Chapter 2

Second Quantisation

To facilitate the formulation and analysis of many-body systems, the aim of this section is to introduce and apply the method of second quantisation. The first part of the section focuses on methodology and notation, while the remainder is devoted to applications. Examples of the operator formalism are taken from quantum condensed matter and include the interacting electron gas and quantum magnetism. Specifically, we will investigate the the Mott transition to a magnetic insulator, spin waves in a quantum Heisenberg (anti)ferromagnet, and the weakly interacting Bose gas.

2.1 Notations and Definitions

Second quantisation provides a basic and efficient language in which to formulate many-particle systems. As such, extensive introductions to the concept can be found throughout the literature (see, e.g., Feynman [10]). The first part of this chapter will be concerned with the introduction of the basic elements of second quantisation for bosonic and fermionic degrees of freedom, while the remainder of this section will be concerned with developing fluency in the method by addressing a number of applications.

Let us begin by defining the (normalised) wavefunctions $|\psi_\lambda\rangle$ and corresponding eigenvalues ϵ_λ of the single-particle Hamiltonian $\hat{H}$, viz.

$$\hat{H}|\psi_\lambda\rangle = \epsilon_\lambda|\psi_\lambda\rangle.$$

With this definition, populating states 1 and 2, the symmetrised (and normalised) 2-particle wavefunction for fermions and bosons is respectively given by

$$\begin{aligned}
\psi_F(x_1, x_2) &= \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\right) \\
\psi_B(x_1, x_2) &= \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)\right).
\end{aligned}$$

In the Dirac bracket representation, we can write

$$\begin{aligned}
|1,2\rangle_F &\equiv \frac{1}{\sqrt{2}}\left(|\psi_1\rangle\otimes|\psi_2\rangle - |\psi_2\rangle\otimes|\psi_1\rangle\right),\\
|1,2\rangle_B &\equiv \frac{1}{\sqrt{2}}\left(|\psi_1\rangle\otimes|\psi_2\rangle + |\psi_2\rangle\otimes|\psi_1\rangle\right).
\end{aligned}$$

More generally, a *symmetrised* N-particle wavefunction of fermions ($\zeta = -1$) or bosons ($\zeta = +1$) is expressed in the form

$$\boxed{|\lambda_1,\lambda_2,\ldots\lambda_N\rangle \equiv \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty} n_\lambda!}}\sum_{\mathcal{P}} \zeta^{\mathcal{P}} |\psi_{\lambda_{\mathcal{P}1}}\rangle\otimes|\psi_{\lambda_{\mathcal{P}2}}\rangle\ldots\otimes|\psi_{\lambda_{\mathcal{P}N}}\rangle}$$

where n_λ is the total number of particles in state λ (for fermions, Pauli exclusion enforces the constraint $n_\lambda = 1$) – see Fig. 2.1. The summation runs over all $N!$ permutations of the set of quantum numbers $\{\lambda_1,\ldots\lambda_N\}$, and $\mathcal{P}$ denotes the parity, defined as the number of transpositions of two elements which brings the permutation $(\mathcal{P}_1,\mathcal{P}_2,\cdots\mathcal{P}_N)$ back to the ordered sequence $(1,2,\cdots N)$. Note that the summation over permutations is necessitated by quantum mechanical **indistinguishability**: for bosons/fermions[1] the wave function has to be symmetric/anti-symmetric under particle exchange. It is straightforward to confirm that the prefactor $1/\sqrt{N!\prod_\lambda n_\lambda!}$ normalises the many-body wave function. In the fermionic case, the many-body wavefunction is known as a **Slater determinant**.

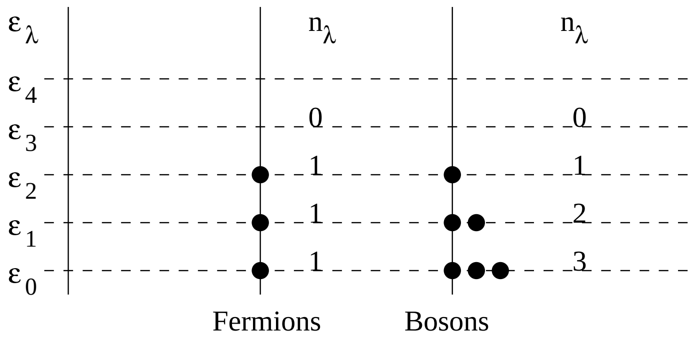
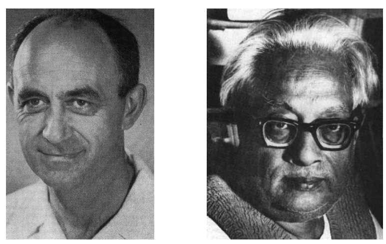


Figure 2.1: Schematic diagram showing occupation numbers for a generic fermion and boson system.

The expression above makes it clear that this 'first quantised' representation of the many-body wavefunction is clumsy. The formalism of second quantisation affords the possibility to heavily condense the representation. To this end, let us define the **vacuum**

[1] **Enrico Fermi** 1901-1954 (left) and **Satyendranath Bose** 1894-1974 (right): Fermi was made 1938 Nobel Laureate in Physics for his demonstrations of the existence of new radioactive elements produced by neutron irradiation, and for his related discovery of nuclear reactions brought about by slow neutrons.



state $|\Omega\rangle$, and introduce a set of **field operators** a_λ together with their adjoints $a^\dagger_\lambda$, as follows:[2]

$$\boxed{a_\lambda|\Omega\rangle = 0, \qquad \frac{1}{\sqrt{\prod_\lambda n_\lambda!}}\prod_{i=1}^{N} a^\dagger_{\lambda_i}|\Omega\rangle = |\lambda_1,\lambda_2,\ldots\lambda_N\rangle} \tag{2.1}$$

Physically, the operator $a^\dagger_\lambda$ creates a particle in state λ while the operate a_λ annhilates it. These definitions are far from innocent and deserve some qualification. Firstly, in order not to be at conflict with the symmetry of the wavefunction, the operators a_λ have to fulfill the commutation relations

$$\boxed{\left[a_\lambda, a^\dagger_\mu\right]_{-\zeta} = \delta_{\lambda,\mu}, \qquad \left[a_\lambda, a_\mu\right]_{-\zeta} = 0, \qquad \left[a^\dagger_\lambda, a^\dagger_\mu\right]_{-\zeta} = 0} \tag{2.2}$$

where $[\hat{A},\hat{B}]_{-\zeta} \equiv \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$ is the commutator $\zeta = 1$ (anti-commutator $\zeta = -1$) for bosons (fermions).[3] The most straightforward way to understand this condition is to check that the definition $|\lambda,\mu\rangle = a^\dagger_\lambda a^\dagger_\mu|\Omega\rangle$ and property $|\lambda,\mu\rangle = \zeta|\mu,\lambda\rangle$ in fact necessitate Eqs. (2.2). Yet even if (2.2) is understood, the definitions above remain non-trivial. Actually, quite a strong statement has been made: for *any* N, the N-body wavefunction can be generated by an application of a set of N-*independent* operators to a unique vacuum state. In order to check that Eqs. (2.1) and (2.2) actually represent a valid definition, including, for instance, the right symmetrisation and normalisation properties of N-body wave functions, various consistency checks have to be made.

Based on Eqs. (2.1) and (2.2), a formal definition of the general many-body or **Fock space** can now be given as follows. First define $\mathcal{F}_N$ to be the linear span of all N-particle states $|\lambda_1,\cdots\lambda_N\rangle = (1/\sqrt{\prod_\lambda n_\lambda})\prod_{i=1}^N a^\dagger_{\lambda_i}|\Omega\rangle$. The Fock space $\mathcal{F}$ is then defined as the direct sum $\oplus_{N=0}^\infty \mathcal{F}_N$ (see Fig. 2.2).[4] A general state $|\phi\rangle$ of the Fock space is, therefore, a

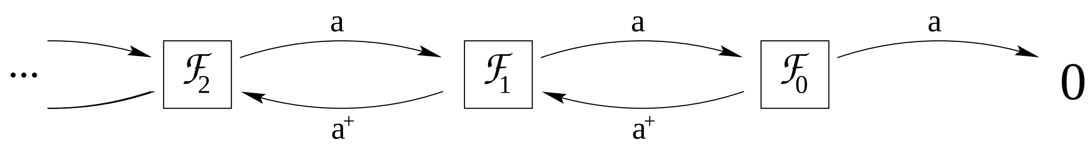


Figure 2.2: Visualisation of the generation of the Fock-subspaces $\mathcal{F}_N$ by repeated action of creation operators onto the vacuum space $\mathcal{F}_0$.

linear combination of states with any number of particles. To turn these rather abstract definitions into a valuable tool for practical computations we need to put them into relation with standard operations performed in quantum mechanics. In particular we have to specify how changes from one single particle basis $\{\lambda\}$ to another $\{\tilde{\lambda}\}$ affect the operator algebra $\{a_\lambda\}$, and in which way standard operators of (many-body) quantum mechanics can be represented in terms of the as:

[2]As before, it will be convenient to represent these operators without a circumflex.

[3]As a convention, when unspecified by ζ, the notation $[\cdot,\cdot]$ will be used to denote the commutator and $\{\cdot,\cdot\}$ the anticommutator.

[4]Here, the symbol of the direct sum $\oplus$ is used to show that each "submodule" $\mathcal{F}_N$ is linearly independent.

▷ **Change of basis:** Using the resolution of identity, id $= \sum_{\lambda=0}^{\infty} |\lambda\rangle\langle\lambda|$, the relations $|\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle$, $|\lambda\rangle \equiv a_\lambda^\dagger|\Omega\rangle$, and $|\tilde{\lambda}\rangle \equiv a_{\tilde{\lambda}}^\dagger|\Omega\rangle$ immediately give rise to the transformation law

$$\boxed{a_{\tilde{\lambda}}^\dagger = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a_\lambda^\dagger, \qquad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda} \tag{2.3}$$

In many applications we are not dealing with a set of discrete quantum numbers (spin, quantised momenta, etc.), but rather with a continuum (a continuous position coordinate, say). In these cases, the quantum numbers are commonly denoted in a bracket notation $a_\lambda \rightsquigarrow a(x) = \sum_\lambda \langle x|\lambda\rangle a_\lambda$ and the summations appearing in the transformation formula above become integrals.

