Problem set 2 - Many-body theory SFI7534

1. **Weakly interacting Fermions.** Consider a system of N interacting spin-1/2 fermions the Hamiltonian of which is

$$H=\sum_i \frac{p_i^2}{2m}+\frac{g}{2}\sum_{i\neq j} f\left(\mathbf{r}_i-\mathbf{r}_j\right),$$

where $f(\mathbf{r})=f\left(r\right)$ parameterizes the interaction between the particles which are spin independent and depends only on the distance between the particles. The constant g parameterizes the strength of the interactions.

   (a) Write H in second quantization. (*Hint*: Recall that the field operator $\psi\left(\mathbf{r}\right)=\left(2\pi\right)^{-3/2}\int d\mathbf{p}e^{i\mathbf{p}\cdot\mathbf{r}}a_{\mathbf{p}}$ annihilates a particle at position $\mathbf{r}$ and that $\left|\mathbf{r}\right\rangle=\psi^{\dagger}\left(\mathbf{r}\right)\left|0\right\rangle$.)

   (b) For $f\left(\mathbf{r}\right)=\delta\left(\mathbf{r}\right)$, compute the ground state energy up to first order in perturbation theory for g.

   (c) Show that, unlike the Jellium model, the weak interacting regime corresponds to the low-density limit. Why is that so?

   (d) Show that the spin density operator

$$\mathbf{S}\left(\mathbf{r}\right)=\left(\begin{array}{cc}\psi_{\uparrow}^{\dagger} & \psi_{\downarrow}^{\dagger}\end{array}\right)\frac{\boldsymbol{\sigma}}{2}\left(\begin{array}{c}\psi_{\uparrow}\\ \psi_{\downarrow}\end{array}\right)=\frac{1}{2}\sum_{\alpha,\beta}\psi_{\alpha}^{\dagger}\left(\mathbf{r}\right)\boldsymbol{\sigma}_{\alpha,\beta}\psi_{\beta}\left(\mathbf{r}\right),$$

   where $\boldsymbol{\sigma}=\left(\sigma^{x},\sigma^{y},\sigma^{z}\right)$ are the Pauli matrices, satisfies the SU(2) algebra $\left[S^{a}\left(\mathbf{r}\right),S^{b}\left(\mathbf{r}'\right)\right]=i\varepsilon_{abc}S^{c}\left(\mathbf{r}\right)\delta\left(\mathbf{r}-\mathbf{r}'\right)$, where ε_{abc} is the Levi-Civita tensor and the sum over the c index is implicit.

   (e) Show that the total spin $\mathbf{S}_{\mathrm{Tot}}=\int d\mathbf{r}\mathbf{S}\left(\mathbf{r}\right)$ commutes with H. Why is this expected?

2. **Hubbard model I.** Consider the Hubbard model given by

$$H=-t\sum_{\sigma}\sum_{\langle i,j\rangle}\left(c_{i,\sigma}^{\dagger}c_{j,\sigma}+\text{h.c.}\right)+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow},$$

where $n_{i,\sigma}=c_{i,\sigma}^{\dagger}c_{i,\sigma}$.

   (a) In the Heisenberg picture, obtain the equation of motion for $c_{i,\sigma}(t)$.

   (b) Obtain the equation of motion for $A_{j,\sigma}(t)$, where $A_{j,\sigma}=n_{i,-\sigma}c_{i,\sigma}$.

   (c) Consider the following approximations

$$\begin{aligned}n_{i,-\sigma}(t)c_{j,\sigma}(t)&\approx\left\langle n_{i,-\sigma}\right\rangle c_{j,\sigma}(t),\\ c_{j,-\sigma}^{\dagger}(t)c_{i,-\sigma}(t)c_{i,\sigma}(t)&\approx\left\langle c_{j,-\sigma}^{\dagger}c_{i,-\sigma}\right\rangle c_{i,\sigma}(t),\\ c_{i,-\sigma}^{\dagger}(t)c_{j,-\sigma}(t)c_{i,\sigma}(t)&\approx\left\langle c_{i,-\sigma}^{\dagger}c_{j,-\sigma}\right\rangle c_{i,\sigma}(t),\end{aligned}$$

   where $\langle\cdots\rangle$ means the ground-state mean value. (Why are these mean values time independent?) Apply these approximation on the equation of motion for $A_{j,\sigma}(t)$ and show that it depends only on $A_{j,\sigma}(t)$ and $c_{i,\sigma}(t)$.

