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UNIVERSITY COLLEGE LONDON
DEPARTMENT OF PHYSICS AND ASTRONOMY

PHASM/G048 CONDENSED MATTER THEORY

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Contents

Chapter 1

From the Harmonic Oscillator to Phonons

In this chapter, we start with a review of the harmonic oscillator and its description using raising and lowering operators. We note in particular how all of its properties - expectations of operators in arbitrary states or even thermal distributions - can be calculated in terms of these raising and lowering operators without ever having to write down the wavefunction explicitly.

Next, we will proceed to couple two such oscillators and then a whole chain. The latter provides a simple model for quantum oscillations of a lattice - known as phonons. In working through this problem, we will have introduced the central ideas of quantum field theory. These will be formulated as a book-keeping tool to describe many-particle quantum systems in chapter 2 and we will use them throughout the course.

1.1 The Harmonic Oscillator

Consider a quantum particle whose motion is described by the Hamiltonian

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{1.1}$$

We solve this by introducing raising and lowering operators

$$\begin{aligned}\mathcal{H} &= \hbar\omega \underbrace{\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)}_{\hat{a}^\dagger}\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)}_{\hat{a}}}_{\text{complete square}} - \underbrace{i\hbar\omega\frac{m\omega}{2\hbar}\frac{1}{m\omega}[\hat{x},\hat{p}]}_{\text{allow for } \hat{x},\hat{p} \text{ not commuting}} \\ &= \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2).\end{aligned} \tag{1.2}$$

The constant $\hbar\omega/2$ is the zero-point energy. It follows directly from the Heisenberg uncertainty principle, since the classical groundstate is forbidden as it would give perfect knowledge about both the position and momentum of the operator.

Commutation Relations:
The definitions of $\hat{a}$ and $\hat{a}^\dagger$ given above ($\hat{a}/\hat{a}^\dagger = \sqrt{m\omega/(2\hbar)}\left(\hat{x} \pm i\frac{\hat{p}}{m\omega}\right)$) imply the commutation relations

$$[\hat{x}, \hat{p}] = i\hbar \quad \Leftrightarrow \quad [\hat{a}, \hat{a}^\dagger] = 1. \tag{1.3}$$

The Quantum groundstate is given by

$$\hat{a}|0\rangle = 0.$$

We could in principle express $\hat{a}$ as a differential operator (in real space, for example) and solve for a (real space) wavefunction. The beauty of raising and lowering operators is that we can calculate every single property of the state without ever having to obtain an explicit representation in this way.

Excitations are created by the action of the raising operator on the groundstate. The state

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$$

is a state that contains n excitations (the action of the number operator $\hat{n} = \hat{a}^\dagger\hat{a}$ on this state is $\hat{n}|n\rangle = n|n\rangle$). It has energy $\hbar\omega(n + 1/2)$. The action of the raising and lowering operators on this state are

$$\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}|n-1\rangle, \\ \hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle. \end{aligned}$$

These follow directly from the commutation relations, Eq.(1.3).

Calculations with Raising and Lowering Operators:
We can calculate all of the observable properties of the harmonic oscillator using the above relations and without ever having to obtain explicit expressions for the wavefunction. The following are a few instructive examples:

a) Average in the n^{th} excited state:

$$\begin{aligned} \langle\hat{x}^2\rangle &= \langle n|\hat{x}^2|n\rangle \\ &= \frac{\hbar}{2m\omega}\langle n|(\hat{a} + \hat{a}^\dagger)^2|n\rangle \\ &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}^2 + \hat{a}^\dagger\hat{a}^\dagger + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n\rangle \\ &\quad \text{Using } \langle n|\hat{a}^2|n\rangle \propto \langle n|n-2\rangle = 0 \text{ and } \langle n|\hat{a}^\dagger\hat{a}^\dagger|n\rangle \propto \langle n|n+2\rangle = 0 \\ &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n\rangle \\ &\quad \text{Using } \hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a} \\ &= \frac{\hbar}{2m\omega}\langle n|(2\hat{a}^\dagger\hat{a} + 1)|n\rangle \\ &= \frac{\hbar}{m\omega}(n + 1/2) \end{aligned}$$

b) The partition function :

$$\begin{aligned}\mathcal{Z} &= \sum_n e^{-\beta\epsilon_n}\langle n|n\rangle \\ &= \sum_n e^{-\beta\hbar\omega(n+1/2)} \\ &= \frac{1}{1-e^{-\beta\hbar\omega}}e^{-\beta\hbar\omega/2}\end{aligned}$$

