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Quantum Many-Body Systems

7. Exercise Sheet

20 Generating functional for time-ordered correlation functions of the fermionic oscillator – Operator approach

In this exercise, we will compute the generating functional of a fermionic harmonic oscillator (equivalent to a fermionic single mode system). The Hamiltonian operator that defines such a system is given by

$$\hat{H}_0 = \hbar\omega_0\big(\hat{c}^\dagger\hat{c} - \frac{1}{2}\big), \tag{20.1}$$

where the annihilation and creation operators obey the anti-commutation relations $[\hat{c},\hat{c}]_+ = [\hat{c}^\dagger,\hat{c}^\dagger]_+ = 0$, $[\hat{c},\hat{c}^\dagger]_+ = 1$. Note that the first two relations also imply that $\hat{c}^2 = (\hat{c}^\dagger)^2 = 0$. From such identities and the remaining anti-commutation relation, it is trivial to show that the particle number operator $\hat{n} = \hat{c}^\dagger\hat{c}$ satisfies the equation $\hat{n}^2 = \hat{n}$ and thus that such operator has two possible eigenvalues, namely 0 or 1 (the Hilbert space that describes the problem is thus two-dimensional), with the corresponding eigenstates being designated by $|0\rangle$ and $|1\rangle$. The Hamiltonian $\hat{H}_0$ is diagonal in such states, with eigenvalues $\hat{H}_0|0\rangle = -\frac{\hbar\omega_0}{2}|0\rangle$, $\hat{H}_0|1\rangle = \frac{\hbar\omega_0}{2}|1\rangle$.

(a) Show that $\hat{n}^2 = \hat{n}$
(2 points)

(b) Show that $|1\rangle = \hat{c}^\dagger|0\rangle$ and that $|0\rangle = \hat{c}|1\rangle$.
(2 points)
Hint: what is $\hat{c}\hat{c}^\dagger$?

(c) Show that the partition function $Z_\beta = \mathrm{Tr}\big(e^{-\beta \hat{H}_0}\big)$ is given by $Z_\beta = 2\cosh(\beta\hbar\omega_0/2)$.
(2 points)
Hint: Compute the trace in the eigenbasis of the Hamiltonian.

(d) From the expression for the free energy of such a system $F(T) = -k_B T \ln Z_\beta$, compute the entropy $S(T) = \frac{dF}{dT}$ and show that the expression obtained satisfies the third law of thermodynamics.
(2 points)

(e) The annihilation and creation operators are given in the Heisenberg representation by

$$\hat{c}(t) = e^{i\hat{H}_0 t/\hbar}\hat{c}e^{-i\hat{H}_0 t/\hbar}, \tag{20.2}$$

$$\hat{c}^\dagger(t) = e^{i\hat{H}_0 t/\hbar}\hat{c}^\dagger e^{-i\hat{H}_0 t/\hbar}. \tag{20.3}$$

Show that these operators are related to $\hat{c}$ and $\hat{c}^\dagger$ by

$$\hat{c}(t) = \hat{c}e^{-i\omega_0 t}, \tag{20.4}$$

$$\hat{c}^\dagger(t) = \hat{c}^\dagger e^{i\omega_0 t}. \tag{20.5}$$

(4 points)
Hint: Have a look at the solution of exercise **6(a)** and adapt it accordingly.

(f) Consider the more general case in which the Hamiltonian is given, in the Schrödinger picture, by $\hat{H}(t) = \hat{H}_0 + \hat{H}_I(t)$, with $\hat{H}_I(t) = -[\bar{\eta}(t)\hat{c} + \hat{c}^\dagger\eta(t)]$, where $\eta(t)$ and $\bar{\eta}(t)$ are Grassmann fields that *anti-commute* with each other and with the annihilation and creation operators $\hat{c}$ and $\hat{c}^\dagger$. In other words, for arbitrary times t and u, $[\eta(t), \eta(u)]_+ = 0$, $[\bar{\eta}(t), \bar{\eta}(u)]_+ = 0$, $[\eta(t), \bar{\eta}(u)]_+ = 0$, and $[\eta(t), \hat{c}]_+ = 0$, $[\eta(t), \hat{c}^\dagger]_+ = 0$, $[\bar{\eta}(t), \hat{c}]_+ = 0$, $[\bar{\eta}(t), \hat{c}^\dagger]_+ = 0$. Moreover, these Grassmann variables commute with any *c-number*.

