ZHEJIANG UNIVERSITY
Center for Correlated Matter
Stefan Kirchner
kirchner@correlated-matter.com

Quantum Many-Body Systems

1. Exercise Sheet

Mini-Review

Before we ask you to perform any calculations, let us first briefly review some notions of second quantisation. The Hilbert space of a system composed of N (for the moment distinguishable) sub-systems is given by the tensor product of individual Hilbert spaces

$$\mathcal{H}_N = \mathcal{H}_{S_1} \otimes \mathcal{H}_{S_2} \otimes \ldots \otimes \mathcal{H}_{S_N}. \tag{0.1}$$

A complete basis for this space is given by the tensor product

$$\{|\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle\}, \tag{0.2}$$

where $\{|\alpha_{i_n}\rangle\}$ is a complete set of orthonormal vectors that span the Hilbert space of the system n.
The closure relation for $\mathcal{H}$ is given by

$$\begin{aligned}\sum_{i_1,i_2,\ldots,i_N} |\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle\langle\alpha_{i_1}| \otimes \langle\alpha_{i_2}| \otimes \ldots \otimes \langle\alpha_{i_N}| = \\ \Big(\sum_{i_1} |\alpha_{i_1}\rangle\langle\alpha_{i_1}|\Big) \ldots \Big(\sum_{i_N} |\alpha_{i_N}\rangle\langle\alpha_{i_N}|\Big)\& = \\ \mathbf{1}_1 \otimes \ldots \otimes \mathbf{1}_N.\end{aligned} \tag{0.3}$$

As short-hand for the tensor product above, we will write

$$|\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_N}\rangle = |\alpha_{i_1}\rangle \otimes |\alpha_{i_2}\rangle \otimes \ldots \otimes |\alpha_{i_N}\rangle. \tag{0.4}$$

In the case of indistinguishable particles, it can be shown in relativistic quantum field theory that, in three dimensions, the joint wave-function of such a system can have one of two possible symmetries under the interchange of two particles:

- it is symmetric in the case of particles of integer spin (bosons), or
- it is anti-symmetric in the case of particles of half-integer spin (fermions).

This so-called spin-statistics theorem has to be accepted at our level as a fact of life and moreover, it does not hold in two dimensions (the particles with strange interchange properties that are found in certain two-dimensional electron gases are called anyons). If one takes this observation into account, one concludes that the (un-normalised) wave-function of such systems of indistinguishable particles has to have the form

$$\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_P \xi^{\sigma(P)} \big|\alpha_{P(1)}, \alpha_{P(2)}, \ldots, \alpha_{P(N)}\big), \tag{0.5}$$

where P represents one of the $N!$ possible permutations of the numbers $\{1, 2, \ldots, N\}$ and $\xi = \pm 1$, having the plus sign for bosons and the minus sign for fermions. The function $\sigma(P)$ is the order of the permutation, i.e. the number, modulo 2, of transpositions of two numbers at a time that is necessary to perform in order to bring the N numbers in that permutation to their natural order $1 < 2 < ... < N$. It can be shown, e.g. by induction, that a given permutation can always be decomposed into a product of transpositions. Such a decomposition is not unique, but the number of transpositions necessary is either even or odd and thus the order of a permutation is a well-defined quantity. Using the orthonormal character of the basis of each individual particle, it is easy to convince oneself that a second state $\big|\alpha'_1, \alpha'_2, \ldots, \alpha'_N\big\}$ is orthogonal to $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ unless the set of the α's constitute a permutation of $\alpha_1, \ldots, \alpha_N$. Thus, one has

$$\big\{\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha'_1, \alpha'_2, \ldots, \alpha'_N\big\} = \sum_P \prod_i^N \delta_{\alpha_i, \alpha'_{P(i)}} \parallel \big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} \parallel^2 , \tag{0.6}$$

where only one of the terms in the summation above is non-zero. Applying the definition given in (0.5), one obtains for the square of the norm of $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ the result

$$\begin{aligned}
&\big\{\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} \\
&= \frac{1}{N!}\sum_{P,P'} \xi^{\sigma(P)+\sigma(P')} \big(\alpha_{P'(1)}, \alpha_{P'(2)}, \ldots, \alpha_{P'(N)}\big|\alpha_{P(1)}, \alpha_{P(2)}, \ldots, \alpha_{P(N)}\big) \qquad (0.7)\\
&= \frac{1}{N!}\sum_{P,P'} \xi^{\sigma(P)+\sigma(P')} \big(\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_{P'.P^{-1}(1)}, \alpha_{P.P'^{-1}(2)}, \ldots, \alpha_{P.P'^{-1}(N)}\big)\\
&= \sum_{\tilde{P}} \xi^{\sigma(\tilde{P})} \Big(\alpha_1, \alpha_2, \ldots, \alpha_N\big|\alpha_{\tilde{P}(1)}, \alpha_{\tilde{P}(2)}, \ldots, \alpha_{\tilde{P}(N)}\Big)\\
&= \sum_{\tilde{P}} \xi^{\sigma(\tilde{P})} \langle\alpha_1|\alpha_{\tilde{P}(1)}\rangle\langle\alpha_2|\alpha_{\tilde{P}(2)}\rangle \ldots \langle\alpha_N|\alpha_{\tilde{P}(N)}\rangle\\
&= \begin{cases} \det\left[\langle\alpha_i|\alpha_j\rangle\right], & \text{for fermions}\\ \operatorname{per}\left[\langle\alpha_i|\alpha_j\rangle\right], & \text{for bosons}\end{cases}, \qquad (0.8)
\end{aligned}$$

