with additional onsite interactions)

$$H = t \sum_{i=1}^{N-1} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma} \right) + \sum_{i=1\sigma}^{N} \varepsilon_i c_{i\sigma}^{\dagger} c_{i,\sigma} + \sum_{i=1}^{N} U_i \, c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}. \qquad (1)$$

Here, ε_i is the on-site energy and U_i the on-site interaction representing a short range Coulomb repulsion. For simplicity, let's first take

a) $\varepsilon_i = \varepsilon \delta_{i,1}$ and $U_i = U \delta_{i,1}$: Anderson model

b) $\varepsilon_i = \varepsilon$ and $U_i = U$: homogeneous Hubbard model

The Hilbert space of the system grows by a factor of four for each additional site we include. For a 6 site system, the Hamiltonian matrix would be of dimension $4^6 = 4096$, which would take a while to diagonalize numerically (but it is possible). But 10 sites is completely out of reach. To help, we can fortunately exploit symmetries of the systems: in this case charge and spin conservation. The Hamiltonian can then be block-diagonalized. Since the time for diagonalization goes as $\sim N^3$, each of the smaller matrices can be treated much more efficiently. Here we divide the full system in subsystems labelled by quantum numbers Q and S_z. At first use $U + 2\varepsilon = 0$, which corresponds to half-filling. The parameters ε_i and U_i for all the sites can be changed later to explore the resulting physics.

First, download from the course webpage the archive with the code for the template program `exactDiagonalization_f.tar.gz` (for a FORTRAN version) or `exactDiagonalization_c.tar.gz` (for a C++ version). From the console, type:

```
wget http://www.thp.uni-koeln.de/~mitchell/day3/<file>
```

To unzip the archives write `tar -zxvf <file>.tar.gz` in the console. Those programs constitute a template from which you will construct working exact diagonalization code. As before, crucial parts of the algorithm are left out for you to program yourself.

Problem 1:

Try to understand the working steps of the program. How are the many-particle basis states set up, and what information do they store? What do `qszcount` and `states` describe?

Problem 2:

In the `exactDiagonalization`-program, there is a large block of if-statements (written out in full here for clarity). They correspond to the off-diagonal elements of the Hamiltonian. What do these statements mean, and what do the off-diagonal terms correspond to in Eq. (1)? Where in the code should the diagonal elements be entered? What terms of Eq. (1) do they correspond to? Write code to populate the diagonal parts of the Hamiltonian matrix in each sub-block for both task (a) and (b).
c) Work out on paper what the off-diagonal parts of the Hamiltonian should be. Hint: beware of commutation relations! Modify the code to describe correctly these terms.

Problem 3:

Run the code to block-diagonalize the Hamiltonian. First take an even-chain. In which Q, S_z subspace is the ground state? Why is it different from the ground state of a system with an odd chain length? Now implement a numerical search for the ground state quantum numbers.

Problem 4:

Diagonalization of the Hamiltonian matrix provides eigenenergies and eigenvectors. This allows to calculate matrix elements of any operator. For the spectrum of a given site, we will need matrix elements between many-particle eigenstates of the destruction operator for that site. The exact configuration of the system is enumerated in the old basis. In this basis, the matrix elements ${}_{old}\langle Q, S_z, r|c_{i\sigma}|Q', S_z', r'\rangle_{old}$ can be easily evaluated. But for the spectrum we need the matrix elements ${}_{diag}\langle Q, S_z, r|c_{i\sigma}|Q', S_z', r'\rangle_{diag}$ in the new basis. Evaluate these elements using their expansion in terms of the old basis states.
For even chain systems, calculate matrix elements from the ground state ${}_{diag}\langle 0, 0, 0|c_{1,\sigma}|Q, S_z, r\rangle_{diag}$.

Problem 5:

Calculate the spectral function for site 1,

$$A_{1,\sigma}(\omega) = \sum_{Q,S_z,r} |{}_{diag}\langle 0, 0, 0|c_{1,\sigma}|Q, S_z, r\rangle_{diag}|^2 \, \delta(\omega - E_{Q,S_z,r}).$$

Once you have the discrete spectrum, use your code from yesterday (or the one provided) to broaden the poles and recover a continuous spectrum.

Problem 6:

Explore the physics of the models through the spectral functions. In the Hubbard chain (b), start with a small Coulomb interaction and maintain particle-hole symmetry ($U = -2\varepsilon$). A chain length of 6 should suffice (but you can vary it, if you like). Since we have only a small number of large poles, take a rather large broadening `b` and investigate the spectral function upon increasing U. What behaviour do you expect; what do you see? What would you get if you could do the calculation for a Hubbard chain of 10 sites, or 20? Try this for the Anderson model, (a).