FI 002 – Mecânica Quântica II – Lista 4

P.01. P.1.8, Schwabl:
A system of N interacting particles is described by the Hamiltonian

$$H = \sum_{i,j} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} \langle i\, j|V|k\, l\rangle a_i^\dagger a_j^\dagger a_l a_k.$$

a) For a system of N interacting bosons, show that the Hamiltonian H commutes with the total particle-number operator $\hat{N} = \sum_i a_i^\dagger a_i$.

b) For a system of N interacting fermions, show that $[H, \hat{N}] = 0$.

Hint: Identity $[AB, CD] = [A, C]BD + A[B, C]D + C[A, D]B + CA[B, D]$ and the equivalent in terms of anticommutators.

P.02. P.22.3, Merzbacher:
Consider the unperturbed states

$$a_{n\, m_n}^\dagger \ldots a_{k\, m_k}^\dagger \ldots a_{1\, m_1}^\dagger |0\rangle$$

of n spin one-half particles, each occupying one of n equivalent, degenerate orthogonal orbitals labeled by the quantum number k, and with $m_k = \pm 1/2$ denoting the spin quantum number associated with the orbital k. Show that, in the space of the 2^n unperturbed states, a spin-independent two-body interaction may, in first-order perturbation theory, be replaced by the effective exchange (or Heisenberg) Hamiltonian

$$H_{eff} = -\frac{1}{\hbar^2} \sum_{i,j} \langle i\, j|V|j\, i\rangle \mathbf{S}_i \cdot \mathbf{S}_j + \mathrm{cte} = \sum_{i,j} J_{i,j}\, \mathbf{S}_i \cdot \mathbf{S}_j + \mathrm{cte},$$

where $\mathbf{S}_i$ is the localized spin operator

$$\mathbf{S}_i = \frac{\hbar}{2} \sum_{m_i, m_i'} a_{i\, m_i}^\dagger a_{i\, m_i'} \langle m_i|\hat{\sigma}|m_i'\rangle.$$

Alternative: Consider a system of N electrons hopping on the sites of a given lattice and described by the model (for more details about the Hamiltonian, see P.1.7, Schwabl)

$$\hat{H} = \hat{T} + \hat{V} = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{1}{2} \sum_{\alpha,\beta} \sum_{i,j,k,l} \langle i\, j|V|k\, l\rangle c^\dagger_{i,\alpha} c^\dagger_{j,\beta} c_{l,\beta} c_{k,\alpha},$$

where t_{ij} is the hopping energy between sites i and j and $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) creates (destroys) an electron with spin $\sigma =\uparrow, \downarrow$ on site i of the lattice. The interacting term $\hat{V}$ can be written as

$$\hat{V} = \hat{V}_D + \hat{V}_E + \ldots,$$

where the direct term $\hat{V}_D$ and the exchange term $\hat{V}_E$ are given by

$$\hat{V}_D = \frac{1}{2} \sum_{\alpha,\beta} \sum_{i \neq j} \langle i\, j|V|i\, j\rangle c^\dagger_{i,\alpha} c^\dagger_{j,\beta} c_{j,\beta} c_{i,\alpha},$$

$$\hat{V}_E = \frac{1}{2} \sum_{\alpha,\beta} \sum_{i \neq j} \langle i\, j|V|j\, i\rangle c^\dagger_{i,\alpha} c^\dagger_{j,\beta} c_{i,\beta} c_{j,\alpha}.$$

a) Show that $\hat{V}_D$ can be written in terms of the number operator $\hat{n}_i = \sum_\alpha c^\dagger_{i,\alpha} c_{i,\alpha}$.

b) Show that $\hat{V}_E$ can be written in terms of the number operator $\hat{n}_i$ and the spin operators

$$S^\mu_i = \frac{1}{2} \sum_{\alpha,\beta} c^\dagger_{i,\alpha} \sigma^\mu_{\alpha\beta} c_{i,\beta}, \qquad \mu = x, y, z,$$

where $\sigma^\mu_{\alpha\beta} = \langle \alpha|\sigma^\mu|\beta\rangle$ with σ^μ being a Pauli matrix.

