FI 193 – Teoria Quântica de Sistemas de Muitos Corpos – Lista 2

P.01. P.3.3, Miranda: Jordan-Wigner representation for spin-$1/2$ operators.
Consider a one-dimensional system of N localized spins-$1/2$ described by the Heisenberg model

$$H = \sum_j \left(J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z \right), \tag{1}$$

where S_j^α is the α component of a spin operator associated with a spin $S = 1/2$ localized at site j of the (one-dimensional) spin chain, J_α are the exchange constants with $\alpha = x$, y, z. The Heisenberg model (1) can be studied with the aid of the Jordan-Wigner representation, where spin-$1/2$ operators are expanded in terms of fermions operators d and $d^\dagger$,

$$d_j = e^{i\phi_j} S_j^-, \qquad d_j^\dagger = e^{-i\phi_j} S_j^+, \qquad \text{where} \qquad \phi_j = \pi \sum_{l=-\infty}^{j-1} \left(\frac{1}{2} + S_l^z \right). \tag{2}$$

The operator $e^{i\phi_j}$ is the so-called string operator.

(a) Show that the fermion operators d_j defined in Eq. (2) satisfy the anticommutation algebra of fermions. Note that the string operator provides the appropriated algebra for the fermion operators d_j.

(b) Show that the number operator for the fermions d_j is given by

$$\hat{n}_j = d_j^\dagger d_j = \frac{1}{2} + S_j^z. \tag{3}$$

Note that Eq. (3) allow us to identify the states $|\uparrow\rangle_j \equiv d_j^\dagger|0\rangle$ and $|\downarrow\rangle \equiv |0\rangle$, where $|0\rangle$ is the vacuum state for the fermions d. Moreover, note that the string operator can be written in terms of the number operators $\hat{n}_l$.

(c) Determine the inverse of the representation (2) (note that a spin $=$ fermion $\times$ string) and express the Hamiltonian (1) in terms of the fermions d_j. Note that the spin Hamiltonian is mapped into an interacting model for spinless fermions.

(d) Consider now the Heisenberg model (1) with $J_x \neq 0$, $J_y \neq 0$, and $J_z = 0$, the so-called XY-model, and determine the excitation spectrum. Moreover, comment on the particular cases (i) $J_x = J_y$ (XX-model) and (ii) $J_x \neq 0$ and $J_y = 0$ (Ising model).
Hint: It is useful to perform a gauge transformation before the diagonalization of the fermionic Hamiltonian via a canonical transformation.

02. P.3.3, Fetter and Walecka: Two-particle Green's function.
Define the two-particle Green's function by

$$G_{\alpha\beta;\gamma\lambda}(\mathbf{r}_1\, t_1, \mathbf{r}_2\, t_2; \mathbf{r}_1'\, t_1', \mathbf{r}_2'\, t_2') = (-i)^2 \frac{\langle\Psi_0|T\left[\psi_\alpha(\mathbf{r}_1, t_1)\psi_\alpha(\mathbf{r}_2, t_2)\psi_\lambda^\dagger(\mathbf{r}_2', t_2')\psi_\gamma^\dagger(\mathbf{r}_1', t_1')\right]|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}.$$

Prove that the expectation value of the two-body interaction in the exact ground state is given by

$$\langle\hat{V}\rangle = -\frac{1}{2}\int d^3r\, d^3r'\, V_{\mu'\lambda',\mu\lambda}(\mathbf{r}, \mathbf{r}')G_{\lambda\lambda';\mu\mu'}(\mathbf{r}'\, t, \mathbf{r}\, t; \mathbf{r}'\, t^+, \mathbf{r}\, t^+).$$

03. P.3.4, Fetter and Walecka: Equation of motion for single-particle Green's function.
Consider a many-body system in the presence of an external potential $U(\mathbf{r})$ with a spin-independent interaction potential $V(\mathbf{r}-\mathbf{r}')$. Show that the exact one-particle Green's function obeys the equation of motion

$$\left[i\hbar\frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m}\nabla_1^2 - U(\mathbf{r}_1)\right] G_{\alpha\beta}(\mathbf{r}_1\, t_1, \mathbf{r}_1'\, t_1')$$
$$\pm i\int d^3r_2\, V(\mathbf{r}_1-\mathbf{r}_2)G_{\alpha\gamma;\beta\gamma}(\mathbf{r}_1\, t_1, \mathbf{r}_2\, t_2; \mathbf{r}_1'\, t_1', \mathbf{r}_2\, t_1^+) = \hbar\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(t_1-t_1')\delta_{\alpha\beta},$$

where the upper (lower) sign refers to bosons (fermions) and the two-particle Green's function is defined in Prob. 3.3, Fetter and Walecka.