where we have reordered the terms in the summation over P' on going from the first to the second line of this equation, and have reordered the summation over P such that it is performed over the permutation $\tilde{P} = P \cdot P'^{-1}$, with $\sigma(\tilde{P}) = \sigma(P) + \sigma(P')$, on going from the second to the third line. The summation over P' can then be performed and gives a simple factor $N!$. Since the vectors are supposed to be orthonormal, the determinant in (0.7) is equal to one if all α_i's are different and zero otherwise. The calculation of the permanent is a bit more involved but is nevertheless trivial.
Suppose there are k different αs, $\alpha_1, \ldots, \alpha_k$, such that $n_{\alpha_1} + \ldots + n_{\alpha_k} = N$. Since the wave-function for bosons is symmetric, one can reorder the αs that are equal in a contiguous fashion, *i.e.* we can write the wave-function as $|\alpha_1, \ldots, \alpha_1, \alpha_2, \ldots, \alpha_2, \ldots, \alpha_k, \ldots, \alpha_k\}$, where α_1 appears n_{α_1} times, etc. From this construction, it is now easy to see that the permanent that we wish to compute is that of a block-diagonal matrix in which each block is solely constituted of 1s. Since the permanent of a matrix that is composed of 1s is equal to the factorial of its dimension and the dimensions of each block matrix are $n_{\alpha_1}, \ldots, n_{\alpha_k}$, one sees that $\operatorname{per}[\langle\alpha_i|\alpha_j\rangle] = \prod_{i=1}^k n_{\alpha_i}!$.

One now defines the creation operator through the relation

$$\big|\mu, \alpha_1, \ldots, \alpha_N\big\} = c_\mu^\dagger\big|\alpha_1, \ldots, \alpha_N\big\}, \qquad (0.9)$$

i.e., this operator adds a particle in state μ to the many-particle state. If one wishes to add two particles to the system, to states μ and ν ($\mu \neq \nu$), say, one may apply first $c_\mu^\dagger$ and then $c_\nu^\dagger$, obtaining $|\mu, \nu, \alpha_1, \ldots, \alpha_N\}$ or the other way around, obtaining instead $|\nu, \mu, \alpha_1, \ldots, \alpha_N\}$. However, since $|\nu, \mu, \alpha_1, \ldots, \alpha_N\} = \xi|\mu, \nu, \alpha_1, \ldots, \alpha_N\}$, one concludes that

$$c_\mu^\dagger c_\nu^\dagger - \xi c_\nu^\dagger c_\mu^\dagger = 0, \qquad (0.10)$$

i.e. the creation operators commute in the case of bosons, but they anti-commute in the case of fermions. The same rule has to apply to the adjoint operators c_μ and c_ν, as results from considering the adjoint of the above equation.
It follows from (0.9) that

$$\big\{\alpha_1, \alpha_2, \ldots, \alpha_N \big| c_\mu \big| \mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} = \| \, \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} \, \|^2 . \tag{0.11}$$

Since the above scalar product is non-zero (in the case of fermions, one assumes that μ is different from all the αs), this implies that $c_\mu \alpha_1, \ldots, \alpha_N = C(\mu, \alpha_1, \ldots, \alpha_N)\big|\alpha_1, \ldots, \alpha_N\big\}$, with

$$C(\mu, \alpha_1, \ldots, \alpha_N) = \frac{\| \, \big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} \, \|^2}{\| \, \big|\alpha_1, \alpha_2, \ldots, \alpha_N \big\} \, \|^2} = n_\mu(\mu, \alpha_1, \alpha_2, \ldots, \alpha_N), \tag{0.12}$$

where $n_\nu(\mu, \alpha_1, \alpha_2, \ldots, \alpha_N)$ is the number of times the index μ appears in the series $\mu, \alpha_1, \alpha_2, \ldots, \alpha_N$.