Example: The transformation from the coordinate to the momentum representation in a finite one-dimensional system of length L would read

$$a_k = \int_0^L dx\ \langle k|x\rangle a(x), \qquad \langle k|x\rangle \equiv \langle x|k\rangle^* = \frac{1}{L^{1/2}} e^{-ikx}.$$

▷ **Representation of operators (one-body):** Single particle or one-body operators $\hat{\mathcal{O}}_1$ acting in a N-particle **Hilbert space**[5] $\mathcal{F}_N$ generally take the form $\hat{\mathcal{O}}_1 = \sum_{n=1}^N \hat{o}_n$, where $\hat{o}_n$ is an ordinary single particle operator acting on the nth particle. A typical example is the kinetic energy operator $\hat{T} = \sum_n \hat{p}_n^2/2m$, where $\hat{p}_n$ is the momentum operator acting on the nth particle. Other examples include the one-particle potential operator $\hat{V} = \sum_n V(\hat{x}_n)$, where $V(x)$ is a scalar potential, the total spin-operator $\sum_n \hat{\mathbf{S}}_n$, etc. Since we have seen that, by applying field operators to the vacuum space, we can generate the Fock space in general and any N-particle Hilbert space in particular, it must be possible to represent any operator $\hat{\mathcal{O}}_1$ in an a-representation.

Now, although the representation of n-body operators is afterall quite straightforward, the construction can, at first sight seem daunting. A convenient way of finding such a representation is to express the operator in terms of a basis in which it is diagonal, and only later transform to an arbitrary basis. For this purpose it is useful to define the **occupation number operator**

$$\boxed{\hat{n}_\lambda = a_\lambda^\dagger a_\lambda} \tag{2.4}$$

with the property that, for bosons or fermions (exercise), $\hat{n}_\lambda\ (a_\lambda^\dagger)^n|\Omega\rangle = n\ (a_\lambda^\dagger)^n|\Omega\rangle$, i.e. the state $(a_\lambda^\dagger)^n|\Omega\rangle$ is an eigenstate of the number operator with eigenvalue n.

5

David Hilbert 1862-1943; His work in geometry had the greatest influence in that area after Euclid. A systematic study of the axioms of Euclidean geometry led Hilbert to propose 21 such axioms and he analysed their significance. He contributed to many areas of mathematics.

When acting upon a state $|\lambda_1, \lambda_2, \cdots \lambda_N\rangle$, it is a straightforward exercise to confirm that the number operator simply counts the number of particles in state λ,

$$\hat{n}_\lambda|\lambda_1, \lambda_2, \cdots \lambda_N\rangle = a^\dagger_\lambda a_\lambda \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} \prod_{i=1}^N a^\dagger_{\lambda_i}|\Omega\rangle = \sum_{i=1}^N \delta_{\lambda\lambda_i}|\lambda_1, \lambda_2, \cdots \lambda_N\rangle.$$

Let us now consider a one-body operator, $\hat{\mathcal{O}}_1$, which is diagonal in the orthonormal basis $|\lambda\rangle$, $\hat{o} = \sum_\lambda o_\lambda|\lambda\rangle\langle\lambda|$, $o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$. With this definition, one finds

$$\begin{aligned}
\langle\lambda'_1, \cdots \lambda'_N|\hat{\mathcal{O}}_1|\lambda_1, \cdots \lambda_N\rangle &= \left(\sum_{i=1}^N o_{\lambda_i}\right)\langle\lambda'_1, \cdots \lambda'_N|\lambda_1, \cdots \lambda_N\rangle \\
&= \langle\lambda'_1, \cdots \lambda'_N|\sum_{\lambda=0}^\infty o_\lambda \hat{n}_\lambda|\lambda_1, \cdots \lambda_N\rangle.
\end{aligned}$$

Since this equality holds for any set of states, we obtain the operator or second quantised representation

$$\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^\infty o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^\infty \langle\lambda|\hat{o}|\lambda\rangle a^\dagger_\lambda a_\lambda.$$

The result is straightforward; a one-body operator engages a single particle at a time — the others are just spectators. In the diagonal representation, one simply counts the number of particles in a state λ and multiplies by the corresponding eigenvalue of the one-body operator. Finally, by transforming from the diagonal representation to a general basis, one obtains the result,

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\lambda\mu\nu}\langle\mu|\lambda\rangle o_\lambda\langle\lambda|\nu\rangle a^\dagger_\mu a_\nu = \sum_{\mu\nu}\langle\mu|\hat{o}|\nu\rangle a^\dagger_\mu a_\nu} \tag{2.5}$$

Examples: The **total spin operator** is given by

$$\hat{\mathbf{S}} = \sum_{\lambda\alpha\alpha'} a^\dagger_{\lambda\alpha'}\mathbf{S}_{\alpha'\alpha}a_{\lambda\alpha}, \qquad \mathbf{S}_{\alpha\alpha'} = \frac{1}{2}\sigma_{\alpha\alpha'} \tag{2.6}$$

where $\alpha =\uparrow, \downarrow$ is the spin-quantum number, λ denotes the set of additional quantum numbers (e.g. coordinate), and σ denotes the vector of Pauli[6] spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.7}$$

6

Wolfgang Pauli 1900-1958: 1945 Nobel Laureate in Physics for the discovery of the Exclusion Principle, also called the Pauli Principle.

i.e. $\hat{S}^z = \sum_\lambda (\hat{n}_{\lambda\uparrow} - \hat{n}_{\lambda\downarrow})/2$, and $\hat{S}^+ = \sum_\lambda a^\dagger_{\lambda\uparrow} a_{\lambda\downarrow}$.

Second quantised in the position representation, the **one-body Hamiltonian** is given as a sum of kinetic and potential energy as (exercise)

$$\boxed{\hat{H} = \hat{T} + \hat{V} = \int dx\; a^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] a(x)}$$

where $\hat{p} = -i\hbar\partial_x$. (Note that the latter is easily proved by expressing the kinetic energy in the diagonal (i.e. momentum) representation.)

Finally, the **total occupation number operator** is defined as $\hat{N} = \int dx\; a^\dagger(x) a(x)$.

▷ **Representation of operators (two-body):** Two-body operators $\hat{\mathcal{O}}_2$ are needed to describe *pairwise interactions* between particles. Although pair-interaction potentials are straightforwardly included into *classical* many-body theories, their embedding into conventional many-body quantum mechanics is made awkwardly cumbersome by particle indistinguishability. As compared to the conventional description, the formulation of interaction processes within the language of second quantisation is *considerably* more straightforward.

Initially, let us consider particles subject to the symmetric two-body potential $V(x_m, x_n) \equiv V(x_n, x_m)$ between two particles at position x_m and x_n. Acting on two-particle states, the operator is then given by

$$\hat{V}^{(2)} = \frac{1}{2} \int dx \int dx'\; |x, x'\rangle V(x, x') \langle x, x'|. \tag{2.8}$$

Our aim is to find an operator $\hat{V}$ in second quantised form whose action on a many-body state gives

$$\hat{V}|x_1, x_2, \cdots x_N\rangle = \sum_{n<m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle.$$

Comparing this expressions with (2.8) one might immediately guess that

$$\hat{V} = \frac{1}{2} \int dx \int dx'\; a^\dagger(x) a^\dagger(x') V(x, x') a(x') a(x).$$

That this is the correct answer can be confirmed by applying the operator to a many-body state. We first note that

$$\begin{aligned}
&a(x')a(x)|x_1, x_2, \cdots x_N\rangle \\
&= a(x') \sum_{n=1}^{N} \zeta^{n-1} \delta(x - x_n) |x_1, x_2, \cdots (\text{no } x_n) \cdots x_N\rangle \\
&= \sum_{n=1}^{N} \zeta^{n-1} \delta(x - x_n) \sum_{m=1,(m\neq n)}^{N} \eta_{mn} \delta(x' - x_m) |x_1, x_2, \cdots (\text{no } x_n, x_m) \cdots x_N\rangle
\end{aligned}$$

where

$$\eta_{mn} = \begin{cases} \zeta^{m-1} & \text{if } m < n \\ \zeta^{m} & \text{if } m > n \end{cases}.$$

Then, making use of the identity

$$\begin{aligned}
&a^\dagger(x)a^\dagger(x')a(x')a(x)|x_1, x_2, \cdots x_N\rangle \\
&= \sum_{m\neq n}^{N} \zeta^{n-1}\eta_{mn}\delta(x-x_n)\delta(x'-x_m)|x, x', x_1, x_2, \cdots (\text{no } x_n, x_m) \cdots x_N\rangle \\
&= \sum_{m\neq n}^{N} \zeta^{n-1}\eta_{mn}\delta(x-x_n)\delta(x'-x_m)|x_n, x_m, x_1, x_2, \cdots (\text{no } x_n, x_m) \cdots x_N\rangle \\
&= \sum_{m\neq n}^{N} \delta(x-x_n)\delta(x'-x_m)|x_1, x_2, \cdots x_N\rangle,
\end{aligned}$$

multiplying by $V(x,x')/2$, and integrating over x and x', one confirms the validity of the expression. It is left as an exercise to confirm that the expression, although a plausible candidate, $\frac{1}{2}\int dx \int dx'\, V(x,x')\hat{n}(x)\hat{n}(x')$ does *not* reproduce the two-body operator.

More generally, turning to a non-diagonal basis, it is easy to confirm that a general two-body operator can be expressed in the form

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu,\mu',\lambda,\lambda'} a^\dagger_\mu a^\dagger_{\mu'} a_\lambda a_{\lambda'}} \tag{2.9}$$

where $\mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle \mu, \mu'|\hat{\mathcal{O}}_2|\lambda, \lambda'\rangle$.

In principle one may proceed in the same manner and represent general n-body interactions in terms of second quantised operators. However, as $n > 2$ interactions rarely appear, and certainly not in this lecture course, we refer to the literature for discussion.

