2

Quantum Theory of Spin Waves

In Chapter 1, we discussed the angular momenta and magnetic moments of individual atoms and ions. When these atoms or ions are constituents of a solid, it is important to take into consideration the ways in which the angular momenta on different sites interact with one another. For simplicity, we will restrict our attention to the case when the angular momentum on each site is entirely due to spin.

The elementary excitations of coupled spin systems in solids are called *spin waves*. In this chapter, we will introduce the quantum theory of these excitations at low temperatures. The two primary interaction mechanisms for spins are magnetic dipole–dipole coupling and a mechanism of quantum mechanical origin referred to as the *exchange interaction*. The dipolar interactions are of importance when the spin wavelength is very long compared to the spacing between spins, and the exchange interaction dominates when the spacing between spins becomes significant on the scale of a wavelength. In this chapter, we focus on exchange-dominated spin waves, while dipolar spin waves are the primary topic of subsequent chapters.

We begin this chapter with a quantum mechanical treatment of a single electron in a uniform field and follow it with the derivations of Zeeman energy and Larmor precession. We then consider one of the simplest exchange-coupled spin systems, molecular hydrogen. Exchange plays a crucial role in the existence of ordered spin systems. The ground state of H_2 is a two-electron exchange-coupled system in an embryonic antiferromagnetic state. It serves to illustrate the origins of the exchange interaction and also provides a vehicle for our discussion on the Heisenberg spin Hamiltonian in ferromagnetic solids.

2.1 Charged Particle in an Electromagnetic Field

We obtained the time-independent Schrödinger equation (1.46) by quantizing the total energy of a particle moving in an electrostatic potential. Since we also want to understand the effects of a magnetic field, we now concern

ourselves with understanding the interactions of a charged particle in a general electromagnetic field. Maxwell's equation from Gauss' Law specifies the divergence of the magnetic flux density as

$$\nabla \cdot \mathbf{B} = 0. \tag{2.1}$$

This allows us to express $\mathbf{B}$ as the curl of a vector

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{2.2}$$

where $\mathbf{A}$ is known as the vector potential.[1] If we substitute this into Maxwell's equation from Faraday's law

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{2.3}$$

we obtain

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0. \tag{2.4}$$

Thus, we can set

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi, \tag{2.5}$$

where ϕ is known as the scalar potential.

Now, consider the motion of a particle with charge q in an electromagnetic field. The force acting on the particle is given by

$$\mathbf{F} = q[\mathbf{E} + \mathbf{v} \times \mathbf{B}] \tag{2.6}$$

or

$$m\frac{d\mathbf{v}}{dt} = q \left(-\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi + \mathbf{v} \times (\nabla \times \mathbf{A}) \right). \tag{2.7}$$

Since

$$\frac{dA_x}{dt} = \frac{\partial A_x}{\partial t} + \left(v_x \frac{\partial A_x}{\partial x} + v_y \frac{\partial A_x}{\partial y} + v_z \frac{\partial A_x}{\partial z} \right), \tag{2.8}$$

we can write

$$\begin{aligned}
(\mathbf{v} \times \nabla \times \mathbf{A})_x &= v_y \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) - v_z \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \\
&= \frac{\partial}{\partial x}(\mathbf{v} \cdot \mathbf{A}) - \frac{dA_x}{dt} + \frac{\partial A_x}{\partial t}.
\end{aligned} \tag{2.9}$$

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[1] Note that (2.2) gives us the freedom to write $\mathbf{A} = \mathbf{A}' + \nabla \phi$, since $\nabla \times (\nabla \phi) = 0$ for any scalar function ϕ. Further, we must specify the divergence as well as the curl to uniquely define a vector function. Generally, the choice of $\nabla \cdot \mathbf{A}$ is made for convenience. The choice $\nabla \cdot \mathbf{A} = 0$ is known as the *Coulomb gauge* [1].

With some simple algebra, we simplify Eq. (2.7) to

$$\frac{d}{dt}[m\mathbf{v} + q\mathbf{A}] = \nabla[-q\phi + q(\mathbf{v} \cdot \mathbf{A})]. \tag{2.10}$$

Let us borrow the concept of a *Lagrangian* from classical mechanics, to aid us in the interpretation of Eq. (2.10). Consider the motion of a particle, in three dimensions, in a potential $V(\mathbf{x})$. The Lagrangian for the particle is defined as the difference between the kinetic and potential energies:

$$\begin{aligned}\mathcal{L} &= T - V \\ &= \frac{1}{2}m|\dot{\mathbf{x}}|^2 - V(\mathbf{x}).\end{aligned} \tag{2.11}$$

The motion of the particle is given by the *Euler–Lagrange* equation (cf. Goldstein [2])

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}}\right) = \frac{\partial \mathcal{L}}{\partial \mathbf{x}}. \tag{2.12}$$

Substituting (2.11) into (2.12) yields $m\ddot{\mathbf{x}} + \nabla V = 0$. If we define the force exerted on the particle as $\mathbf{F} = -\nabla V$, we recover the first law of Newtonian mechanics, $\mathbf{F} = m\ddot{\mathbf{x}}$. We can also identify the *canonical variable* $\mathbf{p} = m\dot{\mathbf{x}}$ as the momentum of the particle in consonance with Newton's second law $\mathbf{F} = d\mathbf{p}/dt$.

Returning to our discussion of a charged particle in an electromagnetic field, consider the x component of (2.10),

$$\frac{d}{dt}[m\mathbf{v}_x + q\mathbf{A}_x] = \frac{\partial}{\partial x}\left[-q\phi + q(\mathbf{v} \cdot \mathbf{A})\right]. \tag{2.13}$$

If we identify the Lagrangian as

$$\mathcal{L} = \frac{1}{2}m\mathbf{v} \cdot \mathbf{v} - q\phi + q\mathbf{A} \cdot \mathbf{v}, \tag{2.14}$$

we observe that (2.13) is the Euler–Lagrange equation in one dimension,

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = \frac{\partial \mathcal{L}}{\partial x}. \tag{2.15}$$

We can also identify the conjugate momentum variable for x,

$$p_x = \frac{\partial \mathcal{L}}{\partial \dot{x}} = mv_x + qA_x. \tag{2.16}$$

Performing a similar analysis for the y and z-components of (2.12) leads to

$$\mathbf{p} = m\mathbf{v} + q\mathbf{A}. \tag{2.17}$$

A reformulation of Lagrangian mechanics, introduced by the Irish mathematician W. R. Hamilton, allows us to express the equations of motion as first

order differential equations in a phase space defined by $\mathbf{x}$ and $\mathbf{p}$. The Hamiltonian of a system, introduced in Eq. (1.43), is defined as the sum of the kinetic and potential energies. A particle with velocity $\mathbf{v}$ has kinetic energy $T = (\mathbf{p} \cdot \mathbf{v})/2$. To study the interaction of the particle with an electromagnetic field, we use (2.11) and rewrite the Hamiltonian as

$$
\begin{aligned}
\mathcal{H} &= T + V \\
&= \mathbf{p} \cdot \mathbf{v} - \mathcal{L} \\
&= \mathbf{p} \cdot \left[\frac{1}{m}(\mathbf{p} - q\mathbf{A}) \right] - \frac{m}{2} \left[\frac{1}{m}(\mathbf{p} - q\mathbf{A}) \right]^2 + q\phi - q\mathbf{A} \cdot \frac{1}{m}(\mathbf{p} - q\mathbf{A}) \\
&= \frac{1}{2m}[\mathbf{p} - q\mathbf{A}]^2 + q\phi,
\end{aligned}
\tag{2.18}
$$

where we have used (2.17) to eliminate $\mathbf{v}$. We make the transition to quantum mechanics, following the procedure adopted in Section 1.4.2, by replacing the operator $\mathbf{p}$ with $(\hbar/i)\nabla$ to yield

$$
\mathcal{H} = \frac{1}{2m} \left[\frac{\hbar}{i}\nabla - q\mathbf{A} \right]^2 + q\phi.
\tag{2.19}
$$

Finally, we postulate that the particle is described by a wavefunction $\Psi(\mathbf{r}, t)$, which is a solution to the *time-dependent Schrödinger equation*

$$
i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi.
\tag{2.20}
$$

The Schrödinger equation (2.20) is an operator equation that describes how the wavefunction Ψ evolves with time, while $\mathcal{H}$ is time independent. Other interpretations of time evolution in quantum mechanics, such as the Heisenberg and the interaction pictures [3], allow operators like $\mathcal{H}$ to become time dependent. We shall confine our present discussions to the Schrödinger picture of quantum mechanics.

2.2 Zeeman Energy

Let us write the wavefunction of the particle in a static electromagnetic field as

$$
\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-i\mathcal{E}t/\hbar}.
\tag{2.21}
$$

Substituting $\Psi(\mathbf{r}, t)$ into Eq. (2.20), we find that $\psi(\mathbf{r})$ must satisfy the equation

$$
\frac{1}{2m} \left[\frac{\hbar}{i}\nabla - q\mathbf{A} \right]^2 \psi + q\phi\psi = \mathcal{E}\psi
\tag{2.22}
$$

or

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{\hbar}{i}\frac{q}{2m}\left[\nabla\cdot(\mathbf{A}\psi) + \mathbf{A}\cdot\nabla\psi\right] + \left[\frac{q^2}{2m}A^2 + q\phi\right]\psi = \mathcal{E}\psi. \quad (2.23)$$

Recall that we had some flexibility in our definition of the vector potential $\mathbf{A}$, and in particular we can specify $\nabla\cdot\mathbf{A}$ to our convenience. A common choice is $\nabla\cdot\mathbf{A} = 0$, referred to as the Coulomb gauge. Hence,

$$\nabla\cdot(\mathbf{A}\psi) = (\nabla\cdot\mathbf{A})\psi + \mathbf{A}\cdot\nabla\psi = \mathbf{A}\cdot\nabla\psi. \quad (2.24)$$

Furthermore, for a uniform magnetic field, since

$$\begin{aligned}
\nabla\times(\mathbf{B}\times\mathbf{r}) &= \mathbf{B}\,\nabla\cdot\mathbf{r} - \mathbf{r}\,\nabla\cdot\mathbf{B} + (\mathbf{r}\cdot\nabla)\mathbf{B} - (\mathbf{B}\cdot\nabla)\mathbf{r} \\
&= (\nabla\cdot\mathbf{r})\mathbf{B} - (\mathbf{B}\cdot\nabla)\mathbf{r} \\
&= [3\mathbf{B} - \mathbf{B}] \\
&= 2\mathbf{B},
\end{aligned} \quad (2.25)$$

we can write

$$\nabla\times\mathbf{A} = \frac{1}{2}\nabla\times(\mathbf{B}\times\mathbf{r}). \quad (2.26)$$

Using Eqs. (2.24) and (2.26), we find that the second term on the left of Eq. (2.23) can be simplified and written as[2]

$$\begin{aligned}
-\frac{\hbar}{i}\frac{q}{m}\mathbf{A}\cdot\nabla\psi &= -\frac{\hbar}{i}\frac{q}{2m}(\mathbf{B}\times\mathbf{r})\cdot\nabla\psi \\
&= -\frac{q}{2m}\mathbf{B}\cdot\left[\mathbf{r}\times\left(\frac{\hbar}{i}\nabla\right)\right]\psi \\
&= -\frac{q}{2m}\mathbf{B}\cdot(\mathbf{r}\times\mathbf{p})\psi \\
&= -\frac{q}{2m}(\mathbf{B}\cdot\mathbf{L})\psi \\
&= -\boldsymbol{\mu}\cdot\mathbf{B}\,\psi,
\end{aligned} \quad (2.27)$$

where we have used the classical definition of angular momentum $\mathbf{L} = \mathbf{r}\times\mathbf{p}$. We define the *Zeeman energy* as

$$\mathcal{E}_z = -\boldsymbol{\mu}\cdot\mathbf{B}, \quad (2.28)$$

and note that it yields a lower energy when the magnetic moment $\boldsymbol{\mu}$ is parallel to the applied magnetic field.