P.04. P.3.8, Fetter and Walecka: Density-density correlation function.
Derive the Lehmann representation for $D(\mathbf{k}, \omega)$, which is the Fourier transform of

$$iD(x, y) = \frac{\langle\Psi_0|T\left[\tilde{n}_H(x)\tilde{n}_H(y)\right]|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle},$$

with the density fluctuation operator defined by

$$\tilde{n}(\mathbf{r}) \equiv \psi_\alpha^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r}) - \frac{\langle\Psi_0|\psi_\alpha^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r})|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}.$$

Show that $D(\mathbf{k}, \omega)$ is a meromorphic function with poles in the second and fourth quadrant of the complex ω plane. Introduce the corresponding retarded and advanced functions, and construct a Lehmann representation for their Fourier transforms. Discuss the analytic properties and derive the dispersion relations analogous to Eq. (7.70), Fetter and Walecka.
Hint: See Eqs. (223.2) and (224.1) from the lecture notes.

P.05. P.3.11, Fetter and Walecka and P.4.2, Miranda: Free fermions on a external potential. Consider a system of noninteracting spin-$1/2$ fermions in an external static potential with a Hamiltonian

$$H^{ex} = \sum_{\alpha,\beta} \int d^3r \, \psi_\alpha^\dagger V_{\alpha\beta}(\mathbf{r}) \psi_\beta(\mathbf{r}).$$

(a) Use Wick's theorem to find the Feynman rules (in coordinate spaces) for the single-particle Green's function in the presence of an external potential.

(b) Show that Dyson's equation becomes

$$G^{ex}_{\alpha\beta}(x,y) = G^0_{\alpha\beta}(x-y) + \frac{1}{\hbar} \sum_{\mu,\nu} \int d^4z \, G^0_{\alpha\mu}(x-z) V_{\mu\nu}(\mathbf{z}) G^{ex}_{\nu\beta}(z,y).$$

(c) Consider a spin independent potential,

$$V_{\alpha\beta}(\mathbf{r}) = \delta_{\alpha\beta} V(\mathbf{r}),$$

and derive the Dyson equation in momentum space. In this case, the Fourier transform of the Green's function $G^{ex}(x,x')$ assumes the form

$$G^{ex}(x,x') = \int \frac{d^3k \, d^3q \, d\omega}{(2\pi)^7} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}'} e^{-i\omega(t-t')} G^{ex}(\mathbf{k},\mathbf{q},\omega),$$

since spatial translation invariance is broken due to the external potential. Show that

$$G^{ex}(\mathbf{k},\mathbf{q},\omega) = G^{(0)}(\mathbf{k},\omega)\delta_{\mathbf{k},\mathbf{q}} + G^{(0)}(\mathbf{k},\omega) T(\mathbf{k},\mathbf{q},\omega) G^{(0)}(\mathbf{q},\omega)$$

where $T(\mathbf{k},\mathbf{q},\omega)$ is the T-matrix for the scattering potential, and determine an equation for $T(\mathbf{k},\mathbf{q},\omega)$.

(d) Consider the local potential

$$V(\mathbf{r}) = U\delta^{(d)}(\mathbf{r})$$

in d-dimensions and determine the T-matrix, which, in this particular case, is momentum independent. For $d \leq 2$ and $U < 0$, show that there is a bound state, regardless the value of U.
Hint: In order to calculate the momentum integrals, it is necessary to introduce a cut-off $k < \Lambda$; recall that the energy spectrum is related to the poles of the T-matrix.

P.06. P.3.12, Fetter and Walecka: Second-order contributions to the self-energy.
Consider a uniform system of spin-$1/2$ fermions with spin-independent interactions.