P.03. P.1.3 and P.1.4, Mahan:

a) Solve the Hamiltonian below with a canonical transformation:

$$\begin{aligned} H &= E_0 a^\dagger a + F\left(a + a^\dagger\right), \\ \bar{H} &= e^S H e^{-S}, \qquad\qquad S = \lambda\left(a - a^\dagger\right), \end{aligned}$$

where a and $a^\dagger$ are boson operators:
(a) Show that $\lambda = \lambda^*$ since H is Hermitian;
(b) Use the Baker-Hausdorff identity, and show that only a few terms in the series are finite (the remainder vanish);
(c) Find the choice of λ which reduces H to a diagonal form.

b) Find the exact solution to

$$H = \epsilon a^\dagger a + \frac{1}{2}\Delta\left(a^\dagger a^\dagger + aa\right),$$

where ϵ and Δ are constants and a and $a^\dagger$ are boson operators.
Show that:
(1) the Hamiltonian H can be written as

$$H = E_0 + \frac{1}{2}\epsilon\left(a^\dagger a + aa^\dagger\right) + \frac{1}{2}\Delta\left(a^\dagger a^\dagger + aa\right)$$

and determine the constant E_0;
(2) Express the boson operators a in terms of new bosons operators b, $a = \mu b + \lambda b^\dagger$;
(3) Determine the relation between the constants μ and λ such that the boson operators b satisfy bosonic commutation relations;
(4) Verify that the constants μ and λ can be written as $\mu = \cosh\xi$ and $\lambda = \sinh\xi$;
(5) Determine the constants μ and λ such that H is now diagonal;
(6) Determine the ground-state of the system and the ground-state energy.

P.04. P1.13, Mahan and P.1.6, Schwabl:

a) Consider a system of N spinless particles. The density operator is defined as

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i),$$

where $\mathbf{r}_i$ is the position of the particle i. Show that $\rho(\mathbf{r}) = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})$, where $\Psi^\dagger(\mathbf{r})$ and $\Psi(\mathbf{r})$ are field operators, and

$$\rho(\mathbf{q}) = \int d^3r \, e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}) = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}-\mathbf{q}} c_{\mathbf{k}}.$$

b) Repeat item (a) for the current-density operator

$$\mathbf{J}(\mathbf{r}) = \frac{1}{2} \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i}{m} \delta\left(\mathbf{r} - \mathbf{r}_i\right) + \delta\left(\mathbf{r} - \mathbf{r}_i\right) \frac{\mathbf{p}_i}{m} \right].$$

c) Consider now a system of N spin-$1/2$ particles and determine the density operator $\rho(\mathbf{r})$ and the current-density operator $\mathbf{J}(\mathbf{r})$ in terms of the fermion operators $c^\dagger_{\mathbf{k}\,\sigma}$ and $c_{\mathbf{k}\,\sigma}$. For a system of free fermions described by the Hamiltonian

$$H = \sum_{\mathbf{k}\,\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\,\sigma} c_{\mathbf{k}\,\sigma},$$

where $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}/2m$, determine $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$, and show that they satisfy the continuity equation

$$\partial_t \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0.$$

d) Consider a system of N spin-$1/2$ particles and repeat item (a) for the components of the spin-density operator

$$S^\alpha = \sum_{i=1}^{N} \delta\left(\mathbf{r} - \mathbf{r}_i\right) S^\alpha_i,$$

where $\alpha = x$, y, and z.

P.05. Single-particle Green's function:
The single-particle Green's function for spinless fermions at temperature $T = 0$ is defined as

$$G(\mathbf{r}-\mathbf{r}', t-t') = -i\langle\Phi_0|T\Psi(\mathbf{r},t)\Psi^\dagger(\mathbf{r}',t')|\Phi_0\rangle,$$

where $|\Phi_0\rangle$ is the many-body ground state, $\Psi(\mathbf{r},t)$ is the field operator in the Heisenberg picture,

$$\Psi(\mathbf{r},t) = U^\dagger(t,0)\Psi(\mathbf{r})\Psi(t,0) = e^{iHt/\hbar}\Psi(\mathbf{r})e^{-iHt/\hbar},$$

and

$$T\Psi(\mathbf{r},t)\Psi^\dagger(\mathbf{r}',t) = \begin{cases} +\Psi(\mathbf{r},t)\Psi^\dagger(\mathbf{r}',t'), & t > t', \\ -\Psi^\dagger(\mathbf{r}',t')\Psi(\mathbf{r},t), & t' > t \end{cases}$$

defines the time-ordering for fermions. In the following, we considere a system of non-interacting spinless fermions described by the Hamiltonian

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}},$$

where $c^\dagger_{\mathbf{k}}$ and $c_{\mathbf{k}}$ respectively creates and destroys a fermion with momentum $\mathbf{p} = \hbar\mathbf{k}$ and energy $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$. The ground state of the Hamiltonian H is given by

$$|\Phi_0\rangle = \prod_{\mathbf{k},k<k_F} c^\dagger_{\mathbf{k}}|0\rangle,$$

where $|0\rangle$ is the fermion vacuum.