This completes our formal introduction to the method of second quantisation. To make these concepts seem less abstract, the remainder of this section applies this method to a variety of problems.

2.2 Applications of Second Quantisation

Although the second quantisation is a representation and not a solution, its application often leads to a considerable simplification of the analysis of many-particle systems. To emphasize this fact, and to practice the manipulation of second quantised operators, we turn to several applications. The first novel example is taken from the physics of strongly correlated electron systems, and will engage the manipulation of fermionic creation and annihilation operators. The second example involves the study of models of quantum magnetism within the framework of boson creation and annihilation operators. However, before getting to these applications, let us first go back and reinterpret our analysis of *phonon modes* in the quantum chain.

2.2.1 Phonons

Although, at the time, we did not specify in which Hilbert space the field operators a_k act, the answer is that the representation space is again a Fock space; this time a Fock space of phonons or, more formally, of oscillator states. In contrast to what we'll find for the fermion case below, the Fock space in the phonon problem does not have an *a priori* interpretation as a unification of physical N-particle spaces. However, outgoing from a vacuum state, it can be constructively generated by applying the oscillator creation operators $a_k^\dagger$ to a unique vacuum space:

▷ INFO. *Define* a ground or vacuum state $|\Omega\rangle$ by requiring that all operators a_k annihilate it. Next define $\mathcal{F}_0$ to be the space generated by $|\Omega\rangle$. We may then introduce a set of states $|k\rangle \equiv a_k^\dagger|\Omega\rangle$, $k = 0, 2\pi/L, \ldots$ by applying oscillator creation operators to the vacuum. Physically, the state $|k\rangle$ has the significance of a single harmonic oscillator quantum excited in mode k. In other words, all oscillator states $k' \neq k$ are in their ground state, whilst mode k is in the first exited state. The vector space generated by linear combinations of states $|k\rangle$ is called $\mathcal{F}_1$. This procedure can be iterated in an obvious manner. Simply define the space $\mathcal{F}_N$ to be generated by all states $a_{k_1}^\dagger \ldots a_{k_N}^\dagger|\Omega\rangle \equiv |k_1, \ldots, k_N\rangle$. The spaces $\mathcal{F}_N$ can be defined more concisely by saying that they are the eigenspaces of the occupation number operator with eigenvalue N. Finally, the Fock space is just the sum of all $\mathcal{F}_N$, $\mathcal{F} \equiv \oplus_{N=0}^{\infty}\mathcal{F}_N$. By construction, the application of any one $a_k^\dagger$ or a_k to states $\in \mathcal{F}$ does not leave $\mathcal{F}$. A closer analysis actually shows that the corresponding Fock space $\mathcal{F}$ represents a proper representation space for the operators a_k. A particle interpretation of the phonon states can now be naturally introduced by saying that the Fock space sector $\mathcal{F}_N$ represents a space of bosonic N-particle states. Application of $a_k^\dagger$ (a_k) to a state $\in \mathcal{F}_N$ creates (annihilates) a particle (cf. Fig. 2.2)).

2.2.2 Interacting Electron Gas

As a second example, we will cast the interacting electron gas as a second quantised Hamiltonian. To emphasize the utility of this approach, in the next section we will use it to explore an unusual part of the electronic phase diagram of a *strongly interacting* gas of electrons. In doing so, we will uncover the limitations of the "nearly free electron theory" of metals.

As we have seen, in second quantised notation, the non-interacting Hamiltonian of a one-dimensional system of electrons subject to a lattice potential is given by

$$\hat{H}^{(0)} = \int dx \sum_\sigma c_\sigma^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right] c_\sigma(x),$$

where the electron field operators obey the anticommutation relations $[c_\sigma(x), c^\dagger_{\sigma'}(x')]_+ = \delta(x-x')\,\delta_{\sigma\sigma'}$ appropriate for spinfull fermions. The field operators act on the 'big' many-particle Fock space, $\mathcal{F} = \oplus_{N=0}^{\infty}\mathcal{F}_N$. Each N-particle space $\mathcal{F}_N$ is spanned by states of the form $\prod_{i=1}^N c^\dagger_{\sigma_i}(x_i)|\Omega\rangle$ where the 'no-particle' state or vacuum $|\Omega\rangle$ is annihilated by all operators $c_\sigma(x)$.

Applying a two-body Coulomb interaction potential, $\frac{1}{2}\sum_{i\neq j} e^2/|\hat{x}_i - \hat{x}_j|$, where $\hat{x}_i$ is the position operator of the i-th electron, the total many-body Hamiltonian takes the second quantised form

$$\boxed{\hat{H} = \hat{H}^{(0)} + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c^\dagger_\sigma(x) c^\dagger_{\sigma'}(x') \frac{e^2}{|x-x'|} c_{\sigma'}(x') c_\sigma(x)} \tag{2.10}$$

(Exercise: Setting $V = 0$ and switching to the Fourier basis in which the non-interacting Hamiltonian is diagonal, reexpress the Coulomb interaction. Show that the latter is non-diagonal, and scatters electrons between different quasi-momentum states — see Fig. 2.3.)

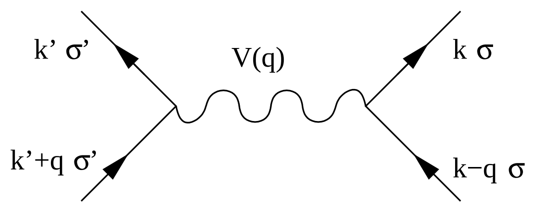


Figure 2.3: Feynman diagrammatic representation of the two-body Coulomb interaction.

Having introduced both the field operators themselves and their representation spaces, we are in a position to point out certain conceptual analogies between the model theories discussed above. In each case we have described a physical system in terms of a theory involving a continuum of operators, $\hat{\phi}(x)$ (phonons) and $c_\sigma(x)$ (electrons). Of course there are also important differences between the examples discussed in this section. Obviously, in the phonon theory, we are dealing with bosons whilst the electron gas is fermionic. However, by far the most important difference is that the first example has been a **free field theory**. That means that the Hamiltonian contained field operators at quadratic order but no higher. As a rule, free field theories can be solved (in a sense that will become clear later on) straightforwardly. The fermionic model, however, represents a typical example of an interacting field theory. There are terms of fourth order in the field operators which arose from the Coulomb interaction term. As compared to free theories, the analysis of interacting theories is infinitely harder, a fact that will surely become evident later on.

To develop some fluency in the manipulation of second quantised field operators we will continue by exploring the '**atomic limit**' of a strongly interacting electron gas. In doing so, we will derive a model Hamiltonian which has served as a paradigm for strongly correlated electronic systems.

2.2.3 Tight-Binding Theory and the Mott Transition

According to the conventional band picture of *non-interacting* electrons, a system with a half-filled band of valence states is metallic. However, the strong interaction of electrons can induce a phase transition to a (magnetic) insulating electron 'solid' phase (much as interactions can drive the condensation of a classical liquid into a solid). To understand the nature of this phenomenon, which, after Sir Neville Mott, is known as the **Mott transition**, it is convenient to reexpress the interacting Hamiltonian in a **tight-binding approximation**.

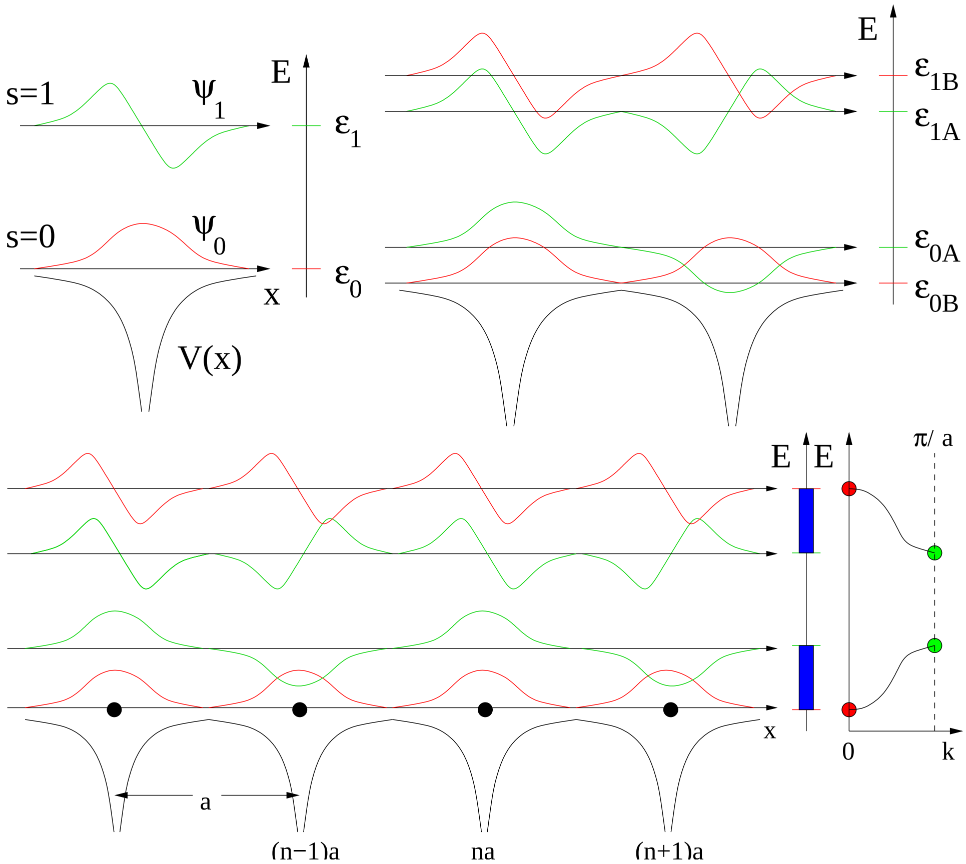


Figure 2.4: Infinitely separated, each lattice site is associated with a set of states, $s = 0, 1, \cdots$, bound to the potential core. Bringing together just two atoms, the orbitals weakly overlap and hybridise into bonding and anti-bonding combinations. Bringing together a well-separated lattice of atoms, each atomic orbital broadens into a delocalised band of Bloch states indexed by a quasi-momentum k from the Brillouin zone and a orbital or band index s.

