LMU München
WS 2013/2014
Lehrstuhl für Theoretische Nanophysik
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8. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, November 13, 2013.

Exercise 1: Two-body potential

Consider a two-body potential of the form $V = V(\boldsymbol{r} - \boldsymbol{r}')$.

a. Write down the interaction term in real space in 2nd quantization.

b. Transform to momentum space.

c. Show that the matrix elements of a two-body operator can be evaluated either in the direct product of single-particle states or in the symmetrized form.

d. Compute $V(q)$ for (i) Coulomb potential, (ii) contact interactions, (iii) Yukawa potential.

Exercise 2: Commutators

a. Derive the commutation relations for bosons and fermions from the definitions of the creation and annihilation operators that were given in the lecture.

b. Compute the following fermionic commutators:

$$\left[c^\dagger_\alpha c_\alpha \ , \ c_\alpha\right] = ? \quad (1)$$

$$\left[c^\dagger_\alpha c_\alpha \ , \ c^\dagger_\alpha\right] = ? \quad (2)$$

$$\left[c^\dagger_\alpha c_\alpha \ , \ c^\dagger_\beta c_\alpha\right] = ? \quad (3)$$

Exercise 3: 1D Tight-binding model

We consider a Hamiltonian with periodic boundary conditions (PBC) and L sites:

$$H = -t \sum_{l=1}^{L} (c^\dagger_l c_{l+1} + h.c.)$$

a. Find the local current operator j_l from the discretized continuity equation:

$$-(j_{l+1} - j_l) = i[H, n_l]$$

where $n_l = c_l^\dagger c_l$.

b. Show that $[H, J] = 0$ where $J = \sum_{l=1}^{L} j_l$

c. Show that J can be written as:

$$J = \sum_k v_k c_k^\dagger c_k \,.$$

d. Derive the local energy current-operator j_l^e from the equation of continuity of energy $-(j_{l+1}^e - j_l^e) = i[H, h_l]$ where $h_l = -t(c_l^\dagger c_{l+1} + h.c.)$. Show that the total energy current can be written as,

$$J = \sum_k \epsilon_k v_k n_k \,.$$

e. What is $\langle n_k \rangle$ at (i) $T = 0$ and (ii) $T > 0$?

f. Consider a system with $L = 10$ and $N = 4$. Write down the g.s. in 2nd quantization. What is the g.s. energy?

Exercise 4: Hartree-Fock again

We consider a one-dimensional one-band model with a two-body interactions, L sites and periodic boundary conditions:

$$H = -t\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + h.c.) + V\sum_{i=1}^{L} n_i n_{i+1}$$

Rederive the energy $\langle \psi_{\mathrm{HF}} | H | \psi_{\mathrm{HF}} \rangle$ in Hartree Fock approximation by using the ansatz

$$|\psi\rangle = \prod_{\mu=1}^{N} c_\mu^\dagger |0\rangle \,.$$

Proceed as follows:

a. Express the original c_i through the c_μ:

$$c_i = \sum_\alpha a_{i\alpha} c_\alpha \,.$$

b. Compute the expectation value of the kinetic energy. Verify that you obtain the known dispersion of a 1D tight binding lattice by choosing the index μ to be the quasi-momentum.

c. First, bring the interaction term into the standard form with creation operators to the left and annihilation operators to the right. Identify the Hartree and the Fock term.

d. What are the variational parameters? Derive the Hartree-Fock equations.

e. Now consider a 3D gas in free space. Compute the following correlation function:

$$\sum_{\sigma\sigma'} \langle FS | \hat{\Psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\Psi}_{\sigma'}^\dagger(\boldsymbol{r'}) \hat{\Psi}_{\sigma'}(\boldsymbol{r'}) \hat{\Psi}_\sigma(\boldsymbol{r}) | FS \rangle$$

where $|FS\rangle$ is the Fermi sea of non-interacting electrons.