a) The coordinate-space $G(\mathbf{r}-\mathbf{r}', t-t')$ and momentum-space $G(\mathbf{k}, t-t')$ Green's functions are related via a Fourier transform

$$G(\mathbf{r}-\mathbf{r}', t-t') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} G(\mathbf{k}, t-t').$$

Since the field operator $\Psi(\mathbf{r})$ can be expanded in terms of the fermion operator $c_{\mathbf{k}}$ as

$$\Psi(\mathbf{r}) = \frac{1}{L^{3/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}} = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}},$$

show that

$$G(\mathbf{k}, t-t') = -i\langle\Phi_0|Tc_{\mathbf{k}}(t)c^\dagger_{\mathbf{k}}(t')|\Phi_0\rangle.$$

b) Determine $c^\dagger_{\mathbf{k}}(t)$ and $c_{\mathbf{k}}(t)$ in terms of $\epsilon_{\mathbf{k}}$.

c) In the following, we set $t' = 0$. Show that

$$G(\mathbf{k}, t) = -i\left[(1-n_{\mathbf{k}})\theta(t) - n_{\mathbf{k}}\theta(-t)\right] e^{-i\epsilon_{\mathbf{k}}t/\hbar},$$

where $n_{\mathbf{k}} = \Theta(k_F - k)$ with $\hbar k_F$ being the Fermi momentum.

d) It is convenient to introduce the Fourier transform in time of $G(\mathbf{k}, t)$:

$$G(\mathbf{k}, \omega) = \int dt\, e^{i\omega t} G(\mathbf{k}, t).$$

Show that

$$G(\mathbf{k}, \omega) = \frac{\theta(k - k_F)}{\omega - \epsilon_{\mathbf{k}}/\hbar + i\delta} + \frac{\theta(k_F - k)}{\omega - \epsilon_{\mathbf{k}}/\hbar - i\delta} = \frac{1}{\omega - \epsilon_{\mathbf{k}}/\hbar + i\delta_{\mathbf{k}}},$$

where $\delta_{\mathbf{k}} = \delta \mathrm{sgn}(k - k_F)$. Comment about the poles of $G(\mathbf{k}, \omega)$.

P.06. P.1.6, Mahan:
Consider a system of $N_e = N$ free spinless electrons hopping on the sites of a square lattice and described by the tight-binding model (for more details about the Hamiltonian, see P.1.7, Schwabl)

$$H = -t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) = -t \sum_{i,\delta} \left(c_i^\dagger c_{i+\delta} + c_{i+\delta}^\dagger c_i \right),$$

where t is the nearest-neighbor hopping energy, $c_i^\dagger$ and c_i respectively creates and destroys an electron on site i of the square lattice, and $\delta = a\hat{x}$ and $a\hat{y}$ are the nearest-neighbor vectors with a being the lattice spacing. Show that the fermion operators $c_{\mathbf{k}}^\dagger$ and $c_{\mathbf{k}}$ defined via the Fourier transform

$$c_i^\dagger = \frac{1}{N_s^{1/2}} \sum_{\mathbf{k} \in BZ} e^{-i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}}^\dagger,$$

where $N_S = N$ is the number of sites of the square lattice and $\mathbf{R}_i$ is a vector of the square lattice, obey fermion anticommutation relations. Show that the Hamiltonian H can be diagonalized with the aid of the above Fourier transform, i.e.,

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}},$$

and determine the energy $\epsilon_{\mathbf{k}}$ of the electrons.
Hint: Identity $\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i} = N_s \delta_{\mathbf{k},0}$.

P.07. P.1.16, Mahan:
Consider a ferromagnet system of N spins $S = 1/2$ localized on the sites of a square lattice and described by the Heisenberg model (see P.22.3, Merzbacher)

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where i and j are nearest neighbor sites on the square lattice and the exchange constant $J > 0$. The ferromagnetic Heisenberg model can be studied with the aid of the so-called the Holstein-Primakoff transformation,

$$S_i^+ = (1 - \hat{n}_i)^{1/2} \, a_i, \qquad S_i^- = a_i^\dagger \, (1 - \hat{n}_i)^{1/2}, \qquad S_i^z = \frac{1}{2} - \hat{n}_i,$$

where $S_i^\pm = S_i^x \pm i S_i^y$ and $\hat{n}_i = a_i^\dagger a_i$.