To develop an effective Hamiltonian of the strongly interacting electron system we begin by considering a lattice of very widely spaced (almost isolated) atoms — the atomic limit. In the simplest, *non-interacting*, picture, the overlap of the outermost electrons (albeit exponentially weak) leads to a hybridisation of the electronic orbitals and induces the 'delocalisation' of a *narrow* band of extended states (see Fig. 2.4). These Bloch states[7] $\psi_{ks}(x)$ of $\hat{H}^{(0)}$, which carry a quasi-momentum index k and a band or orbital index $s = 0, 1, \cdots$, provide a convenient basis in which to expand the interaction. We can, in turn, define a set of local **Wannier orbitals**

$$\overbrace{|\psi_{ns}\rangle}^{c^\dagger_{ns}|\Omega\rangle} \equiv \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{ikna} \overbrace{|\psi_{ks}\rangle}^{c^\dagger_{ks}|\Omega\rangle}, \qquad |\psi_{ks}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-ikna} |\psi_{ns}\rangle$$

where N denotes the total number of primitive lattice sites (with periodic boundary conditions). Here the sum on k runs over the N k-points spanning the Brillouin zone, i.e. $k = 2\pi m/aN$ with integers $-N/2 < m \leq N/2$. If the lattice is very widely spaced, the Wannier state ψ_{ns} will differ little from the sth bound state of an isolated atom at $x = na$ (see Fig. 2.5).

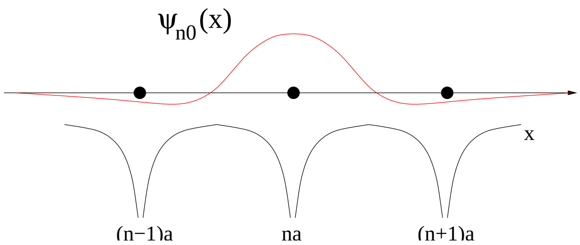


Figure 2.5: Diagram showing the weak overlap of Wannier states in the atomic limit.

Restricting attention to the lowest band $s = 0$, and restoring the spin degrees of freedom σ, the field operators associated with the Wannier functions are defined by

$$\overbrace{|\psi_n\rangle}^{c^\dagger_{n\sigma}|\Omega\rangle} = \int_0^{L=Na} dx \overbrace{|x\rangle}^{c^\dagger_\sigma(x)|\Omega\rangle} \langle x|\psi_n\rangle,$$

i.e.

$$c^\dagger_{n\sigma} \equiv \int_0^L dx\; \psi_n(x) c^\dagger_\sigma(x), \qquad c^\dagger_\sigma(x) = \sum_{n=1}^{N} \psi^*_n(x) c^\dagger_{n\sigma}. \tag{2.11}$$

Physically, $c^\dagger_{n\sigma}$ can be interpreted as an operator creating an electron with spin σ at site n in the lowest band. Since the transformation (2.11) is unitary, it is straightforward to confirm that the operators $c_{n\sigma}$, and $c^\dagger_{n\sigma}$ obey fermionic anticommutation relations $[c_{n\sigma}, c^\dagger_{m\sigma'}]_+ = \delta_{\sigma\sigma'}\delta_{nm}$.

[7] **Felix Bloch** 1905-1983: 1952 Nobel Laureate in Physics for the development (with Edward M. Purcell) of new methods for nuclear magnetic precision measurements and discoveries in connection therewith.

In the presence of a two-body Coulomb interaction, a substitution of the field operators in Eq. (2.10) by Wannier operators generates the generalised tight-binding Hamiltonian (exercise)

$$\boxed{\hat{H} = -\sum_{mn}\sum_{\sigma} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \sum_{mnrs}\sum_{\sigma\sigma'} U_{mnrs}\; c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{r\sigma'} c_{s\sigma'}}$$

where the "hopping" matrix elements are given by

$$t_{mn} = -\left\langle \psi_m | \hat{H}^{(0)} | \psi_n \right\rangle = \frac{1}{N}\sum_k e^{i(n-m)ka}\epsilon_k = t^*_{nm},$$

and the interaction parameters are set by

$$U_{mnrs} = \frac{1}{2}\int_0^L dx \int_0^L dx'\; \psi^*_m(x)\psi^*_n(x')\frac{e^2}{|x-x'|}\psi_r(x')\psi_s(x).$$

Physically t_{mn} represents the probability amplitude for an electron to transfer (hop) from a site m to a site n. (Exercise: show that, in the momentum basis, $c_{n\sigma} = N^{-1/2}\sum_k^{\text{B.Z.}} e^{inka} c_{k\sigma}$, the non-interacting Hamiltonian is diagonalised as $\hat{H}^{(0)} = \sum_k^{\text{B.Z.}} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$.)

Expressed in the Wannier basis, the representation above is exact (at least for states contained entirely within the lowest band). However, for a widely spaced lattice, most of the matrix elements of the general tight-binding model are small and can be neglected. Focusing on the most relevant:

▷ The **direct terms** $U_{mnnm} \equiv V_{mn}$ involve integrals over square moduli of Wannier functions and couple *density fluctuations* at different sites,

$$\sum_{m\neq n} V_{mn}\hat{n}_m\hat{n}_n,$$

where $\hat{n}_m = \sum_\sigma c^\dagger_{m\sigma} c_{m\sigma}$. Such terms have the capacity to induce *charge density* instabilities. Here we will focus on transitions to a magnetic phase where such contributions are inconsequential and can be safely neglected.

▷ A second important contribution derives from the **exchange coupling** which induce magnetic correlations among the electronic spins. Setting $J^F_{ij} \equiv U_{ijij}$, and making use of the identity $\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$, one obtains (exercise)

$$\sum_{m\neq n}\sum_\sigma U_{mnmn} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{m\sigma'} c_{n\sigma} = -2\sum_{m\neq n} J^F_{mn}\left(\hat{\mathbf{S}}_m\cdot\hat{\mathbf{S}}_n + \frac{1}{4}\hat{n}_m\hat{n}_n\right).$$

Such contributions tend to induce weak **ferromagnetic coupling** of neighbouring spins (i.e. $J_F > 0$). Physically, the origin of the coupling is easily understood as deriving from a competition between kinetic and potential energies. By aligning with each other and forming a symmetric spin state, two electrons can reduce their potential energy arising from their mutual Coulomb repulsion. To enforce the anti-symmetry of the two-electron state, the orbital wavefunction would have to vanish at $x = x'$ where the Coulomb potential is largest. This mechanism is familiar from atomic physics where it is manifest as **Hund's rule**.

▷ However, in the **atomic limit** where the atoms are well-separated and the overlap between neighbouring orbitals is weak, the matrix elements t_{ij} and J_{ij}^F are exponentially small in the interatomic separation. By contrast the 'on-site' Coulomb or **Hubbard interaction**

$$\sum_m \sum_\sigma U_{mmmm} c^\dagger_{m\sigma} c^\dagger_{m\sigma'} c_{m\sigma'} c_{m\sigma} = U \sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow},$$

where $U \equiv 2U_{mmmm}$, increases as the atomic wavefunctions become more localised.

Therefore, dropping the constant energy off-set $\epsilon_0 = t_{nn}$, in the atomic limit, a strongly interacting many-body system of electrons can be described effectively by the (single-band) **Hubbard Hamiltonian**

$$\boxed{\hat{H} = -t \sum_{\langle mn \rangle} \sum_\sigma c^\dagger_{m\sigma} c_{n\sigma} + U \sum_m \hat{n}_{m\uparrow}\hat{n}_{m\downarrow}} \tag{2.12}$$

where we have introduced the notation $\langle mn \rangle$ to indicate a sum over neighbouring lattice sites, and $t = t_{mn}$ (assumed real and usually positive). In hindsight, a model of this structure could have been guessed on phenomenological grounds from the outset. Electrons tunnel between atomic orbitals localised on individual lattice sites and experience a local Coulomb interaction with other electrons.

Deceptive in its simplicity, the Hubbard model is acknowledged as a paradigm of strong electron correlation in condensed matter. Yet, after forty years of intense investigation, the properties of this seemingly simple model system — the character of the ground state and nature of the quasi-particle excitations — is still the subject of heated controversey (at least in dimensions higher than one — see below). Nevertheless, given the importance attached to this system, we will close this section with a brief discussion of the remarkable phenomenology that is believed to characterise the Hubbard system.

As well as dimensionality, the phase behaviour of the Hubbard Hamiltonian is characterised by three dimensionless parameters; the ratio of the Coulomb interaction scale to the bandwidth U/t, the particle density or filling fraction n (i.e. the average number of electrons per site), and the (dimensionless) temperature, T/t. The symmetry of the Hamiltonian under particle–hole interchange (exercise) allows one to limit consideration to densities in the range $0 \leq n \leq 1$ while densities $1 < n \leq 2$ can be inferred by 'reflection'.

Focussing first on the low temperature system, in the dilute limit $n \ll 1$, the typical electron wavelength is greatly in excess of the particle separation and the dynamics is free. Here the local interaction presents only a weak perturbation and one can expect the properties of the Hubbard system to mirror those of the weakly interacting nearly free electron system. Here, while the interaction remains weak one expects a metallic behaviour to persist.

By contrast, let us consider the half–filled system where the average site occupancy is unity. Here, if the interaction is weak $U/t \ll 1$, one may again expect properties reminiscent of the weakly interacting electron system.[8] If, on the other hand, the interaction is very strong $U/t \gg 1$, site double occupancy is inhibited and electrons in the half–filled

[8]In fact, one has to exercise some caution since the commensurability of the Fermi wavelength with

system become 'jammed': migration of an electron to a neighbouring lattice site necessitates site double occupancy incurring an energy cost U. Here, in this strongly correlated state, the mutual Coulomb interaction between the electrons drives the system from a metallic to an insulating phase with properties very different from those of a conventional band insulator.

