
2.2 Applications of second quantization

Figure 2.10 Showing the spin configuration of an elementary spin-wave excitation from the spin polarized ground state.

The Heisenberg model is a set of quantum mechanical spins $\hat{S}_m$ located at fixed lattice points with
exchange interactions between nearest-neighbors

\[ \hat{H} = -J \sum_{\langle mn \rangle} \hat{S}_m \cdot \hat{S}_n , \]

It was introduced by W. Heisenberg, *Zur Theorie des Ferromagnetismus*, Z. f. Phys. 49, 619-636 (1928), who studied the properties of the ground state and low-lying excitations based on the commutation relations

\[ \left[ \hat{S}_j^i, \hat{S}_k^j \right] = -i\delta_{mn}\epsilon^{jk}_\ell \hat{S}_\ell^\ell , \quad \hat{S}^2 = S(S+1) . \]

The figure from Altland-Simons shows a spin-wave or Magnon excitation of a one-dimensional chain of spins.

If the coupling \( J > 0 \), neighboring spins will prefer to align. The ground state of a chain of \( N \) spins will have all spins aligned, for example in the \( z \) direction of spin space. This is an eigenstate of total \( z \) component \( \hat{S}^z = \sum_m \hat{S}_m^z \) with eigenvalue \( NS \) and energy \( E_0 = -J(NS)^2 \).

The ground state is highly degenerate because the Hamiltonian is invariant under global rotation in spin-space of all spins simultaneously. This symmetry results in zero-mass excitations called spin waves, similar to the density (sound) waves in the continuum limit of the oscillator chain.

To find the low-lying excitations of the system, define spin ladder operators

\[ \hat{S}_m^\pm \equiv \hat{S}_m^x \pm i\hat{S}_m^y , \quad \left[ \hat{S}_m^z, \hat{S}_n^\pm \right] = i\delta_{mn}\hat{S}_n^\pm , \quad \left[ \hat{S}_m^+, \hat{S}_n^- \right] = 2\delta_{mn}\hat{S}_m^z . \]
This algebra can be simplified by introducing bosonic ladder operators with commutation relations

\[ [a_m, a_n^\dagger] = \delta_{mn}, \]

and making a Holstein-Primakoff transformation

\[
\hat{S}_m^- = a_m^\dagger (2S - a_m^\dagger a_m)^{1/2}, \quad \hat{S}_m^+ = (2S - a_m^\dagger a_m)^{1/2} a_m, \quad \hat{S}_m^z = S - a_m^\dagger a_m,
\]


**Low Energy Excitations**

The Holstein-Primakoff transformation is exact but non-linear in the number operator \( a_m^\dagger a_m \). In the low-energy and long-wavelength limit, there are a small number of spin wave excitations, and their wavefunctions are spread out over the chain. The expectation value \( \langle a_m^\dagger a_m \rangle \) will be a small fraction of the spin \( S \), and the non-linear square root operator can be approximated

\[
(2S - a_m^\dagger a_m)^{1/2} \simeq \sqrt{2S} + \frac{1}{2\sqrt{2S}} a_m^\dagger a_m + \cdots
\]
The Hamiltonian operator can be expanded in powers of \(1/S\)

\[
\hat{H} = -J \sum_{m} \left[ \hat{S}_{m}^{z} \hat{S}_{m+1}^{z} + \frac{1}{2} \left( \hat{S}_{m}^{+} \hat{S}_{m+1}^{-} + \hat{S}_{m}^{-} \hat{S}_{m+1}^{+} \right) \right]
\]

\[
= -JNS^2 - JS \sum_{m} \left[ (a_{m}^\dagger a_{m+1} + a_{m+1}^\dagger a_{m} - 2a_{m}^\dagger a_{m}) \right] + \mathcal{O}(S^0)
\]

\[
= -JNS^2 - JS \sum_{m} \left( a_{m+1}^\dagger - a_{m}^\dagger \right) \left( a_{m+1} - a_{m} \right) + \mathcal{O}(S^0)
\]

The quadratic operator sum can be diagonalized by Fourier transforming to wavenumber space and imposing periodic boundary conditions for convenience

\[
a_k = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} a_m e^{ikm}, \quad k = 0, \pm 1, \ldots, \pm K,
\]

where \(K = \pi N/2\) is the Brioullin zone (B.Z.) boundary. The spin-wave Hamiltonian is

\[
\hat{H} = -JNS^2 + \sum_{k} \hbar \omega_k a_k^\dagger a_k + \mathcal{O}(S^0), \quad [a_k, a_{k'}^\dagger] = \delta_{kk'},
\]

with dispersion relation

\[
\hbar \omega_k = 2JS(1 - \cos k) = 4JS \sin^2 \left( \frac{k}{2} \right).
\]
The Bethe Ansatz


The webpage, G. Müller et al., *Introduction to the Bethe Ansatz*, has a series of tutorial articles on Bethe’s method.

The Bethe ansatz is an exact method for the calculation of eigenvalues and eigenvectors of a class of quantum many-body model systems. It is useful for two reasons. (1) The eigenstates are characterized by a set of quantum numbers which can be used to distinguish them according to specific physical properties. (2) In many cases the eigenvalues and the physical properties derived from them can be evaluated in the thermodynamic limit.

The Ansatz was applied by Bethe to the Heisenberg model of spins $S_n = (S^x_n, S^y_n, S^z_n)$ with quantum number $S = 1/2$ on a 1-dimensional lattice of $N$ sites with periodic boundary conditions $S_{N+1} = S_1$ and Hamiltonian

$$H = -J \sum_{n=1}^{N} S_n \cdot S_{n+1} = -J \sum_{n=1}^{N} \left[ \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + S_n^z S_{n+1}^z \right].$$

$H$ acts on a Hilbert space of dimension $2^N$ spanned by the orthogonal basis vectors $|\sigma_1 \ldots \sigma_N\rangle$, where $\sigma_n = \uparrow$ represents an up spin and $\sigma_n = \downarrow$ a down spin at site $n$.

