Exercise 1 - Fermionic Commutation Relations (2 points)

Consider the Hamiltonian for the H^{2+} molecule in second quantization

$$H = E_0(c_1^\dagger c_1 + c_2^\dagger c_2) - t(c_1^\dagger c_2 + c_2^\dagger c_1), \tag{1}$$

where $c_{1,2}$ are Fermionic annihilation operators for electrons at the proton positions $1, 2$, E_0 is the ground state energy of the system when the two protons are infinitely apart, and t is the hopping of electrons between positions 1 and 2.

(a) Define new Fermionic (A)nti-bonding and (B)onding operators as

$$c_A = \frac{1}{\sqrt{2}}(c_1 - c_2), \tag{2}$$

$$c_B = \frac{1}{\sqrt{2}}(c_1 + c_2), \tag{3}$$

and show that they obey anti-commutation relations;

(b) Prove that in terms of the new variables the Hamiltonian reads

$$H = (E_0 + t)c_A^\dagger c_A + (E_0 - t)c_B^\dagger c_B. \tag{4}$$

Exercise 2 - Tight binding chain in second quantization (4 points)

Consider a $1D$ tight binding model with N sites and periodic boundary conditions. The Hamiltonian is given by

$$H = -t\sum_{n=1}^{N}\left(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n\right) \tag{5}$$

where t is the hopping matrix element between neighbouring sites. $a_n^\dagger$ and a_n are creation- and annihilation operators for (spinless) Fermions at site n.

(a) Show that the particle number operator $N = \sum_n a_n^\dagger\, a_n$ commutes with the Hamiltonian.

(b) Diagonalize the Hamiltonian by means of an appropriate operator transformation.

(c) Check that the new creation and annihilation operators $c_k^\dagger, c_k$ also satisfy canonical anti-commutation relations.

(d) Show that $[n_k, c_{k'}^\dagger] = \delta_{k,k'}c_k^\dagger$ and derive the commutator of H with $c_k^\dagger$.

(e) Using (d), show that if $|E\rangle$ is an eigenstate of H with energy E, then $c_k^\dagger|E\rangle$ is also an eigenstate with energy $E + \epsilon(k)$, where $\epsilon(k)$ is the single particle tight binding dispersion.

Solutions due on: 1 July, 2011