▷ INFO. Despite the ubiquity of the experimental phenomenon (first predicted in a celebrated work by Mott[9]) the nature of the **Mott–Hubbard transtion** from the metallic to the insulating phase in the half–filled system has been the subject of considerable discussion and debate. In the original formulation, following a suggestion of Peierls, Mott conceived of an insulator characterised by two 'Hubbard bands' with a bandwidth $\sim t$ separated by a charge gap U.[10] States of the upper band engage site double occupancy while those states that make up the lower band do not. The transition between the metallic and insulating phase was predicted to occur when the interaction was sufficiently strong that a charge gap develops between the bands. Later, starting from the weakly interacting Fermi–liquid, Brinkman and Rice[11] proposed that the transition was associated with the localisation of quasi–particles created by an interaction driven renormalisation of the effective mass. Finally, a third school considers the transition to the Mott insulating phase as inexorably linked to the development of magnetic correlations in the weak coupling system — the Slater instability.

To summarise, we have shown how the method of second quantisation provides a useful and efficient way of formulating and investigating interacting electron systems. In the next section we will employ methods of second quantisation involving bosonic degrees of freedom to explore the collective excitations of quantum magnets.

2.2.4 Quantum Spin Chains

In the previous section, the emphasis was placed on *charging effects* generated by Coulomb interaction. However, as we have seen, Coulomb interaction may also lead to the indirect generation of *magnetic* interactions of both ferromagnetic and antiferromagnetic character. To address the phenomena brought about by quantum magnetic correlations, it

the lattice can initiate a transition to an insulating **spin density wave** state characterised by a small quasi–particle energy gap. In later chapters, we will discuss the nature of this **Slater Instability** (J. C. Slater, *Magnetic effects and the Hartree–Fock equation*, Phys. Rev. **82**, 538 (1951)) within the framework of the quantum field integral.

[9] **Sir Neville Mott** 1905–1996: 1977 Nobel Laureate in Physics (with Philip W. Anderson and John H. van Vleck) for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems.

[10] N. F. Mott, Proc. Roy. Soc. A **62**, 416 (1949) — for a review see, e.g. N. F. Mott, *Metal–Insulator transition*, Rev. Mod. Phys. **40**, 677 (1968) or N. F. Mott, *Metal–Insulator Transitions*, 2nd ed. (Taylor and Francis, London, 1990).

[11] W. Brinkman and T. M. Rice, *Application of Gutzwiller's variational method to the metal–insulator transition*, Phys. Rev. B **2**, 4302 (1970).

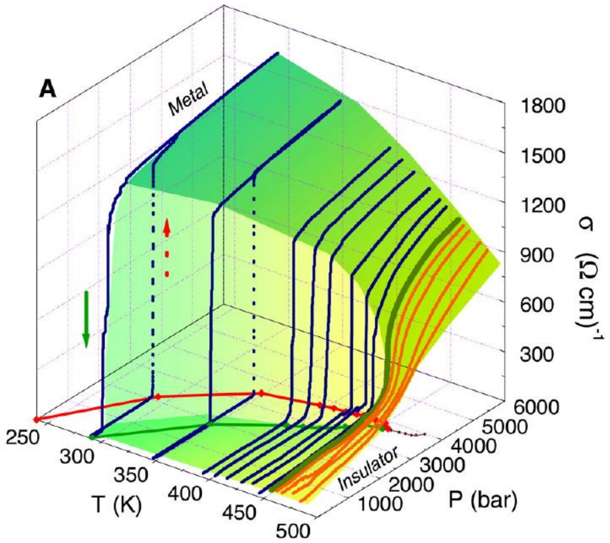


Figure 2.6: Conductivity of Cr–doped V_2O_3 as a function of decreasing pressure and temperature. At temperatures below the Mott–Hubbard transition point ($P_c = 3738\text{bar}, T_c = 457.5\text{K}$) the conductivity reveals hysteretic behaviour characteristic of a first order transition. Figure courtesey of P. Limelette, A. Georges, D. Jérome, P. Wzietek, P. Metcalf, and J. M. Honig, *Universality and critical behavior at the Mott transition*, Science **302**, 89 (2003).

is instructive to begin by considering systems where the charge degrees of freedom are frozen and only spin excitations remain. Such systems are realized, for example, in Mott insulators where magnetic interactions between the local moments of localised electrons is mediated by virtual exchange processes between neighbouring electrons. Here, one can describe the magnetic correlations through models of localised quantum spins — either in chains or, more generally, in higher-dimensional quantum spin lattices. We begin our discussion with the ferromagnetic spin chain.

Quantum Ferromagnet

The quantum Heisenberg[12] ferromagnet is specified by the Hamiltonian

$$\boxed{\hat{H} = -J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n} \tag{2.13}$$

where $J > 0$, $\hat{\mathbf{S}}_m$ represents the quantum mechanical spin operator at lattice site m, and as before, $\langle mn \rangle$ denotes summation over neighbouring sites. In section 2.1 (cf. Eq. (2.6))

12 **Werner Heisenberg** 1901–1976: 1932 Nobel Laureate in Physics "for the creation of quantum mechanics, the application of which has, *inter alia*, led to the discovery of the allotropic forms of hydrogen".

the quantum mechanical spin was represented through an electron basis. However, one can conceive of situations where the spin sitting at site m is carried by a different object (e.g. an atom with non–vanishing magnetic moment). At any rate, for the purposes of our present discussion, we need not specify the microscopic origin of the spin. All we need to know is (i) that the lattice operators $\hat{S}^i_m$ obey the SU(2) commutator algebra (for clarity, we have set $\hbar = 1$ in this section)

$$[\hat{S}^i_m, \hat{S}^j_n] = i\delta_{mn}\epsilon^{ijk}\hat{S}^k_n \tag{2.14}$$

characteristic of quantum mechanical spins, and (ii) that the total spin at each lattice site is S.[13]

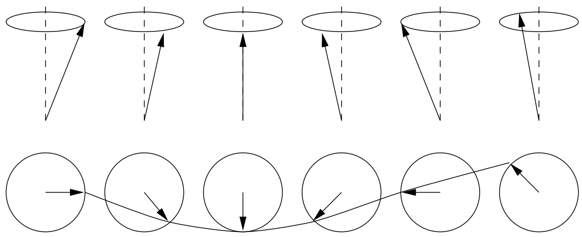


Figure 2.7: Schematic showing the spin configuration of an elementary spin-wave excitation from the spin polarized ground state.

Now, due to the positivity of the coupling constant J, the Hamiltonian favours configurations where the spins at neighbouring sites are aligned in the same direction (cf. Fig. 2.7). A ground state of the system is given by $|\Omega\rangle \equiv \otimes_m |S_m\rangle$, where $|S_m\rangle$ represents a state with maximal spin–z component: $S^z_m|S_m\rangle = S|S_m\rangle$. We have written 'a' ground state instead of 'the' ground state because the system is highly degenerate: A simultaneous change of the orientation of all spins does not change the ground state energy, i.e. the system posesses a global rotation symmetry.

$\triangleright$ Exercise. Compute the energy expectation value of the state $|\Omega\rangle$. Defining *global* spin operators through $\hat{S}^i \equiv \sum_m \hat{S}^i_m$, consider the state $|\alpha\rangle \equiv \exp(i\alpha \cdot \hat{\mathbf{S}})|\Omega\rangle$. Verify that the state α is degenerate with $|\Omega\rangle$. Explicitly compute the state $|(\pi/2, 0, 0)\rangle$. Convince yourself that for general α, $|\alpha\rangle$ can be interpreted as a state with rotated quantisation axis.

As with our previous examples, we expect that a global continuous symmetry will involve the presence of energetically low–lying exciations. Indeed, it is obvious that in the limit of long wavelength λ, a weak distortion of a ground state configuration (cf. Fig. 2.7) will cost vanishingly small energy. To quantitatively explore the physics of these **spin–waves**, we adopt a 'semi–classical' picture, where the spin $S \gg 1$ is assumed to be large. In this limit, the rotation of the spins around the ground state configuration becomes similar to the rotation of a classical magnetic moment.

[13]Remember that the finite–dimensional representations of the spin operator are of dimension $2S + 1$ where S may be integer or half integer. While a single electron has spin $S = 1/2$, the total magnetic moment of electrons bound to an atom may be much larger.

▷ INFO. To better understand the mechanism behind the **semi–classical approximation**, consider the Heisenberg uncertainty relation, $\Delta S^i \Delta S^j \le |\langle[\hat{S}^i, \hat{S}^j]\rangle| = \epsilon^{ijk}|\langle\hat{S}^k\rangle|$, where ΔS^i is the root mean square of the quantum uncertainty of spin component i. Using the fact that $|\langle\hat{S}^k\rangle| \le S$, we obtain for the relative uncertainty, $\Delta S^i/S$,

$$\frac{\Delta S^i}{S}\frac{\Delta S^j}{S} \le \frac{S}{S^2} \xrightarrow{S\gg 1} 0\,.$$

I.e. for $S \gg 1$, quantum fluctuations of the spin become less important.