The term proportional to q^2A^2 in Eq. (2.23) is often ignored since, for typical magnetic field values, it makes a negligible contribution to the total energy. In the absence of an electric field, the Hamiltonian thus reduces to

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{q}{2m}(\mathbf{L}\cdot\mathbf{B}). \quad (2.29)$$

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[2] The *scalar triple product* of three vectors has the identity $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}$.

2.3 Larmor Precession

Let us concentrate on the specific problem of an electron in a uniform magnetic field assumed to be along the $\hat{\mathbf{z}}$ direction. Recall, from Section 1.4.4, that in the presence of both spin and orbital angular momentum, the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. If we neglect all orbital motion, the Hamiltonian representing the interaction of the magnetic field with the magnetic moment of the electron is

$$\mathcal{H}^{\mathrm{spin}} = -\frac{gq}{2m}\mathbf{S}\cdot\mathbf{B}, \tag{2.30}$$

where we have used the Landé g-factor of Eq. (1.81) with $L = 0$. Writing $\mathbf{S}$ in terms of the Pauli spin matrices (cf. Problem 1.5), we have

$$\mathcal{H}^{\mathrm{spin}} = \frac{1}{2}\hbar\omega_0\sigma_z, \tag{2.31}$$

where we have defined the Larmor precession frequency

$$\omega_0 = -\frac{gqB_0}{2m} = \frac{g\mu_{\mathrm{B}}B_0}{\hbar}, \tag{2.32}$$

for a single electron in a magnetic field of magnitude B_0. The eigenvalues of σ_z are ± 1 yielding the corresponding eigenvalues $\pm\frac{1}{2}\hbar\omega_0$ for $\mathcal{H}^{\mathrm{spin}}$ with the spinor eigenstates $\chi_{\uparrow\downarrow}$, respectively. Thus, the general solution to the time-dependent Schrödinger equation (2.20) is

$$\Psi(t) = c_1\, e^{-i\omega_0 t/2}\chi_\uparrow + c_2\, e^{+i\omega_0 t/2}\chi_\downarrow, \tag{2.33}$$

where

$$\chi_\uparrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \chi_\downarrow = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{2.34}$$

A particularly interesting case results when we choose $c_1 = \cos(\theta/2)$ and $c_2 = \sin(\theta/2)$ to yield

$$\Psi(t) = \cos\frac{\theta}{2}\, e^{-i\omega_0 t/2}\chi_\uparrow + \sin\frac{\theta}{2}\, e^{i\omega_0 t/2}\chi_\downarrow. \tag{2.35}$$

To interpret this wavefunction, let us first find the expected value of the x-component of spin using the operator

$$S_x = \frac{\hbar}{2}\sigma_x, \tag{2.36}$$

where (cf. Eq. (1.93))

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{2.37}$$

The expected value of this operator is

$$
\begin{aligned}
\langle S_x \rangle &= \psi^\dagger S_x \psi \\
&= \left(\cos\frac{\theta}{2}\, e^{i\omega_0 t/2} \chi_\uparrow^{\mathrm{T}} + \sin\frac{\theta}{2}\, e^{-i\omega_0 t/2} \chi_\downarrow^{\mathrm{T}} \right) \\
&\quad \times \frac{\hbar}{2}\sigma_x \left(\cos\frac{\theta}{2}\, e^{-i\omega_0 t/2} \chi_\uparrow + \sin\frac{\theta}{2}\, e^{i\omega_0 t/2} \chi_\downarrow \right).
\end{aligned}
\tag{2.38}
$$

Performing the required matrix multiplication and simplifying gives

$$
\langle S_x \rangle = \frac{\hbar}{2} \sin\theta \cos(\omega_0 t).
\tag{2.39}
$$

In a similar manner, we find

$$
\langle S_y \rangle = \frac{\hbar}{2} \sin\theta \sin(\omega_0 t),
\tag{2.40}
$$

$$
\langle S_z \rangle = \frac{\hbar}{2} \cos\theta.
\tag{2.41}
$$

This solution represents a spin making an angle θ with the $\hat{\mathbf{z}}$ axis and precessing about it with angular velocity, ω_0. Thus, we find that a measurement on the quantum mechanical system yields a result analogous to the semi-classical description of a precessing moment adopted in Chapter 1.

## 2.4 Origins of Exchange: The Heisenberg Hamiltonian[3]

To be independent of any coordinate system, the energy of interaction between two spins should depend on $\mathbf{S}_1$ and $\mathbf{S}_2$ only through their relative orientation. Thus, the interaction should be a function of $\mathbf{S}_1 \cdot \mathbf{S}_2$. The simplest form is that of the *Heisenberg Hamiltonian*:

$$
\mathcal{H} = -2\frac{\mathcal{J}}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2 .
\tag{2.42}
$$

Here, $\mathbf{S}_1$ and $\mathbf{S}_2$ are angular momentum operators (see Section 1.4 and Problem 1.5) and $\mathcal{J}$ is referred to as the exchange constant for reasons that will become apparent shortly.

To begin to get an understanding of the origin and meaning of the Heisenberg Hamiltonian, we consider the simplest system of coupled atoms whose spins interact: molecular hydrogen. We would like to calculate the expected energy of the hydrogen molecule, illustrated in Figure 2.1, to gain an understanding of how the energy is affected by the spins of the electrons.

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[3] This section follows a discussion in Mattis [4, Chapter 2]. Treatments of exchange can also be found in Martin [5] and Rado and Suhl [6]. The approach taken here was introduced by Heitler and London [7].
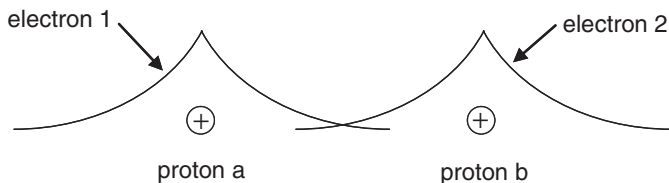
Fig. 2.1. The hydrogen molecule consists of two protons, each with a bound electron. The protons are sufficiently close that the electronic orbitals overlap.

As discussed in Section 1.4.2, we can obtain such an estimate by computing the expectation of the Hamiltonian operator. This operator is obtained by writing down an expression for the total energy of the system (kinetic plus potential), and making the operator substitutions indicated in Table 1.1. The total energy of this system can be written

$$\mathcal{H} = \underbrace{\frac{p_1^2}{2m} + \frac{p_2^2}{2m}}_{\substack{\text{electron} \\ \text{kinetic} \\ \text{energy}}} \underbrace{- \frac{q^2}{cr_{1a}} - \frac{q^2}{cr_{2b}} - \frac{q^2}{cr_{1b}} - \frac{q^2}{cr_{2a}}}_{\substack{\text{potential energy between} \\ \text{opposite charges} \\ \text{(attractive)}}} + \underbrace{\frac{q^2}{cr_{12}} + \frac{q^2}{cR_{ab}}}_{\substack{\text{potential energy} \\ \text{between like} \\ \text{charges (repulsive)}}},$$

(2.43)

where $c = 4\pi\varepsilon_0$, p_i are the electron momenta, m is the electron mass, and r_{ij} is the distance between particles i, j. The separation between the protons R_{ab}, will be considered fixed, as we are primarily interested in how the energy is affected by the electron dynamics. As indicated in the equation, the total energy consists of the kinetic energy associated with the electron motion, the attractive potential energy between each electron and both protons, and the repulsive potential energy between the electrons and between the protons. We have neglected the kinetic energy associated with the motion of the protons, assuming that they are relatively stationary because of their large mass. We have also neglected the magnetic interaction between the electron spins, as this interaction is much weaker than the electrostatic interactions contained in (2.43).

If ψ is the wave function for the system, then the expectation of the energy can be obtained from Schrödinger's equation (1.46) generalized to two particles:

$$\langle \mathcal{E} \rangle = \frac{\int \psi^* \mathcal{H} \psi \, d^3 r_1 \, d^3 r_2}{\int \psi^* \psi \, d^3 r_1 \, d^3 r_2}.$$

(2.44)

Here, two volume integrations are necessary – one for the coordinate of each electron. Since the correct answer will be the minimum value of this expression, a small error in the wave function will result in an error in the energy that is second order in small quantities. Consequently, we should obtain a satisfactory answer with a reasonable approximation to the wave function. Because of

this tolerance to errors in the wave function, this expression is said to be *stationary*.[4] If the atoms are far apart compared to the atomic diameter, we should be able to construct a reasonable wave function using the unperturbed hydrogen atom wave functions φ_a and φ_b. The unperturbed wave functions satisfy the equations

$$\left(\frac{p_1^2}{2m} - \frac{q^2}{cr_{1a}} \right) \varphi_a \left(\mathbf{r}_1 \right) = \mathcal{E}_0 \, \varphi_a \left(\mathbf{r}_1 \right), \tag{2.45}$$

$$\left(\frac{p_2^2}{2m} - \frac{q^2}{cr_{2b}} \right) \varphi_b \left(\mathbf{r}_2 \right) = \mathcal{E}_0 \, \varphi_b \left(\mathbf{r}_2 \right). \tag{2.46}$$

Using these as basis functions, or building blocks, we can construct symmetric and antisymmetric two particle wave functions as follows:

$$\psi_S = \frac{1}{\sqrt{2}} \left[\varphi_a \left(\mathbf{r}_1 \right) \varphi_b \left(\mathbf{r}_2 \right) + \varphi_a \left(\mathbf{r}_2 \right) \varphi_b \left(\mathbf{r}_1 \right) \right], \tag{2.47}$$

$$\psi_A = \frac{1}{\sqrt{2}} \left[\varphi_a \left(\mathbf{r}_1 \right) \varphi_b \left(\mathbf{r}_2 \right) - \varphi_a \left(\mathbf{r}_2 \right) \varphi_b \left(\mathbf{r}_1 \right) \right], \tag{2.48}$$

or

$$\psi_\pm = \frac{1}{\sqrt{2}} \left[\varphi_a \left(\mathbf{r}_1 \right) \varphi_b \left(\mathbf{r}_2 \right) \pm \varphi_a \left(\mathbf{r}_2 \right) \varphi_b \left(\mathbf{r}_1 \right) \right]. \tag{2.49}$$