NB: The zero point term $e^{-\beta\hbar\omega/2}$ is usually omitted as it does not contribute to observables.

c) Finite temperature average of the number operator:

$$\begin{aligned}\langle\langle\hat{n}\rangle\rangle &= \frac{\sum_n e^{-\beta\epsilon_n}\langle n|\hat{n}|n\rangle}{\sum_n e^{-\beta\epsilon_n}\langle n|n\rangle} \\ &= \frac{\sum_n n\, e^{-\beta\hbar\omega n}}{\mathcal{Z}} \\ &= \frac{-\frac{1}{\hbar\omega}\partial_\beta\mathcal{Z}}{\mathcal{Z}} \\ &= \frac{1}{e^{\beta\hbar\omega}-1} \\ &= n_B(\hbar\omega)\end{aligned}$$

d) The finite temperature average of arbitrary operator, $\langle\langle\hat{\theta}\rangle\rangle$, follows similarly: i. write the operator in terms of numer operators $\hat{n}$ using commutation relations; ii. calculate averages as above (often this amounts to the replacement $\hat{n} \to n_B$ although sometimes a bit more care is required).

Problems:

Q1. What is $\langle\hat{x}^4\rangle$ in the n^{th} excited state of the harmonic oscillator?

Q2. What is $\langle\langle\hat{x}^4\rangle\rangle$ for a thermal distribution of harmonic oscillators?

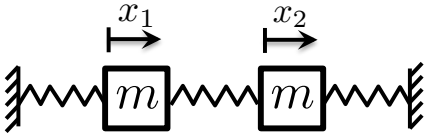
1.2 Two Coupled Oscillators

Up to now this has hopefully been revision. Now lets turn to something new. We will consider a simple problem of two coupled quantum harmonic oscillators. In doing so, we will see many of the techniques that underpin quantum field theory.

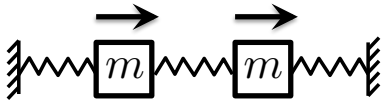
Consider two coupled particles whose motion is described by the Hamiltonian

$$\mathcal{H} = \frac{\hat{p}_1^2}{2m} + \frac{m\omega^2}{2}\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{m\omega^2}{2}\hat{x}_2^2 + \frac{\kappa}{2}\hat{x}_1\hat{x}_2, \tag{1.4}$$

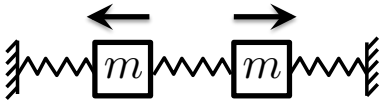
which captures the dynamics of the following configuration:



Sum and Difference Coordinates:
Our physical intuition about this situation suggests two types of periodic motion or *normal modes*:



symmetric normal mode



anti-symmetric normal mode

Accordingly, we make a change of variables to the mean displacement and difference in displacement;

$$\hat{X} = \frac{\hat{x}_1 + \hat{x}_2}{\sqrt{2}} \qquad \text{and} \qquad \hat{x} = \frac{\hat{x}_1 - \hat{x}_2}{\sqrt{2}},$$

with conjugate momenta

$$\hat{P} = \frac{\hat{p}_1 + \hat{p}_2}{\sqrt{2}} \qquad \text{and} \qquad \hat{p} = \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{2}}.$$

In the position representation, $\hat{p}_1 = -i\hbar\partial_{x_1}$ and $\hat{p}_2 = -i\hbar\partial_{x_2}$. The expressions for the momenta $\hat{P}$ and $\hat{p}$ — in particular the factors of $1/\sqrt{2}$ — follow from these.

Preservation of Commutation Relations:
These definitions imply the commutation relations

$$[\hat{x}_1, \hat{p}_1] = [\hat{x}_2, \hat{p}_2] = i\hbar \quad \Leftrightarrow \quad [\hat{X}, \hat{P}] = [\hat{x}, \hat{p}] = i\hbar.$$

The requirement that the commutation relations take this form — *i.e.* that their form is preserved by our change of variables — can be used to fix the expressions (including the factors of $1/\sqrt{2}$) for $\hat{P}$ and $\hat{p}$.

