Physics 561, Fall Semester 2009
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Problem Set No. 2: Green Functions and Perturbation Theory Due Date: October 11, 2009

1 Antiferromagnetic Spin Waves

In this problem you will consider the Heisenberg model of a one-dimensional quantum antiferromagnet. I first give you a brief summary on the Heisenberg model. You **do not** need to have any previous knowledge on magnetism (or the Heisenberg model) to do this problem. You will be able to solve this problem only with the methods that were discussed in class.

The one-dimensional Heisenberg model is defined on a linear chain (a one-dimensional lattice) with N sites. The lattice spacing will be taken to be equal to one (*i.e.,* it is the unit of length). The quantum mechanical Hamiltonian for this system is

$$\hat{H} = J \sum_{n=-N/2+1}^{N/2} \hat{S}_k(n) \cdot \hat{S}_k(n+1) \tag{1}$$

where the exchange constant $J > 0$ (*i.e.,* an antiferromagnet) and the operators $\hat{S}_k$ $(k = 1, 2, 3)$ are the three angular momentum operators in the spin-S representation (S is integer or half-integer) which satisfy the commutation relations

$$[\hat{S}_j, \hat{S}_k] = i\epsilon_{jkl}\hat{S}_l \tag{2}$$

For simplicity we will assume periodic boundary conditions, $\hat{S}_k(n) \equiv \hat{S}_k(n+N)$.

In the semi-classical limit, $S \to \infty$, the operators act like real numbers since the commutators vanish. In this limit, the state with lowest energy has nearby spins which point in opposite (but arbitrary!) directions in spin space. This is the classical Néel state. In this state the spins on one *sub-lattice* (say the *even* sites) point *up* along some direction in space while the spins on the other sub-lattice (the *odd* sites) point down. At finite values of S, the spins can only have a definite projection along one axis but not along all three at the same time. Thus we should expect to see some zero-point motion precessional effect that will depress the net projection of the spin along any axis but, if the state is stable, even sites will have predominantly up spins while odd sites will have predominantly down spins. This observations motivate the following definition of a set of basis states for the full Hilbert space of this system.

The states $|\Psi\rangle$ of the Hilbert space of this chain are spanned by the tensor product of the Hilbert spaces of each individual j^{th} spin $|\Psi_j\rangle$, $|\Psi\rangle = \prod_j \otimes |\Psi_j\rangle$. The latter are simply the $2S+1$ degenerate multiplet of states with angular momentum S of the form $\{|S, M(j)\rangle\}$ ($|M(j)| \leq S$) which satisfy

$$\begin{aligned}
\vec{S}^2(j)|S, M(j)\rangle &= S(S+1)|S, M(j)\rangle \\
S_3(j)|S, M(j)\rangle &= M(j)|S, M(j)\rangle
\end{aligned} \tag{3}$$

The states in this multiplet can be obtained from the *highest weight state* $|S, S\rangle$ by using the lowering operator $\hat{S}^- = \hat{S}_1 - i\hat{S}_2$. Its adjoint is the raising operator $\hat{S}^+(j) = \hat{S}_1(j) + i\hat{S}_2(j)$. For reasons that will become clear below, it is *convenient* to define for j *even* (even site) the *spin-deviation* operator $\hat{n}(j) \equiv S - \hat{S}_3(j)$. For an odd site (j odd) the spin deviation operator is $\hat{n}(j) \equiv S + \hat{S}_3(j)$. For j even, the highest weight state $|S, S\rangle$ is an eigenstate of $\hat{n}(j)$ with eigenvalue zero while the state $|S, -S\rangle$ has eigenvalue $2S$

$$\begin{aligned}
\hat{n}(j)|S, S\rangle &= (S - \hat{S}_3(j))|S, S\rangle = 0 \\
\hat{n}(j)|S, -S\rangle &= (S - \hat{S}_3(j))|S, -S\rangle = 2S\ |S, -S\rangle
\end{aligned} \tag{4}$$

whereas for j odd the state $|S, -S\rangle$ has zero eigenvalue while the state $|S, S\rangle$ has eigenvalue $2S$.

