Simple examples of second quantization 4

In this chapter, we give three examples of the application of second quantization, mainly to non-interacting systems.

4.1 Jordan–Wigner transformation

A non-interacting gas of fermions is still highly correlated: the exclusion principle introduces a *hard-core* interaction between fermions in the same quantum state. This feature is exploited in the Jordan–Wigner representation of spins. A classical spin is represented by a vector pointing in a specific direction. Such a representation is fine for quantum spins with extremely large spin S, but once the spin S becomes small, spins behave as very new kinds of object. Now their spin becomes a quantum variable, subject to its own zero-point motions. Furthermore, the spectrum of excitations becomes discrete or grainy.

Quantum spins are notoriously difficult objects to deal with in many-body physics, because they do not behave as canonical fermions or bosons. In one dimension, however, it turns out that spins with $S = \frac{1}{2}$ actually behave like fermions. We shall show this by writing the quantum spin-$\frac{1}{2}$ Heisenberg chain as an interacting one-dimensional gas of fermions, and we shall actually solve the limiting case of the one-dimensional spin-$\frac{1}{2}$ x-y model, in which the Ising (z) component of the interaction is set to zero.

Jordan and Wigner observed [1] that the "down" and "up" states of a single spin can be thought of as empty and singly occupied fermion states (Figure 4.1.), enabling them to make the mapping (see Figure 4.1)

$$| \uparrow\rangle \equiv f^{\dagger}|0\rangle, \qquad | \downarrow\rangle \equiv |0\rangle. \tag{4.1}$$

An explicit representation of the spin-raising and spin-lowering operators is then

$$\begin{aligned} S^{+} &= f^{\dagger} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ S^{-} &= f \equiv \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}. \end{aligned} \tag{4.2}$$

The z component of the spin operator can be written

$$S_z = \frac{1}{2}\Big[| \uparrow\rangle\langle\uparrow | - | \downarrow\rangle\langle\downarrow |\Big] \equiv f^{\dagger}f - \frac{1}{2}. \tag{4.3}$$

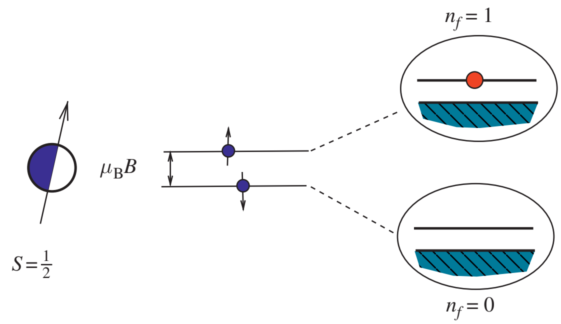

Fig. 4.1 The "up" and "down" states of a spin $\frac{1}{2}$ can be treated as a one-particle state which is either full or empty.

We can also reconstruct the transverse spin operators

$$\begin{aligned} S_x &= \frac{1}{2}(S^+ + S^-) = \frac{1}{2}(f^\dagger + f) \\ S_y &= \frac{1}{2i}(S^+ - S^-) = \frac{1}{2i}(f^\dagger - f). \end{aligned} \tag{4.4}$$

The explicit matrix representation of these operators makes it clear that they satisfy the same algebra:

$$[S_a, S_b] = i\epsilon_{abc}S_c. \tag{4.5}$$

Curiously, due to a hidden supersymmetry, they also satisfy an anticommuting algebra:

$$\{S_a, S_b\} = \frac{1}{4}\{\sigma_a, \sigma_b\} = \frac{1}{2}\delta_{ab}. \tag{4.6}$$

In this way, the Pauli spin operators provided Jordan and Wigner with an elementary model of a fermion.

Unfortunately the represeentation needs to be modified if there is more than one spin, for independent spin operators commute but independent fermions anticommute. Jordan and Wigner discovered a way to fix this difficulty in one dimension by attaching a phase factor called a *string* to the fermions [1]. For a chain of spins in one dimension, the Jordan–Wigner representation of the spin operator at site j is defined as

$$S_j^+ = f_j^\dagger e^{i\phi_j}, \tag{4.7}$$

where the phase operator ϕ_j contains the sum over all fermion occupancies at sites to the left of j:

$$\phi_j = \pi \sum_{l<j} n_j. \tag{4.8}$$

The operator $e^{i\hat{\phi}_j}$ is known as a *string operator*.

