1 Bosons

1.a Hamiltonian diagonalization

i. $h = h^\dagger = S^\dagger D S$ with $D = \mathrm{diag}(\varepsilon_1, \varepsilon_2, \ldots)$ and S orthogonal

ii. $\hat{H} = \boldsymbol{a}^\dagger h \boldsymbol{a} = (S\boldsymbol{a})^\dagger D (S\boldsymbol{a}) = \tilde{\boldsymbol{a}}^\dagger D \tilde{\boldsymbol{a}}$ with $\tilde{a}_i = S_{ij} a_j$, $\tilde{a}_i^\dagger = S_{ij}^\dagger a_j^\dagger$

We can check the canonicity of a transformation by direct substitution. Taking into account the known commutation relations and orthogonality of S

$$[a_i, a_j^\dagger] = \delta_{ij}, \qquad [a_i, a_j] = 0, \qquad s_{ik} S_{kj}^\dagger = \delta_{ij},$$

we could check

$$[\tilde{a}_i,\, \tilde{a}_j^\dagger] = \left[S_{ki} a_i,\, a_j^\dagger S_{jp}^\dagger\right] = S_{ki}(\delta_{ij} + a_j^\dagger a_i) S_{jp}^\dagger - a_j^\dagger S_{jp}^\dagger S_{ki} a_i = S_{ki} \delta_{ij} S_{jp}^\dagger + (S_{ki} S_{jp}^\dagger - S_{jp}^\dagger S_{ki}) a_j^\dagger a_i = \delta_{kp}.$$

Similarly $[\tilde{a}_i,\, \tilde{a}_j]$ will be reduced to 0.

iii. Since $\varepsilon_k > 0$ ground state will be reduced to the absence of excitations, namely $|0\rangle$.

1.b Heisenberg representation

i. Let's start with calculating the commutator in diagonal case

$$[a_q,\, a_k^\dagger a_k] = (\delta_{qk} + a_k^\dagger a_q) a_k - a_k^\dagger a_k a_q = a_q, \tag{1}$$

which means the equation of motion can be obtained in the form

$$i\partial_t a(t) = \left[a_q(t),\, \hat{H}\right] = \varepsilon_q a_q(t), \qquad \Rightarrow \qquad a_q(t) = e^{-i\varepsilon_q t} a_q(0).$$

In the off-diagonal case

$$a_q(t) = S_{qk}^\dagger \tilde{a}_k(t) = \sum_k S_{qk}^\dagger e^{-i\varepsilon_k t} \tilde{a}_k(0). \tag{2}$$

ii. Notice, that

$$\left[\hat{H}, a_q\right] = -\varepsilon_q a_q, \qquad \left[\hat{H}, \left[\hat{H}, a_q\right]\right] = (-\varepsilon_q)^2 a_q, \qquad \ldots \qquad \Rightarrow \qquad \left[\hat{H},\, a_q\right]_m = (-\varepsilon_q)^m a_q$$

Using the Baker-Campbell-Hausdorff formula

$$a_q(t) = e^{i\hat{H}t} a_q(0) e^{i-\hat{H}t} = a_q + (-i\varepsilon_q t) a_q + \ldots + \frac{(-i\varepsilon_q t)^m}{m!} a_q + \ldots = e^{-i\varepsilon_q t} a_q(0),$$

which is in accordance with the previous result.

iii. $a_q^\dagger(t) = a_q(t)^\dagger = e^{i\varepsilon_q t} a_q^\dagger(0)$

iv. Expression (1) will not change for fermions, so evolution will occur according to the same law.

1.c Correlation function

Let's consider the correlation function

$$f_{qk}(t) = \langle 0 | a_q(t) a_k^\dagger(0) | 0 \rangle.$$

Using (2), we get

$$f_{qk}(t) = S_{qp}^\dagger S_{kj} e^{-i\varepsilon_p t} \delta_{pj} = \sum_j S_{qj}^\dagger S_{kj} e^{-i\varepsilon_j t},$$

and with $h_{qk} = \delta_{qk} \varepsilon_k$

$$f_{qk}(t) = \delta_{qk} e^{-i\varepsilon_q t}.$$

2 Fermions

We work in the grand canonical ensemble and assume periodic boundary conditions:

$$\hat{H} = -J \sum_l (c_l^\dagger c_{l+1} + \mathrm{h.c.}) - \mu \sum_j c_j^\dagger c_j.$$

(a) Let's do a discrete Fourier transform

$$|j\rangle = \frac{1}{\sqrt{L}} \sum_{n=0}^{N-1} e^{-i\frac{2\pi}{L}nj} |n\rangle ,$$

which corresponds to impulses $k = \frac{2\pi}{La}n$. Using the ortonality of the chosen system of functions, we obtain

$$\hat{H} = \sum_{n=0}^{L-1} (\varepsilon_n - \mu) c_n^\dagger c_n, \qquad \varepsilon_n = -2J\cos\left(\tfrac{2\pi}{L}n\right) = -2J\cos(ka).$$

