Quantum Theory of Condensed Matter

Prof. Milena Grifoni
Dr. Andrea Donarini

Room H33
Wednesdays at 13:15

Sheet 8

1. The discrete jellium model

Consider e set of spinless fermions on a crystal lattice described by the Hamiltonian in the Wannier basis:

$$H = -t \sum_{<i,j>} c_i^\dagger c_j + U \sum_{<i,j>} \hat{n}_i \hat{n}_j$$

where $< i, j >$ are the nearest neighbours sites i and j, $\hat{n}_i$ is the counting operator $c_i^\dagger c_i$. Prove that, in the same spirit of the continuous jellium model, the Hamiltonian should be modified in order to include charge neutrality and thus should read:

$$H = -t \sum_{<i,j>} c_i^\dagger c_j + U \sum_{<i,j>} (\hat{n}_i - 1)(\hat{n}_j - 1)$$

2. Wick's theorem

1. Show that, for a system of non-interacting fermions described by the Hamiltonian in the eigenvalue basis

   $$H = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha,$$

   the following relation for the many-body grancanonical expectation values holds:

   $$\langle c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger c_{\alpha_3} c_{\alpha_4} \rangle = \langle c_{\alpha_1}^\dagger c_{\alpha_4} \rangle \langle c_{\alpha_2}^\dagger c_{\alpha_3} \rangle \delta_{\alpha_1\alpha_4} \delta_{\alpha_2\alpha_3} - \langle c_{\alpha_1}^\dagger c_{\alpha_3} \rangle \langle c_{\alpha_2}^\dagger c_{\alpha_4} \rangle \delta_{\alpha_1\alpha_3} \delta_{\alpha_2\alpha_4},$$

   where

   $$\langle c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger c_{\alpha_3} c_{\alpha_4} \rangle \equiv \frac{1}{Z} \mathrm{Tr} \left\{ c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger c_{\alpha_3} c_{\alpha_4} \exp[-\beta(H - \mu N)] \right\}$$

   and Z is the grancanonical partition function. The trace is taken over the full Fock space.

2. Derive from point (a) that, for non-interacting fermions, in every other given single particle basis $\{|n\rangle\}$ the following relation holds:

   $$\langle c_{n_1}^\dagger c_{n_2}^\dagger c_{n_3} c_{n_4} \rangle = \langle c_{n_1}^\dagger c_{n_4} \rangle \langle c_{n_2}^\dagger c_{n_3} \rangle - \langle c_{n_1}^\dagger c_{n_3} \rangle \langle c_{n_2}^\dagger c_{n_4} \rangle.$$

   Note that this is valid even if in this basis the Hamiltonian

   $$H = \sum_{n,m} t_{nm} c_n^\dagger c_m$$

   would contain non-diagonal terms t_{nm} for $n \neq m$.

   Hint: Diagonalize first H using a unitary transformation $c_n = \sum_\alpha u_{n\alpha} c_\alpha$. Apply then the equation proved in point (a). Finally perform the canonical transformation in the opposite direction.

Frohes Schaffen!