In the general case of a series of labels $\alpha_1, \ldots, \alpha_N$, in which the first is not necessarily equal to μ, the rule that generalizes this result and takes into account the symmetry of the wave-function is

$$c_\mu \big| \mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} = \sum_{i=1}^{N} \xi^{i-1} \delta_{\mu, \alpha_i} \big| \alpha_1, \ldots, \alpha_{i-1}, \alpha_{i+1}, \ldots, \alpha_N \big\}. \tag{0.13}$$

Note in particular that the state with no particles, the vacuum, is annihilated by each one of the operators c_μ, *i.e.* $c_\mu|0\rangle = 0$. Using (0.13), we now have

$$\big[c_\mu c_\nu^\dagger - \xi c_\nu^\dagger c_\mu\big] \big| \mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\} = \delta_{\mu,\nu} \big| \mu, \alpha_1, \alpha_2, \ldots, \alpha_N \big\}. \tag{0.14}$$

Since the state $\big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ is arbitrary, we conclude that

$$\big[c_\mu c_\nu^\dagger\big]_{-\xi} = \delta_{\mu,\nu}, \tag{0.15}$$

i.e. these operators also obey commutation ($\xi = 1$) or anti-commutation ($\xi = -1$) relations among themselves, but with a commutator or anti-commutator that is non-zero, unlike above.
Note that the state that arises from the normalisation of $\big|\mu, \alpha_1, \alpha_2, \ldots, \alpha_N\big\} = c_{\alpha_1}^\dagger \ldots c_{\alpha_N}^\dagger |0\rangle$ can be written, up to a reordering of the operators, as

$$\big| n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k} \big\rangle = \frac{(c_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \cdots \frac{(c_{\alpha_k}^\dagger)^{n_{\alpha_k}}}{\sqrt{n_{\alpha_k}!}} \big|0\big\rangle, \tag{0.16}$$

where solely the occupation number of each mode is displayed. This form is valid both for bosons and fermions (but in the latter case, $n_\alpha = 0, 1$). It is relatively simple to show from the closure relation (0.3), after symmetrisation or anti-symmetrisation, that this set of states obeys the closure relation

$$\sum_{\{n_\alpha\}} \big| n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k} \big\rangle \big\langle n_{\alpha_1}, n_{\alpha_2}, \ldots, n_{\alpha_k} \big| = \mathcal{P}_\xi, \tag{0.17}$$

where the sum is over all possible particle numbers on all possible modes and

$$\mathcal{P}_\xi = \sum_N \frac{1}{N!} \sum_{\alpha_1,\ldots,\alpha_N} \sum_P \xi^{\sigma(P)} \big|\alpha_1, \alpha_2, \ldots, \alpha_N\big)\big(\mu, \alpha_{P_1}, \alpha_{P_2}, \ldots, \alpha_{P_N}\big| \tag{0.18}$$

is the symmetrisation or anti-symmetrisation operator of the wave-functions.

One last note on a change of basis in second quantisation. It is known from elementary quantum mechanics that if $\{|\alpha_i\rangle\}$ is a complete basis of the one-particle Hilbert space and $\{|\beta_j\rangle\}$ is another complete basis, the two are related by an unitary transformation, *i.e.* $|\beta_j\rangle = \sum_i |\alpha_i\rangle U^\dagger_{ij}$, where $U_{ji} = \langle\beta_j|\alpha_i\rangle$. Since $|\alpha_i\rangle = c^\dagger_{\alpha_i}|0\rangle$ and $\beta_j\rangle = c^\dagger_{\beta_j}|0\rangle$, we conclude that $c^\dagger_{\beta_j} = \sum_i c^\dagger_{\alpha_i} U^\dagger_{ij}$. The adjoint of this equation is the desired transformation law

$$c_{\beta_j} = \sum_i U_{ji} c_{\alpha_i}. \tag{0.19}$$

This ends our crash course on second quantisation.

1 One-particle operators in second quantization

A one-particle operator in a many-body system is an operator that acts on the state of a single particle at a time. It is defined as $\hat{B} = \sum_{i=1}^{N} \hat{B}_i$ where $\hat{B}_i$ is given by

$$\hat{B}_i = \mathbb{1}_1 \otimes \ldots \otimes \mathbb{1}_{i-1} \otimes \sum_{\nu,\mu} \langle \nu | \hat{b} | \mu \rangle |\nu\rangle\langle\mu|_i \otimes \mathbb{1}_{i+1} \otimes \ldots \otimes \mathbb{1}_N, \tag{1.1}$$

where $\langle \nu | \hat{b} | \mu \rangle$ are the matrix elements in one-particle quantum mechanics. In other words, $\hat{B}_i$ acts trivially in all Hilbert spaces, except in that of particle i.

(a) Applying $\hat{B}$ to the state $\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\}$ introduced above, show that one obtains

$$\hat{B}\big|\alpha_1, \alpha_2, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_{\mu,\nu} \langle \nu | \hat{b} | \mu \rangle \times \sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.2}$$

Note that we have explicitly labeled the one-particle states with a subscript to identify the subspace they belong to within the tensor product (0.2), *e.g.* $|\nu\rangle_i$belongs to the subspace of particle i.
(2 points)

(b) Show that one can write the last summation in (1.2) as

$$\sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N = \tag{1.3}$$

$$\sum_{j,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_j} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_{P^{-1}(j)} \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.4}$$

(2 points)
Hint: Note that $\sum_j \delta_{j,P(i)} = 1$ for fixed i, as $P(i) = j$ for some $j, \varepsilon\{1, \ldots, N\}$ since any P is a bijective mapping of $\{1, \ldots, N\}$ in itself.