(a) Use the Feynman rules in momentum space to write out the second-order contributions to the proper self-energy; evaluate the frequency integrals (some of them will vanish).

(b) Hence show that the second-order contribution to the ground-state energy can be written as [see Eq. (9.38), Fetter and Walecka]

$$\begin{aligned}\frac{E^{(2)}}{V} &= \frac{2m}{\hbar^2}\int \frac{d^3k\, d^3p\, d^3q\, d^3q'}{(2\pi)^9}\delta(\mathbf{k}+\mathbf{p}-\mathbf{q}-\mathbf{q}') \\ &\quad \times \left[2V(\mathbf{q}-\mathbf{k})^2 - V(\mathbf{q}-\mathbf{k})V(\mathbf{p}-\mathbf{q})\right] \\ &\quad \times \frac{\theta(k_F-p)\theta(k_F-k)\theta(q'-k_F)\theta(q-k_F)}{p^2+k^2-q^2-q'^2+i\eta}.\end{aligned}$$

(c) Specialize to an electron gas and rederive the results of Prob. 1.4, Fetter and Walecka.

P.07. P.3.14, Fetter and Walecka: Poles of the single-particle Green's function.
From the expression of the exact single-particle Green's function,

$$G_{\alpha\beta}(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon^0_{\mathbf{k}}/\hbar - \Sigma^*(\mathbf{k},\omega)}\delta_{\alpha\beta},$$

show that the energy $\epsilon_{\mathbf{k}}$ and the damping $|\gamma_{\mathbf{k}}|$ of the long-lived single-particle excitations are given by

$$\epsilon_{\mathbf{k}} = \epsilon^0_{\mathbf{k}} + \mathrm{Re}\,\hbar\Sigma^*(\mathbf{k},\epsilon_{\mathbf{k}}/\hbar)$$

and

$$\gamma_{\mathbf{k}} = \left[1 - \frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma^*(\mathbf{k},\omega)|_{\epsilon_{\mathbf{k}}/\hbar}\right]^{-1}\,\mathrm{Im}\,\Sigma^*(\mathbf{k},\epsilon_{\mathbf{k}}/\hbar).$$

08. P.x.x, Cologne: From the Hubbard to the t-J model
Let us consider the single-band Hubbard model

$$\hat{H} = \hat{T} + \hat{V} = -t \sum_{\langle i,j \rangle\, \sigma} c^{\dagger}_{i\,\sigma} c_{j\,\sigma} + U \sum_{i} \hat{n}_{i\,\uparrow} \hat{n}_{i\,\downarrow}, \tag{4}$$

where $c^{\dagger}_{i\,\sigma}$ ($c_{i\,\sigma}$) creates (annihilates) an electron with spin $\sigma = \uparrow, \downarrow$ on a lattice site i, $\hat{n}_{i\,\sigma} = c^{\dagger}_{i\,\sigma} c_{i\,\sigma}$ is the electron density operator, t is the hopping energy, and $U > 0$ is the on-site repulsion energy. Notice that U is the amount of energy that should be paid if two electrons are on the same lattice site. We want to study the model (4) in the limit $U \gg t$. An effective Hamiltonian ($\hat{H}_{eff}$), which describes the low-energy sector of the model (4), can be derived using second order perturbation theory which can be implemented via a canonical transformation.

(a) The Hilbert space of the model (4) can be divided into two subspaces $\mathcal{S}$ and $\mathcal{D}$, where the former contains configurations in which there is either zero or one electron per lattice site, while the latter contains at least one doubly occupied lattice site. Show that the hopping term $\hat{T}$ can be written as $\hat{T} = \hat{T}_0 + \hat{T}_+ + \hat{T}_-$, where