We first calculate the normalization integral in the denominator of (2.44). For the two-particle wave functions, we must perform a double integration over the coordinates of both electrons:

$$\iint \psi_\pm^* (\mathbf{r}_1, \mathbf{r}_2) \, \psi_\pm (\mathbf{r}_1, \mathbf{r}_2) \, d^3 r_1 \, d^3 r_2 = 1 \pm \alpha^2, \tag{2.50}$$

where we have used

$$\int |\varphi_a \left(\mathbf{r} \right)| \, d^3 r = \int |\varphi_b \left(\mathbf{r} \right)| \, d^3 r = 1, \tag{2.51}$$

and α is defined to be the overlap integral

$$\alpha = \int \varphi_a^* (\mathbf{r}) \varphi_b (\mathbf{r}) \, d^3 r. \tag{2.52}$$

After some manipulation, the numerator of Eq. (2.44) is found in a similar manner to be

$$\int \psi_\pm^* (\mathbf{r}_1, \mathbf{r}_2) \, \mathcal{H} (\mathbf{r}_1, \mathbf{r}_2) \, \psi_\pm (\mathbf{r}_1, \mathbf{r}_2) \, d^3 r_1 \, d^3 r_2 = 2\mathcal{E}_0 (1 \pm \alpha^2) + V \pm U \tag{2.53}$$

where V and U are a "coulomb integral" and an "exchange integral", respectively, defined by

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[4] We provide a more detailed discussion of stationary formulas and variational formulations in Chapter 7.

$$V = \int \varphi_a^* \left(\mathbf{r}_1\right) \varphi_b^* \left(\mathbf{r}_2\right) \mathcal{H}_i \left(\mathbf{r}_1, \mathbf{r}_2\right) \varphi_a \left(\mathbf{r}_1\right) \varphi_b \left(\mathbf{r}_2\right) d^3 r_1 \, d^3 r_2, \qquad (2.54)$$

$$U = \int \varphi_a^* \left(\mathbf{r}_2\right) \varphi_b^* \left(\mathbf{r}_1\right) \mathcal{H}_i \left(\mathbf{r}_1, \mathbf{r}_2\right) \varphi_a \left(\mathbf{r}_1\right) \varphi_b \left(\mathbf{r}_2\right) d^3 r_1 \, d^3 r_2, \qquad (2.55)$$

and $\mathcal{H}_i$ is the interaction part of the Hamiltonian given by

$$\mathcal{H}_i = \frac{q^2}{c r_{12}} + \frac{q^2}{c R_{ab}} - \frac{q^2}{c r_{1b}} - \frac{q^2}{c r_{2a}}. \qquad (2.56)$$

To understand why U is called the exchange integral, note that it gives the probability of the system making a transition from the state $\varphi_a(\mathbf{r}_1) \varphi_b(\mathbf{r}_2)$ to the state $\varphi_a(\mathbf{r}_2) \varphi_b(\mathbf{r}_1)$ owing to the presence of the interaction Hamiltonian. Since these two states differ only by the interchange of the electrons, this integral is a measure of the rate at which the electrons will exchange places. The energies of the symmetric and antisymmetric states are, therefore,

$$\mathcal{E}_\pm = 2\mathcal{E}_0 + \frac{V \pm U}{1 \pm \alpha^2}. \qquad (2.57)$$

The difference in energy between the two states is

$$\mathcal{E}_S - \mathcal{E}_A = -2 \frac{V\alpha^2 - U}{1 - \alpha^4}. \qquad (2.58)$$

The actual value of this difference will clearly depend on the relative magnitudes of α, V, and U.

So far so good, but what about spin? None of these calculations has explicitly taken spin into account, so how can the spin affect the energy? We have seen that the energy difference between the symmetric and antisymmetric states can be thought of as arising from the overlap of electronic wave functions along with the possibility of the electrons exchanging positions. It can also be thought of as depending on the spin orientations through the *Pauli exclusion principle*, as we will now show.

First, we need to show that the complete two-particle wave function (by complete we mean including spin) must be antisymmetric. This follows from the Pauli exclusion principle: no two electrons can be in the same state at the same time. To see that this principle requires an antisymmetric wave function, consider what would happen if we interchanged the electrons.

- If the wave function is antisymmetric, then interchanging them should give the negative of the wave function $(-\psi)$.
- If the electrons were in the same state, then interchanging them will leave the wave function (ψ) unchanged.

The only way that both conditions can be satisfied is for the trivial case of $\psi = 0$. Consequently, we conclude that the use of antisymmetric wave functions ensures that no two electrons can be in the same state, and the

Pauli exclusion principle is satisfied. In statistical mechanics, the behavior of particles that obey the Pauli exclusion principle is described by the *Fermi–Dirac statistics*, and are referred to as *fermions*. In contrast, a moment's consideration of the same interchange operation on a symmetric wave function would again leave the wave function ψ_S unchanged, but ψ_S would not have to vanish. Consequently, symmetric wave functions *do* allow multiple particles to be in the same state. Particles that do not obey the Pauli exclusion principle obey *Bose–Einstein statistics*, and are called *bosons*. We will return to the topic of bosons in a later section.

Having established that the complete wave function for a multiple electron system must be antisymmetric, we must assign a symmetric spin function to ψ_A, and an antisymmetric spin function to ψ_S. The possibilities are shown in Table 2.1. As discussed in Section 1.4, the angular momentum (in this case spin only) can be characterized by the total angular momentum and the component along a single direction. Consequently, we have also listed the total spin and the z-component of spin for the corresponding states in Table 2.1.

Since any of the three symmetric spin eigenfunctions could be used without changing the energy (the energy is determined by ψ_A), we will use the symbols χ_A and χ_S to represent antisymmetric and symmetric spin eigenfunctions, respectively.

At this point, we note that the singlet state $\psi_S\chi_A$ has a total spin 0, whereas each of the triplet states $\psi_A\chi_S$ has spin 1. Since these two states have different energy, we should be able to construct an operator that could give us the energy of the state by "sniffing out" the spin orientations without regard to spatial coordinate symmetries. Before considering such operators, let us consider how the spin orientation affects the energy.

If the two spins are lined up, the Pauli exclusion principle requires them to stay away from each other thereby reducing the Coulomb repulsion energy between them. Based on this argument alone, one would conclude that the ground state of H_2 should be the triplet state. However, in hydrogen, the increase in kinetic energy associated with the parallel spin configuration outweighs the decrease in coulomb potential energy and the antiparallel configuration turns out to be more favorable. The result is that the difference in energy may be viewed as depending on the spin orientations through the

Table 2.1. Two electron spin eigenfunctions.

Function	Parity	Total spin	z-Component of spin
$\frac{1}{\sqrt{2}}[\chi_{\uparrow\downarrow} - \chi_{\downarrow\uparrow}]$	antisymm	0	0
$\chi_{\uparrow\uparrow}$	symm	1	1
$\frac{1}{\sqrt{2}}[\chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow}]$	symm	1	0
$\chi_{\downarrow\downarrow}$	symm	1	−1

exclusion principle. Thus, although the hydrogen molecule exhibits antifer-romagnetic rather than ferromagnetic order, it does illustrate how energy can depend on spin orientation, and hence helps to motivate the form of the Heisenberg Hamiltonian. It is interesting that the interactions that give rise to magnetic ordering are actually electrostatic in origin!

The task at hand, then, is to find an operator that can sense the spin orientations and thereby give us the energy of the state. Clearly, one choice would be the square of the total spin operator S^2 since it has the properties (see Section 1.4)[5]

$$S^2 \psi_S \chi_A = \hbar^2 s(s+1) \psi_S \chi_A = 0, \tag{2.59}$$

$$S^2 \psi_A \chi_S = \hbar^2 s(s+1) \psi_A \chi_S = 2\hbar^2 \psi_A \chi_S. \tag{2.60}$$

A suitable operator would be

$$\mathcal{H}^{\text{spin}} = \mathcal{E}_S + \frac{1}{2\hbar^2} [\mathcal{E}_T - \mathcal{E}_S] S^2, \tag{2.61}$$

where the subscripts now indicate singlet and triplet states rather than symmetric and antisymmetric (e.g., $\mathcal{E}_T = \mathcal{E}_A$), respectively. The dependence on the relative orientations of the two electron spins can be made more apparent by expanding the operator as $S^2 = (\mathbf{S}_1 + \mathbf{S}_2) \cdot (\mathbf{S}_1 + \mathbf{S}_2)$ such that

$$\begin{aligned}
\mathcal{H}^{\text{spin}} &= \mathcal{E}_S + \frac{1}{2\hbar^2} [\mathcal{E}_T - \mathcal{E}_S] \left[S_1^2 + S_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \right] \\
&= \mathcal{E}_S + \frac{1}{2\hbar^2} [\mathcal{E}_T - \mathcal{E}_S] \left[2\hbar^2 s(s+1) + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \right] \\
&= \frac{1}{4} [\mathcal{E}_S + 3\mathcal{E}_T] + \frac{1}{\hbar^2} [\mathcal{E}_T - \mathcal{E}_S] \mathbf{S}_1 \cdot \mathbf{S}_2.
\end{aligned} \tag{2.62}$$

In the last line, we have made use of the fact that $s = 1/2$ for an electron.[6]

Since we are interested in low-lying excitations above the ground state, the zero of energy is not important. We can, therefore, write Eq. (2.62) in the form of a Heisenberg spin Hamiltonian (cf. Eq. (2.42))

$$\mathcal{H} = -2\frac{\mathcal{J}}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2, \tag{2.63}$$

where

$$\mathcal{J} = \frac{1}{2} (\mathcal{E}_S - \mathcal{E}_T) = \frac{U - V\alpha^2}{1 - \alpha^4}. \tag{2.64}$$

---

[5] Note that the spin operator only operates on the spin eigenfunction χ_A or χ_S.

[6] In (2.62), $s = 1/2$ since it results from the single electron operators $S_{1,2}^2$. In contrast, $s = 1$ in (2.60), since it results from the square of the total spin operator $\mathbf{S}$.

One last item and we will be over the hump of hydrogen molecule Hamiltonians and we can go on to bigger and better things.