(c) Consider again

$$\big|\alpha_1, \ldots, \alpha_j, \ldots, \alpha_N\big\} = \frac{1}{\sqrt{N!}} \sum_P \xi^{\sigma(P)} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu_{P(j)}\rangle_j \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N. \tag{1.5}$$

In which position in each of these terms is α_j located? Note that I am not asking where $\alpha_{P(j)}$ is located, which is obviously at position j. From this observation and using (1.3), prove the identity

$$\frac{1}{\sqrt{N!}} \sum_{i,P} \xi^{\sigma(P)} \delta_{\mu,\alpha_{P(i)}} |\alpha_{P(1)}\rangle_1 \otimes \ldots \otimes |\nu\rangle_i \otimes \ldots \otimes |\alpha_{P(N)}\rangle_N = \tag{1.6}$$

$$\sum_j \delta_{\mu,\alpha_j} \big|\alpha_1, \ldots, \alpha_{j-1}, \nu, \alpha_{j+1} \ldots, \alpha_N\big\}. \tag{1.7}$$

(2 points)

(d) Show that

$$c_\nu^\dagger c_\mu \big|\alpha_1, \ldots, \alpha_N\big\} = \sum_j \delta_{\mu,\alpha_j} \big|\alpha_1, \ldots, \alpha_{j-1}, \nu, \alpha_{j+1} \ldots, \alpha_N\big\}. \tag{1.8}$$

(2 points)
Hint: Use (0.13) and the symmetry properties of the wave-function under interchange of particles.

(e) Thus, show that

$$\hat{B}\big|\alpha_1, \ldots, \alpha_N\big\} = \sum_{\mu,\nu} \langle \nu|\hat{b}|\mu\rangle c_\nu^\dagger c_\mu \big|\alpha_1, \ldots, \alpha_N\big\}. \tag{1.9}$$

(1 point)

Since the state $\big|\alpha_1, \ldots, \alpha_N\big\}$ is arbitrary, we conclude that a one-particle operator is given, in second quantisation, by

$$\hat{B} = \sum_{\mu,\nu} \langle \nu|\hat{b}|\mu\rangle c_\nu^\dagger c_\mu. \tag{1.10}$$

2 The density operator in second quantization (revision)

For a system of N identical particles (fermions) enclosed in a volume V with periodic boundary conditions, the density operator at position r is defined (in its first quantised form), as

$$\hat{\rho}(\boldsymbol{r}) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i), \tag{2.1}$$

where $\hat{\boldsymbol{r}}_i$ is the position operator of particle i. Note that $\boldsymbol{r}$ is not an operator.

(a) Show that the Fourier transform $\hat{\rho}_q = \int_V d^3r e^{-iq\cdot r} \hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}_q = \sum_{i=1}^{N} e^{-iq\cdot\hat{r}_i}. \tag{2.2}$$

(1 point)

(b) The second quantisation representation of $\hat{\rho}(\boldsymbol{r})$, as follows from (1.10), is given by

$$\hat{\rho}(\boldsymbol{r}) = \sum_{\sigma',\sigma} \int_V d^3x' \int_V d^3x \langle \boldsymbol{x}'\sigma'|\delta(\boldsymbol{r} - \hat{\boldsymbol{r}})|\boldsymbol{x}\sigma\rangle \hat{\psi}_{\sigma'}^\dagger(\boldsymbol{x}')\hat{\psi}_\sigma(\boldsymbol{x}), \tag{2.3}$$

where $\hat{\psi}_\sigma(\boldsymbol{x})$ and $\hat{\psi}^\dagger_\sigma(\boldsymbol{x})$ are the annihilation and creation operators for a fermion, with spin projection along z equal to σ, at point $\boldsymbol{x}$. Show from (2.3) that $\hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}(\boldsymbol{r}) = \sum_\sigma \hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}). \tag{2.4}$$

(2 points)

(c) Show that in second quantization the FT of $\hat{\rho}(\boldsymbol{r})$ is given by

$$\hat{\rho}_q = \sum_{i=1}^{N} \hat{c}^\dagger_{k-q,\sigma}\hat{c}_{k,\sigma}. \tag{2.5}$$

(2 points)
Hint: Substitute the relations $\hat{\psi}_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_k e^{ik\cdot r}\hat{c}_{\boldsymbol{k},\sigma}$, $\hat{\psi}^\dagger_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_k e^{-ik\cdot r}\hat{c}^\dagger_{\boldsymbol{k},\sigma}$, see (0.19), in the definition of the Fourier transform given above. Note that $\int_V d^3r e^{-i(k-k')\cdot r} = V\delta_{k,k'}$.

(d) Show that $\hat{\rho}^\dagger_q = \hat{\rho}_{-q}$.
(1 point)

(e) Show that $\left[\hat{\rho}_q, \hat{\rho}_{q'}\right] = 0$.
(2 points)
Hint: Use the identities $\left[\hat{A}, \hat{B}, \hat{C}\right]_- = \left[\hat{A}, \hat{B}\right]_{-\xi}\hat{C} + \xi\hat{B}\left[\hat{A}, \hat{C}\right]_{-\xi}$ where $\xi = \pm 1$.