In terms of the operators $\hat{n}(j)$, the basis states are $\{|S, M(j)\rangle\} \equiv \{|n(j)\rangle\}$, where $M(j) = S \mp n(j)$. For even sites, the raising and lowering operators $\hat{S}(j)^{\pm}$ act on the states of this basis like

$$\begin{aligned}
\hat{S}^+|n\rangle &= \left[2S\left(1 - \frac{n-1}{2S}\right)\ n\right]^{\frac{1}{2}} |n-1\rangle \\
\hat{S}^-|n\rangle &= \left[2S(n+1)\left(1 - \frac{n}{2S}\right)\right]^{\frac{1}{2}} |n+1\rangle
\end{aligned} \tag{5}$$

For odd sites the action of the above two operators is interchanged.

The action of the operators $\hat{S}^{\pm}$ is somewhat similar to that of annihilation and creation operators in harmonic oscillator states. For this reason we define a set of creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ such that

$$\begin{aligned}
\hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\
\hat{a}|n\rangle &= \sqrt{n}|n-1\rangle
\end{aligned} \tag{6}$$

which satisfy the conventional algebra $[\hat{a}, \hat{a}^\dagger] = 1$. Since we have two sub-lattices and the operators $\hat{S}^{\pm}$ are different on each sub-lattice, it is useful to introduce two types of creation and annihilation operators: the operators $\hat{a}^\dagger(j)$ and $\hat{a}(j)$ which act on even sites, and $\hat{b}^\dagger(j)$ and $\hat{b}(j)$ which act on odd sites. They obey the commutation relations

$$\begin{aligned}
\left[\hat{a}(j), \hat{a}^\dagger(k)\right] &= \left[\hat{b}(j), \hat{b}^\dagger(k)\right] = \delta_{jk} \\
\left[\hat{a}(j), \hat{a}(k)\right] &= \left[\hat{b}(j), \hat{b}(k)\right] = \left[\hat{a}(j), \hat{b}(k)\right] = 0
\end{aligned} \tag{7}$$

and similar equations for their hermitian conjugates. It is easy to check that the action of raising and lowering operators on the states $\{|n\rangle\}$ is the *same* as the action of the following operators on the same states

1. On even sites:

$$
\begin{aligned}
\hat{S}^{+}(j) &= \sqrt{2S}\left[1-\frac{\hat{n}(j)}{2S}\right]^{\frac{1}{2}} \hat{a}(j) \\
\hat{S}^{-}(j) &= \sqrt{2S}\hat{a}^{\dagger}(j)\left[1-\frac{\hat{n}(j)}{2S}\right]^{\frac{1}{2}} \\
\hat{S}_3(j) &= S-\hat{n}(j) \\
\hat{n}(j) &= \hat{a}^{\dagger}(j)\hat{a}(j)
\end{aligned}
\tag{8}
$$

2. On odd sites:

$$
\begin{aligned}
\hat{S}^{-}(j) &= \sqrt{2S}\left[1-\frac{\hat{n}(j)}{2S}\right]^{\frac{1}{2}} \hat{b}(j) \\
\hat{S}^{+}(j) &= \sqrt{2S}\hat{b}^{\dagger}(j)\left[1-\frac{\hat{n}(j)}{2S}\right]^{\frac{1}{2}} \\
\hat{S}_3(j) &= -S+\hat{n}(j) \\
\hat{n}(j) &= \hat{b}^{\dagger}(j)\hat{b}(j)
\end{aligned}
\tag{9}
$$

Notice that although the integers n can now range from 0 to infinity, the Hilbert space is still finite since (for even sites) $\hat{S}^{-}|n=2S\rangle = 0$. Similarly, for odd sites, the state $|n=2S\rangle$ is anihilated by the operator $\hat{S}^{+}$.

