LMU München
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Lehrstuhl für Theoretische Nanophysik
PD Dr. F. Heidrich-Meisner
Jan Stolpp, *Questions: jan.stolpp@physik.uni-muenchen.de*

11. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, January 20, 2017.

Exercise 1: 1D Tight-binding model

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

$$H = -t \sum_{l=1}^{L} \left(c_l^\dagger c_{l+1} + \text{h.c.} \right) .$$

a. Compute the local current operator j_l, which is defined through 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 $J = \sum_{l=1}^{L} j_l$ is the total current.

c. Show that J can be written

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

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

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

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

f. Consider a system with $L = 10$ and $N = 4$ electrons. Write down the ground state in 2^{nd} quantization. What is the ground state energy ?

Exercise 2: The polaron problem – Lang-Firsov transformation

We consider the 1-dimensional Holstein model

$$H = \omega \sum_{j=0}^{L-1} b_j^\dagger b_j + \gamma \sum_{j=0}^{L-1} (b_j^\dagger + b_j) n_j - t \sum_{j,\sigma} \left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.} \right)$$

where b_j ($b_j^\dagger$) and c_j ($c_j^\dagger$) represent annihilation (creation) operators for phonons (which are bosons) and electrons with spin $\sigma = \uparrow, \downarrow$ and $n_j = c_{j,\uparrow}^\dagger c_{j,\uparrow} + c_{j,\downarrow}^\dagger c_{j,\downarrow}$ gives the electron number on site j. The parameters of the model are the phonon frequency ω, the electron-phonon coupling parameter γ and the electron hopping integral t in units of energy.

We consider the strong coupling limit ($t = 0$) and that only one electron is present. We define $H_0 = \sum_j H_{0,j}$ where the on-site Hamiltonian is

$$H_{0,j} = \omega b_j^\dagger b_j + \gamma(b_j^\dagger + b_j)n_j \, .$$

a. Write $H_{0,j}$ in the case where there is no electron on site j. Show that it is diagonal.

b. Write the on-site Hamiltonian for the phonons in the case where one electron is present on site j. What is the ground state energy ?
Hint: $H_{0,j}$ can be diagonalized by a simple shift of the $b^\dagger$.

c. Show that in the case of (b) the ground state can be written as a coherent state

$$|\tilde{0}_j\rangle = e^{-|g|^2/2} e^{g b_j^\dagger} |0_j\rangle \, . \tag{1}$$

d. Compute the average phonon number in that state.

e. What is the ground state of H_0 in the strong coupling limit ?

We now want to find the unitary transformation that diagonalizes H_0. We therefore define

$$|\tilde{0}_j\rangle = e^{S_j}|0_j\rangle \qquad \text{with} \qquad S_j = g(b_j^\dagger - b_j) \tag{2}$$

f. Show that transformation (2) is unitary and that is has the desired effect when one electron sits on site j.

We now define the global Lang-Firsov transformation

$$\tilde{A} = e^S A e^{-S} \qquad \text{with} \qquad S = g\sum_j (b_j^\dagger - b_j)n_j \, . \tag{3}$$

which takes into account that (2) should hold only on sites where one electron sits.

g. Transform the bosonic operators.
Hint: You can use the Baker-Campbell-Hausdorff relation:

$$\tilde{A} = A + [S, A] + \frac{1}{2}[S,[S,A]] + \frac{1}{6}[S,[S,[S,A]]] + \dots \, .$$

h. Transform the fermionic operators.
Hint: You can derive and formally integrate the following equation of motion:

$$\frac{\partial \tilde{A}(\eta)}{\partial \eta} = [S, \tilde{A}(\eta)] \qquad \text{where} \qquad \tilde{A}(\eta) = e^{\eta S} A e^{-\eta S} \, .$$

Note: You can also derive the Baker-Campbell-Hausdorff relation in that way.

i. Show that the commutation relations are preserved, and in particular that $[\tilde{c}_i, \tilde{b_j}] = 0$.

j. Write Hamiltonian H_0 in terms of the transformed operators. Under which condition is it diagonal ?

k. The electron and the phonons constitute a quasi-particle called polaron. Can you guess what the qualitative effect of a finite t will be ?