The exchange phenomenon can be further clarified by introducing the Pauli spin exchange operator P. This operator simply interchanges the two electron spins: $P\chi_{\uparrow\downarrow} = \chi_{\downarrow\uparrow}$. Using this property, it is apparent that

$$P\chi_S = \chi_S, \quad P\chi_A = -\chi_A. \tag{2.65}$$

Since this operator obviously senses the spin orientations, it should be no surprise that the Hamiltonian can also be written in terms of it:

$$\mathcal{H}^P = -\frac{\mathcal{J}}{2}(2P - 1). \tag{2.66}$$

To verify the equivalence, we first need to find the expected value of the Hamiltonian (2.63), then compare with the expected value of (2.66). From (2.62) we have

$$\frac{1}{\hbar^2}[\mathcal{E}_T - \mathcal{E}_S]\,\mathbf{S}_1 \cdot \mathbf{S}_2 = -2\frac{\mathcal{J}}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2 = \mathcal{H}^{\text{spin}} - \frac{1}{4}[\mathcal{E}_S + 3\mathcal{E}_T]. \tag{2.67}$$

Applying this operator to the singlet state gives

$$
\begin{aligned}
-2\frac{\mathcal{J}}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\psi_S\chi_A &= \left(\mathcal{H}^{\text{spin}} - \frac{1}{4}[\mathcal{E}_S + 3\mathcal{E}_T]\right)\psi_S\chi_A \\
&= \left(\mathcal{E}_S - \frac{1}{4}[\mathcal{E}_S + 3\mathcal{E}_T]\right)\psi_S\chi_A \\
&= \frac{3}{4}(\mathcal{E}_S - \mathcal{E}_T)\psi_S\chi_A \\
&= \frac{3}{2}\mathcal{J}\psi_S\chi_A.
\end{aligned}
\tag{2.68}
$$

Examination of the Hamiltonian expressed in terms of the spin exchange operator (2.66) shows that it gives the identical result:

$$
\begin{aligned}
\mathcal{H}^P\psi_S\chi_A &= -\frac{\mathcal{J}}{2}(2P - 1)\psi_S\chi_A = -\frac{\mathcal{J}}{2}(-2 - 1)\psi_S\chi_A \\
&= \frac{3}{2}\mathcal{J}\psi_S\chi_A.
\end{aligned}
\tag{2.69}
$$

Following a similar procedure for the triplet state, we find that

$$\mathcal{H}^P\psi_A\chi_S = \mathcal{H}\psi_A\chi_S = -\frac{1}{2}\mathcal{J}\psi_A\chi_S \tag{2.70}$$

from both the Heisenberg form (2.63) and the spin exchange form (2.66) (see Problem 2.1). Thus, we have established the equivalence between the Heisenberg and the Pauli spin exchange operator forms of the Hamiltonian.

2.5 Spin Wave on a Linear Ferromagnetic Chain: Spin Exchange Operator Method[7]

It is a great leap from the hydrogen molecule to a linear chain of coupled spins. The fact that a Heisenberg Hamiltonian can be written for two coupled spins is no guarantee that the Hamiltonian for N-coupled spins can be written in a similar form. It is an even greater leap to postulate a Heisenberg Hamiltonian for a 3D solid. In actual solids, the interactions are often so complex that the concept of an exchange interaction ceases to be well defined. Nevertheless, it turns out that many phenomena described by the Heisenberg Hamiltonian are observed in magnetic materials so that it has been found to be a simple model rich in physical insight. We, therefore, postulate the Hamiltonian for a chain of N spins to be

$$\mathcal{H} = -2\frac{\mathcal{J}}{\hbar^2} \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \tag{2.71}$$

where we have made the additional assumptions that only nearest neighbor interactions are important, and all nearest neighbor exchange interactions are equal. We will further assume $s = 1/2$ and $\mathcal{J} > 0$.

Using the Pauli spin exchange operator introduced in Section 2.4 we can also write this Hamiltonian in the form

$$\mathcal{H}^P = -\frac{\mathcal{J}}{2} \sum_n (2P_{n,n+1} - 1). \tag{2.72}$$

Before continuing with the calculation of the expected energy, it is convenient to introduce a compact notation introduced by Dirac. Instead of representing a state with a wave function, the state is represented by the symbol

$$\psi \leftrightarrow |\psi\rangle. \tag{2.73}$$

The Hermitian transpose (simply the complex conjugate for a scalar function) is written

$$\psi^* \leftrightarrow \langle\psi|. \tag{2.74}$$

When the symbols are juxtaposed, an *inner product* is indicated. If the state is represented by a vector, then the inner product is simply the vector dot product. If the state is represented by a continuous function, then the inner product implies integration:

$$\langle\psi|\psi\rangle = \int \psi^*\psi d^3r. \tag{2.75}$$

As a joke on the word "bracket," the symbol $\langle\psi|$ is called a "bra" and the symbol $|\psi\rangle$ is called a "ket" (note that the terminology does *not* refer to any

---

[7] This section draws heavily on [8, Section 15-2].

articles of clothing!). The inner product between two states represents the probability amplitude that the system will transition between the states:

$$\langle \varphi | \, \psi \rangle = \int \varphi^* \psi d^3 r. \tag{2.76}$$

Finally, if an operator is placed between a "bra" and a "ket," it represents the expected value of the operator if the bra and ket represent the same state, and a transition probability amplitude if the bra and ket states are different:

$$\langle \varphi | \, A \, | \psi \rangle = \int \varphi^* A \psi d^3 r. \tag{2.77}$$

Returning now to the linear chain of spins, with $\mathcal{J} > 0$, the lowest energy will clearly be that with all spins aligned. We will call this the ground state and denote it $|G\rangle$. The spin exchange operator leaves the ground state unchanged, so that

$$\langle G | \, \mathcal{H}^P \, | G \rangle = -\mathcal{J} N / 2. \tag{2.78}$$

As before, we are not interested in the constant energy offset, so we can subtract this energy and refer all excitation energies to the ground state. The Hamiltonian (2.72) then becomes

$$\mathcal{H}^P = -\mathcal{J} \sum_n \left(P_{n,n+1} - 1 \right). \tag{2.79}$$

This clearly gives zero for the ground state energy.

The lowest excited states of this system are those for which one spin is flipped. One possible choice of basis states to use is the set of all possible states in which only one spin is flipped. We will denote the state in which the spin on the mth site is flipped by $|m\rangle$. The actual state of the system $|\psi\rangle$ can be expressed as a sum over all possible states with one flipped spin

$$|\psi\rangle = \sum_m |m\rangle \langle m | \, \psi \rangle, \tag{2.80}$$

where $\langle m | \, \psi \rangle$ is the probability amplitude that the system is in the state with a flipped spin at location m. The Schrödinger equation can be written

$$\mathcal{H} \, |\psi\rangle = \mathcal{E} \, |\psi\rangle,$$
$$\langle n | \, \mathcal{H} \, |\psi\rangle = \mathcal{E} \, \langle n \, |\psi\rangle,$$
$$\sum_m \langle n | \, \mathcal{H} \, |m\rangle \langle m \, |\psi\rangle = \mathcal{E} \, \langle n \, |\psi\rangle, \tag{2.81}$$
$$-\mathcal{J} \sum_i \sum_m \langle n | \, (P_{i,i+1} - 1) \, |m\rangle \langle m \, |\psi\rangle = \mathcal{E} \, \langle n \, |\psi\rangle.$$

Now consider what happens when the spin exchange operator is applied to the state $|m\rangle$. If neither i nor $i+1$ are equal to m, then two parallel spins

are flipped leaving the state unchanged and $(P_{i,i+1} - 1) |m\rangle = 0$. However, if $i = m$, then the flipped spin at location m is transferred to location $m + 1$ so that

$$(P_{m,m+1} - 1) |m\rangle = |m + 1\rangle - |m\rangle. \tag{2.82}$$

Similarly, if $i + 1 = m$, then the flipped spin is transferred to location $m - 1$:

$$(P_{m-1,m} - 1) |m\rangle = |m - 1\rangle - |m\rangle. \tag{2.83}$$

Substitution of Eqs. (2.82) and (2.83) into (2.81) leads to

$$-\mathcal{J} \sum_m \langle n| (|m + 1\rangle - |m\rangle + |m - 1\rangle - |m\rangle) \langle m |\psi\rangle = \mathcal{E} \langle n |\psi\rangle. \tag{2.84}$$

To simplify this, we use the fact that the state with a flipped spin at location m is orthogonal to the state with a flipped spin at location n unless $m = n$. We further take the states to be normalized so that

$$\langle m| n\rangle = \delta_{m,n}, \tag{2.85}$$

and $\delta_{m,n}$ is the Kronecker delta. Consider the first term on the left-hand side of (2.84):

$$-\mathcal{J} \sum_m \langle n|m + 1\rangle \langle m|\psi\rangle = -\mathcal{J} \sum_m \delta_{n,m+1} \langle m|\psi\rangle$$
$$= -\mathcal{J} \langle n - 1|\psi\rangle. \tag{2.86}$$

Simplifying the remaining terms in (2.84) in a similar manner gives

$$-\mathcal{J} (\langle n - 1 |\psi\rangle + \langle n + 1 |\psi\rangle - 2 \langle n |\psi\rangle) = \mathcal{E} \langle n |\psi\rangle. \tag{2.87}$$

If the location of the nth spin is x_n and the spacing between spins is a, let us write

$$\langle n| \psi\rangle \equiv C (x_n), \tag{2.88a}$$
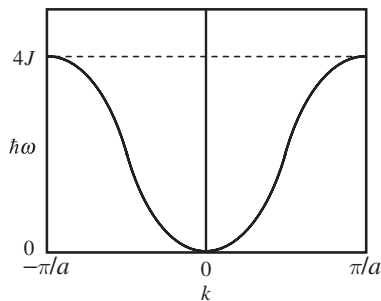$$\langle n \pm 1| \psi\rangle \equiv C (x_n \pm a). \tag{2.88b}$$

Equation (2.87) can now be written as

$$-\frac{\mathcal{E}}{\mathcal{J}} C (x_n) = C (x_n - a) + C (x_n + a) - 2C (x_n) \tag{2.89}$$

which is a difference equation with a solution of the form

$$C (x_n) = e^{ikx_n}. \tag{2.90}$$

Fig. 2.2. Dispersion relation for a spin wave on a linear chain of spins. The points $k = \pm\pi/a$ represent the edges of the *Brillouin zone*. Because the spacing between spins is a, any value of k outside this range is indistinguishable from the point within this range obtained by adding or subtracting an integer multiple of $G = 2\pi/a$, referred to as a *reciprocal lattice vector*.

Substituting this trial solution into (2.89) and simplifying yields

$$-\frac{\mathcal{E}}{\mathcal{J}}e^{ikx_n} = e^{ik(x_n-a)} + e^{ik(x_n+a)} - 2e^{ikx_n},$$

$$-\frac{\mathcal{E}}{\mathcal{J}} = 2\left(\frac{e^{ika} + e^{-ika}}{2}\right) - 2, \qquad (2.91)$$

$$\mathcal{E} = 2\mathcal{J}\left(1 - \cos ka\right).$$

Associating the energy $\mathcal{E}$ with the frequency $\hbar\omega$ gives the *dispersion relation* (Figure 2.2)

$$\omega = \frac{2\mathcal{J}}{\hbar}\left(1 - \cos ka\right). \qquad (2.92)$$

If the wavelength is long compared to the spacing between spins so that $ka \ll 1$, the dispersion relation reduces to

$$\omega \approx \frac{\mathcal{J}a^2}{\hbar}k^2. \qquad (2.93)$$

Recall that $\langle n| \psi\rangle \equiv C\left(x_n\right) = \exp(ikx_n)$ represents the probability amplitude that the flipped spin is located on site n. Referring to the semi-classical picture of a precessing spin introduced in Section 1.4, we can interpret the spin wave as an excitation in which the precession phase varies linearly from site-to-site as illustrated in Figure 2.3.