The generating functional of the correlation functions of the annihilation and creation operators is defined as

$$\mathcal{Z}[\eta(t), \bar{\eta}(t)] = \frac{1}{Z_\beta}\mathrm{Tr}\Big(e^{-\beta\hat{H}_0} T e^{-\frac{i}{\hbar}\int_0^T dt\, \hat{H}_I^{\mathrm{int}}(t)}\Big), \tag{20.6}$$

where $\hat{H}_I^{\mathrm{int}}(t) = e^{i\hat{H}_0 t/\hbar}\hat{H}_I(t)e^{-i\hat{H}_0 t/\hbar}$ is the interaction Hamiltonian in the interaction representation. Show that it can be written as

$$\mathcal{Z}[\eta(t), \bar{\eta}(t)] = \frac{1}{Z_\beta}\mathrm{Tr}\Big(e^{-\beta\hat{H}_0} e^{-\frac{i}{\hbar}\int_0^T dt\, \hat{H}_I^{\mathrm{int}}(t)}\Big)\, e^{-\frac{1}{2\hbar^2}\int_)^T dt\, \int_)^t du\, [\hat{H}_I^{\mathrm{int}}(t), \hat{H}_I^{\mathrm{int}}(u)]_-}. \tag{20.7}$$

(2 points)
Hint: Check that $[\hat{H}_I^{\mathrm{int}}(t), \hat{H}_I^{\mathrm{int}}(u)]_-$ commutes with $\hat{H}_I^{\mathrm{int}}(t')$ for arbitrary t, u, and t' and then apply (??).

(g) Using the time-evolution of the annihilation and creation operators in the interaction representation, show that one can write $\mathcal{Z}[\eta(t), \bar{\eta}(t)]$ as

$$\mathcal{Z}[\eta(t), \bar{\eta}(t)] = \frac{1}{Z_\beta} \mathrm{Tr}\Big(e^{-\beta \hat{H}_0} e^{\hat{c}^\dagger \gamma - \bar{\gamma}\hat{c}}\Big)\, e^{-\frac{1}{2\hbar^2}\int_)^T dt\, \int_)^t du\, [\hat{H}_I^{\mathrm{int}}(t), \hat{H}_I^{\mathrm{int}}(u)]_-}, \tag{20.8}$$

where $\gamma = \frac{i}{\hbar}\int_0^T dt\, e^{i\omega_0 t}\eta(t)$ and $\bar{\gamma} = -\frac{i}{\hbar}\int_0^T dt\, e^{-i\omega_0 t}\bar{\eta}(t)$ are Grassmann variables.
(2 points)

(h) Show that

$$\frac{1}{Z_\beta}\mathrm{Tr}\Big(e^{-\beta\hat{H}_0} e^{\hat{c}^\dagger\gamma - \bar{\gamma}\hat{c}}\Big) = (1 + e^{-\beta\hbar\omega_0})^{-1} \sum_{n=0}^{1} e^{-\beta\hbar\omega_0 n} \langle n | e^{\hat{c}^\dagger\gamma - \bar{\gamma}\hat{c}} | n \rangle. \tag{20.9}$$

(2 points)

(i) Show that

$$\langle 0 | e^{\hat{c}^\dagger\gamma - \bar{\gamma}\hat{c}} | 0 \rangle = 1 - \frac{1}{2}\bar{\gamma}\gamma \tag{20.10}$$

$$\langle 1 | e^{\hat{c}^\dagger\gamma - \bar{\gamma}\hat{c}} | 1 \rangle = 1 + \frac{1}{2}\bar{\gamma}\gamma \tag{20.11}$$

(3 points)
Hint: Taking into account that γ and $\bar{\gamma}$ are Grassmann variables and that $\hat{c}$ and $\hat{c}^\dagger$ are fermion operators, expand the exponentials on the left-hand side of equation (20.10) and (20.11) as a power series in these variables.

(j) Substitute (20.9) in (20.8) and, taking into account (20.10) and (20.11), with γ and $\bar{\gamma}$ given by their definition above, show that

$$\mathcal{Z}[\eta(t), \bar{\eta}(t)] = e^{-\frac{1}{\hbar^2}\int_0^T dt\, \int_0^T du\, \bar{\eta}(t)\eta(u)\tilde{G}(t-u)}, \tag{20.12}$$

where $\tilde{G}(t-u) = \frac{1}{2}e^{-i\omega_0(t-u)}[\tanh(\beta\hbar\omega_0/2) + \Theta(t-u) - \Theta(u-t)]$.
(3 points)
Hint: $e^{\frac{1}{2}\tanh(\beta\omega_0/2)\bar{\gamma}\gamma} = 1 - \frac{1}{2}\tanh(\beta\omega_0/2)\bar{\gamma}\gamma$.