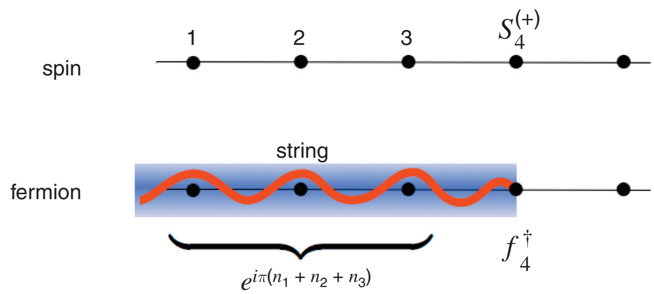

Fig. 4.2 Illustrating the Jordan–Wigner transformation. The spin-raising operator at site $j = 4$ is decomposed into a product of a fermion operator and a string operator.

The complete transformation is then

$$\left.\begin{array}{rcl} S_j^z & = & f_j^\dagger f_j - \frac{1}{2} \\ S_j^+ & = & f_j^\dagger e^{i\pi \sum_{l<j} n_l} \\ S_j^- & = & f_j e^{-i\pi \sum_{l<j} n_l}. \end{array}\right\} \text{Jordan–Wigner transformation} \tag{4.9}$$

(Notice that $e^{i\pi n_j} = e^{-i\pi n_j}$ is a Hermitian operator so that the overall sign of the phase factors can be reversed without changing the spin operator.) In words (Figure 4.2):

spin = fermion × string.

The important property of the string is that it *anticommutes* with any fermion operator to the left of its free end. To see this, note first that the operator $e^{i\pi n_j}$ anticommutes with f_j. This follows because f_j reduces n_j from unity to zero so that, acting to the right of f_j, since $n_j = 1$, $e^{i\pi n_j} = -1$ and hence $f_j\, e^{i\pi n_j} = -f_j$; whereas, acting to the left of f_j, since $n_j = 0$, $e^{i\pi n_j} f_j = f_j$. It follows that

$$\{e^{i\pi n_j}, f_j\} = e^{i\pi n_j} f_j + f e^{i\pi n_j} = f_j - f_j = 0 \tag{4.10}$$

and similarly, from the conjugate of this expression, $\{e^{i\pi n_j}, f_j^\dagger\} = 0$. Now the phase factor $e^{i\pi n_l}$ at any other site $l \neq j$ commutes with f_j and $f_j^\dagger$, so that the string operator $e^{i\hat{\phi}_j}$ anticommutes with all fermions at all sites l to the left of j, i.e. $l < j$:

$$\{e^{i\phi_j}, f_l^{(\dagger)}\} = 0 \qquad (l < j),$$

while commuting with fermions at all other sites $l \geq j$:

$$[e^{i\phi_j}, f_l^{(\dagger)}] = 0 \qquad (l \geq j).$$

We can now verify that the transverse spin operators satisfy the correct commutation algebra. Suppose $j < k$; then $e^{i\phi_j}$ commutes with fermions at sites j and k, so that

$$[S_j^{(\pm)}, S_k^{(\pm)}] = [f_j^{(\dagger)} e^{i\phi_j}, f_k^{(\dagger)} e^{i\phi_k}] = e^{i\phi_j}[f_j^{(\dagger)}, f_k^{(\dagger)} e^{i\phi_k}].$$

But $f_j^{(\dagger)}$ antcommutes with both $f_k^{(\dagger)}$ and $e^{i\phi_k}$ so it commutes with their product $f_k^{(\dagger)}e^{i\phi_k}$, and hence

$$[S_j^{(\pm)}, S_k^{(\pm)}] \propto [f_j^{(\dagger)}, f_k^{(\dagger)}e^{i\phi_k}] = 0. \tag{4.11}$$

So we see that by multiplying a fermion by the string operator, it is transformed into a boson.

As an example of the application of this method, we shall now discuss the one-dimensional Heisenberg model,

$$H = -J\sum[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y] - J_z \sum_j S_j^z S_{j+1}^z. \tag{4.12}$$

In real magnetic systems, local moments can interact via ferromagnetic or antiferromagnetic interactions. Ferromagnetic interactions generally arise as a result of *direct exchange*, in which the Coulomb repulsion energy is lowered when electrons are in a triplet state because the wavefunction is then spatially antisymmetric. Antiferromagnetic interactions are generally produced by the mechanism of *super exchange*, in which electrons on neighboring sites that form singlets (antiparallel spin) lower their energy through virtual quantum fluctuations into high-energy states in which they occupy the same orbital. Here we have written the model as if the interactions are ferromagnetic.