$$\begin{aligned}
\hat{T}_0 &= -t \sum_{\langle i,j \rangle\, \sigma} (1 - \hat{n}_{i\,-\sigma}) c^{\dagger}_{i\,\sigma} c_{j\,\sigma} (1 - \hat{n}_{j\,-\sigma}) + \hat{n}_{i\,-\sigma} c^{\dagger}_{i\,\sigma} c_{j\,\sigma} \hat{n}_{j\,-\sigma}, \\
\hat{T}_+ &= -t \sum_{\langle i,j \rangle\, \sigma} \hat{n}_{i\,-\sigma} c^{\dagger}_{i\,\sigma} c_{j\,\sigma} (1 - \hat{n}_{j\,-\sigma}), \\
\hat{T}_- &= -t \sum_{\langle i,j \rangle\, \sigma} (1 - \hat{n}_{i\,-\sigma}) c^{\dagger}_{i\,\sigma} c_{j\,\sigma} \hat{n}_{j\,-\sigma}.
\end{aligned} \tag{5}$$

Here $-\sigma = \uparrow$ if $\sigma = \downarrow$ and vice-versa. What kind of process does each of the three terms in Eq. (5) describe? Why can we treat $\hat{H}_1 = \hat{T}_+ + \hat{T}_-$ as a perturbation to $\hat{H}_0 = \hat{T}_0 + \hat{V}$ in the limit $U \gg t$?

(b) In order to calculate the effective Hamiltonian $\hat{H}_{eff}$ described above, we perform the following canonical transformation

$$\begin{aligned}
\hat{H}_{eff} = e^{\hat{S}} \hat{H} e^{-\hat{S}} &= \hat{H} + [\hat{S}, \hat{H}] + \frac{1}{2!}[\hat{S}, [\hat{S}, \hat{H}]] + \ldots \\
&= \hat{H}_0 + \hat{H}_1 + [\hat{S}, \hat{H}_0] + [\hat{S}, \hat{H}_1] + \frac{1}{2!}[\hat{S}, [\hat{S}, \hat{H}_0]] + \ldots,
\end{aligned} \tag{6}$$

where the operator $\hat{S}$ is determined by imposing that the term linear in t in Eq. (6) vanishes, i.e.,

$$\hat{H}_1 + [\hat{S}, \hat{H}_0] = 0, \tag{7}$$

The effective Hamiltonian then reads

$$\hat{H}_{eff} = \hat{H}_0 + \frac{1}{2}[\hat{S}, \hat{H}_1] + \mathcal{O}(t^3). \tag{8}$$

Show that the condition (7) is fullfiled in first order in t/U if we choose

$$\hat{S} = \frac{1}{U}\left(a^{+}\hat{T}_{+} + a^{-}\hat{T}_{-}\right). \tag{9}$$

Calculate the constants a^{+} and a^{-}. Verify that $\hat{S}$ is anti-hermitian.

(c) Before we continue, prove the following identity

$$\sum_{\sigma,\sigma'} c^{\dagger}_{i\,\sigma} c^{\dagger}_{j\,\sigma'} c_{i\,\sigma'} c_{j\,\sigma} = -\frac{1}{2}\left(\hat{n}_i \hat{n}_j + 4\mathbf{S}_i \cdot \mathbf{S}_j\right), \qquad\qquad i \neq j \tag{10}$$

where the spin operator is defined as

$$\mathbf{S}_i = \frac{1}{2}\sum_{\sigma,\sigma'} c^{\dagger}_{i\,\sigma} \hat{\tau}_{\sigma,\sigma'} c_{i\,\sigma'} \tag{11}$$

with $\hat{\tau} = (\tau_x, \tau_y, \tau_z)$ a vector of Pauli matrices.

(d) Suppose that we are at half-filling, i.e., $\langle \hat{n}_i \rangle = \langle \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \rangle = 1$. Using the results of item (b), calculate $\hat{H}_{eff}$. Project the resulting Hamiltonian into the subspace $\mathcal{S}$ and explain why some terms drop out after the projection. Use the identity (10) and show that $\hat{H}_{eff}$ can be written as

$$\hat{H}_{eff} = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}\right), \tag{12}$$

where the exchange constant $J = 4t^2/U$.

(e) Suppose we now move away from half-filling by introducing some holes in the system. In this case, Eq. (12) should be modified, i.e., some extras terms should be added to it. The final result is the so-called t-J model, which is relevant for the description of the high-T$_c$ superconductors. Using the results of the previous items, derive the Hamiltonian of the t-J model.