Problem set 4

1. **Spin-waves in an AFM:** assume a 1D chain with $2N$ sites described by the Heisenberg Hamiltonian:

$$\mathcal{H} = J \sum_i \vec{S}_i \vec{S}_{i+1}$$

where $\vec{S}_i$ is the spin at site i, and cyclic boundary conditions are implied and $J > 0$. For simplicity, we assume that only nearest-neighbors are coupled (one can easily generalize the problem for higher dimensions and/or longer-range couplings, provided that they do not introduce frustration).

Let us assume that the Hartree-Fock ground-state is $|HF\rangle = |+S, -S, +S, -S, ..., +S, -S\rangle$ where S is the value of the spin ($S = 1/2$ for electrons). It can be easily shown that $|HF\rangle$ is self-consistent, although it is clearly not an eigenstate of $\mathcal{H}$. We would like to use RPA techniques to find the low-energy excitations above this HF ground-state describing a long-range ordered AFM.

In order to excite the system, we need to either lower a spin at an odd site, $S^-_{2i+1}|HF\rangle$, or raise a spin at an even site $S^+_{2i}|HF\rangle$. Since neither of these kinds of states are eigenvectors of H, we have to assume that the proper operators to create low-energy excited states are a linear combinations of such raising and lowering operators. In order to figure out the most general combination we need to consider, we have to analyze the "interaction" Hamiltonian. For this case,

(a) show that one can rewrite

$$\mathcal{H} = J \sum_i S^z_i S^z_{i+1} + \frac{J}{2} \sum_i \left(S^+_i S^-_{i+1} + S^-_i S^+_{i+1} \right)$$

where $S^\pm = S^x \pm i S^y$.

It should now become apparent that a simple choice for the collective operators $Q^\dagger_\alpha = \sum_{i=1}^N (a_i S^+_{2i} + b_i S^-_{2i+1})$ cannot diagonalize an interaction that contains terms like $S^+_{2i} S^-_{2i+1}$ and $S^-_{2i} S^+_{2i+1}$ (if this is not obvious to you, then try it). It follows that we must use the more general case, and try for

$$Q^\dagger_\alpha = \sum_{i=1}^N (a_i S^+_{2i} + b_i S^-_{2i+1} + c_i S^-_{2i} + d_i S^+_{2i+1})$$

We proceed now with the RPA scheme, trying to find the coefficients a, b, c, d and the energies of the collective modes that satisfy

$$[\mathcal{H}, Q^\dagger_\alpha] \approx \hbar \Omega_\alpha Q^\dagger_\alpha$$

We know that the equality can only hold "in average". Compute the commutator. You should get a result which is a linear combination of two-spin operator terms, while on the right-hand side we have a linear combination of one-spin operator terms. We can now proceed in two ways; either take an extra commutator (as discussed in class) and average the result over the $|HF\rangle$ state, to isolate all 4 possible terms on the right hand side. Or, equivalently, we can "linearize" the two-spin operators on the left-hand side, using $S^\alpha_i S^\beta_j \to \langle S^\alpha_i \rangle S^\beta_j + S^\alpha_i \langle S^\beta_j \rangle$, where $\langle\rangle$ is the expectation value of the corresponding spin operator in the $|HF\rangle$ ground state, and then we can identify term by term operators from left and right hand sides. Both approaches lead to the same results.

You should now solve the linear systems and find the eigenenergies $\hbar\Omega_\alpha$ of the spin-waves. What is the meaning of the quantum number α, and why is that (not) surprising?

Extra questions:

(i). is the spectrum of collective excitations gapless (i.e. one can have $\hbar\Omega$ arbitrarily close to zero) or is it gaped (i.e., there is a minimum non-zero value that $\hbar\Omega$ must take)?

(ii) are these excitations indeed "collective", i.e. do different spins along the chain participate "equally" in them, or not?

(iii). if you did the calculation correctly, it should follow that the general formula for $Q_\alpha^\dagger$ that we used is actually more general than needed. Why is that, and what arguments should one use to start with the simpler overall form? (think of possible good quantum numbers to characterize eigenstates).

2. Let's do the same problem using the Hostein-Primakoff representation for spins. This way you can check your results.

a) Assume $\hat{S}_x, \hat{S}_y, \hat{S}_z$ are the spin operators corresponding to a spin S, satisfying the usual algebra (take $\hbar = 1$) $[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma$. Assume that $a, a^\dagger$ are a pair of bosonic operators, $[a, a^\dagger] = 1$. Show that we can then represent the spin operators as:

$$\hat{S}_z = S - a^\dagger a; \hat{S}_+ = \sqrt{(2S - a^\dagger a)}a; \hat{S}_- = a^\dagger\sqrt{2S - a^\dagger a}$$

i.e., that in this case the proper commutation relations are satisfied and that you get the expected eigenstates with the usual raising and lowering action of S_+ and S_-.

b) show that the same can be achieved by using the representation

$$\hat{S}_z = -S + b^\dagger b; \hat{S}_+ = b^\dagger\sqrt{2S - b^\dagger b}; \hat{S}_- = \sqrt{(2S - b^\dagger b)}b$$

Either of these are called Hostein-Primakoff representations. We use one or the other depending on whether we expect the spin to be closer to "up"$= |S, +S\rangle$ state, or closer to 'down"$= |S, -S\rangle$ state.