1. Derive the quantum mechanical equations of motion obeyed by the the spin operators $\hat{S}^{\pm}(j), \hat{S}_3(j)$ in the Heisenberg representation, for both j even and j odd. Are these equations linear? Explain your result.

2. Verify that the definition for the operators $S^{\pm}$ and S_3 of equations 7 and 8 are consistent with those of equation 4.

3. Use the definitions given above to show that the Heisenberg Hamiltonian can be written in terms of two sets of creation and annihilation operators $\hat{a}^{\dagger}(j)$ and $\hat{a}(j)$ (which act on even sites), and $\hat{b}^{\dagger}(j)$ and $\hat{b}(j)$ which act on odd sites.

4. Find an approximate form for the Hamiltonian which is valid in the semi-classical limit $S \to \infty$ (or $\frac{1}{S} \to 0$). Include terms which are of order $\frac{1}{S}$ (relative to the leading order term). Show that the approximate Hamiltonian is quadratic in the operators a and b.

5. Make the approximations of section (4) on the equations of motion of section (1). Show that the equations of motion are now linear. Of what order in $\frac{1}{S}$ are the terms that have been neglected?

6. Show that the Fourier transform

$$\begin{aligned} \hat{a}(q) &= \sqrt{\frac{2}{N}} \sum_{j \text{ even}} e^{iqj}\, \hat{a}(j) \\ \hat{b}(q) &= \sqrt{\frac{2}{N}} \sum_{j \text{ odd}} e^{-iqj}\, \hat{b}(j) \end{aligned} \tag{10}$$

   followed by the canonical (Bogoliubov) transformation

$$\begin{aligned} \hat{c}(q) &= \cosh(\theta(q))\, \hat{a}(q) + \sinh(\theta(q))\, \hat{b}^\dagger(q) \\ \hat{d}(q) &= \cosh(\theta(q))\, \hat{b}(q) + \sinh(\theta(q))\, \hat{a}^\dagger(q) \end{aligned} \tag{11}$$

   yields a *diagonal* Hamiltonian H_{SW} of the form

$$H_{\text{SW}} = E_0 + \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \frac{dq}{2\pi}\, \omega(q)(\hat{n}_c(q) + \hat{n}_d(q)) \tag{12}$$

   where $\hat{n}_c(q) = \hat{c}^\dagger(q)\hat{c}(q), \hat{n}_d(q) = \hat{d}^\dagger(q)\hat{d}(q)$, provided that the angle $\theta(q)$ is chosen properly. The operators $\hat{c}(q)$ and $\hat{d}(q)$ and their hermitian conjugates obey the algebra of eq (6). Derive an explicit expression for the angle $\theta(q)$ and for the frequency $\omega(q)$.

7. Find the ground state for this system in this approximation (usually called the *spin-wave* approximation).

8. Find the single particle eigenstates within this approximation. Determine the quantum numbers of the excitations. Find their dispersion (or energy-momentum) relations. Find a set of values of the momentum q for which the energy of the excited states goes to zero. Show that the energy of these states vanish linearly as the momentum approaches the special points and determine the spin-wave velocity v_s at these points. Note: This is the semi-classical or spin-wave approximation. The identities of eq (8) and eq (9) are known as the Holstein-Primakoff identities.

9. Derive an expression for the following propagators in terms of time-ordered expectation values of the bosonic a and b operators introduced above

   (a)
$$D_{33}(nt, n't') = -i\langle \text{gnd}|T\ \hat{S}_3(n,t)\hat{S}_3(n',t')|\text{gnd}\rangle \tag{13}$$

   (b)
$$D_{+-}(nt, n't') = -i\langle \text{gnd}|T\ \hat{S}^+(n,t)\hat{S}^-(n',t')|\text{gnd}\rangle \tag{14}$$

   in momentum and frequency space. Be very careful and very explicit in the way you treat the poles of these propagators. Show that your choice of frequency integration contour yields a propagator which satisfies the correct boundary conditions.