In the limit of large spin S, and at low excitation energies, it is natural to describe the ordered phase in terms of small fluctuations of the spins around their expectation values (cf. the description of the ordered phase of a crystal in terms of small fluctuations of the atoms around the ordered lattice sites). These fluctuations are conveniently represented in terms of spin raising and lowering operators: with $\hat{S}^{\pm}_m \equiv \frac{1}{2}(S^1_m \pm iS^2_m)$, it is straightforward to verify that

$$[\hat{S}^z_m, \hat{S}^{\pm}_n] = \pm\delta_{mn}S^{\pm}_m, \qquad [\hat{S}^+_m, \hat{S}^-_n] = 2\delta_{mn}S^z_m. \tag{2.15}$$

Application of $\hat{S}^{-(+)}_m$ lowers (raises) the z–component of the spin at site m by one. To actually make use of the fact that deviations around $|\Omega\rangle$ are small, a representation known as the **Holstein–Primakoff transformation**[14] was introduced in which the spin operators $\hat{S}^{\pm}, \hat{S}$ are specified in terms of bosonic creation and annihilation operators $a^\dagger$ and a:

$$\boxed{\hat{S}^-_m = a^\dagger_m(2S - a^\dagger_m a_m)^{1/2}, \qquad \hat{S}^+_m = (2S - a^\dagger_m a_m)^{1/2}a_m, \qquad \hat{S}^z_m = S - a^\dagger_m a_m}$$

The utility of this representation is clear: When the spin is large $S \gg 1$, an expansion in powers of $1/S$ gives $\hat{S}^z_m = S - a^\dagger_m a_m$, $\hat{S}^-_m \simeq (2S)^{1/2}a^\dagger_m$, and $\hat{S}^+_m \simeq (2S)^{1/2}a_m$. In this approximation, the one-dimensional Heisenberg Hamiltonian takes the form

$$\begin{aligned}
\hat{H} &= -J\sum_m \left\{\hat{S}^z_m\hat{S}^z_{m+1} + \frac{1}{2}\left(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1}\right)\right\} \\
&= -JNS^2 - JS\sum_m \left\{-2a^\dagger_m a_m + \left(a^\dagger_m a_{m+1} + \text{h.c.}\right)\right\} + \mathcal{O}(S^0) \\
&= -JNS^2 + S\sum_m (a^\dagger_{m+1} - a^\dagger_m)(a_{m+1} - a_m) + \mathcal{O}(S^0).
\end{aligned}$$

Keeping fluctuations at leading order in S, the quadratic Hamiltonian can be diagonalised by Fourier transformation. In this case, it is convenient to impose periodic boundary conditions: $\hat{S}_{m+N} = \hat{S}_m$, and $a_{m+N} = a_m$, where N denotes the total number of lattice sites. Defining

$$a_k = \frac{1}{\sqrt{N}}\sum_{m=1}^{N} e^{ikm}a_m, \qquad a_m = \frac{1}{\sqrt{N}}\sum_{k}^{\text{B.Z.}} e^{-ikm}a_k, \qquad [a_k, a^\dagger_{k'}] = \delta_{kk'},$$

[14]T. Holstein and H. Primakoff, *Field dependence of the intrinsic domain magnetisation of a ferromagnet*, Phys. Rev. **58**, 1098 (1940).

the Hamiltonian for the one dimensional lattice system takes the form (exercise)

$$\boxed{\hat{H} = -JNS^2 + \sum_k^{\text{B.Z.}} \omega_k a_k^\dagger a_k + \mathcal{O}(S^0)} \tag{2.16}$$

where $\omega_k = 2JS(1 - \cos k) = 4JS\sin^2(k/2)$ represents the dispersion relation of the spin excitations. In particular, in the limit $k \to 0$, the energy of the elementary excitations vanishes, $\omega_k \to JSk^2$. These massless low–energy excitations, known as **magnons**, describe the elementary spin–wave excitations of the ferromagnet. Taking into account terms at higher order in the parameter $1/S$, one finds interactions between the magnons.

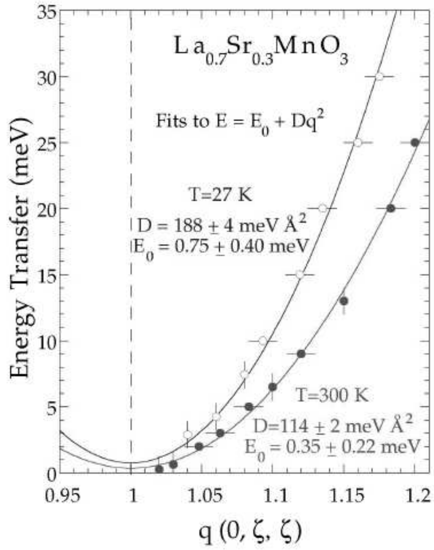


Figure 2.8: Measurements of the spin-wave dispersion relations for the ferromagnet $La_{0.7}Sr_{0.3}MnO_3$.

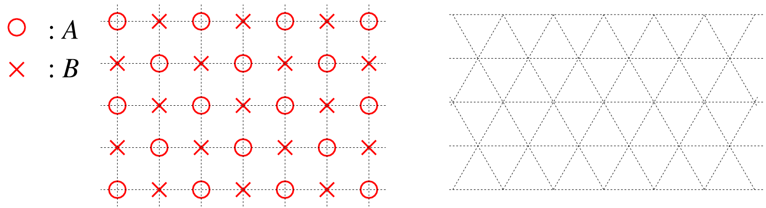
Quantum Antiferromagnet

Having explored the elementary excitation spectrum of the ferromagnet, we now turn to the discussion of the spin S Heisenberg antiferromagnetic Hamiltonian

$$\boxed{\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n}$$

where, once again, $J > 0$. Such local moment antiferromagnetic phases frequently occur in the arena of strongly correlated electron systems. Although the Hamiltonian differs from its ferromagnetic relative 'only' by a change of sign, the differences in the physics are drastic. Firstly, the phenomenology displayed by the antiferromagnetic Hamiltonian $\hat{H}$ depend sensitively on the geometry of the underlying lattice: For a **bipartite lattice**, i.e. one in which the neighbours of one sublattice A belong to the other sublattice B

(cf. Fig. 2.9(a)), the ground states of the Heisenberg antiferromagnet are close[15] to a staggered spin configuration, known as a **Néel state**,[16] where *all* neighbouring spins are antiparallel. Again the ground state is degenerate, i.e. a global rotation of all spins by the same amount does not change the energy. By contrast, on non–bipartite lattices such as the triangular lattice shown in Fig. 2.9(b), no spin arrangement can be found wherein which each and every bond can recover the full exchange energy J. Spin models of this kind are said to be **frustrated**.



a) b)

Figure 2.9: (a) Example of a two–dimensional bipartite lattice and (b) a non–bipartite lattice. Notice that, with the latter, no antiferromagnetic arrangement of the spins can be made that recovers the maximum exchange energy from each and every bond.

Returning to the one–dimensional system, we first note that a chain is trivially bipartite. As before, our strategy will be to expand the Hamiltonian in terms of bosonic operators. However, before doing so, it is convenient to apply a canonical transformation to the Hamiltonian in which the spins on one sublattice, say B, are rotated through 180^o about the x–axis, i.e. $S_B^x \to \widetilde{S}_B^x = S_B^x$, $S_B^y \to \widetilde{S}_B^y = -S_B^y$, and $S_B^z \to \widetilde{S}_B^z = -S_B^z$. I.e. when represented in terms of the new operators, the Néel ground state looks like a ferromagnetic state, with all spins aligned. We expect that a gradual distortion of this state will produce the antiferromagnetic analogue of the spin–waves discussed in the previous section.

Represented in terms of the transformed operators, the Hamiltonian takes the form

$$\hat{H} = -J \sum_m \left[S_m^z \widetilde{S}_{m+1}^z - \frac{1}{2}\left(S_m^+ \widetilde{S}_{m+1}^+ + S_m^- \widetilde{S}_{m+1}^- \right) \right].$$

Once again, applying an expansion of the Holstein–Primakoff representation, $S_m^- \simeq (2S)^{1/2} a_m^\dagger$,

[15]It is straightforward to verify that the classical ground state — the Néel state — is now not an exact eigenstate of the quantum Hamiltonian. The true ground state exhibits zero–point fluctuations reminiscent of the quantum harmonic oscillator or atomic chain. However, when $S \gg 1$, it serves as a useful reference state from which fluctuations can be examined.

[16] **Louis Néel** 1904–: 1970 Nobel Laureate in physics for fundamental work and discoveries concerning antiferromagnetism and ferrimagnetism which have led to important applications in solid state physics

etc., one obtains the Hamiltonian

$$\hat{H} = -NJS^2 + JS\sum_m \left[a_m^\dagger a_m + a_{m+1}^\dagger a_{m+1} + a_m a_{m+1} + a_m^\dagger a_{m+1}^\dagger\right] + \mathcal{O}(S^0)\,.$$

At first sight the structure of this Hamiltonian, albeit quadratic in the Bose operators, looks akward. However, after Fourier transformation, $a_m = N^{-1/2}\sum_k e^{-ikm} a_k$ it assumes the more accessible form

$$\hat{H} = -NJS(S+1) + JS\sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} + \mathcal{O}(S^0),$$

where $\gamma_k = \cos k$.

Quadratic in the bosonic operators, the Hamiltonian can be again diagonalised by canonical transformation. However, to preserve the commutation relations, the transformation must preserve the metric $g = \mathrm{diag}(1, -1)$ (cf. the Lorentz transformation). In the present context, such a transformation is known as a **Bogoliubov transformation**[17] .

$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}. \tag{2.17}$$

Applying (2.17), and setting $\tanh 2\theta_k = \gamma_k$, the Hamiltonian assumes the diagonal form (exercise)

$$\boxed{\hat{H} = -NJS^2 + 2JS\sum_k |\sin k| \left[\alpha_k^\dagger \alpha_k + \frac{1}{2}\right]} \tag{2.18}$$

Thus, in contrast to the ferromagnet, the spin–wave excitations of the antiferromagnet display a *linear spectrum* in the limit $k \to 0$. Surprisingly, although developed in the limit of large spin, experiment shows that even for $S = 1/2$ spin chains, the integrity of the linear dispersion is maintained (see Fig. 2.10).

2.2.5 Bogoluibov Theory of the Dilute Bose Gas

Ealier, we explored the influence of interactions on the electron gas. When interactions are weak, it was noted that the elementary collective excitations are reminiscent of the excitations of the free electron gas — the Fermi-liquid phase. When the interactions are strong, we discussed a scenario in which the electron liquid can condense into a solid insulating phase — the Mott transition. In the following section, we will discuss the

[17] **N. N. Bogoliubov** 1909-1992: Theoretical physcists aclaimed for his works in nonlinear mechanics, statistical physics, theory of superfluidity and superconductivity, Quantum field theory, renormalization group theory, proof of dispersion relations, and elementary particle theory.

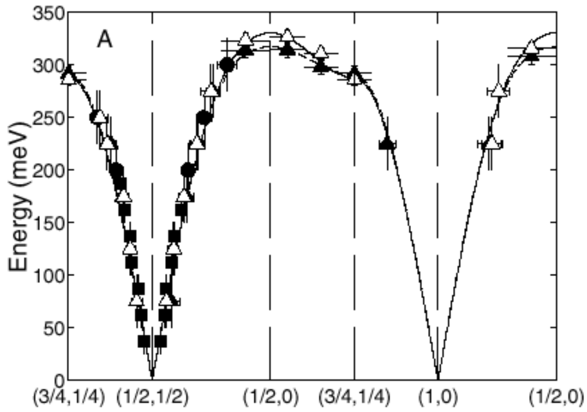


Figure 2.10: Experimentally obtained spin–wave dispersion of the high–T_c parent compound $LaCuO_4$ — a prominent spin 1/2 antiferromagnet. (Courtesy of R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001).)

properties of a quantum liquid comprised of Bose particles — the weakly interacting dilute Bose gas.