Consider now a 1D AFM chain with spins of magnitude S. Assuming that in the ground-state, even site spins are "up", and odd site spins are "down", rewrite the Heisenberg Hamiltonian in terms of operators a_{2i} and b_{2i+1} associated with spins at even/odd sites. Now, in the ground-state we expect the spins to be close to full polarization, and therefore $< a_{2i}^\dagger a_{2i} >= S - < S_{2i}^z > \to 0$, etc. (i.e., very few spins are flipped). If this is true, we can use Taylor expansion to simplify $\sqrt{2S - a_{2i}^\dagger a_{2i}} \approx \sqrt{2S}$, and same for b's. After this approximation, you should be left with a Hamiltonian that is quadratic in a and b operators, and can be diagonalized. Find its spectrum and explain why this is (hopefully) just the spin-wave spectrum you found in the previous problem.

Comments:

These mean-field type approximations always find gapless spin-wave excitations (spin-waves) for a 1D AFM. In reality, it turns out that if the spins are integer, then the excitation spectrum is gapped. Only for half-spin integers the gap is closed and we have such spin-wave excitations. This is a purely quantum 1D effect and can be understood in terms of spin path integrals.

3. **Spin waves in a double-exchange or Zener Hamiltonian**: Let's consider the following Hamiltonian

$$H = -t\sum_{i,\sigma}(c_{i\sigma}^\dagger c_{i+1,\sigma} + h.c.) - J\sum_i \vec{s}_i \cdot \vec{S}_i$$

which describes electrons hopping along a $1D$ chain with N sites (cyclic boundary conditions assumed). At each site along the chain there is a spin $\vec{S}_i$, and there is on-site ferromagnetic coupling ($J > 0$) between the spin of the electrons $\vec{s}_i = 1/2\sum_{\alpha,\beta} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$ and these "lattice" spins. (Such Hamiltonians appear, for instance, in the study of manganites).

Let us assume that the number of electrons is $N_0 = pN$, where $p << 1$ (i.e., we are well below half-filling).

(1). Find the true ground-state of the system (hint: we know from problem 1 of Set 3 that at low densities, metallic systems have a tendency towards ferromagnetism - so start with a reasonable "guess" for what a FM ground-state might look like, and show that it is indeed an eigenstate of the full Hamiltonian). What do you think that the ground-state might look like if $p \approx 1$? (speculate, no need for detailed calculations).

(2). What is the ground-state energy per site, E_0/N? (hint: since the electron concentration is low, and therefore k_F is small, you can expand $2t\cos(ka) \approx 2t(1 - k^2a^2/2)$.)

(3). What is the spectrum of collective spin-wave excitations for this system? I'll help you by telling you that if all symmetries as well as the form of the Hamiltonian are taken into consideration, the most general form for the creation operator of a spin-wave with momentum q is

$$Q_q^\dagger = \alpha \sum_{n=1}^{N} \frac{1}{\sqrt{N}} e^{iqna} S_n^- + \sum_k \beta_k c_{k\downarrow}^\dagger c_{k-q,\uparrow}$$

Can you justify this general form? (and by the way, are there other types of collective excitations possible?) Find the system of equations relating α, β_k and $\hbar\Omega_q$. Solve it. You should find a final equation for $\hbar\Omega_q$ of the form

$$\hbar\Omega_q = a + b \sum_{|k|<k_F} \frac{1}{\hbar\Omega_q - JS + \epsilon_{k+q} - \epsilon_k}$$

where $\epsilon_k = 2tcos(ka)$. What are the constants a and b?

(4). Perform the integral assuming again that you can expand ϵ_k up to quadratic terms for all $|k| < k_F$. Find the long wave-length spectrum $\hbar\Omega_q$ in the limit $q \to 0$ (hint: this is a ferromagnet).

4. And finally: **the one-particle Green's function for a free bosonic system**. Consider a non-interacting, bosonic Hamiltonian:

$$\mathcal{H} = \sum_q \hbar\omega_q b_q^\dagger b_q$$

(for example, this could describe phonons in a crystals). In turns out that in most Hamiltonians involving phonons, the phonon operators usually appear in the combination:

$$\hat{\phi}_q = b_q^\dagger + b_{-q}$$

(see for instance the electron-phonon Hamiltonian discussion). Because of this, instead of working with Green's functions defined in direct analogy with the ones for fermions, it is more convenient to use the definition:

$$D(k_1, t_1; k_2, t_2) = -i\langle\Psi_0|T\{\hat{\phi}_{k1}^\dagger(t_1)\hat{\phi}_{k_2}(t_2)\}|\Psi_0\rangle$$

where $\hat{\phi}_q(t) = \exp(\frac{i}{\hbar}\mathcal{H}t)\hat{\phi}_q \exp(-\frac{i}{\hbar}\mathcal{H}t)$ and $|\Psi_0\rangle$ is the ground-state. Calculate the Fourier transform of this propagator, $D(k_1, k_2, \omega)$, for the non-interacting Hamiltonian given above.