If we were to add together several closely spaced frequency components, we can form a "wave packet" that moves along the chain in the same manner as a particle. Comparing $\hbar^2 k^2/(2m^*)$ with $\mathcal{J}a^2k^2$ suggests a particle with an effective mass

$$m^* = \frac{\hbar^2}{2\mathcal{J}a^2}. \qquad (2.94)$$
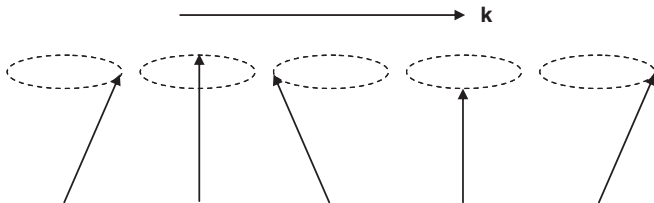
Fig. 2.3. Visualization of a spin wave as a disturbance in which the angle of precession varies linearly from spin-to-spin in the direction of propagation.

This "particle" is sometimes called a *magnon*, and represents the movement along the chain of a region where the likelihood of a flipped spin is high. The movement is enabled by the probability that spins will exchange places with a nearest neighbor, effectively moving the location of the flipped spin.

2.6 Harmonic Oscillator[8]

In Section 2.5, we considered the properties of a single spin wave on a linear chain. Clearly, we would like to be able to discuss the properties of multiple spin waves in 3D solids. To enable this more ambitious discussion, it is helpful to briefly make a side trip into a very important model in quantum mechanics: the *harmonic oscillator*. We will see that the concepts introduced by the model play an important role in the description of magnons.

2.6.1 Harmonic Oscillator Eigenfunctions

We begin by considering the solution to the Schrödinger equation for a charged particle in one dimension (cf. Eq. (1.46)):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = \mathcal{E}\psi(x). \tag{2.95}$$

The classical harmonic oscillator consists of a mass on the end of a spring. In this case, the potential energy is that of a stretched spring, or $V = Kx^2/2$, where K is the spring constant. We know from the classical problem that there is a natural resonant frequency of oscillation of the spring given by $\omega = \sqrt{K/m}$. In terms of the resonant frequency, the potential energy can be expressed $V = m\omega^2 x^2/2$. Substituting this expression for the potential into Schrödinger's equation (2.95) gives the equation describing the quantum mechanical harmonic oscillator:

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[8] For a more detailed discussion of the quantum mechanical harmonic oscillator, see [3, Chapter 5].

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = \mathcal{E}\psi. \tag{2.96}$$

To obtain solutions to this equation, it is helpful to make the change of variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x. \tag{2.97}$$

After making this substitution, Schrödinger's equation becomes

$$\frac{d^2\psi'}{d\xi^2} + \left(\frac{2\mathcal{E}}{\hbar\omega} - \xi^2\right)\psi' = 0. \tag{2.98}$$

Next, we introduce a new function f such that

$$\psi'(\xi) = e^{-\xi^2/2}f(\xi). \tag{2.99}$$

The equation for f is found to be

$$\frac{d^2 f}{d\xi^2} - 2\xi\frac{df}{d\xi} + 2nf = 0, \tag{2.100}$$

where $2n \equiv 2\mathcal{E}/\hbar\omega - 1$ or

$$\mathcal{E} = \hbar\omega\left(n + \frac{1}{2}\right). \tag{2.101}$$

It turns out that the solutions to (2.100) diverge as $\xi \to \infty$ in such a way that ψ' also diverges unless n is a positive integer. Since the wave function for a real particle must be bounded, we conclude that physically meaningful solutions only exist when n is a positive integer. In this case, the solutions to (2.100) are given by the *Hermite polynomials* $H_n(\xi)$. The first few polynomials are

$$\begin{aligned} H_0(\xi) &= 1, \\ H_1(\xi) &= 2\xi, \\ H_2(\xi) &= -2 + 4\xi^2. \end{aligned} \tag{2.102}$$

These polynomials have the following useful recurrence relations:

$$\frac{dH_n}{d\xi} = 2nH_{n-1}, \tag{2.103}$$

$$H_{n+1} = 2\xi H_n - 2nH_{n-1}. \tag{2.104}$$

The eigenfunctions for the original harmonic oscillator problem are, therefore

$$\psi_n(x) = C_n \exp\left(-\frac{x^2}{2\alpha^2}\right) H_n\left(\frac{x}{\alpha}\right), \tag{2.105}$$

where α is a characteristic length given by $\alpha = \sqrt{\hbar/(m\omega)}$. The constant C_n is normally chosen so that the eigenfunctions are orthonormal, i.e.,

$$\int_{-\infty}^{\infty} \psi_n(x)\,\psi_m(x)\,dx = \delta_{m,n}. \tag{2.106}$$

Using the integral

$$\int_{-\infty}^{\infty} H_m(\xi)\,H_n(\xi)e^{-\xi^2}\,d\xi = 2^n n!\,\sqrt{\pi}\,\delta_{m,n}, \tag{2.107}$$

the normalization coefficient is found to be

$$C_n = \left(\alpha 2^n n!\sqrt{\pi}\right)^{-1/2}. \tag{2.108}$$

The normalized eigenfunctions are finally

$$\psi_n(x) = \frac{e^{-x^2/(2\alpha^2)}H_n\left(\frac{x}{\alpha}\right)}{\sqrt{\alpha 2^n n!\sqrt{\pi}}}. \tag{2.109}$$

Using this expression along with the recurrence relations (2.103) and (2.104) leads to a property that we will need in the next section:

$$\frac{d\psi_n}{dx} = \frac{1}{\alpha}\left(\psi_{n-1}\sqrt{\frac{n}{2}} - \psi_{n+1}\sqrt{\frac{n+1}{2}}\right). \tag{2.110}$$

2.6.2 Raising and Lowering Operators

It is convenient to introduce a new operator defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + i\frac{p}{m\omega}\right), \tag{2.111}$$

where $p = (\hbar/i)d/dx$ is the 1D momentum operator from Table 1.1. Making this substitution and again introducing the characteristic length α, the operator can be expressed as

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{\alpha} + \alpha\frac{d}{dx}\right). \tag{2.112}$$

To understand the significance of this operator, we apply it to the nth harmonic oscillator eigenfunction:

$$a\psi_n = \frac{1}{\sqrt{2}}\left(\frac{x}{\alpha} + \alpha\frac{d}{dx}\right)\psi_n$$
$$= \frac{1}{\sqrt{2}}\left(\frac{x}{\alpha}\psi_n + \psi_{n-1}\sqrt{\frac{n}{2}} - \psi_{n+1}\sqrt{\frac{n+1}{2}}\right). \tag{2.113}$$

Here, we have expanded the derivative using (2.110). Using the recurrence relation (2.104) along with the normalized eigenfunctions (2.109), we can show that

$$\frac{x}{\alpha}\psi_n - \sqrt{\frac{n+1}{2}}\,\psi_{n+1} = \sqrt{\frac{n}{2}}\,\psi_{n-1}. \tag{2.114}$$

Making this substitution into (2.113) gives

$$a\psi_n = \sqrt{n}\,\psi_{n-1}. \tag{2.115}$$

We see that the effect of the operator a is to lower the state from n to $n-1$. For this reason, a is referred to as a *lowering operator*. Similarly, let us define the operator

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{p}{m\omega}\right) = \frac{1}{\sqrt{2}}\left(\frac{x}{\alpha} - \alpha\frac{d}{dx}\right). \tag{2.116}$$

Following a similar procedure as before, we find that (Problem 2.2)

$$a^\dagger\psi_n = \sqrt{n+1}\,\psi_{n+1}. \tag{2.117}$$

We refer to $a^\dagger$ as a *raising operator* since it raises the state n to $n+1$. It is also interesting to consider the effect of consecutively applying the operators:

$$a^\dagger a\psi_n = a^\dagger\sqrt{n}\,\psi_{n-1} = \sqrt{n}\,a^\dagger\psi_{n-1} = n\psi_n. \tag{2.118}$$

We observe that the expected value of the operator $a^\dagger a$ is simply the state number n. What if we were to apply the operators in the reverse order? We have:

$$aa^\dagger\psi_n = a\sqrt{n+1}\,\psi_{n+1} = \sqrt{n+1}\,a\,\psi_{n+1} = (n+1)\,\psi_n. \tag{2.119}$$

It is clear, then, that the operators do not commute. We encountered non-commuting operators when we discussed angular momentum in Section 1.4, and we found it useful to specify their properties with commutators. In the present case, (2.118) and (2.119) imply

$$\left[a, a^\dagger\right]\psi_n \equiv \left(aa^\dagger - a^\dagger a\right)\psi_n = \psi_n, \tag{2.120}$$

or equivalently

$$\left[a, a^\dagger\right] = 1. \tag{2.121}$$

It is often useful to generalize the notion from the specific case of a charged particle in a quadratic potential well to an abstract state labeled by n for which raising and lowering operators can be defined. In this case, we define

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(q + i\frac{p}{m\omega} \right), \tag{2.122}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(q - i\frac{p}{m\omega} \right), \tag{2.123}$$

where q and p are canonical position and momentum operators, respectively, and m is a canonical effective mass. The Hamiltonian expressed in terms of these canonical variables takes the form

$$\mathcal{H} = \frac{|p|^2}{2m} + \frac{m\omega^2}{2} |q|^2. \tag{2.124}$$

The canonical variables can also be expressed in terms of the raising and lowering operators:

$$q = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger \right), \tag{2.125}$$

$$p = -i\sqrt{\frac{m\omega\hbar}{2}} \left(a - a^\dagger \right). \tag{2.126}$$

Substituting these relations into (2.124) leads to the Hamiltonian expressed in terms of raising and lowering operators:

$$\begin{aligned}
H &= \frac{|p|^2}{2m} + \frac{m\omega^2}{2} |q|^2 \\
&= \frac{1}{2m} \frac{m\omega\hbar}{2} \left(a - a^\dagger \right) \left(a^\dagger - a \right) + \frac{m\omega^2}{2} \frac{\hbar}{2m\omega} \left(a + a^\dagger \right) \left(a^\dagger + a \right) \tag{2.127} \\
&= \frac{\hbar\omega}{2} \left(aa^\dagger + a^\dagger a \right).
\end{aligned}$$

Using the commutation relation (2.121), this can be written as

$$\mathcal{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right). \tag{2.128}$$

Let $|n\rangle$ represent an abstract state with state number n. The actions of the raising and lowering operators on these states are given by

$$\begin{aligned}
a|n\rangle &= \sqrt{n}|n - 1\rangle, \\
a^\dagger|n\rangle &= \sqrt{n + 1}|n + 1\rangle, \\
a^\dagger a|n\rangle &= n|n\rangle, \\
\mathcal{H}|n\rangle &= \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle.
\end{aligned} \tag{2.129}$$

Note that the action of the Hamiltonian operator on the state $|n\rangle$ gives the energy of the state as given in Eq. (2.101).