(b) In the thermodynamic limit $L \to \infty$ the Hamiltonian can be rewritten as

$$\hat{H} = \int_0^{2\pi} \frac{dk}{2\pi} (\varepsilon_k - \mu) c_k^\dagger c_k, \qquad \varepsilon_k = -2J\cos(ka).$$

So we could introduce DOS (density of states)

$$g(\varepsilon) = \int \frac{dk}{2\pi} \delta(\varepsilon - \varepsilon_k) \propto \int \frac{d\varepsilon_k}{\sqrt{(2J)^2 - \varepsilon_k^2}} \delta(\varepsilon - \varepsilon_k) = \frac{1}{\sqrt{4J^2 - \varepsilon^2}},$$

with characteristic behavior $g(\varepsilon \to \pm 2J) \to \infty$.

(c) The population of the state can be written as

$$\bar{n}_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1},$$

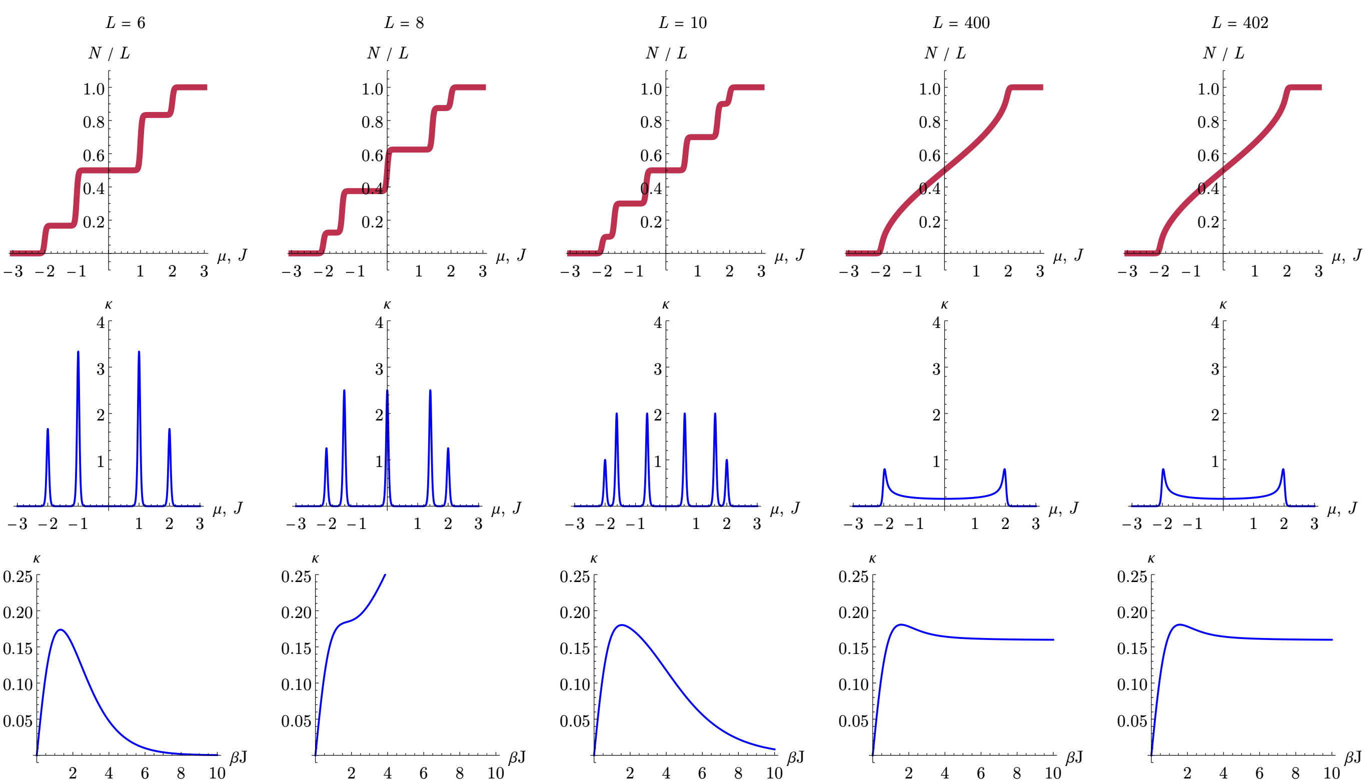
Substituting the energy value, we find

$$\tfrac{1}{L}\langle N(\mu)\rangle = \frac{1}{L} \sum_k \frac{1}{\exp\left(-2\beta J\cos(ka) - \beta\mu\right)},$$

And, rewriting through the density of states

$$\tfrac{1}{L}\langle N(\mu)\rangle = \int_{-2J}^{2J} \frac{g(\varepsilon)\, d\varepsilon}{e^{\beta(\varepsilon - \mu)} + 1}.$$

(d) For $\beta J = 40$ let's plot $\langle \hat{N}\rangle(\mu)$ and $\kappa = \partial_\mu \langle \hat{N}\rangle$. For a small L, characteristic steps are noticeable, corresponding to the population of a new state.



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