   (d) Within these approximations, solve the equation of motion for $c_{\mathbf{k},\sigma}(\omega)$. The corresponding frequencies are associated to the system normal modes. The approximation used gives us two bands. Discuss on the nature of these bands, investigate if and when there are gaps, etc. Make schematic diagrams and plots. Physically, when this approximation is reasonable or not? Which aspects of your results do you expect to change in a more sophisticate approximation?

3. **Hubbard model II.** Consider the attractive Hubbard model in the low-density limit, i.e., $U<0$ and $N\ll N_s$, where N is the total number of electrons and N_s is the number of sites. For simplicity, consider that N is even. In the following, consider the strongly interacting limit $-U\gg t$.

(a) The lowest energy sector is that in which a site is either completely empty or doubly occupied. How many states are there in this sector?

(b) Let $B_j = c_{j,\uparrow}c_{j,\downarrow}$ be the electron pair annihilation operator. Show that $[B_i, B_j] = 0$ and that $\left[B_i, B_j^\dagger\right] \approx \delta_{i,j}$. Why the B operators are not exactly bosonic operators?

(c) Using perturbation theory in the lowest energy sector, obtain the effective Hamiltonian for the B operators and interpret each term.

(d) *Optional*: Analyze the effective Hamiltonian obtained and conclude if the system is a metal, a insulator, or something else. In which dimensions do you think your conclusion is valid?

4. **Bose-Hubbard model.** In cold atomic systems, it is possible to experimentally realize the Hubbard model for bosons (often called Bose-Hubbard model) with two internal states (often called bosons with pseudospin-1/2). In addition, the hopping amplitude depend on these internal states [see L.-M. Dual et al., Phys. Rev. Lett. **91**, 090402 (2003)]. Consider the Hamiltonian

$$H = -\sum_{\langle i,j\rangle}\sum_{\sigma} t_\sigma \left(b_{i,\sigma}^\dagger b_{j,\sigma} + \text{h.c.}\right) + \frac{1}{2}U\sum_i n_i\left(n_i - 1\right),$$

where $b_{j,\sigma}$ annihilates a boson at site j in the internal state σ (which is either $\uparrow$ or $\downarrow$), $n_j = \sum_\sigma b_{j,\sigma}^\dagger b_{j,\sigma}$, and $t_\uparrow \neq t_\downarrow$.

(a) Show that the effective spin Hamiltonian for the corresponding Mott insulator $U \gg t_\sigma$ (in the filling of one boson per site) is (up to an irrelevant constant) the XXZ spin-1/2 model

$$H_{\text{eff}} = \sum_{\langle i,j\rangle}\left[J^x\left(S_i^x S_j^x + S_i^y S_j^y\right) + J^z S_i^z S_j^z\right],$$

where the exchange constants $J^{x,z}$ are to be computed.

(b) *Optional*: What is the corresponding model for $t_\uparrow = t_\downarrow$? Could this result be obtained based on the symmetries of the Bose-Hubbard model? What is the physical interpretation of the sign of the coupling constants? What is the symmetry of the model when $t_\uparrow \neq t_\downarrow$?

5. **Direct exchange.** Consider the following term which was neglected in the Hubbard model:

$$H_{\text{DE}} = \sum_{i,j}\sum_{\sigma_1,\sigma_2}\langle i,j\left|V(\mathbf{r}_1 - \mathbf{r}_2)\right|j,i\rangle\, c_{i,\sigma_1}^\dagger c_{j,\sigma_2}^\dagger c_{i,\sigma_2} c_{j,\sigma_1},$$

where

$$\langle i,j\left|V\right|j,i\rangle = e^2\int \mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\frac{\phi_i^*(\mathbf{r}_1)\phi_j(\mathbf{r}_1)\phi_j^*(\mathbf{r}_2)\phi_i(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \equiv J_{\text{DE}} > 0$$

is the Coulombian exchange integral between orbital ϕ_i and ϕ_j.

(a) What is the physical process described by H_{DE}?

(b) In the strong interaction limit $U \gg |t|, J_{\text{DE}}$ and at half-filling $n_{i,\uparrow} + n_{i,\downarrow} = 1$, show that H_{DE} gives rise to the ferromagnetic Heisenberg model.

6. **Magnon interaction.** Keeping up to quadratic terms in the bosonic operators of the Holstein-Primakoff transformation in the Heisenberg ferromagnet, obtain the magnon interaction given by

$$H_{\text{int}} = \frac{1}{N}\sum_{\mathbf{p},\mathbf{k},\mathbf{q}} V(\mathbf{p},\mathbf{k},\mathbf{q})a_{\mathbf{p}+\mathbf{q}}^\dagger a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}} a_{\mathbf{p}}.$$

Compute the scattering amplitude $V(\mathbf{p},\mathbf{k},\mathbf{q})$ and discuss its behavior in the limit when the momentum of one of the magnons vanishes.