(f) Use the first quantisation representation of $\hat{\rho}_q$, as given in equation (2.2), to show the previous identity.
(2 points)
Hint: What is $\left[\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{r}}_j\right]$ for arbitrary i, j?

(g) What is $\hat{\rho}_{q=0}$?
(1 point)

In the following exercise, we will consider a many-body system (enclosed in a volume V with periodic boundary conditions), whose dynamics is described by an Hamiltonian $\hat{H}_0$ that is given by

$$\hat{H}_0 = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m}\hat{c}^\dagger_{k,\sigma}\hat{c}_{k,\sigma} + \frac{1}{2}\sum_{q,k,k',\sigma,\sigma'} V(\boldsymbol{q})\hat{c}^\dagger_{k-q,\sigma}\hat{c}^\dagger_{k'+q,\sigma'}\hat{c}_{k',\sigma'}\hat{c}_{k,\sigma} \tag{2.6}$$

where $\hat{c}_{k,\sigma}$, $\hat{c}^\dagger_{k,\sigma}$ are fermion operators, in the plane-wave basis, with a definite projection σ of the spin along the z direction, satisfying anti-commutation relations. The function $V(q)$ is the Fourier transform of the two-body inter-electron (Coulomb) interaction, but with the condition $V(0) = 0$, which takes into account in an approximate manner the presence of the attractive potential due to the ions (jellium model). If one goes beyond such an approximation, the appropriate basis to express the Hamiltonian is no longer the plane-wave basis, but it is instead the Bloch basis of states, which modifies the form of the one-particle and two-particle terms. More importantly, the assumption of translation invariance, made below, is no longer valid. A description of such a many-body system in contact with an external environment is provided by the density-matrix, which generalises the concept of wave-function to open systems. It is an Hermitian operator, which implies that an orthonormal basis can be found that diagonalises such operator. In such a basis, one has that

$$\hat{\rho}_0 = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{2.7}$$

where $0 \leq p_i \leq 1$ are the eigenvalues of $\hat{\rho}_0$, which can be chosen such that $\sum_i p_i = 1$ (normalisation of probability). If the system is in equilibrium with a thermal bath at temperature T and with a reservoir of particles with the chemical potential μ (grand canonical ensemble), $\hat{\rho}_0 = \frac{1}{Z_0} e^{-\beta(\hat{H}_0 - \mu\hat{N})}$, where $N = \sum_{k,\sigma} \hat{c}^\dagger_{k,\sigma}\hat{c}_{k,\sigma}$ is the particle-number operator of the system and $Z_0 = \mathrm{Tr}(e^{-\beta(\hat{H}_0-\mu\hat{N})})$ is the grand canonical partition function of the system, which acts as normalisation factor of the density matrix. Incidentally, $\Omega_0 = -k_B T \ln Z_0$ is the so-called grand canonical potential, which encodes all thermodynamic information regarding the many-body system. Moreover, the thermal average of any operator $\hat{B}$ is defined as $\langle\hat{B}\rangle_0 = \mathrm{Tr}(\hat{B}\hat{\rho}_0)$ and is a time-independent quantity, since $\hat{\rho}_0$ commutes with the Hamiltonian $\hat{H}_0$. Finally, note that in equilibrium, the basis that diagonalises $\hat{\rho}_0$ is just the joint basis of eigenstates of $\hat{H}_0$ and $\hat{N}$ (see also below).

3 Lehmann representation of the density-density response function. Sum rules

Consider now that the many-body system is perturbed by a weak, space dependent potential, which couples to the (local) density of particles. The full Hamiltonian $\hat{H}(t)$ (in the Schrödinger representation) is given by

$$\hat{H}(t) = \hat{H}_0 - \int_V d^3r' \phi(\boldsymbol{r}', t)\hat{\rho}(\boldsymbol{r}'), \tag{3.1}$$

where $\phi(\boldsymbol{r}, t)$ is a weak scalar potential.

(a) Repeating the steps performed in the lecture, show that to linear order in the scalar potential, the change in the density of the system is given by

$$\langle\delta\hat{\rho}(\boldsymbol{r})\rangle_t = \int_V d^3r' \int_{-\infty}^{\infty} dt' \chi(\boldsymbol{r}, t-t'; \boldsymbol{r}', 0)\phi(\boldsymbol{r}', t'), \tag{3.2}$$

where $\chi(\boldsymbol{r}, t; \boldsymbol{r}', t') = \frac{i}{\hbar}\mathrm{Tr}([\delta\hat{\rho}(\boldsymbol{r}, t), \delta\hat{\rho}(\boldsymbol{r}', 0)])\Theta(t)$ is the density-density linear response function, where $\delta\hat{\rho}(\boldsymbol{r}, t) = e^{i\hat{H}_0 t/\hbar}\delta\hat{\rho}(\boldsymbol{r})e^{-i\hat{H}_0 t/\hbar}$ with $\delta\hat{\rho}(\boldsymbol{r}) = \hat{\rho}(\boldsymbol{r}) - \langle\hat{\rho}(\boldsymbol{r})\rangle_0$. **(3 points)**