a) Show that the commutation relations for the spin operators,

$$[S_i^z, S_j^+] = \delta_{i,j} S_i^+, \qquad [S_i^z, S_j^-] = -\delta_{i,j} S_i^-, \qquad [S_i^+, S_j^-] = 2\delta_{i,j} S_i^z,$$

are satisfied by the above bosonic representation.

b) Express the Heisenberg Hamiltonian in terms of the boson operators a_i.

c) At low temperatures, the Hamiltonian derived in item (b) can be simplified since $n_i = \langle \hat{n}_i \rangle$ is a small quantity. Derive an approximate expression for the Hamiltonian up to second order in terms of the boson operators a_i (harmonic approximation).

d) Show that the approximate Hamiltonian derived in item (c) can be diagonalized via a Fourier transformation, i.e.,

$$H = E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}},$$

and determine the constant E_0 and the energy $\omega_{\mathbf{k}}$ of the bosons $a_{\mathbf{k}}$ (magnons). Determine the ground-state of the system $|\Psi\rangle$ and the ground-state energy.

P.08. P.2.1, Schwabl:
Consider a system of N noninteracting fermions at $T = 0$ and determine the static structure factor

$$S^0(\mathbf{q}) = \frac{1}{N} \langle \phi_0 | \hat{n}_{\mathbf{q}} \hat{n}_{-\mathbf{q}} | \phi_0 \rangle.$$

Here, $\hat{n}_{\mathbf{q}} = \sum_{\mathbf{k},\sigma} a_{\mathbf{k}\,\sigma}^\dagger a_{\mathbf{k}+\mathbf{q}\,\sigma}$ is the particle density operator in the momentum representation and $|\phi_0\rangle$ is the ground state of the system. Take the continuum limit $\sum_{\mathbf{k},\sigma} = 2V \int d^3k/(2\pi)^3$ and calculate $S^0(\mathbf{q})$ explicitly.
Hint: Consider the cases $\mathbf{q} = 0$ and $\mathbf{q} \neq 0$ separately.

09. P.1.3 and P.2.6, Schwabl:

a) Derive the following relations for boson operators:

$$[a, e^{\alpha a^\dagger}] = \alpha e^{\alpha a^\dagger}, \qquad e^{-\alpha a^\dagger} a e^{\alpha a^\dagger} = a + \alpha,$$

$$e^{-\alpha a^\dagger} e^{\beta a} e^{\alpha a^\dagger} = e^{\beta\alpha} e^{\beta a}, \qquad e^{\alpha a^\dagger a} a e^{-\alpha a^\dagger a} = e^{-\alpha} a.$$

b) Derive the following relations for fermion operators:

$$e^{-\alpha a^\dagger} a e^{\alpha a^\dagger} = a - \alpha^2 a^\dagger + \alpha \left(a a^\dagger - a^\dagger a \right),$$

$$e^{-\alpha a} a^\dagger e^{\alpha a} = a^\dagger - \alpha^2 a + \alpha \left(a a^\dagger - a^\dagger a \right),$$

$$e^{\alpha a^\dagger a} a e^{-\alpha a^\dagger a} = e^{-\alpha} a, \qquad e^{\alpha a^\dagger a} a^\dagger e^{-\alpha a^\dagger a} = e^{-\alpha} a^\dagger.$$

10. P.22.2, Merzbacher:

a) Using the fermion creation operators $a^\dagger_{jm}$, appropriate to particles with angular momentum j, form the closed-shell state in which all one-particle states $m = -j$ to $m = +j$ are occupied.

b) Prove that the closed shell has zero total angular momentum.

c) If a fermion with magnetic quantum number m is missing from a closed shell of particles with angular momentum j, show that, for coupling angular momenta, the hole state may be treated like a one-particle state with magnetic quantum number $-m$ and an effective creation operator $(-1)^{j-m} a_{jm}$.

11. P.1.6, Mahan:

Consider now a tight-binding solid which has alternate atoms of type A and B. The electron Hamittonian in the nearest neighbor model has the form

$$H = t \sum_i \sum_\delta \left(a_i^\dagger b_{i+\delta} + b_{i+\delta}^\dagger a_i \right) + \sum_i \left(\epsilon_a a_i^\dagger a_i + \epsilon_b b_i^\dagger b_i \right),$$

where a_i and b_j are electron operators for atoms of type A and B. Find the exact eigenvalues of this Hamiltonian.