For convenience, the model can be rewritten as

$$H = -\frac{J}{2}\sum[S_{j+1}^+ S_j^- + \text{H.c.}] - J_z \sum_j S_j^z S_{j+1}^z, \tag{4.13}$$

where "H.c." denotes the Hermitian conjugate. To "fermionize" the first term, we note that all terms in the strings cancel except for $e^{i\pi n_j}$, which has no effect:

$$\frac{J}{2}\sum_j S_{j+1}^+ S_j^- = \frac{J}{2}\sum_j f_{j+1}^\dagger e^{i\pi n_j} f_j = \frac{J}{2}\sum_j f_{j+1}^\dagger f_j, \tag{4.14}$$

so that the transverse component of the interaction induces a "hopping" term in the fermionized Hamiltonian. Notice that the string terms would enter if the spin interaction involved next-nearest neighbors. The z component of the Hamiltonian becomes

$$-J_z \sum_j S_{j+1}^z S_j^z = -J_z \sum_j \left(n_{j+1} - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right). \tag{4.15}$$

Notice how the ferromagnetic interaction means that spin fermions attract one another. The transformed Hamiltonian is then

$$H = -\frac{J}{2}\sum_j (f_{j+1}^\dagger f_j + f_j^\dagger f_{j+1}) + J_z \sum_j n_j - J_z \sum_j n_j n_{j+1}. \tag{4.16}$$

Interestingly enough, the pure x-y model has no interaction term in it, so this case can be mapped onto a non-interacting fermion problem, a discovery made by Lieb, Schulz and Mattis in 1961 [2].

To write out the fermionized Hamiltonian in its most compact form, let us transform to momentum space, writing

$$f_j = \frac{1}{\sqrt{N}} \sum_k s_k e^{ikR_j}, \tag{4.17}$$

where $s_k^\dagger$ creates a spin excitation in momentum space, with momentum k. In this case, the one-particle terms become

$$J_z \sum_j n_j = J_z \sum_k s_k^\dagger s_k$$

$$\begin{aligned} -\frac{J}{2} \sum_j (f_{j+1}^\dagger f_j + \text{H.c.}) &= -\frac{J}{2N_s} \sum_k (e^{-ika} + e^{ika}) s_k^\dagger s_{k'} \overbrace{\sum_j e^{-i(k-k')R_j}}^{N\delta_{kk'}s} \\ &= -J \sum_k \cos(ka) s_k^\dagger s_k. \end{aligned} \tag{4.18}$$

The anisotropic Heisenberg Hamiltonian can thus be written

$$H = \sum_k \omega_k s_k^\dagger s_k - J_z \sum_j n_j n_{j+1}, \tag{4.19}$$

where

$$\omega_k = (J_z - J \cos ka) \tag{4.20}$$

defines a *magnon excitation energy*. We can also cast the second term in momentum space by noticing that the interaction is a function of $i - j$, which is $-J_z/2$ for $i - j = \pm 1$ but zero otherwise. The Fourier transform of this short-range interaction is $V(q) = -J_z \cos qa$, so that Fourier transforming the interaction term gives

$$H = \sum_k \omega_k s_k^\dagger s_k - \frac{J_z}{N_s} \sum_{k,k',q} \cos(qa)\, s_{k-q}^\dagger s_{k'+q}^\dagger s_{k'} s_k. \tag{4.21}$$

This transformation holds for both the ferromagnet and the antiferromagnet. In the former case, the fermionic spin excitations correspond to the magnons of the ferromagnet. In the latter case, the fermionic spin excitations are often called *spinons*.

To see what this Hamiltonian means, let us first neglect the interactions. This is a reasonable thing to do in the limiting cases of (i) the Heisenberg ferromagnet, $J_z = J$, and (ii) the x-y model, $J_z = 0$.

- *Heisenberg ferromagnet*, $J_z = J$ (Figure 4.3)
  In this case, the spectrum

  $$\omega_k = 2J \sin^2(ka/2) \tag{4.22}$$

  is always positive, so that there are no magnons present in the ground state. The ground state can thus be written

  $$|0\rangle = |\downarrow\downarrow\downarrow\cdots\rangle, \tag{4.23}$$

  corresponding to a state with a spontaneous magnetization $M = -N_s/2$.

  Curiously, since $\omega_{k=0} = 0$, it costs no energy to add a magnon of arbitrarily long wavelength. This is an example of a *Goldstone mode*, and the reason it arises is that the

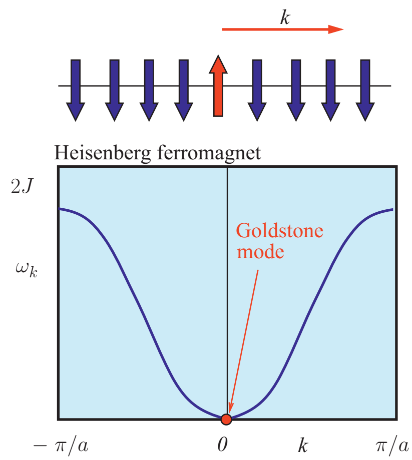

Fig. 4.3 Excitation spectrum of the one-dimensional Heisenberg ferromagnet.