(b) A system is said to possess translational invariance if a translation by an arbitrary vector $\boldsymbol{v}$ of every argument of an N -point correlation function leaves such a function invariant. In mathematical terms, this means that

$$G_N(\boldsymbol{r}_1+\boldsymbol{v},\boldsymbol{r}_2+\boldsymbol{v},\dots,\boldsymbol{r}_N+\boldsymbol{v}) = G_N(\boldsymbol{r}_1,\boldsymbol{r}_2,\dots,\boldsymbol{r}_N) \tag{3.3}$$

(i) Show that the previous definition implies that $G_1(\boldsymbol{r}) = g_1$, where g_1 is a constant independent of the position.
(1 point)

(ii) Show, by the same token, that $G_2(\boldsymbol{r}_1,\boldsymbol{r}_2) = g_2(\boldsymbol{r}_1-\boldsymbol{r}_2)$ where $g_2(\boldsymbol{r})$ is a function depending on a single argument.
(1 point)
Hint: Choose the vector $\boldsymbol{v}$ appropriately in one case and the other.

(iii) Show that the FT $G_2(\boldsymbol{q}_1,\boldsymbol{q}_2) = \int_V d^3r_1 \int_V d^3r_2 e^{-i(q_1\cdot r_1+q_2\cdot r_2)} G_2(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is given, in the case of translational invariance, by $G_2(\boldsymbol{q}_1,\boldsymbol{q}_2) = V\delta_{q_1+q_2,0}\, g_2(\boldsymbol{q}_1)$, where $g_2(\boldsymbol{q}) = \int_V d^3r e^{-iq\cdot r} g_2(\boldsymbol{r})$.
(2 points)

(iv) Hence, show that for a system with translational invariance, the FT $\chi(\boldsymbol{q},t;\boldsymbol{q}',0) = V\delta_{q+q',0}\chi(\boldsymbol{q},t)$, where $\chi(\boldsymbol{q},t) = \frac{i}{\hbar V}\mathrm{Tr}([\delta\hat{\rho}_q(t),\delta\hat{\rho}_{-q}(0)]\hat{\rho}_0)\Theta(t)$.
(2 points)

(c) Using the completeness relation for the set of the eigenstates of $\hat{H}_0$, show that $\chi(\boldsymbol{q},t)$ has the following Lehmann representation

$$\chi(\boldsymbol{q},t) = \frac{i}{\hbar V Z_0}\sum_{n,m}\big|\langle n|\delta\hat{\rho}_{-q}|m\rangle\big|^2 e^{-i\omega_{n,m}t}(1-e^{-\beta\hbar\omega_{nm}})e^{-\beta(E_m-\mu N_m)}\Theta(t), \tag{3.4}$$

where $\omega_{nm} = \frac{1}{\hbar}(E_n - E_m)$.
(4 points)
Hint: Note that $\delta\hat{\rho}_q^\dagger = \delta\hat{\rho}_{-q}$. Moreover, do note that the eigenstates of $\hat{H}_0$ can be chosen to be simultaneous eigenstates of $\hat{N}$, *i.e.*, $\hat{N}|n\rangle = N_n|n\rangle$, as $[\hat{N},\hat{H}_0] = 0$, since the total number of particles is conserved by the dynamics. Thus, show that $\langle n|\delta\hat{\rho}_{-q}|m\rangle = 0$ unless $N_n = N_m$, using the results of the previous exercise, items e and g.

(d) Show from (3.4) that the Fourier transform of $\chi(\boldsymbol{q},t)$ is given by

$$\chi(\boldsymbol{q},\omega) = \frac{i}{\hbar V Z_0}\sum_{n,m}\frac{\big|\langle n|\delta\hat{\rho}_{-q}|m\rangle\big|^2}{\omega-\omega_{nm}+i\epsilon}(1-e^{-\beta\hbar\omega_{nm}})e^{-\beta(E_m-\mu N_m)}. \tag{3.5}$$

(2 points)

(e) Show that one can write (3.5) also as

$$\chi(\boldsymbol{q},\omega) = \int_{-\infty}^{\infty} d\omega' \frac{1-e^{-\beta\hbar\omega'}}{\omega'-\omega-i\epsilon} S(\boldsymbol{q},\omega'), \tag{3.6}$$

where $S(\boldsymbol{q},\omega)$ is the so-called dynamic structure factor and is given by

$$S(\boldsymbol{q},\omega) = \frac{i}{\hbar V Z_0} \sum_{n,m} \left|\langle n|\delta\hat{\rho}_{-q}|m\rangle\right|^2 e^{-\beta(E_m-\mu N_m)}\delta(\omega-\omega_{nm}). \tag{3.7}$$

(2 points)