(k) Finally, by performing the functional derivatives with respect to $\eta(t)$ and $\bar{\eta}(t)$, show that $\langle T\{\hat{c}(t_1)\hat{c}^\dagger(t_2)\}\rangle = \tilde{G}(t_1 - t_2)$.
(2 points)

21 Bogoliubov transformation for a fermion two-mode problem – Generating functional

Consider a Hamiltonian $\hat{H}_0$ that describes a fermion two-mode problem in which hopping between the two modes can occur

$$\hat{H}_0 = \hbar\omega_L \hat{c}_L^\dagger \hat{c}_L + \hbar\omega_R \hat{c}_R^\dagger \hat{c}_R - t(\hat{c}_L^\dagger \hat{c}_R + \hat{c}_R^\dagger \hat{c}_L), \tag{21.1}$$

where t is a real quantity. Assume for definiteness that $\omega_L > \omega_R$ (if the opposite is true, simply interchange L and R). The annihilation and creation operators satisfy the canonical anti-commutation relations $[\hat{c}_\mu, \hat{c}_\nu]_+ = 0$, $[\hat{c}_\mu^\dagger, \hat{c}_\nu^\dagger]_+ = 0$, and $[\hat{c}_\mu, \hat{c}_\nu^\dagger]_+ = \delta_{\mu,\nu}$, where $\mu, \nu = L, R$.

(a) Define the operators $\hat{c}_+$,

(b) Define the operators $\hat{c}_+$, $\hat{c}_+^\dagger$, $\hat{c}_-$, $\hat{c}_-^\dagger$ through the following relations

$$\hat{c}_L = \cos\theta \hat{c}_+ + \sin\theta \hat{c}_-, \tag{21.2}$$

$$\hat{c}_L = -\sin\theta \hat{c}_+ + \cos\theta \hat{c}_-, \tag{21.3}$$

where θ is a real number. The hermitian conjugate of these equations give us the relation between the operators $\hat{c}_L^\dagger$, $\hat{c}_R^\dagger$ and $\hat{c}_+^\dagger$, $\hat{c}_-^\dagger$.

Show that the new operators $\hat{c}_+$, $\hat{c}_+^\dagger$, $\hat{c}_-$, $\hat{c}_-^\dagger$ also obey canonical anti-commutation relations among themselves.
(2 points)
Hint: Express the new operators in terms of the old ones and use the known anti-commutation relations.

(c) Show that it one chooses θ such that $\tan(2\theta) = \frac{2t}{\hbar(\omega_L - \omega_R)}$, one can write $\hat{H}_0$ in terms of the operators $\hat{c}_+$, $\hat{c}_+^\dagger$, $\hat{c}_-$, $\hat{c}_-^\dagger$ as

$$\hat{H}_0 = \hbar\omega_+ \hat{c}_+^\dagger \hat{c}_+ + \hbar\omega_- \hat{c}_-^\dagger \hat{c}_-, \tag{21.4}$$

i.e., $\hat{H}_0$ is diagonal in the new set of operators. The eigenfrequencies $\omega_\pm$ are given by $\omega_\pm = \frac{1}{2}[(\omega_L + \omega_R) \pm \sqrt{(\omega_L - \omega_R)^2 + 4t^2}]$. Note that apart from an overall constant, $\hat{H}_0$ can be written as the sum of two independent fermionic harmonic oscillators.
(4 points)
Hint: Substitute (21.2),(**??**) and their complex conjugates in (21.1) and ask yourself what is the condition that θ must obey in order that the cross terms involving $\hat{c}_+^\dagger \hat{c}_-$ and $\hat{c}_-^\dagger \hat{c}_+$ ar exactly zero.

(d) Show that the partition function $Z_\beta = \mathrm{Tr}\big(e^{-\beta \hat{H}_0}\big)$ is given by

$$Z_\beta = Z_\beta^+ Z_\beta^- = 4\cosh(\beta\omega_+/2)\cosh(\beta\omega_-/2)e^{-\beta\hbar(\omega_+ + \omega_-)/2}, \tag{21.5}$$

in which $Z_\beta^\pm$ are the individual partition functions of the independent modes + and −.
(2 points)
Hint: Write the trace in terms of the eigenstates that diagonalise the Hamiltonian *i.e.* the eigenstates of the operator $\hat{n}_+ = \hat{c}_+^\dagger \hat{c}_+$ and $\hat{n}_- = \hat{c}_-^\dagger \hat{c}_-$.

(e) Consider the more general case in which the Hamiltonian is given, in the Schrödinger picture, by $\hat{H}(t) = \hat{H}_0 + \hat{H}_I(t)$, with $\hat{H}_I(t) = -\sum_\mu [\bar{\eta}(t)\hat{c}_\mu + \hat{c}_\mu^\dagger \eta_\mu(t)]$, where $\eta_\mu(t)$ and $\bar{\eta}_\mu(t)$ are Grassmann fields that *anti-commute* with each other and with the annihilation and creation operators $\hat{c}_\mu$ and $\hat{c}_\mu^\dagger$. In other words, for arbitrary times t and u, $[\eta(t), \eta(u)]_+ = 0$, $[\bar{\eta}(t), \bar{\eta}(u)]_+ = 0$, $[\eta(t), \bar{\eta}(u)]_+ = 0$, and $[\eta(t), \hat{c}]_+ = 0$, $[\eta(t), \hat{c}^\dagger]_+ = 0$, $[\bar{\eta}(t), \hat{c}]_+ = 0$, $[\bar{\eta}(t), \hat{c}^\dagger]_+ = 0$. Moreover, these Grassmann variables commute with any *c-number*.