Let us consider a *dilute* system of N Bose particles confined to a volume L^d and subject to the Hamiltonian

$$\boxed{\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2}\int d^d\mathbf{x} \int d^d\mathbf{x}' a^\dagger(\mathbf{x}) a^\dagger(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') a(\mathbf{x}') a(\mathbf{x})}$$

where $V(\mathbf{x})$ denotes a weak *repulsive* pairwise interaction between the particles. In the case of a Bose gas, this assumption is connected with the fact that even for infinitesimal attractive forces, a Bose gas cannot stay dilute at low temperatures. In Fourier space, the corresponding two-body interaction can be expressed as (exercise)

$$\hat{H}_I = \frac{1}{2L^d} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V(\mathbf{q})\, a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'} a_{\mathbf{k}} a_{\mathbf{k}'+\mathbf{q}},$$

where $a_{\mathbf{k}} = L^{-d/2}\int d^d\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{x})$, and $V(\mathbf{q}) = \int d^d\mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x})$. In the following, we will be interested in the ground state and low-lying excitations of the dilute system. In this case, we may distill the relevant components of the interaction and considerably simplify the model.

In the ground state, the particles of an ideal (i.e. non-interacting) Bose gas *condense* into the lowest energy level. In a dilute gas, because of the weakness of the interactions, the ground state will differ only slightly from the ground state of the ideal gas, i.e. the number of particles N_0 in the condensate will still greatly exceed the number of particles in other levels, so that $N - N_0 \ll N$. Since the number of particles in the condensate is specified by the number operator $\hat{N}_0 = a^\dagger_{k=0} a_{k=0} = \mathcal{O}(N) \gg 1$, matrix elements of the Bose operators scale as $a_0 \sim O(\sqrt{N_0})$.[18] This means that, from the whole sum in the

[18]Note that the commutator $[a_0, a^\dagger_0] = 1$ is small as compared to a_0 and $a^\dagger_0$ allowing the field operators to be replaced by the ordinary c-number $\sqrt{N_0}$.

interaction, it is sufficient to retain only those terms which involve interaction with the condensate itself. Taking $V(\mathbf{q}) = V$ constant, one obtains (exercise)

$$\hat{H}_I = \frac{V}{2L^d}\hat{N}_0^2 + \frac{V}{L^d}\hat{N}_0 \sum_{\mathbf{k}\neq 0}\left[a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}} a_{-\mathbf{k}} + \frac{1}{2}\left(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}}\right)\right] + \mathcal{O}(N_0^0).$$

Terms involving the excited states of the ideal gas have the following physical interpretation:

- ▷ $V a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ represents the 'Hartree-Fock energy' of excited particles interacting with the condensate;[19]
- ▷ $V(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}})$ represents creation or annihilation of excited particles from the condensate. Note that, in the present approximation, the total number of particles is not conserved.

Now, using the identity $N = \hat{N}_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ to trade for $\hat{N}_0$, the total Hamiltonian takes the form

$$\hat{H} = \frac{VnN}{2} + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^{(0)}_{\mathbf{k}} + Vn\right)\left(a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}} a_{-\mathbf{k}}\right) + \frac{Vn}{2}\left(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}}\right)\right],$$

where $n = N/L^d$ represents the total number density and $\epsilon^{(0)}_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$ denotes the free particle dispersion. This result may be compared with that obtained for the Hamiltonian of the quantum antiferromagnet in the spin wave approximation. Applying the Bogoluibov transformation (2.17): $a_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}\alpha_{\mathbf{k}} - \sinh\theta_{\mathbf{k}}\alpha^\dagger_{-\mathbf{k}}$, etc., with (exercise)

$$\sinh^2\theta_{\mathbf{k}} = \frac{1}{2}\left(\frac{\epsilon^{(0)}_{\mathbf{k}} + Vn}{\epsilon_{\mathbf{k}}} - 1\right),$$

where $\epsilon_{\mathbf{k}} = [(\epsilon^{(0)}_{\mathbf{k}} + Vn)^2 - (Vn)^2]^{1/2}$, one obtains

$$\hat{H} = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^{(0)}_{\mathbf{k}} + nV - \epsilon_{\mathbf{k}}) + \sum_{\mathbf{k}\neq 0}\epsilon_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}.$$

From this result, we find that the spectrum of low energy excitations scales linearly as $\epsilon_{\mathbf{k}} \simeq \hbar c|\mathbf{k}|$ where the velocity is given by $c = (Vn/m)^{1/2}$ while, at high energies (when $k \sim k_0 = mc/\hbar$), the spectrum becomes free particle-like.[20]

▷ INFO. Since the number operator $\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}$ can assume only positive values, one can infer the ground state wavefunction from the condition $\alpha_{\mathbf{k}}|\text{g.s.}\rangle = 0$. Specifically, noting that the Bogoluibov transformation can be written as $\alpha_{\mathbf{k}} = U a_{\mathbf{k}} U^{-1}$, with (exercise)

$$U = \exp\left[\sum_{\mathbf{k}\neq 0}\frac{\theta_{\mathbf{k}}}{2}(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} - a_{\mathbf{k}} a_{-\mathbf{k}})\right],$$

[19] Note that the contact nature of the interaction disguises the presence of the direct and exchange contributions.

[20] Physically, the effect of the interaction is to displace particles from the condensate even at $T = 0$.

one can obtain the ground state as $|\text{g.s.}\rangle = U|\Phi\rangle$, where $|\Phi\rangle = (a^\dagger_{\mathbf{k}=0})^N|\Omega\rangle$ denotes the ground state of the ideal Bose gas and $|\Omega\rangle$ the vacuum. The proof follows as

$$0 = a_{\mathbf{k}\neq 0}|\Phi\rangle = U^{-1}\overbrace{Ua_{\mathbf{k}}U^{-1}}^{\alpha_{\mathbf{k}}}U|\Phi\rangle.$$

For the contact interaction, the corresponding ground state energy diverges and must be 'regularised'.[21] In doing so, one obtains $E_0 = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^{(0)}_{\mathbf{k}} + nV - \epsilon_{\mathbf{k}} - \frac{(nV)^2}{2\epsilon^{(0)}_{\mathbf{k}}})$ which, when summed over $\mathbf{k}$, translates to the energy density

$$\frac{E_0}{L^d} = \frac{n^2V}{2}\left[1 + \frac{128}{15\sqrt{\pi}}(na^3)^{1/2}\right],$$

where $a \simeq (m/4\pi\hbar^2)V$ denotes the scattering length of the interaction.

Finally, one may estimate the depletion of the condensate due to interaction.

$$\frac{N-N_0}{N} = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\langle \text{g.s.}|a^\dagger_{\mathbf{k}}a_{\mathbf{k}}|\text{g.s.}\rangle = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\sinh^2\theta_{\mathbf{k}} = \frac{1}{n}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\sinh^2\theta_{\mathbf{k}} = \frac{1}{3\pi^2 n}k_0^3,$$

i.e. ca. one particle per "coherence length" $\xi \sim 1/k_0$. Recast using the scattering length, one obtains

$$\frac{N-N_0}{N} = \frac{8}{3\sqrt{\pi}}(na^3)^{1/2}.$$

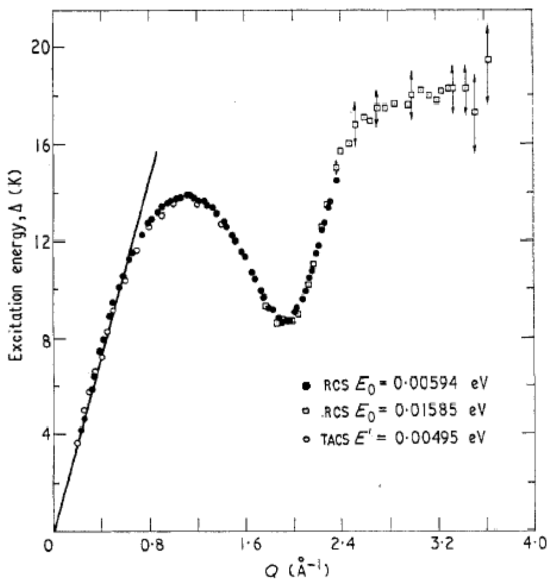
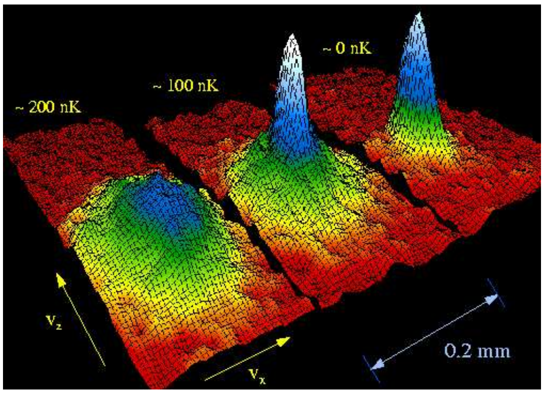


Figure 2.11: The dispersion curve for ^{4}He for the elementary excitations at 1.1K (from Cowley and Woods 1971).

[21] For details see, e.g., Ref. [1].

How do these prediction compare with experiment?[22] When cooled to temperatures below $4K$, ^{4}He condenses from a gas into a liquid. The ^{4}He atoms obey Bose statistics and, on cooling still further, the liquid undergoes a transition to a superfluid phase in which a fraction of the Helium atoms undergo Bose-Einstein condensation. Within this phase, neutron scattering can be used to probe the elementary excitations of the system. Fig. 2.11 shows the excitation spectrum below the transition temperature. As predicted by the Bogoluibov theory, the spectrum of low-energy excitations is clearly linear. The data also shows the limitations of the weakly interacting theory. In Helium, the steric interactions are strong. At higher energy scales an important second branch of excitations known as rotons appear. The latter lie outside the simple hydrodynamic scheme described above.