(f) Show, taking into account the properties of $S(\boldsymbol{q},\omega)$, that

$$\mathrm{Re}\chi(\boldsymbol{q},\omega) = P\int_{-\infty}^{\infty} d\omega' \frac{1-e^{\beta\hbar\omega'}}{\omega'-\omega} S(\boldsymbol{q},\omega), \tag{3.8}$$

$$\mathrm{Im}\chi(\boldsymbol{q},\omega) = \pi(1-e^{\beta\hbar\omega'})S(\boldsymbol{q},\omega), \tag{3.9}$$

and hence show that these two equations imply the first Kramers-Kronig relation for $\chi(\boldsymbol{q},\omega)$.
(3 points)

(g) Show from (3.7) that $S(\boldsymbol{q},-\omega) = e^{-\beta\hbar\omega}S(-\boldsymbol{q},\omega)$. If the Hamiltonian of the system is invariant under time-reversal or space-inversion (or both) $S(-\boldsymbol{q},\omega) = S(\boldsymbol{q},\omega)$. Conclude that in such a case $S(\boldsymbol{q},-\omega) = e^{-\beta\hbar\omega}S(\boldsymbol{q},\omega)$. This relation is known as the *detailed-balance relation* (already derived in the lecture using a different method).
(2 points)
Hint: Note that one may relabel the summation indices in (3.7).

(h) Show, using the previous result and (3.9), that $\mathrm{Im}\chi(\boldsymbol{q},\omega) = \pi(S(\boldsymbol{q},\omega) - S(-\boldsymbol{q},-\omega))$. If the system is invariant under time-reversal or space-inversion, show that $\mathrm{Im}\chi(\boldsymbol{q},-\omega) = \pi(S(\boldsymbol{q},\omega) - S(\boldsymbol{q},-\omega))$.
(1 point)

(i) Show, using (3.9), as well as the definition of $S(\boldsymbol{q},\omega)$, that

$$\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\chi(\boldsymbol{q},\omega')}{\omega'} = \frac{\pi}{\hbar V Z_0}\sum_{n,m} \frac{\left|\langle n|\delta\hat{\rho}_{-q}|m\rangle\right|^2}{\omega'_{nm}} \left(1-e^{-\beta\hbar\omega_{nm}}\right)e^{-\beta(E_m-\mu N_m)}. \tag{3.10}$$

(2 points)

(j) Show that one can rewrite the RHS of (3.10) such that it now reads

$$\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\chi(\boldsymbol{q},\omega')}{\omega'} = \frac{\pi}{V}\int_0^\beta d\lambda \mathrm{Tr}(\delta\hat{\rho}_q(-i\hbar\lambda)\delta\hat{\rho}_{-q}(0)\hat{\rho}_0), \tag{3.11}$$

where $\delta\hat{\rho}_q(-i\hbar\lambda) = e^{\lambda\hat{H}_0}\delta\hat{\rho}_q e^{-\lambda\hat{H}_0}$
(2 points)
Hint: $\int_0^\beta d\lambda e^{-\lambda\hbar\omega_{nm}} = \frac{1-e^{-\beta\hbar\omega_{nm}}}{\hbar\omega_{nm}}$.

(k) Finally, show that in the limit $\boldsymbol{q} \to 0$, one has

$$\lim_{q\to 0} \int_{-\infty}^{\infty} d\omega' \frac{\mathrm{Im}\chi(\boldsymbol{q},\omega')}{\omega'} = \frac{\pi\beta}{V} \langle (\hat{N} - \langle \hat{N} \rangle_0)^2 \rangle_0. \tag{3.12}$$

(3 points)
Hint: What is $[\hat{N}, \hat{H}_0]$?

(l) Show that

$$\frac{\partial \langle \hat{N} \rangle_0}{\partial \mu}\Big|_{T,V} = \beta \langle (\hat{N} - \langle \hat{N} \rangle_0)^2 \rangle_0. \tag{3.13}$$

(2 points)
Hint: Use the definition $\langle \hat{N}_0 \rangle = \frac{1}{Z_0} \sum_m N_m e^{-\beta(E_m - \mu N_m)}$ and differentiate with respect to μ.

(m) Consider the case in which the system is invariant under time-reversal or space-inversion. Use the thermodynamic identity $\frac{\partial \langle \hat{N} \rangle_0}{\partial \mu}\big|_{T,V} = V n^2 \kappa_T$ where $n = \langle \hat{N} \rangle_0 / V$ is the density of electrons and $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial P}\big|_{T,N}$ is the isothermal compressibility of the system, to show that

$$\lim_{q\to 0} \int_{-\infty}^{\infty} d\omega' \frac{S(\boldsymbol{q},\omega')}{\omega'} = \frac{1}{2} n^2 \kappa_T. \tag{3.14}$$

This relation is known as the *compressibility sum rule.*
(2 points)

(n) Show that

$$\mathrm{Tr}\big([\delta\hat{\rho}_q, [\hat{H}_0, \delta\hat{\rho}_{-q}]]\hat{\rho}_0\big) = \frac{\hbar}{Z_0} \sum_{n,m} \omega_{nm} \big[\big| \langle n | \delta\hat{\rho}_{-q} | m \rangle \big|^2 + \big| \langle n | \delta\hat{\rho}_q | m \rangle \big|^2 \big] \tag{3.15}$$

$$\times\, e^{-\beta(E_m - \mu N_m)}. \tag{3.16}$$

(2 points)