$$[\hat{X}, \hat{P}] = [\frac{\hat{x}_1 + \hat{x}_2}{\sqrt{2}}, \frac{\hat{p}_1 + \hat{p}_2}{\sqrt{2}}] = [\hat{x}_1, \hat{p}_1]/2 + [\hat{x}_2, \hat{p}_2]/2 + \underbrace{[\hat{x}_1, \hat{p}_2]/2}_{=0} + \underbrace{[\hat{x}_2, \hat{p}_1]/2}_{=0} = i\hbar.$$

$$[\hat{x}, \hat{p}] = [\frac{\hat{x}_1 - \hat{x}_2}{\sqrt{2}}, \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{2}}] = [\hat{x}_1, \hat{p}_1]/2 + [\hat{x}_2, \hat{p}_2]/2 - \underbrace{[\hat{x}_1, \hat{p}_2]/2}_{=0} - \underbrace{[\hat{x}_2, \hat{p}_1]/2}_{=0} = i\hbar.$$

Substituting into the Hamiltonian(1.4), we find

$$\begin{aligned} \mathcal{H} &= = \frac{1}{4m}(\hat{P} + \hat{p})^2 + \frac{m\omega^2}{4}(\hat{X} + \hat{x})^2 + \frac{1}{4m}(\hat{P} - \hat{p})^2 + \frac{m\omega^2}{4}(\hat{X} - \hat{x})^2 + \frac{\kappa}{4}(\hat{X} + \hat{x})(\hat{X} - \hat{x}) \\ &= \frac{\hat{P}^2}{2m} + \frac{1}{2}\left(m\omega^2 + \frac{\kappa}{2}\right)\hat{X}^2 + \frac{\hat{p}^2}{2m} + \frac{1}{2}\left(m\omega^2 - \frac{\kappa}{2}\right)\hat{x}^2 \end{aligned}$$

We have reduced the motion to two *independent* harmonic motions with masses $2m$ and $m/2$, and frequencies

$$\omega_\pm = \omega\sqrt{1 \pm \frac{\kappa}{2m\omega^2}}.$$

We may introduce creation and annihilation operators to calculate the properties of this 2-particle system.

This method of separating — or *diagonalising* — a Hamiltonian into independent harmonic oscillators is more general. As we shall see in the next section, it is related to a Fourier transform for a translationally invarient system; for a 2-site chain, the allowed Fourier components have wavevector 0 and $2\pi/2a$ — we have used a Fourier transform to diagonalize our Hamiltonian.

Problems:

For the system of two coupled harmonic oscillators described above:

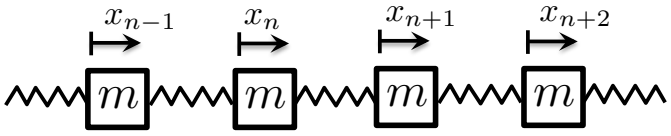
Q1. What is the r.m.s. zero-point fluctuations in the position of the 1st particle?

Q2. What is the thermal expectation of $x_1 - x_2$ at temperature T?

Q3. What is the heat capacity ($\partial_T \langle\langle \hat{\mathcal{H}} \rangle\rangle$) at temperature T?

1.3 The Harmonic Chain

Next, we consider a harmonic chain consisting of quantum particles whose Hamiltonian is given by the elastic energy due to coupling to nearest neighbours.



The Hamiltonian is given by

$$\mathcal{H} = \sum_{n=1}^{N} \left[\frac{\hat{p}_n^2}{2m} + \frac{1}{2}\kappa(\hat{x}_n - \hat{x}_{n-1})^2 \right] \tag{1.5}$$

and we will use periodic boundary conditions corresponding to taking $\hat{x}_0 = \hat{x}_N$. Our solution is going to follow essentially the same steps as we used for two coupled oscillators.

1.3.1 Diagonalising by Fourier Transform

The first step is to reduce the problem to a set of independent harmonic oscillators. We achieve this by using a discrete Fourier transform. Many problems in physics are translationally invariant (or can be treated as such) and in these cases the Fourier transform takes us much of the way towards diagonalising our system.