spontaneous magnetization could actually point in any direction. Suppose we want to rotate the magnetization through an infinitesimal angle $\delta\theta$ about the x-axis; then the new state is given by

$$\begin{aligned}|\psi\rangle' &= e^{i\delta\theta S_x}|\downarrow\downarrow\cdots\rangle \\ &= |\downarrow\downarrow\cdots\rangle + i\frac{\delta\theta}{2}\sum_j S_j^+|\downarrow\downarrow\cdots\rangle + O(\delta\theta^2).\end{aligned} \tag{4.24}$$

The change in the wavefunction is proportional to the state

$$\begin{aligned}S^+_{TOT}|\downarrow\downarrow\cdots\rangle &\equiv \sum_j f_j^\dagger e^{i\phi_j}|0\rangle \\ &= \sum_j f_j^\dagger|0\rangle = \sqrt{N_s}s^\dagger_{k=0}|0\rangle.\end{aligned} \tag{4.25}$$

In other words, the action of adding a single magnon at $q = 0$ rotates the magnetization infinitesimally upwards. Rotating the magnetization should cost no energy, and this is the reason why the $k = 0$ magnon is a zero-energy excitation.

- *x-y ferromagnet* (Figure 4.4)
  As J_z is reduced from J, the spectrum develops a negative part, and magnon states with negative energy will become occupied. For the pure x-y model, where $J_z = 0$, the interaction identically vanishes, and the excitation spectrum of the magnons is given by $\omega_k = -J\cos ka$, as sketched in Figure 4.4. All the negative-energy fermion states with $|k| < \pi/2a$ are occupied, so the ground state is given by

$$|\Psi_g\rangle = \prod_{|k|<\pi/2a} s_k^\dagger|0\rangle. \tag{4.26}$$

The band of magnon states is thus precisely half-filled, so that

$$\langle S_z\rangle = \left\langle n_f - \frac{1}{2}\right\rangle = 0, \tag{4.27}$$

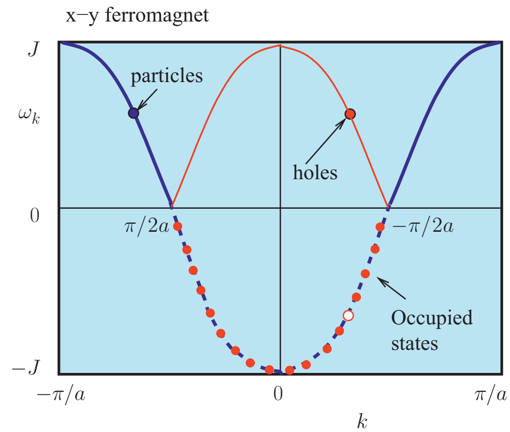

Fig. 4.4 Excitation spectrum of the one-dimensional x-y ferromagnet, showing how the negative energy states are filled. The negative-energy dispersion curve is "folded over" to describe the positive hole excitation energy.

so that, remarkably, there is no ground-state magnetization. We may interpret this loss of ground-state magnetization as a consequence of the growth of quantum spin fluctuations in going from the Heisenberg to the x-y ferromagnet.

Excitations of the ground state can be made, either by adding a magnon at wavevectors $|k| > \pi/2a$ or by annihilating a magnon at wavevectors $|k| < \pi/2a$, to form a *hole*. The energy to form a hole is $-\omega_k$. To represent the hole excitations, we make a *particle–hole transformation* for the occupied states, writing

$$\tilde{s}_k = \begin{cases} s_k & (|k| > \pi/2a) \\ s^\dagger_{-k}, & (|k| < \pi/2a). \end{cases} \tag{4.28}$$

These are the "physical" excitation operators. Since $s^\dagger_k s_k = 1 - s_k s^\dagger_k$, the Hamiltonian of the pure x-y ferromagnet can be written

$$H_{xy} = \sum_k J|\cos ka|(\tilde{s}^\dagger_k \tilde{s}_k - \frac{1}{2}). \tag{4.29}$$

Notice that, unlike the Heisenberg ferromagnet, the magnon excitation spectrum is now linear. The ground-state energy is evidently

$$\begin{aligned} E_g &= -\frac{1}{2}\sum_k J|\cos ka| \\ &= -a\int_{-\pi/2a}^{\pi/2a} \frac{dk}{2\pi} J\cos(ka) = -\frac{J}{\pi}. \end{aligned} \tag{4.30}$$

But if there is no magnetization, why are there zero-energy magnon modes at $q = \pm\pi/a$? Although there is no true long-range order, it turns out that the spin correlations in the x-y model display power-law correlations with an infinite spin correlation length, generated by the gapless magnons in the vicinity of $q = \pm\pi/a$.