1 Equations of motion for creation and annihilation operators

Consider non-interacting bosons described by the Hamiltonian

$$\hat{H} = \sum_{k,p} h_{k,p} a_k^\dagger a_p, \tag{1}$$

in the single particle basis $|k\rangle$ of the Hilbert space with $h_{k,p} = \langle k|\underline{h}|p\rangle$.

(a) Let us diagonalize the Hamiltonian $\hat{H}$.

(i) What are the requirements on the single particle matrix $\underline{h}$ for $\hat{H}$ to be self-adjoint?

(ii) Bring the Hamiltonian to diagonal form $\hat{H} = \sum_k \varepsilon_k \tilde{a}_k^\dagger \tilde{a}_k$ diagonalizing $\underline{h}$. What is the relation between the two set of creation and annihilation operators $\langle \tilde{a}_k, \tilde{a}_k^\dagger \rangle$ and $\langle a_k, a_k^\dagger \rangle$? Make sure the set $\langle \tilde{a}_k, \tilde{a}_k^\dagger \rangle$ still satisfies the canonical commutation relations.

> Hint: As you have shown in (i), $\underline{h}$ can be written as $\underline{h} = S^\dagger D S$ with D a diagonal matrix.

(iii) Obtain the ground state of $\hat{H}$ assuming all its eigenvalues are positive, i.e., $\varepsilon_k > 0$.

> Hint: Use that $\tilde{a}_k |\tilde{0}\rangle = 0$.

(b) Compute the annihilation operator in the Heisenberg representation $a_q(t) = e^{i\hat{H}t} a_q e^{-iHt}$ by

(i) solving the equations of motion $i\frac{\partial}{\partial t} a_q(t) = [a_q(t), \hat{H}]$.

(ii) directly using the Baker-Campbell-Hausdorff formula $e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \ldots$ to resolve $a_q(t) = e^{i\hat{H}t} a_q e^{-iHt}$.

> Hint: You can define $[A, B]_m := [A, [A, B]_{m-1}]$ for $m \geq 1$ and $[A, B]_0 = B$ and prove it by induction.

(iii) Calculate $a_q^\dagger(t)$.

(iv) What would change in your previous (i-iii) derivations if a_k were fermionic operators?

(c) Using (b), compute the evolution of the correlation function $\langle 0|a_{k'}(t) a_k^\dagger(0)|0\rangle$ with $a_{k'}|0\rangle = 0$. Evaluate the result for $h_{k,p} = \varepsilon_k \delta_{k,p}$.

2 Non-interacting lattice fermions

Consider fermions hopping on a one-dimensional lattice with L sites and lattice constant a. We work in the grand canonical ensemble and assume periodic boundary conditions:

$$\hat{H} = -J \sum_{l} (c_l^\dagger c_{l+1} + \text{h.c.}) - \mu \sum_{l} c_l^\dagger c_l \tag{2}$$

(a) Diagonalize (2) by a basis transformation to momentum states ($\langle l|k\rangle = L^{-1/2} e^{ikla}$). Your result should have the form

$$\hat{H} = \sum_{k} (\epsilon_k - \mu) c_k^\dagger c_k \tag{3}$$

with ϵ_k the energy dispersion. Provide a sketch of ϵ_k. What values can k have?

(b) In the thermodynamic Limit, $L \longrightarrow \infty$, it is convenient to introduce the density of states (DOS)

$$g(\epsilon) = \int \frac{dk}{2\pi} \delta(\epsilon - \epsilon_k). \tag{4}$$

Calculate $g(\epsilon)$, how does it behave near the edges of the band $\epsilon \sim \pm 2J$?

(c) Compute the expectation value of the total particle number operator $\langle \hat{N} \rangle$ and from that the compressibility $\kappa = \partial \langle \hat{N} \rangle / \partial \mu$ in thermal equilibrium. Give the formulas both for finite L and in the thermodynamic limit.

(d) Evaluate the formulas you derived above numerically and plot $\langle \hat{N} \rangle / L$ and κ / L (i) as a function of μ for $\beta J = 40$ and $L = 6, 8, 10, 400, 402$ and (ii) as a function of βJ for $\mu = 0$ and $L = 6, 8, 10, 400, 402$. Interpret your results. Compare the finite L results to the thermodynamic limit. How large has L to be, to mimic $L = \infty$? What is special about system sizes ($L \mod 4) = 0$ when $\mu = 0$.