The Fourier components of the particle displacements are given by

$$\hat{x}_k = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \hat{x}_n \quad \text{with inverse} \quad \hat{x}_n = \frac{1}{\sqrt{N}} \sum_k e^{-ikna} \hat{x}_k, \tag{1.6}$$

for the position operators and

$$\hat{p}_k = \frac{1}{\sqrt{N}} \sum_n e^{-ikna} \hat{p}_n \quad \text{with inverse} \quad \hat{p}_n = \frac{1}{\sqrt{N}} \sum_k e^{ikna} \hat{p}_k, \tag{1.7}$$

for the momentum operators. N is the length of the chain, a is the separation of the particles, $k = \frac{2\pi}{Na} m_k$ and m_k is an integer taking values from $-N/2$ to $N/2$. We could

have written this in terms of cos and sin rather than taking the real part, but I prefer to keep things closer to the Fourier transform. Since $\hat{x}_n$ is real (or has only real expectations) $\hat{x}_k = \hat{x}^*_{-k}$. This fixes the number of degrees of freedom to be correct — otherwise there would appear to be twice as many components of $\hat{x}_k$ due to the real and imaginary parts. Note the opposite sign of wavevector k in the transformations of $\hat{x}$ and $\hat{p}$. The reasons for this will become clear shortly.

The restriction of k to values $\frac{2\pi}{Na}m_k$ with m_k an integer between $-N/2$ and $N/2$ occurs because a wavevector $k' = k + 2\pi/a$ leads to the same displacements of the particles; $e^{ik'na} = e^{iknа+2\pi n} = e^{iknа}$. This is known as the *first Brillouin zone.*

The Hamiltonian expressed in terms of these transformed operators is given by

$$\mathcal{H} = \sum_k \left[\frac{\hat{p}_k \hat{p}_{-k}}{2m} + 2\kappa \sin^2(ka/2) \hat{x}_k \hat{x}_{-k} \right]. \tag{1.8}$$

Except for the presence of both $\hat{p}_k$ and $\hat{p}_{-k}$ (and $\hat{x}_k$ and $\hat{x}_{-k}$) this a Hamiltonian for one independent oscillator for each value of k. We can make it look exactly like independent harmonic oscillators by separating $\hat{x}_k$ and $\hat{p}_k$ into parts that are symmetric and anti-symmetric in k;

$$\hat{x}^c_k = \frac{\hat{x}_k + \hat{x}_{-k}}{\sqrt{2}} \quad \text{and} \quad \hat{x}^s_k = \frac{\hat{x}_k - \hat{x}_{-k}}{i\sqrt{2}}, \quad \text{and} \quad \hat{p}^c_k = \frac{\hat{p}_k + \hat{p}_{-k}}{\sqrt{2}} \quad \text{and} \quad \hat{p}^s_k = \frac{\hat{p}_k - \hat{p}_{-k}}{i\sqrt{2}}.$$

As implied by the notation, these are the coefficients of $\cos(ka)$ and $\sin(ka)$ in a real Fourier expansion. In terms of these

$$\mathcal{H} = \sum_{k>0, \sigma=c,s} \left[\frac{\hat{p}^\sigma_k \hat{p}^\sigma_k}{2m} + 2\kappa \sin^2(ka/2) \hat{x}^\sigma_k \hat{x}^\sigma_k \right] \tag{1.9}$$

The system has been reduced to a set of independent harmonic oscillators with frequencies given by $m\omega_k^2/2 = 2\kappa \sin^2(ka/2)$ or $\omega_k = 2\sqrt{\kappa/m}\sin(ka/2)$, which in the limit of small frequencies reduces to $\omega_k \approx ka\sqrt{\kappa/m}$.

Commutation relations:
Just as in the case of the two coupled oscillators, the commutation relations are preserved by our Fourier transformation;

$$[\hat{x}_n, \hat{p}_m] = i\hbar\delta_{n,m} \quad \Leftrightarrow [\hat{x}_p, \hat{p}_q] = i\hbar\delta_{p,q}$$

Details of Fourier Transform

A. Forwards and Backwards Transforms

This can be verified using the identity

$$\delta_{n,m} = \frac{1}{N}\sum_k e^{ik(n-m)a}$$

which is the discrete equivalent of the integer representation of the delta function $\delta(x-y) = \int_{-\infty}^{\infty} dk e^{ik(x-y)}/(2\pi)$. Substituting into the Fourier transformed operators, we find

$$\begin{aligned}
\hat{x}_n &= \frac{1}{\sqrt{N}}\sum_k e^{-ikna}\hat{x}_k \\
&= \frac{1}{N}\sum_k e^{-ikna}\left(\sum_m e^{ikma}\hat{x}_m\right) \\
&= \frac{1}{N}\sum_{k,m} e^{-ik(n-m)a}\hat{x}_m \\
&= \frac{1}{2}\sum_m \delta_{n,m}\hat{x}_m \\
&= \hat{x}_n
\end{aligned}$$