2.7 Magnons in a 3D Ferromagnet: Method of Holstein and Primakoff [9]

For our discussion of a 3D ferromagnet, we will again assume that only nearest-neighbor interactions are important. We will also add the Zeeman energy from a static bias magnetic field. The Hamiltonian in this case can be expressed

$$\mathcal{H} = -2\frac{\mathcal{J}}{\hbar^2} \sum_{j,\boldsymbol{\delta}} \mathbf{S}_j \cdot \mathbf{S}_{j+\boldsymbol{\delta}} - \frac{g\mu_{\mathrm{B}}B_0}{\hbar} \sum_j S_{jz}. \tag{2.130}$$

In this expression, j represents a specific spin site in the crystal, $\boldsymbol{\delta}$ represents a vector to one of the nearest-neighbors of j, and we have chosen the sign of B_0 so that the lowest energy configuration occurs when all spins are "up."

2.7.1 Magnon Dispersion Relation

It is computationally convenient to re-express the first term of (2.130) in terms of the spin raising and lowering operators introduced in Section 1.4.3. For the jth spin site, we define

$$S_j^+ = S_{jx} + iS_{jy}, \tag{2.131a}$$

$$S_j^- = S_{jx} - iS_{jy}. \tag{2.131b}$$

In terms of these operators, the Hamiltonian (2.130) can be written as

$$\mathcal{H} = -2\frac{\mathcal{J}}{\hbar^2} \sum_{j,\boldsymbol{\delta}} \left[\frac{1}{2}\left(S_j^- S_{j+\boldsymbol{\delta}}^+ + S_j^+ S_{j+\boldsymbol{\delta}}^- \right) + S_{jz}S_{j+\boldsymbol{\delta},z} \right] - \frac{g\mu_{\mathrm{B}}B_0}{\hbar} \sum_j S_{jz}. \tag{2.132}$$

Now consider a state $|s_{jz}\rangle$, where the z-quantum number on site j is s_{jz}. We know that (cf. Eq. (1.62))

$$S_{jz}|s_{jz}\rangle = s_{jz}|s_{jz}\rangle, \tag{2.133}$$

but we need to evaluate

$$S_j^\pm|s_{jz}\rangle = \lambda|s_{jz} \pm 1\rangle, \tag{2.134}$$

or its Hermitian adjoint

$$\langle s_{jz}|S_j^\mp = \langle s_{jz} \pm 1|\lambda^*. \tag{2.135}$$

Taking the inner product of (2.134) and (2.135) gives

$$\langle s_{jz}|S_j^\mp S_j^\pm|s_{jz}\rangle = \langle s_{jz} \pm 1|\lambda^*\lambda|s_{jz} \pm 1\rangle = |\lambda|^2, \tag{2.136}$$

---

[9] In addition to the original paper [9], discussions of this topic can be found in Sparks [10, Section 3.2] and Kittel [11, Chapter 4].

where we have assumed the states are normalized so that $\langle s_{jz}| s_{jz} \rangle = 1$. To find λ, we make use of the relation

$$S_j^2 = \frac{1}{2} \left(S_j^+ S_j^- + S_j^- S_j^+ \right) + S_{jz}^2. \tag{2.137}$$

The quantity $S_j^+ S_j^-$ can be eliminated from (2.137) using the commutator (cf. Eq. (1.58c))

$$\left[S_j^+, S_j^- \right] = S_j^+ S_j^- - S_j^- S_j^+ = 2\hbar S_{jz}. \tag{2.138}$$

The result is

$$S_j^- S_j^+ = S_j^2 - S_{jz} \left(S_{jz} + \hbar \right). \tag{2.139}$$

The inner product can now be evaluated:

$$\begin{aligned}
\langle s_{jz}|S_j^- S_j^+|s_{jz}\rangle &= \langle s_{jz}| \left(S_j^2 - S_{jz} \left(S_{jz} + \hbar \right) \right) |s_{jz}\rangle \\
&= \langle s_{jz}| \left(\hbar^2 s(s+1) - \hbar^2 s_{jz} \left(s_{jz} + 1 \right) \right) |s_{jz}\rangle \\
&= \hbar^2 \left(s(s+1) - s_{jz} \left(s_{jz} + 1 \right) \right) \\
&= |\lambda|^2 .
\end{aligned} \tag{2.140}$$

We conclude that

$$\lambda = \hbar \left(s(s+1) - s_{jz} \left(s_{jz} + 1 \right) \right)^{1/2} \tag{2.141}$$

and

$$S_j^+|s_{jz}\rangle = \lambda|s_{jz} + 1\rangle = \hbar \left(s(s+1) - s_{jz} \left(s_{jz} + 1 \right) \right)^{1/2} |s_{jz} + 1\rangle. \tag{2.142}$$

Following a similar procedure, we find (Problem 2.3)

$$S_j^-|s_{jz}\rangle = \hbar \left(s(s+1) - s_{jz} \left(s_{jz} - 1 \right) \right)^{1/2} |s_{jz} - 1\rangle. \tag{2.143}$$

We next introduce the basis states $|n_j\rangle$, where n_j is the number of spin deviations (flipped spins) at site j. Increasing n_j by 1 decreases s_{jz} by 1. We also introduce raising and lowering operators similar to those for the harmonic oscillator with the properties

$$\begin{aligned}
\left[a_i, a_j^+ \right] &= \delta_{i,j}, \\
\left[a_i^\pm, a_j^\pm \right] &= 0.
\end{aligned} \tag{2.144}$$

When these operators are applied to the basis states, we obtain (cf. Eq. (2.129))

$$\begin{aligned}
a_j |n_j\rangle &= \sqrt{n_j} |n_j - 1\rangle, \\
a_j^+ |n_j\rangle &= \sqrt{n_j + 1} |n_j + 1\rangle, \\
a_j^+ a_j |n_j\rangle &= n_j |n_j\rangle.
\end{aligned} \tag{2.145}$$

Since flipping a spin reduces the z-component of the spin on the site, we have

$$S_{jz}|s_{jz}\rangle = \hbar\left(s - n_j\right)|s_{jz}\rangle \tag{2.146}$$

or

$$s_{jz} = s - n_j, \tag{2.147}$$

where s is the total spin on the site. Since we saw previously that a flipped spin distributed over a group of sites corresponds to a quasi-particle called a magnon, the operators a_j^+ and a_j can also be viewed as magnon (or spin deviation) *creation* and *annihilation* operators, respectively. Since more than one flipped spin can exist on a site (depending on the total spin), it is possible for multiple magnons to exist at the same location, and we conclude that the quasi-particles do not obey the Pauli exclusion principle. This means that magnons behave as bosons.

Using Eqs. (2.147) and (2.142), the effect of the raising operator on the new basis states can be written as

$$\begin{aligned}
S_j^+ |n_j\rangle &= \hbar\left(s(s+1) - (s - n_j)(s - n_j + 1)\right)^{1/2}|n_j - 1\rangle \\
&= \hbar\left(2sn_j - n_j^2 + n_j\right)^{1/2}|n_j - 1\rangle \\
&= \hbar\sqrt{2s}\left(1 - \frac{(n_j - 1)}{2s}\right)\sqrt{n_j}\,|n_j - 1\rangle.
\end{aligned} \tag{2.148}$$

Comparison with (2.145) suggests that the spin raising operator S_j^+ can be expressed in terms of the new harmonic oscillator raising and lowering operators as follows:

$$S_j^+ = \hbar\sqrt{2s}\left(1 - \frac{a_j^+ a_j}{2s}\right)^{1/2} a_j. \tag{2.149}$$

Following a similar procedure, we find that

$$S_j^- = \hbar\sqrt{2s}\,a_j^+\left(1 - \frac{a_j^+ a_j}{2s}\right)^{1/2}. \tag{2.150}$$

Equations (2.149) and (2.150) are known as the *Holstein–Primakoff transformation* [9].

We now make the low-temperature approximation that makes this problem solvable. Specifically, we assume that the total number of flipped spins in the system is small compared to the total number of spins. In this case

$$\left\langle \sum_j \left(1 - \frac{a_j^+ a_j}{2s}\right)^{1/2}\right\rangle \approx N, \tag{2.151}$$

where the brackets indicate the expected value. This suggests that we can approximate the radical by

$$\left(1 - \frac{a_j^+ a_j}{2s}\right)^{1/2} \approx 1. \tag{2.152}$$

If s is small, this may introduce considerable error in the term for the jth site, but since the operator is averaged over the entire sample, the overall error in the energy will be small provided

$$\frac{\left\langle \sum_j (a_j^+ a_j) \right\rangle}{2Ns} \ll 1. \tag{2.153}$$

We can then approximate the spin raising and lowering operators as

$$S_j^+ \approx \hbar\sqrt{2s}\, a_j, \tag{2.154}$$

$$S_j^- \approx \hbar\sqrt{2s}\, a_j^+. \tag{2.155}$$

Substituting these approximations into the Hamiltonian (2.132) and keeping terms up to second-order in creation/annihilation operators gives

$$
\begin{aligned}
\mathcal{H} = &- 2\mathcal{J}s \sum_{j,\boldsymbol{\delta}} \left[a_j^+ a_{j+\boldsymbol{\delta}} + a_j a_{j+\boldsymbol{\delta}}^+ - a_j^+ a_j - a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}} + s \right] \\
&- g\mu_{\mathrm{B}} B_0 \sum_j \left(s - a_j^+ a_j \right).
\end{aligned}
\tag{2.156}
$$

We would now like to diagonalize this Hamiltonian. Since the form of Eq. (2.156) clearly shows the coupling between adjacent spins, we suspect the basis states that will diagonalize the Hamiltonian will involve collective excitations of all the spins in the system. The transformation to collective excitations can be made through the use of the *Fourier transforms* of the a_j's. We therefore introduce the operators[10] $a_{\mathbf{k}}^+$ and $a_{\mathbf{k}}$ which create and annihilate magnons of wavevector $\mathbf{k}$, respectively:

$$
\begin{aligned}
a_{\mathbf{k}}^+ &= N^{-1/2} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} a_j^+, \\
a_{\mathbf{k}} &= N^{-1/2} \sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} a_j.
\end{aligned}
\tag{2.157}
$$

Here, $\mathbf{r}_j$ is the vector locating the jth site in the crystal. The inverse transform is

$$
\begin{aligned}
a_j^+ &= N^{-1/2} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}^+ \\
a_j &= N^{-1/2} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}.
\end{aligned}
\tag{2.158}
$$

---

[10] Our choice of sign convention in the exponent is that of Oguchi [12] and opposite to that of Holstein and Primakoff [9].