(o) Thus, show that

$$\frac{1}{\hbar^2 V} \mathrm{Tr}\big([\delta\hat{\rho}_q, [\hat{H}_0, \delta\hat{\rho}_{-q}]]\hat{\rho}_0\big) = \int_{-\infty}^{\infty} d\omega' \omega' [S(\boldsymbol{q},\omega') + S(-\boldsymbol{q},\omega')]. \tag{3.17}$$

(2 points)

(p) Show that this relation is equivalent to

$$\frac{1}{\hbar^2 V} \mathrm{Tr}\big([\delta\hat{\rho}_q, [\hat{H}_0, \delta\hat{\rho}_{-q}]]\hat{\rho}_0\big) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' \omega' \mathrm{Im}\chi(\boldsymbol{q},\omega'). \tag{3.18}$$

This is of course just a particular case of the *series of sum-rules* derived in the lecture.
(1 point)

(q) Now, show that $[\delta\hat{\rho}_q, [\hat{H}_0, \delta\hat{\rho}_{-q}]] = \frac{\hbar^2 q^2}{m}\hat{N}$.
(3 points)
Hint: Write the second term of (2.6) as an expression involving a sum of products of densities $\hat{\rho}_{q'}\hat{\rho}_{-q'}$ and use the result of Exercise 2e to show that such a term commutes with $\delta\hat{\rho}_{-q}$. The terms in the commutator arising from the first term of (2.6) yield the desired result.

(r) Thus, show that

$$\int_{-\infty}^{\infty} d\omega' \omega' \mathrm{Im}\chi(\boldsymbol{q}, \omega') = \frac{\pi n q^2}{m}, \tag{3.19}$$

where n is, as above, the electron density of the system.
(1 point)

(s) Show that for a system that is invariant under time-reversal or space-inversion, one has

$$\int_{-\infty}^{\infty} d\omega' \omega' S(\boldsymbol{q}, \omega') = \frac{n q^2}{m}, \tag{3.20}$$

This relation is know as the *f-sum rule.*
(2 points)

4 The single mode approximation

In the previous exercise, we derived the sum rules assuming a many-body system where fermions interact through the Coulomb interaction. However, a little thought shows that the same conclusions will hold with a different form of the interaction provided that it involves only the density of particles of the system (in fact, we did not even use a definite form for $V(\boldsymbol{q})$). Moreover, the same results would have followed if we had considered interacting bosons, rather than fermions (you may wish to check that explicitly). We now consider an uncharged system and postulate a specific form for $S(\boldsymbol{q}, \omega)$, namely

$$S(\boldsymbol{q}, \omega) = F(\boldsymbol{q})\left[\delta(\omega - \omega_q) + e^{\beta\hbar\omega}\delta(\omega + \omega_q)\right], \tag{4.1}$$

where $\omega_q > 0$ is the frequency of the excitations and $F(\boldsymbol{q})$ is an unknown amplitude.

(a) Show that $S(\boldsymbol{q}, \omega)$ obeys the detailed-balance relation.
(2 points)

(b) Show that $F(\boldsymbol{q})$ is related to the static structure factor $S(\boldsymbol{q}) = \int_{-\infty}^{\infty} d\omega S(\boldsymbol{q}, \omega)$ by $F(\boldsymbol{q}) = S(\boldsymbol{q})/(1 + e^{-\beta\hbar\omega_q})$.
(1 point)

(c) Show from the *f-sum rule* that ω_q is related to $S(\boldsymbol{q})$ by $\omega_q \tanh\left(\frac{\beta\hbar\omega_q}{2}\right) = \frac{nq^2}{2mS(\boldsymbol{q})}$.
(2 points)

(d) Show that from the *compressibility sum rule* that $\lim_{q\to 0}\frac{S(\boldsymbol{q})}{\omega_q}\tanh\left(\frac{\beta\hbar\omega_q}{2}\right)=\frac{1}{2}n^2\kappa_T$.
(2 points)

(e) Show that these two relations imply that at small $\boldsymbol{q}$,$\omega_q=c_s|\boldsymbol{q}|$, where $c_s^{-2}=nm\kappa_T$. What is the physical meaning of c_s?
(2 points) Hint: What are the units of c_s?

(f) Show that at small $\boldsymbol{q}$, $S(\boldsymbol{q})=\frac{n|\boldsymbol{q}|}{2mc_s}\tanh^{-1}\left(\frac{\beta\hbar c_s|\boldsymbol{q}|}{2}\right)$. Study the different limits $T=0$ ($\beta\to\infty$) and $T\neq 0$.
(3 points)

(g) Finally, use (3.6) with the postulated form for $S(\boldsymbol{q},\omega)$, to show that

$$\chi(\boldsymbol{q},\omega)=-\frac{nq^2}{m}\frac{1}{(\omega+i\epsilon)^2-\omega_q^2}. \tag{4.2}$$

Discuss in particular the limit of small $\boldsymbol{q}$.
(3 points)

This exercise should illustrate the usefulness of the sum rules derived above.