

Physics 582, Fall Semester 2021
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Problem Set No. 3:

Canonical Quantization

Due Date: Friday October 8, 2021, 9:00 pm US Central Time

1 Spin waves in a quantum Heisenberg antiferromagnet

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 quantum magnets (or the Heisenberg model) to do this problem. You will be able to solve this problem with the methods 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. The quantum mechanical Hamiltonian for this system is

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

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

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

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

In the semi-classical limit, $S \rightarrow \infty$, 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 the even sites sub-lattice point *up* along some direction in space while the spins on the odd sites sub-lattice 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 $|\Psi_j\rangle$, $|\Psi\rangle = \prod_j |\Psi_j\rangle$. 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

$$\hat{S}^2(j)|S, M(j)\rangle = S(S + 1)|S, M(j)\rangle, \quad \hat{S}_3(j)|S, M(j)\rangle = M(j)|S, M(j)\rangle \quad (3)$$

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 $2S$

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

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 as follows

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

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 as follows. 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

$$\begin{aligned} [\hat{a}(j), \hat{a}^\dagger(k)] &= [\hat{b}(j), \hat{b}^\dagger(k)] = \delta_{jk} \\ [\hat{a}(j), \hat{a}(k)] &= [\hat{b}(j), \hat{b}(k)] = [\hat{a}(j), \hat{b}(k)] = 0 \end{aligned} \quad (6)$$

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:

$$\begin{aligned}\hat{S}^+(j) &= \sqrt{2S} \left[1 - \frac{\hat{n}(j)}{2S} \right]^{\frac{1}{2}} \hat{a}(j), & \hat{S}^-(j) &= \sqrt{2S} \hat{a}^\dagger(j) \left[1 - \frac{\hat{n}(j)}{2S} \right]^{\frac{1}{2}} \\ \hat{S}_3(j) &= S - \hat{n}(j), & \hat{n}(j) &= \hat{a}^\dagger(j) \hat{a}(j)\end{aligned}\quad (7)$$

2. On odd sites:

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

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 annihilated 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 (5).
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 $S \rightarrow \infty$ (or $\frac{1}{S} \rightarrow 0$). 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 part 4 on the equations of motion of part 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 transforms

$$\hat{a}(q) = \sqrt{\frac{2}{N}} \sum_{j \text{ even}} e^{iqj} \hat{a}(j), \quad \hat{b}(q) = \sqrt{\frac{2}{N}} \sum_{j \text{ odd}} e^{-iqj} \hat{b}(j) \quad (9)$$

followed by the canonical (Bogoliubov) transformation

$$\begin{aligned}\hat{c}(q) &= \cosh(\theta(q)) \hat{a}(q) + \sinh(\theta(q)) \hat{b}^\dagger(q) \\ \hat{d}(q) &= \cosh(\theta(q)) \hat{b}(q) + \sinh(\theta(q)) \hat{a}^\dagger(q)\end{aligned}\quad (10)$$

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

$$H_{\text{SW}} = E_0 + \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \frac{dq}{2\pi} \omega(q) (\hat{n}_c(q) + \hat{n}_d(q)) \quad (11)$$

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. Here we have rescaled the Fourier transformed operators $c(q)$ and $d(q)$ by a factor of $\sqrt{N/2}$ and taken the thermodynamic limit $N \rightarrow \infty$. Check that the rescaled operators $\hat{c}(q)$ and $\hat{d}(q)$ and their hermitian conjugates obey the algebra $[c(q), c^\dagger(q')] = [d(q), d^\dagger(q')] = 2\pi\delta(q - q')$ (here $\delta(q)$ is the Dirac delta function, not a Kronecker delta!). 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: The approach we used here is the semi-classical (spin-wave) approximation. Eq.(7) and Eq.(8) are known as the Holstein-Primakoff identities.

2 Two-Component Complex Scalar Field

In this problem, you will consider the theory of a two-component complex scalar field $\phi_a(x)$ ($a = 1, 2$) whose Lagrangian is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi_a(x))^* (\partial^\mu \phi_a(x)) - \frac{m_0^2}{2} \phi_a^*(x) \phi_a(x) \quad (12)$$

In class we showed that this theory is invariant under the classical global symmetry

$$\begin{aligned} \phi_a(x) &\rightarrow \phi'_a(x) = U_{ab} \phi_b(x) \\ \phi_a^*(x) &\rightarrow \phi'^*_a(x) = U_{ab}^{-1} \phi_b^*(x) \\ \mathcal{L}(\phi') &= \mathcal{L}(\phi) \end{aligned} \quad (13)$$

where U is a 2×2 unitary matrix, i.e. $U^{-1} = U^\dagger$. This is the symmetry group $SU(2)$. Thus ϕ transforms like the fundamental (spinor) representation of $SU(2)$. The matrices U can be expanded in the basis of 2×2 Pauli matrices $(\sigma_k)_{ab}$ and are parametrized by three Euler angles θ_k ($k = 1, 2, 3$):

$$U_{ab} = [\exp(i\boldsymbol{\theta} \cdot \boldsymbol{\sigma})]_{ab} = \cos(|\boldsymbol{\theta}|)\delta_{ab} + i \frac{\boldsymbol{\theta}}{|\boldsymbol{\theta}|} \cdot \boldsymbol{\sigma}_{ab} \sin(|\boldsymbol{\theta}|) \quad (14)$$

1. Use the classical canonical formalism to find: (a) the canonical momenta Π_a , conjugate to the fields ϕ_a , (b) the Hamiltonian H , and (c) the total momentum P_j .
2. Derive the classical constants of motion associated with the global symmetry $SU(2)$. Relate these constants of motion with the generators of infinitesimal $SU(2)$ transformations. How many constants of motion do you find? Explain your results.
3. Quantize this theory by imposing canonical commutation relations. Write an expression for the quantum mechanical Hamiltonian and total momentum operators in terms of the field and canonical momentum operators.
4. Derive an expression for the *quantum mechanical* generators of global infinitesimal $SU(2)$ transformations in the Hilbert space of states of the system. Explain what relation, if any, do they have with the conserved charges of the classical theory.
5. Derive the quantum mechanical equations of motion of the Heisenberg representation operators.
6. Find an expansion of the field and canonical momentum operators in terms of a suitable set of creation and annihilation operators. How many species of creation and annihilation operators do you need?. Justify your results.
7. Find an expression for the $SU(2)$ generators in terms of creation and annihilation operators.
8. Find the ground state of the system and its quantum numbers. Find the normal ordered Hamiltonian, total momentum and the $SU(2)$ generators relative to this state.
9. Find the spectrum of single particle states. Give an expression for their energies and assign quantum numbers to these states. Do you find any degeneracies?. What is the degree of this degeneracy and why?