The commutation relation for the new operators is

$$
\begin{aligned}
\left[a_{\mathbf{k}}, a_{\mathbf{k}'}^{+}\right] &= \frac{1}{N} \sum_{j,l} e^{-i\mathbf{k}\cdot\mathbf{r}_j} e^{i\mathbf{k}'\cdot\mathbf{r}_l} \left[a_j, a_l^{+}\right] \\
&= \frac{1}{N} \sum_{j,l} e^{-i\mathbf{k}\cdot\mathbf{r}_j} e^{i\mathbf{k}'\cdot\mathbf{r}_l} \delta_{j,l} \\
&= \frac{1}{N} \sum_{j} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_j} \\
&= \delta_{\mathbf{k},\mathbf{k}'} \, .
\end{aligned}
\tag{2.159}
$$

The last step results from the periodicity of the crystal (Problem 2.4). If the site j has Z-nearest neighbors, the Hamiltonian then becomes

$$
\mathcal{H} = -2\mathcal{J}NZs^2 - g\mu_{\mathrm{B}}B_0 Ns + \mathcal{H}_0,
\tag{2.160}
$$

where

$$
\begin{aligned}
\mathcal{H}_0 = &-\frac{2\mathcal{J}s}{N} \sum_{j\boldsymbol{\delta}\mathbf{k}\mathbf{k}'} \Big(e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} e^{i\mathbf{k}'\cdot\boldsymbol{\delta}} a_{\mathbf{k}}^{+} a_{\mathbf{k}'} + e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} e^{-i\mathbf{k}'\cdot\boldsymbol{\delta}} a_{\mathbf{k}} a_{\mathbf{k}'}^{+} \\
&-e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} a_{\mathbf{k}}^{+} a_{\mathbf{k}'} - e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_j+\boldsymbol{\delta})} a_{\mathbf{k}}^{+} a_{\mathbf{k}'} \Big) \\
&+\frac{g\mu_{\mathrm{B}}B_0}{N} \sum_{j\mathbf{k}\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} a_{\mathbf{k}}^{+} a_{\mathbf{k}'} .
\end{aligned}
\tag{2.161}
$$

As before, the sums over j will cause all of the terms to vanish unless $\mathbf{k} = \mathbf{k}'$. We now have

$$
\begin{aligned}
\mathcal{H}_0 = &-2\mathcal{J}s \sum_{\boldsymbol{\delta}\mathbf{k}} \left(e^{i\mathbf{k}\cdot\boldsymbol{\delta}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} a_{\mathbf{k}} a_{\mathbf{k}}^{+} - 2a_{\mathbf{k}}^{+} a_{\mathbf{k}} \right) + g\mu_{\mathrm{B}}B_0 \sum_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} \\
= &-2\mathcal{J}sZ \sum_{\mathbf{k}} \left(\gamma_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} + \gamma_{-\mathbf{k}} a_{\mathbf{k}} a_{\mathbf{k}}^{+} - 2a_{\mathbf{k}}^{+} a_{\mathbf{k}} \right) + g\mu_{\mathrm{B}}B_0 \sum_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}},
\end{aligned}
\tag{2.162}
$$

where we have defined

$$
\gamma_{\mathbf{k}} = \frac{1}{Z} \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}.
\tag{2.163}
$$

For crystals with a center of symmetry $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$ and $\mathcal{H}_0$ can be further simplified with the commutation relation (2.159):

$$
\begin{aligned}
\mathcal{H}_0 &= -2\mathcal{J}sZ \sum_{\mathbf{k}} \left(\gamma_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} + \gamma_{\mathbf{k}} \left(1 + a_{\mathbf{k}}^{+} a_{\mathbf{k}} \right) - 2a_{\mathbf{k}}^{+} a_{\mathbf{k}} \right) + g\mu_{\mathrm{B}}B_0 \sum_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} \\
&= -4\mathcal{J}sZ \sum_{\mathbf{k}} \left(\gamma_{\mathbf{k}} - 1 \right) a_{\mathbf{k}}^{+} a_{\mathbf{k}} + g\mu_{\mathrm{B}}B_0 \sum_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} \\
&= \sum_{\mathbf{k}} \left(4\mathcal{J}sZ \left(1 - \gamma_{\mathbf{k}} \right) + g\mu_{\mathrm{B}}B_0 \right) a_{\mathbf{k}}^{+} a_{\mathbf{k}}.
\end{aligned}
\tag{2.164}
$$

One last simplification allows us to write

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}} \hbar \omega_{\mathbf{k}}, \tag{2.165}$$

where $\hat{n}_{\mathbf{k}} = a_{\mathbf{k}}^+ a_{\mathbf{k}}$ is the operator for the number of magnons with wavevector $\mathbf{k}$, and the frequency is given by

$$\hbar \omega_{\mathbf{k}} = 4 \mathcal{J} s Z \left(1 - \gamma_{\mathbf{k}}\right) + g \mu_{\mathrm{B}} B_0 \,. \tag{2.166}$$

As an example, consider the case of a simple cubic lattice. In this case, the nearest neighbors are along the $\pm x$, $\pm y$, and $\pm z$ axes at a distance a and we have

$$\begin{aligned}
\gamma_{\mathbf{k}} &= \frac{1}{Z} \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}} \\
&= \frac{1}{6} \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a} \right) \\
&= \frac{1}{3} \left(\cos k_x a + \cos k_y a + \cos k_z a \right).
\end{aligned} \tag{2.167}$$

The dispersion relation becomes finally

$$\hbar \omega_{\mathbf{k}} = 24 \mathcal{J} s \left(1 - \frac{1}{3} \left(\cos k_x a + \cos k_y a + \cos k_z a \right) \right) + g \mu_{\mathrm{B}} B_0. \tag{2.168}$$

For small k, this reduces to approximately

$$\hbar \omega_k = g \mu_{\mathrm{B}} B_0 + 4 \mathcal{J} s a^2 k^2. \tag{2.169}$$

2.7.2 Magnon Interactions

The first rigorous calculation of spin wave interactions was done by Dyson [13, 14]. However, in the words of Oguchi [12], "Although Dyson's paper is rigorous, it is not so easy to understand." Consequently, to obtain an understanding of these interactions, we follow Oguchi's approach, which is based on a further expansion of the Holstein–Primakoff transformation. We therefore need to expand the square root in Eq. (2.152) to higher order:

$$\left(1 - \frac{a_j^+ a_j}{2s} \right)^{1/2} \approx 1 - \frac{a_j^+ a_j}{4s}. \tag{2.170}$$

The spin raising and lowering operators then become

$$S_j^+ \approx \hbar \sqrt{2s} \left(a_j - \frac{a_j^+ a_j a_j}{4s} + \cdots \right), \tag{2.171}$$

$$S_j^- \approx \hbar \sqrt{2s} \left(a_j^+ - \frac{a_j^+ a_j^+ a_j}{4s} + \cdots \right). \tag{2.172}$$

Substituting these expressions into (2.132) and keeping terms to fourth order in creation/annihilation operators gives

$$\mathcal{H} = -2\mathcal{J}NZs^2 - g\mu_{\mathrm{B}}B_0Ns + \mathcal{H}_0 + \mathcal{H}_1 \tag{2.173}$$

where

$$\mathcal{H}_1 = \frac{\mathcal{J}}{2}\sum_{j,\boldsymbol{\delta}}\left(a_j^+ a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}} a_{j+\boldsymbol{\delta}} + a_j^+ a_j^+ a_j a_{j+\boldsymbol{\delta}} + a_j a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}}\right.$$
$$\left. + a_j^+ a_j a_j a_{j+\boldsymbol{\delta}}^+ - 4a_j^+ a_j a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}}\right). \tag{2.174}$$

At this point, we again transform this expression to one in terms of $a_{\mathbf{k}}^+$ and $a_{\mathbf{k}}$. The ensuing calculation quickly becomes very tedious, so let us consider the transformation of only the first term to get an idea for what happens:

$$\mathcal{H}_1^{(1)} = \frac{\mathcal{J}}{2}\sum_{j,\boldsymbol{\delta}} a_j^+ a_{j+\boldsymbol{\delta}}^+ a_{j+\boldsymbol{\delta}} a_{j+\boldsymbol{\delta}}$$
$$= \frac{\mathcal{J}}{2N^2}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}\sum_{j,\boldsymbol{\delta}} e^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}_j} e^{-i(\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\boldsymbol{\delta}} a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2}^+ a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \tag{2.175}$$

As before, owing to the periodicity of the crystal, the sum over j gives

$$\sum_j e^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}_j} = N\Delta\left(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4\right), \tag{2.176}$$

where $\Delta(0) = 1$ and $\Delta(x \neq 0) = 0$ (i.e., it is equivalent to the Kronecker delta $\Delta(x) = \delta_{x,0}$). Consequently, the term vanishes unless *momentum is conserved*:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4. \tag{2.177}$$

The sum over nearest neighbors can then be written

$$\sum_{\boldsymbol{\delta}} e^{-i(\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\boldsymbol{\delta}} = \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}_1\cdot\boldsymbol{\delta}} = Z\gamma_{\mathbf{k}_1}, \tag{2.178}$$

where $\gamma_{\mathbf{k}_1}$ is given by (2.163). The first term in the Hamiltonian (i.e., Eq. (2.175)) can now be written

$$\mathcal{H}_1^{(1)} = \frac{\mathcal{J}Z}{2N}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}\Delta\left(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4\right)\gamma_{\mathbf{k}_1} a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2}^+ a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \tag{2.179}$$

When all of the terms are collected, the interaction Hamiltonian becomes

$$\mathcal{H}_1 = \frac{\mathcal{J}Z}{N}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4}\Delta\left(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4\right)\left(\gamma_{\mathbf{k}_1}+\gamma_{\mathbf{k}_3}-2\gamma_{\mathbf{k}_1-\mathbf{k}_3}\right) a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2}^+ a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \tag{2.180}$$

For a simple cubic lattice at long wavelengths ($ka \ll 1$), $\gamma_{\mathbf{k}}$ can be approximated from (2.167) to be

$$\gamma_{\mathbf{k}} \approx 1 - (ka)^2/6, \tag{2.181}$$

and

$$\gamma_{\mathbf{k}_1 - \mathbf{k}_3} \approx 1 - \frac{(k_1 a)^2}{6} - \frac{(k_3 a)^2}{6} + \frac{\mathbf{k}_1 \cdot \mathbf{k}_3 a^2}{3}. \tag{2.182}$$

The magnitude of the interaction Hamiltonian is therefore proportional to

$$\gamma_{\mathbf{k}_1} + \gamma_{\mathbf{k}_3} - 2\gamma_{\mathbf{k}_1 - \mathbf{k}_3} \approx \frac{1}{6} \left(k_1^2 a^2 + k_3^2 a^2 - 4\mathbf{k}_1 \cdot \mathbf{k}_3 a^2 \right). \tag{2.183}$$

The transition probability from a state with magnons $\mathbf{k}_1, \mathbf{k}_2$ to a state with magnons $\mathbf{k}_3, \mathbf{k}_4$ is proportional to $|\langle 3, 4| \mathcal{H}_1 |1, 2\rangle|^2 \sim (ka)^4$, so that the interactions are very weak for long-wavelength magnons.