The Bethe ansatz is a basis transformation of the Hilbert space that diagonalizes the Hamiltonian.
Block Diagonalization

The rotational symmetry about the $z$-axis in spin space implies that the $z$-component of the total spin $S^z_T \equiv \sum_{n=1}^{N} S^z_n$ is conserved: $[H, S^z_T] = 0$. According to Table 1, the operation of $H$ on $|\sigma_1 \ldots \sigma_N\rangle$ yields a linear combination of basis vectors, each of which has the same number of down spins. Sorting the basis vectors according to the quantum number $S^z_T = N/2 - r$, where $r$ is the number of down spins, block diagonalizes $H$.

The block with $r = 0$ (all spins up) consists of a single vector $|F\rangle \equiv |\uparrow \ldots \uparrow\rangle$ eigenstate of $H|F\rangle = E_0|F\rangle$, with $E_0 = -J N/4$.

The $N$ basis vectors in the invariant subspace with $r = 1$ (one down spin) are labeled by the position of the flipped spin:

$$|n\rangle = S^-_n |F\rangle \quad n = 1, \ldots, N.$$ 

It is diagonalized using lattice translation invariance and a wavenumber basis

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn} |n\rangle, \quad k = 2\pi m/N, \quad m = 0, \ldots, N - 1, \quad E - E_0 = J(1 - \cos k).$$
The Bethe ansatz deals with the invariant subspaces with \(2 \leq r \leq N/2\), where the translationally invariant basis does not completely diagonalize the Hamiltonian matrix even if additional symmetries such as the full rotational symmetry in spin space or the reflection symmetry on the lattice are used.

For \(r = 1\), the ansatz (starting point) for any eigenvector \(H|\psi\rangle = E|\psi\rangle\) is a superposition

\[
|\psi\rangle = \sum_{n=1}^{N} a(n)|n\rangle, \quad 2[E - E_0]a(n) = J[2a(n) - a(n - 1) - a(n + 1)] , \quad a(n + N) = a(n).
\]

This system of difference equations has \(N\) linearly independent solutions

\[
a(n) = e^{i kn}, \quad k = \frac{2\pi}{N} m, \quad m = 0, 1, \ldots, N - 1,
\]

which gives the same result as before.

**Bethe ansatz for \(r = 2\)**

The \(r = 2\) subspace has dimension \(N(N - 1)/2\) and an eigenvector can be expanded

\[
|\psi\rangle = \sum_{1 \leq n_1 < n_2 \leq N} a(n_1, n_2)|n_1, n_2\rangle.
\]

Bethe’s ansatz for the coefficients is

\[
a(n_1, n_2) = e^{i(k_1 n_1 + k_2 n_2 + \frac{1}{2} \theta_{12})} + e^{i(k_1 n_2 + k_2 n_1 + \frac{1}{2} \theta_{21})},
\]
where the phase angle \( \theta_{12} = -\theta_{21} \equiv \theta \) depends on two wavevectors \( k_1, k_2 \) that satisfy

\[
2 \cot \frac{\theta}{2} = \cot \frac{k_1}{2} - \cot \frac{k_2}{2}.
\]

Two additional relations between \( k_1, k_2, \) and \( \theta \) follow from the requirement that the wave function be translationally invariant, which implies that \( a(n_1, n_2) = a(n_2, n_1 + N) \). This condition is satisfied provided that

\[
e^{ik_1 N} = e^{i\theta}, \quad e^{ik_2 N} = e^{-i\theta}, \quad Nk_1 = 2\pi \lambda_1 + \theta, \quad Nk_2 = 2\pi \lambda_2 - \theta,
\]

where the integers \( \lambda_i \in \{0, 1, \ldots, N - 1\} \) are called Bethe quantum numbers.

The eigenstates are found by solving this system of algebraic relations. Each solution \( k_1, k_2, \theta \) determines a set of expansion coefficients \( a(n_1, n_2) \), and thus determines an eigenvector with energy

\[
E = E_0 + J \sum_{j=1,2} (1 - \cos k_j), \quad k = k_1 + k_2 = \frac{2\pi}{N} (\lambda_1 + \lambda_2).
\]

For \( r = 2 \), the solutions divide into three classes:

1. A class \( C_1 \) of states for which one of the Bethe quantum numbers is zero, \( \lambda_1 = 0, \lambda_2 = 0, 1, \ldots, N - 1 \).

2. A class \( C_2 \) of states with nonzero \( \lambda_1, \lambda_2 \) which differ by two or more: \( \lambda_2 - \lambda_1 \geq 2 \). There are \( N(N - 5)/2 + 3 \) such pairs.
A class $C_3$ of states has nonzero Bethe quantum numbers $\lambda_1, \lambda_2$ which either are equal or differ by unity. There exist $2N - 3$ such pairs, but only $N - 3$ pairs yield solutions.

The figure shows allowed pairs of Bethe quantum numbers $(\lambda_1, \lambda_2)$ that characterize the $N(N-1)/2$ eigenstates in the $r = 2$ subspace for $N = 32$. The states of class $C_1, C_2,$ and $C_3$ are colored red, white, and blue, respectively.

It is not possible to write down exact analytic formulas for the energies and eigenfunctions. However, the ansatz can be generalized systematically in algorithmic form. Exact solutions for any number of spins can in principle be generated by a computer program, which is straightforward to code.