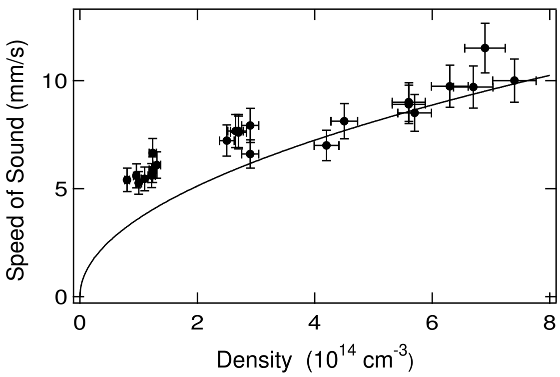


Figure 2.12: Images of the velocity distribution of rubidium atoms by Anderson *et al.* (1995), taken by means of the expansion method. The left frame corresponds to a gas at a temperature just above condensation; the center frame, just after the appearance of the condensate; the right frame, after further evaporation leaves a sample of nearly pure condensate. The field of view is 200μm $\times$ 200μm, and corresponds to the distance the atoms have moved in about 1/20s. Speed of sound, c vs. condensate peak density N_0 for waves propagating along the axial direction in the condensate. Data taken from Kurn *et al.* (1997) compared to theoretical prediction $c \sim N_0^{1/2}$.

While studies of ^{4}He allow only for the indirect manifestations of Bose-Einstein condensation (viz. superfluidity and elementary excitations of the condensate), recent investigations of dilute atomic gases allow momentum distributions to be explored directly. In a remarkable series of experiments,[23] dilute vapours of rubidium, sodium, and (later) Lithium atoms, confined in magnetic traps, were cooled down to extremely low tempera-

[22] For a review of the history of Bose-Einstein condensation see, e.g. Griffin, cond-mat/9901123

[23]

Steven Chu 1948-, Claude Cohen-Tannoudji 1933- and William D. Phillips 1948-: 1997 Nobel Laureates in Physics for development of methods to cool and trap atoms with laser light.

tures, of the order of fractions of microkelvins! Here the atoms in the vapour behave as quantum particles obeying Bose statistics. By abruptly removing the trap, time-of-flight measurements allow the momentum distribution to be inferred directly (see Fig. 2.12a). Below a certain critical temperature, these measurements revealed the development of a sharp peak at low momenta providing a clear signature of Bose-Einstein condensation.

In the condensed phase, one may measure the sound wave velocity by effecting a density fluctuation using the optical dipole force created by a focused, blue-detuned laser beam. By measuring the speed of propagation of the density fluctuation, the sound wave velocity can be inferred. The latter, shown in Fig. 2.12b, shows a good agreement with the theoretical prediction of the Bogoluibov theory.

2.2.6 †Electron-Phonon Interaction

▷ ADDITIONAL EXAMPLE: To close this section, we will address one final application — what is the effect of electron-phonon scattering on the properties of a free electron gas? We will find that, for the majority of electronic states, the scattering induces an effective repulsive interaction of the electrons. However, for a narrow band of states around the Fermi level, electron-phonon scattering can induce an attractive pairwise interaction. Physically, an electron can lower its energy by exploiting a lattice distortion created by the passage of a second electron. This attractive interaction will serve as a microscopic basis for an investigation of the phenomenon of (conventional) superconductivity in subsequent chapters.

The simplest model describing the coupling of electron degrees of freedom to a bath of phonons is expressed through the Hamiltonian

$$\boxed{\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q}} \left(M c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} a_{\mathbf{q}} + \text{h.c.} \right)} \tag{2.19}$$

where $\epsilon_{\mathbf{k}}$ and $\omega_{\mathbf{q}}$ represent the dispersion relations of the electrons and phonons respectively, and M represents the scattering amplitude coupling the degrees of freedom. Note that the electron-phonon interaction conserves momentum. (As usual, summation convention on spin indices σ is assumed.) Here, for simplicity, the matrix element is taken to be independent of $\mathbf{q}$. (As an exercise, one can try to derive the electron-phonon coupling explicitly starting from a suitable microscopic Hamiltonian.)

Treating the coupling as a perturbation $\hat{H}_1$ to the bare non-interacting Hamiltonian $\hat{H}_0$, we can again apply the canonical transformation (??) $\hat{H} \longmapsto \hat{H}' = s^{-\hat{S}} \hat{H} e^{\hat{S}}$ to expand the Hamiltonian to second order (once again, $\hat{S}$ is not to be confused with the spin operator). Terms 1st order in M can be eliminated by setting $\hat{H}_1 + [\hat{H}_0, \hat{S}] = 0$. At second order, we obtain the effective Hamiltonian

$$\hat{H}' = \hat{H}_0 + \frac{1}{2}\left[\hat{H}_1, \hat{S}\right] + O(M^3).$$

The operator S can be determined most easily by expressing the operators as matrix elements on the complete set of basis states of the non-interacting Hamiltonian ($|\{n\}\rangle = |\{\mathbf{k}\}\rangle_{\text{el.}} \otimes |\{\mathbf{q}\}\rangle_{\text{ph.}}$, $\{E_n\} = \{\epsilon_k + \hbar\omega_q\}$). In doing so, one finds (exercise)

$$\langle n|\hat{S}|m\rangle = \frac{\langle n|\hat{H}_1|m\rangle}{E_m - E_n},$$

from which we obtain the effective Hamiltonian

$$\langle n|\hat{H}'|m\rangle = \langle n|\hat{H}_0|m\rangle + \sum_p \langle n|\hat{H}_1|p\rangle\langle p|\hat{H}_1|m\rangle \left[\frac{1}{E_m - E_p} + \frac{1}{E_n - E_p}\right].$$

Rewritten in terms of the electron operators, and projecting onto a state with no phonon excitations, the effective Hamiltonian takes the form

$$\hat{H}' = \hat{H}_0 + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{|M|^2}{2}\left\{\frac{1}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}) - \hbar\omega_{\mathbf{q}}} + \frac{1}{(\epsilon_{\mathbf{k}'+\mathbf{q}} - \epsilon_{\mathbf{k}'}) - \hbar\omega_{\mathbf{q}}}\right\} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c^\dagger_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{k}\sigma}.$$

At second order, the exchange of a phonon excitation between two electrons induces an effective pairwise interaction. A rearrangement of the momenta summations finally gives

$$\hat{H}' = \hat{H}_0 + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} |M|^2 \frac{\hbar\omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2 - \hbar^2\omega_{\mathbf{q}}^2} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c^\dagger_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{k}\sigma}.$$

In particular, the electron-electron interaction is attractive (negative) for excitation energies $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}| < \hbar\omega_{\mathbf{q}}$, and repulsive otherwise. (Even in the attractive region, the interaction is opposed by the screened Coulomb repulsion, but for sufficiently large values of the interaction constant M the phonon interaction is dominant.) In the simplest approximation, we can assume that the attraction is dominant in an interval $\epsilon_F - \hbar\omega_D < \epsilon_{\mathbf{k}}, \epsilon_{\mathbf{k}\pm\mathbf{q}} < \epsilon_F + \hbar\omega_D$ where ω_D represents the Debye frequency[24] of the phonons — note that, as the density of states of the phonons increases with $\mathbf{q}$, most of the phonons are near the Debye limit. Restricting attention to the region in which the interaction is attractive, the momenta $\mathbf{k}$ and $\mathbf{k}'$ are close to k_F and the interaction becomes effectively local in real space and takes the form,

$$\begin{aligned} \hat{H}' &\simeq \hat{H}_0 - V \sum_{|\mathbf{q}|<\hbar\omega_D/c}\sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c^\dagger_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{k}\sigma}, \\ &\simeq \hat{H}_0 - VL\int d\mathbf{r}\, c^\dagger_{\sigma'}(\mathbf{r})c_{\sigma'}(\mathbf{r})c^\dagger_{\sigma}(\mathbf{r})c_{\sigma}(\mathbf{r}), \end{aligned} \tag{2.20}$$

where V is taken to be a positive constant. This model, which is known as the **BCS Hamiltonian** describes an instability of the electron gas towards the formation of a 'paired condensate' and is a paradigm for studies of **superconductivity**.

2.3 Summary

This concludes our preliminary discussion of applications of the second quantisation. In this chapter of the course, we have introduced second quantisation as a tool whereby problems of many–body quantum mechanics can be addressed much more efficiently than by the traditional language of symmetrized many–body wave functions. We have discussed how the two approaches are related to each other and how the standard operations of quantum mechanics can be performed by second quantised methods.

One may note that, beyond qualitative discussions, the list of concrete applications encountered in this chapter involved problems that were either non–interacting from the

[24]The Debye frequency is the energy to which phonons are excited at temperature T.

outset, or could be reduced to a quadratic operator structure by a number of suitable manipulations. However, we carefully avoided dealing with interacting problems were no such reductions are possible. Yet it should be clear already at this stage of our discussion that completely or nearly solvable systems represent only a small minority of the systems encountered in condensed matter physics. What can be done in situations where interactions, i.e. operator contributions of fourth or higher order, are present?

Generically, interacting problems of many–body physics are either fundamentally inaccessible to perturbation theory, or they necessitate perturbative analyses of *infinite* order in the interaction contribution. Situations where a satisfactory result can be obtained by first or second order perturbation theory are exceptional. Within second quantisation, large order perturbative expansions in interaction operators leads to complex polynomials of creation and annihilation operators. Quantum expectation values taken over such structures can be computed by a reductive algorithm, known as **Wick's theorem**. However, from a modern perspective, the formulation of perturbation theory in this way is not very efficient. More importantly, problems that are principally non-perturbative have emerged as the focus of interest.

To understand the language of modern quantum condensed matter, we thus need to develop another layer of theory, known as **field integration**. However, before discussing quantum *field* theory, we should understand how the concept works in principle, i.e. on the level of point particle quantum mechanics. This will be the subject of the next chapter.