In the case of the spin eigenstates $|s_{jz}\rangle$, the z-component of spin can only be raised or lowered until the z-component is equal to the total spin. Further applications of the raising or lowering operators, $S_j^{\pm}$, will give zero. In contrast, the states $|n_j\rangle$ have a harmonic oscillator on each site, so that the number of spin deviations is unlimited. The fact that in reality not more than $2s_j$ spin deviations can exist on a given site gives rise to what Dyson calls the *kinematical interaction*. As we have mentioned, a spin wave is actually a collective excitation; a single spin deviation does not appear on a particular site, but is rather distributed over all of the sites in the crystal. Because of this, the expectation value of the z-component of spin for one spin deviation in a lattice of N sites is of order $s - 1/N$ instead of $s - 1$ (taking the ground state to be all spins up). Speaking classically, the kinematical interaction is caused by the fact that the cone angle of the spin precession can only be opened to π. However, the above z-component of spin suggests a cone angle on the order of $\sqrt{2/(Ns)} \ll 1$ for N large (Problem 2.5). Hence, we expect the effects of the kinematical interaction to be small at low temperatures where the number of magnons present is small compared to the number of sites in the crystal.

In Dyson's analysis, there is another interaction that results from the fact that the spin wave states $|s_j, s_{jz}\rangle$ are not eigenfunctions of the Hamiltonian (2.132). Dyson calls this the *dynamical interaction*. The effects of the simultaneous presence of two spin waves can be modeled by applying two rotations to a given spin vector. The fact that rotations do not commute results in a mutual disturbance that is the dynamical interaction. However, since two very small rotations almost commute, we expect the dynamical interaction to likewise be very small.

The effects of these interactions can be grouped into three categories, namely those due to

(1) the dynamical interaction only,
(2) the kinematical interaction only, and
(3) more complicated effects involving both interactions.

Dyson [14] shows that the contributions from (2) and (3) exactly cancel for all non-negative powers of temperature T. For negative powers of T, he shows that the contribution of the kinematical interaction to the free energy is less than $\exp\left(-T_c/T\right)$, where T_c is the Curie temperature. This interaction, therefore, makes a rigorously negligible contribution for $T \to 0$ when the number of magnons is small. The net result is the following very significant conclusion: the kinematical interaction has no effect on the spin wave scattering probability amplitudes at low temperatures. These processes are governed entirely by the dynamical interaction. Therefore, the scattering probability amplitudes given by our harmonic oscillator model (that does not contain the kinematical interaction) should be entirely satisfactory.

Finally, we note that our Hamiltonian (2.173) does not contain any three wave processes; i.e., terms involving three creation/annihilation operators. This is because we have neglected the magnetic dipole–dipole interactions between the spins in an effort to simplify the discussion. When dipole–dipole interactions are included, it is possible to have magnon splitting and magnon confluence processes as illustrated in Figure 2.4(b),(c). These processes are represented by terms in the Hamiltonian of form

$$\mathcal{H}_1' = \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \Delta\left(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3\right)\left(V\left(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\right)a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2}^+ a_{\mathbf{k}_3} + h.c.\right) \qquad (2.184)$$

where $h.c.$ indicates the Hermitian conjugate.

Dipole–dipole interactions also affect the magnon dispersion relation in the absence of magnon interactions. The net result is to make the dispersion
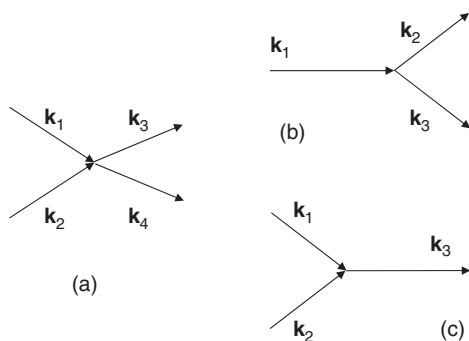
Fig. 2.4. Representative 3- and 4-magnon interactions. Part (a) depicts the scattering process indicated by (2.180), (b) depicts the magnon splitting process described by the first term in (2.184), and (c) illustrates the magnon confluence process described by the Hermitian conjugate term in (2.184).

relation anisotropic even for long-wavelength excitations. To understand the origin of the anisotropy, recall that there is a null in the field from a dipole in directions along its axis, while the field is strongest perpendicular to the axis. If we define θ to be the angle between the direction of propagation and the spin axis, then we expect the shift from dipole coupling to be zero for propagation in the direction $\theta = 0$, and for the shift to be greatest for the direction $\theta = \pi/2$. This spreads the dispersion relation into a band of frequencies for $ka \ll 1$ as illustrated in Figure 2.5. This band of frequencies is referred to as the *spin wave manifold*. Calculations of the effects of dipole–dipole interactions are simpler in a classical formulation for continuous media, so we will defer a more detailed treatment until Chapter 5.
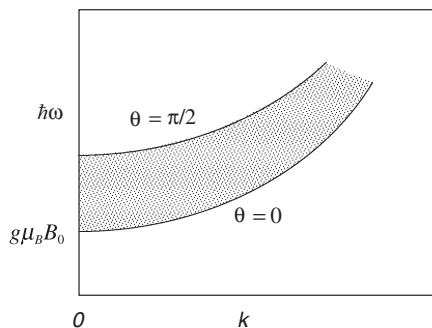
Fig. 2.5. Spin wave dispersion diagram near $k = 0$ with dipolar interactions. The dipole–dipole interactions spread the range of frequencies into a band depending on the direction of propagation with respect to the spin orientation. For $\theta = 0$ the dipolar coupling is zero, and the dispersion relation is given by (2.169). Compared with Figure 2.2, the presence of a bias field raises the frequency for $k = 0$ spin waves.

Problems

2.1. In this problem, we will verify the equivalence of the Heisenberg Hamiltonian and the alternative form expressed in terms of the Pauli spin exchange operator when applied to the hydrogen triplet state $\psi_A \chi_S$.

(a) Calculate the expected value of the Heisenberg Hamiltonian by evaluating

$$-2\frac{\mathcal{J}}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2\, \psi_A \chi_S = \left(\mathcal{H}^{\text{spin}} - \frac{1}{4}\left[\mathcal{E}_S + 3\mathcal{E}_T \right] \right) \psi_A \chi_S, \qquad (2.185)$$

where $\mathcal{J} = (\mathcal{E}_S - \mathcal{E}_T)/2$.

(b) Calculate the expected value of the alternative Hamiltonian by evaluating

$$\mathcal{H}^P \psi_{\text{A}} \chi_{\text{S}} = -\frac{\mathcal{J}}{2}(2P-1)\psi_{\text{A}}\chi_{\text{S}}. \qquad (2.186)$$

2.2. Show that

$$a^\dagger \psi_n = \sqrt{n+1}\,\psi_{n+1}, \qquad (2.187)$$

where

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x}{\alpha} - \alpha\frac{d}{dx}\right) \qquad (2.188)$$

and

$$\psi_n(x) = \frac{e^{-\frac{x^2}{2\alpha^2}} H_n\left(\frac{x}{\alpha}\right)}{\sqrt{\alpha 2^n n!\sqrt{\pi}}}. \qquad (2.189)$$

2.3. Referring to Section 2.7.1, show that

$$S_j^- |s_{jz}\rangle = \hbar\left(s(s+1) - s_{jz}(s_{jz}-1)\right)^{1/2}|s_{jz}-1\rangle. \qquad (2.190)$$

2.4. Consider a linear chain of N spins. The exact solution on a finite chain will depend on the boundary conditions at the ends. A common choice in solid-state physics is the periodic boundary condition, i.e., $\psi(x_1) = \psi(x_{1+N})$.

(a) If $x_n = na$ and $\psi(x) = e^{ikx}$, show that the allowed values of k are $k_m = 2\pi m/Na$, where $m = 0, \pm 1, \pm 2, \ldots, \pm N/2$ (assuming N is even).
(b) With the definitions from Part (a), show that

$$\sum_{j=0}^{N-1} e^{ik_m x_j} = 0, \quad k_m \neq 0 \qquad (2.191)$$

$$\sum_{j=0}^{N-1} e^{ik_m x_j} = N, \quad k_m = 0. \qquad (2.192)$$

$$(2.193)$$

2.5. Consider a classical vector of length s precessing about the z axis. If the z-component of $\mathbf{s}$ is $s-1/N$ with $s \ll N$, show that the cone angle of the precession (i.e., the angle of s with respect to the z-axis) is approximately $\sqrt{2/(Ns)}$.

References

[1] J. D. Jackson, *Classical Electrodynamics*, 3rd ed. Singapore: John Wiley and Sons, 1999.

[2] H. Goldstein, C. P. Poole, and J. L. Safko, *Classical Mechanics*, 3rd ed. Cambridge, MA: Addison-Wesley, 2001.

[3] E. Merzbacher, *Quantum Mechanics*, 3rd ed. New York: John Wiley & Sons, 1998.

[4] D. C. Mattis, *The Theory of Magnetism I: Statics and Dynamics*. New York: Springer-Verlag, Berlin, 1981.

[5] D. H. Martin, *Magnetism in Solids*. Cambridge, MA: M.I.T. Press, 1967.

[6] G. T. Rado and H. Suhl, Eds., *Magnetism I*. New York: Academic Press, 1963.

[7] W. Heitler and F. London, "Reciprocal action of neutral atoms and homopolar combination according to quantum mechanics," Z. Physik, vol. 44, pp. 455–472, 1927.

[8] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics*. Reading, MA: Addison-Wesley, 1964, vol. III.

[9] T. Holstein and H. Primakoff, "Field dependence of the intrinsic domain magnetization of a ferromagnet," *Phys. Rev.*, vol. 58, no. 12, pp. 1098–1113, Dec 1940.

[10] M. Sparks, *Ferromagnetic Relaxation Theory*. New York: McGraw-Hill, 1964.

[11] C. Kittel, *Quantum Theory of Solids*. New York: John Wiley & Sons, 1963.

[12] T. Oguchi, "Theory of spin wave interactions in ferro- and antiferromagnetism," *Phys. Rev.*, vol. 117, pp. 117–123, 1960.

[13] F. J. Dyson, "General theory of spin-wave interactions," *Phys. Rev.*, vol. 102, pp. 1217–1230, 1956.

[14] F. J. Dyson, "Thermodynamic behavior of an ideal ferro-magnet," *Phys. Rev.*, vol. 102, pp. 1230–1244, 1956.

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