7. **Antiferromagnetic spin waves.** Consider the spin-S antiferromagnetic Heisenberg model in a bipartite lattice (a hypercubic one, if you wish). Consider also that its “vacuum” (ground state) is the Néel state in which all spins of one sublattice is in the state $|m^z\rangle = |{+S}\rangle$ while all the spins in the other sublattice is in the “opposite” state $|m^z\rangle = |{-S}\rangle$.

(a) Let $a_j^\dagger$ be the Holstein-Primakoff operator creating an excitation on the vacuum of the "up" sublattice at site j. Comparingt $S^\pm|m^z\rangle = \sqrt{(S \mp m^z)(S \pm m^z + 1)}\,|m^z \pm 1\rangle$ with $a|n\rangle = \sqrt{n}\,|n-1\rangle$ and $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$, write the corresponding transformation between the spins and the a_j bosons.

(b) Likewise, write the corresponding transformation between spins and the b_j bosons, where $b_j^\dagger$ creates an excitation at the jth site of the "down" sublattice.

(c) Using the above Holstein-Primakoff representations, write the antiferromagnetic Heisenberg model in terms of these bosons up to quadratic order. What is the physical meaning of this approximation and when it is expected to be better?

(d) Diagonalize the quadratic Hamiltonian and obtain the dispersion of the antiferromagnons. (*Hint*: use the Bogoliubov transformation.) Expand for small k and compare with that of the ferromagnons.

(e) Obtain the energy correction to that of the classical Néel state. (It is not necessary to compute the integral.)

(f) Obtain the correction to the sublattices magnetization. (Again, it is not necessary to compute the integrals.) Show that, for one spatial dimension $d = 1$, the correction is diverging, suggesting the lost of the validity of the approximation. What else does this result suggest?

(g) Compute the low-temperature dependence of the heat capacity and of the staggered magnetization in d spatial dimensions.

8. Show that the total spin $\mathbf{S}_\mathrm{T} = \sum_{i=1}^N \mathbf{S}_i$ commutes with the Heisenberg Hamiltonian. Thus, the ferromagnetic order parameter (which is the total magnetization) is a conserved quantity. Show however that the operator associated to the antiferromagnetic order parameter, the staggered magnetization operator $\mathbf{M}_\mathrm{AF} = \sum_{j=1}^N e^{i\mathbf{Q}\cdot\mathbf{R}_j}\mathbf{S}_j$, with the ordering vector $\mathbf{Q} = (\pi,\pi,\pi)$ (for a cubic lattice), does not commute with the Heisenberg Hamiltonian and thus, the AF order parameter is not a constant of motion. Nonetheless, in the AF phase, there is a spontaneous symmetry breaking and the staggered magnetization can be considered as a conserved quantity. This is a subtle and important issue at the heart of the spontaneous-symmetry-breaking theory and requires a careful analysis on how the thermodynamic limit is taken in the presence of a vanishing symmetry-breaking term. A careful discussion (and one of the pioneering ones) can be found in P. W. Anderson, Phys. Rev. **86**, 694 (1952).

9. **Fermionization of a spin system.** In one spatial dimension, there is an important transformation between spinless fermions (c_j) and spin-1/2 (S_j) operators known as the Jordan-Wigner transformation given by

$$\begin{aligned} S_j^z &= n_j - \frac{1}{2}, \\ S_j^+ &= e^{i\pi\phi_j} c_j^\dagger, \\ S_j^- &= e^{-i\pi\phi_j} c_j, \end{aligned}$$

where $n_j = c_j^\dagger c_j$ and $\phi_j = \sum_{l<j} n_l$.

(a) Given that the spin operators $\mathbf{S}_j$ obey the angular momentum algebra, show that the fermionic operators obey the anti-commutation relations $\{c_i, c_j\} = 0$ and $\left\{c_i, c_j^\dagger\right\} = \delta_{i,j}$. What is the importance of the string operator (the exponential term)?

(b) What is the correspondence (physical interpretation) between the spins and the spinless fermions?

(c) Fermionize the spin-1/2 XXZ chain

$$H = \sum_{i=1}^{L-1}\left[J^x\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + J^z S_i^z S_{i+1}^z\right],$$

and give an interpretation between each of the terms in the resulting Hamiltonian.

(d) Obtain the spectrum of the spin-1/2 XX chain (the $J^z = 0$ case) in the $L \to \infty$ limit.