10. Use Wick's theorem to find an expression for the corresponding *time-ordered* functions in the *spin-wave approximation* in momentum and frequency space.

11. Use the results of the prvious sections to show that $D_{+-}(p, \omega)$ has, in the limit $\omega \to 0$, a pole at $p = \pi$. Calculate the residue of this pole. The residue is the *square* of the order parameter of the system in this approximation.

2 The Electron Gas

In this problem you will consider the weakly interacting electron gas we discussed in class.

1. Show that the Feynman propagator for the non-interacting system

$$G_0^{\sigma\sigma'}(x, x') = -i_0 \langle G|T\psi_\sigma(x)\psi^\dagger_{\sigma'}(x')|G\rangle_0 \tag{15}$$

where $|G\rangle_0$ is the ground state of the non-interacting system, has the Fourier transform

$$G_0^{\sigma\sigma'}(\vec{p}, \omega) = \frac{\delta_{\sigma\sigma'}}{\omega - \frac{E_0(\vec{p})}{\hbar} + i\text{sign}(\omega)\,\delta} \tag{16}$$

where $E_0(\vec{p}) = \frac{p^2}{2m} - E_F$. Show that this expression is consistent with the propagator being time ordered.

2. The one-particle *density matrix* is defined by the *equal time* ground state expectation value

$$\sum_\sigma \langle G|\psi^\dagger_\sigma(\vec{x})\psi_\sigma(\vec{y})|G\rangle \tag{17}$$

   (a) Find an exact relation between the one-particle density matrix and the Feynman propagator

   (b) Compute the one-particle density matrix for non interacting fermions. Discuss it behavior at both short and long distances $R =| \vec{x} - \vec{y} |$ compared with the Fermi wavelength $\lambda_F = \hbar/p_F$.

3. (a) Draw *all* the Feynman diagrams in momentum space that contribute to the electron propagator *to second order* in the electron-electron interaction potential

   (b) Find the contribution of each diagram and express your result a suitable momentum integral(s). Make sure you indicate the multiplicity of each diagram (*i. e.* how many diagrams have the same weight) and the fermionic sign of each diagram. Do not do the integrals.

   (c) Show that the vacuum diagrams cancel out to this order.

(d) Classify your connected diagrams into one-particle reducible and one particle irreducible diagrams. Indicate the contributions to the electron self-energy $\Sigma^{\sigma\sigma'}(\vec{p}, \omega)$ at second order in the interaction potential.

4. We will imagine that the electron system interacts with an external potential $V_{\text{ext}}(\vec{x})$ which we will take to be static and to correspond to a point charge of strength Q at the origin, $V_{\text{ext}}(\vec{x}) = Q\delta^{(3)}(\vec{x})$. The *change* of the local density $\delta\rho(\vec{x})$ caused by the perturbation $V_{\text{ext}}(\vec{x})$ is obtained by the expression

$$\delta\rho(\vec{x}) = \langle G|\psi^\dagger_\sigma(\vec{x})\psi_\sigma(\vec{x})|G\rangle\big|_{V_{\text{ext}}} - \langle G|\psi^\dagger_\sigma(\vec{x})\psi_\sigma(\vec{x})|G\rangle\big|_{V_{\text{ext}}=0} \tag{18}$$

(a) Use perturbation theory in the external potential to find an expression for $\delta\rho(\vec{x})$ to linear order in the external potential $V_{\text{ext}}(\vec{x})$ in terms of the *density* propagator of the electronic system that we discussed in class. Which regime of the density propagator is of interest in this case?

(b) Use the results discussed in class to draw conclusions on the spacial behavior of the density. You may want to phrase your answer in momentum space using spacial Fourier transforms. Note: you may quote results on any integrals that you may need from my notes or from textbooks.