12. P.3.2, Coleman:
A system is described by the following Hamiltonian

$$H = \epsilon \left(a_1^\dagger a_1 + a_2^\dagger a_2 \right) + \Delta \left(a_1^\dagger a_2^\dagger + a_2 a_1 \right),$$

where ϵ and Δ are constants and a_1 and a_2 are fermion operators.

a) Consider the Bogoliubov transformation

$$a_1 = u c_1 + v c_2^\dagger, \qquad a_2^\dagger = v c_1 - u c_2^\dagger,$$

and determine the condition that the real coefficients u and v should satisfied in order that c_1 and c_2 are fermion operators.

b) Show that the Hamiltonian H can be written as

$$H = E_0 + \epsilon \left(a_1^\dagger a_1 - a_2 a_2^\dagger \right) + \delta \left(a_1^\dagger a_2^\dagger + a_2 a_1 \right)$$

and determine the constant E_0. Use the Bogoliubov transformation discussed in item (a), diagonalize the Hamiltonian, and determine the energy of the new fermions c_1 and c_2.

c) Determine the ground-state energy E_{GS} of the system.

P.13. P.3.3, Schwabl:

a) Consider the following Bogoliubov (canonical) transformation

$$a_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} + v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, \qquad a_{-\mathbf{k}}^\dagger = u_{\mathbf{k}} b_{-\mathbf{k}}^\dagger + v_{\mathbf{k}} b_{\mathbf{k}},$$

where $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are boson operators and $\mathbf{k} \neq 0$. Determine the condition that the functions $u_{\mathbf{k}} = u_{-\mathbf{k}} \in \Re$ and $v_{\mathbf{k}} = v_{-\mathbf{k}} \in \Re$ should satisfy. Show that the previous condition is satisfied if one writes $u_{\mathbf{k}} = \cosh \varphi_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh \varphi_{\mathbf{k}}$. Show that the inverse transformation is is given by

$$b_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger, \qquad b_{-\mathbf{k}}^\dagger = u_{\mathbf{k}} a_{-\mathbf{k}}^\dagger - v_{\mathbf{k}} a_{\mathbf{k}}.$$

Hint: Write the transformation in matrix form.

b) Repeat item (a) for the canonical transformation

$$c_{\mathbf{k}\uparrow} = u_{\mathbf{k}} d_{\mathbf{k}\uparrow} + v_{\mathbf{k}} d_{-\mathbf{k}\downarrow}^\dagger, \qquad c_{-\mathbf{k}\downarrow}^\dagger = u_{\mathbf{k}} d_{-\mathbf{k}\downarrow}^\dagger - v_{\mathbf{k}} d_{\mathbf{k}\uparrow},$$

where $c_{\mathbf{k}\sigma}$ and $d_{\mathbf{k}\sigma}$, with $\sigma = \uparrow, \downarrow$, are fermion operators and $\mathbf{k} \neq 0$.

14. P.14.2, Schwabl:
We denote by S_n, A_n the symmetrizing and antisymmetrizing operators for the particles $1, 2, \ldots, n$ and by S_{n-1}, A_{n-1} the symmetrizing and antisymmetrizing operators for the particles $1, 2, \ldots, n-1$. Show that

$$S_n = \frac{1}{n}\left(1 + \sum_{i=1}^{n-1} P_{in}\right) S_{n-1} = \frac{1}{n} S_{n-1}\left(1 + \sum_{i=1}^{n-1} P_{in}\right),$$

$$A_n = \frac{1}{n}\left(1 - \sum_{i=1}^{n-1} P_{in}\right) A_{n-1} = \frac{1}{n} A_{n-1}\left(1 + \sum_{i=1}^{n-1} P_{in}\right).$$

15. P.1.6, Fetter and Walecka:
Consider a polarized electron gas in which $N_\pm$ denotes the number of electrons with spin-up (-down).

a) Find the ground-state energy to first order in the interaction potential as a function of $N = N_+ + N_-$ and the polarization $\zeta = (N_+ - N_-)/N$.

b) Prove that the ferromagnetic state ($\zeta = 1$) represents a lower energy than the unmagnetized state ($\zeta = 0$) if $r_s > (2\pi/5)(9\pi/4)^{1/3}(2^{1/3} + 1) = 5.45$. Explain why this is so.

c) Show that $\partial^2(E/N)/\partial\zeta^2|_{\zeta=0}$ becomes negative for $r_s > (3\pi^2/2)^{2/3} = 6.03$.

d) Discuss the physical significance of the two critical densities. What happens for $5.45 < r_s < 6.03$?