The generating functional of the correlation functions of the annihilation and creation operators is defined as

$$\mathcal{Z}[\eta_L(t), \eta_R(t), \bar{\eta}_L(t), \bar{\eta}_R(t)] = \frac{1}{Z_\beta} \mathrm{Tr}\Big(e^{-\beta \hat{H}_0} T e^{-\frac{i}{\hbar}\int_0^T dt\, \hat{H}_I^{\mathrm{int}}(t)}\Big), \tag{21.6}$$

where $\hat{H}_I^{\mathrm{int}}(t) = e^{i\hat{H}_0 t/\hbar} \hat{H}_I(t) e^{-i\hat{H}_0 t/\hbar}$ is the interaction Hamiltonian in the interaction representation. Show that it can be written as ($\mu = L, R$)

$$\mathcal{Z}[\eta_L(t), \eta_R(t), \bar{\eta}_L(t), \bar{\eta}_R(t)] = \mathcal{Z}[\eta_+(t), \bar{\eta}_+(t)]\mathcal{Z}[\eta_-(t), \bar{\eta}_-(t)], \tag{21.7}$$

where the Grassmann source fields $\eta_\pm(t)$ are given in terms of the original fields by

$$\eta_+(t) = \cos\theta \eta_L(t) - \sin\theta \eta_R(t), \tag{21.8}$$

$$\eta_-(t) = \sin\theta \eta_L(t) + \cos\theta \eta_R(t), \tag{21.9}$$

with analogous equations for the conjugated fields $\bar{\eta}_\pm(t)$. The generating functionals $\mathcal{Z}_\pm[\eta_\pm(t), \bar{\eta}_\pm(t)]$ are given by

$$\mathcal{Z}_\pm[\eta_\pm(t), \bar{\eta}_\pm(t)] = e^{-\frac{1}{\hbar^2}\int_0^T dt \int_0^T du\, \bar{\eta}_\pm(t)\eta_\pm(u)\tilde{G}_\pm(t-u)}, \tag{21.10}$$

where $\tilde{G}_\pm(t-u) = \frac{1}{2} e^{-i\omega_\pm(t-u)}[\tanh(\beta\hbar\omega_\pm/2) + \Theta(t-u) - \Theta(u-t)]$.
(5 points)
Hint: Express the operator $\hat{H}_I(t)$ in terms of the annihilation and creation operators $\hat{c}_+$, $\hat{c}_+^\dagger$, $\hat{c}_-$, $\hat{c}_-^\dagger$. Show that $\hat{H}_0 = \hat{H}_{0+} + \hat{H}_{0-}$ with $[\hat{H}_{0+}, \hat{H}_{0-}]_- = 0$ and because of that, one can write $\hat{H}_0 = \hat{H}_{I+}^{\mathrm{int}}(t) + \hat{H}_{I-}^{\mathrm{int}}(t)$ such that $\hat{H}_{I+}^{\mathrm{int}}(t)\hat{H}_{I-}^{\mathrm{int}}(u)]_- = 0$ for arbitrary t, u. Once this is done, all you need is to apply the single mode result obtained in **20(j)**.

(f) By writing the functional (21.7) in terms of the original sources $\eta_L(t)$, $\bar{\eta}_L(t)$, $\eta_R(t)$, $\bar{\eta}_R(t)$, show that one has

$$\langle T\{\hat{c}_L(t_1)\hat{c}_L^\dagger(t_2)\}\rangle = \cos^2\theta \tilde{G}_+(t_1 - t_2) + \sin^2\theta \tilde{G}_-(t_1 - t_2), \tag{21.11}$$

$$\langle T\{\hat{c}_R(t_1)\hat{c}_R^\dagger(t_2)\}\rangle = \sin^2\theta \tilde{G}_+(t_1 - t_2) + \cos^2\theta \tilde{G}_-(t_1 - t_2), \tag{21.12}$$

$$\langle T\{\hat{c}_L(t_1)\hat{c}_R^\dagger(t_2)\}\rangle = -\frac{1}{2}\sin(2\theta)[\tilde{G}_+(t_1 - t_2) + \tilde{G}_-(t_1 - t_2)], \tag{21.13}$$

$$\langle T\{\hat{c}_R(t_1)\hat{c}_L^\dagger(t_2)\}\rangle = -\frac{1}{2}\sin(2\theta)[\tilde{G}_+(t_1 - t_2) + \tilde{G}_-(t_1 - t_2)]. \tag{21.14}$$

(4 points)