We can also verify the relationship between the forward and backward transforms using the wavevector version of the delta function summation formula

$$\delta_{k,q+G} = \frac{1}{N}\sum_k e^{-i(k-q)na},$$

where $G = 2\pi \times \text{integer}/a$ is a reciprocal lattice vector. This extra contribution of G effectively allows us to fold back contributions of wavevectors outside of the Brillouin zone into the Brillouin zone, since they give the same displacements. The calculation takes the form

$$\begin{aligned}
\hat{x}_k &= \frac{1}{\sqrt{N}}\sum_n e^{ikna}\hat{x}_n \\
&= \frac{1}{N}\sum_n e^{ikna}\left(\sum_q e^{iqna}\hat{x}_q\right)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{N}\sum_{k,n} e^{-in(q-k)a}\hat{x}_q \\
&= \frac{1}{2}\sum_{k} \delta_{q,k}\hat{x}_q \\
&= \hat{x}_k
\end{aligned}
$$

B. Fourier transforming the Hamiltonian

The Fourier transformation of the Hamiltonian is most easily achieved by splitting it into the kinetic and potential energy parts.

i. Kinetic Energy

$$
\begin{aligned}
\mathcal{H} &= \sum_n \frac{\hat{p}_n^2}{2m} \\
&= \frac{1}{2m}\sum_n \underbrace{\left(\frac{1}{\sqrt{N}}\sum_k e^{ikna}\hat{p}_k\right)\left(\frac{1}{\sqrt{N}}\sum_q e^{iqna}\hat{p}_q\right)}_{\text{NB: different dummy variables}} \\
&= \frac{1}{2m}\sum_{k,q} \underbrace{\frac{1}{N}\sum_n e^{i(k+q)na}}_{=\delta_{k,q}} \hat{p}_k\hat{p}_q \\
&= \frac{1}{2m}\sum_k \hat{p}_k\hat{p}_{-k}
\end{aligned}
$$

ii. Potential Energy

$$
\begin{aligned}
\mathcal{H} &= \frac{\kappa}{2}\sum_n (\hat{x}_n - \hat{x}_{n-1})^2 \\
&= \frac{\kappa}{2}\sum_n \underbrace{\left(\frac{1}{\sqrt{N}}\sum_k e^{-ikna}(1-e^{ika})\hat{x}_k\right)\left(\frac{1}{\sqrt{N}}\sum_q e^{-iqna}(1-e^{iqa})\hat{x}_q\right)}_{\text{NB: different dummy variables}} \\
&= \frac{\kappa}{2}\sum_{k,q} \underbrace{\frac{1}{N}\sum_n e^{-i(k+q)na}}_{=\delta_{k,q}} (1-e^{ika})(1-e^{iqa})\hat{x}_k\hat{x}_q \\
&= \frac{\kappa}{2}\sum_k (1-e^{ika})(1-e^{-ika})\hat{x}_k\hat{x}_{-k} \\
&= 2\kappa\sum_k \sin^2(ka/2)\hat{x}_k\hat{x}_{-k}
\end{aligned}
$$

B. Fourier transforming the commutation relations

The Fourier transform of the commution relations proceeds in a very similar manner to the Fourier transform of the Hamiltonian

$$\begin{aligned}
[\hat{x}_p, \hat{p}_q] &= \frac{1}{N}\left[\sum_n e^{ipna}\hat{x}_n \ , \ \sum_m e^{-iqma}\hat{p}_m\right] \\
&= \frac{1}{N}\sum_{n,m} e^{i(pn-qm)a}\underbrace{[\hat{x}_n, \hat{p}_m]}_{=i\hbar\delta_{n,m}} \\
&= i\hbar\frac{1}{N}\sum_n e^{i(p-q)na} \\
&= i\hbar\delta_{p,q}
\end{aligned}$$

1.3.2 Raising and Lowering Operators

Just as in the case of a single harmonic oscillator, we can now calculate properties of the harmonic chain by introducing ladder operators for each k-mode. These create or destroy quanta of energy in each of the normal modes of oscillation of the harmonic chain. The resulting Hamiltonian is given by

$$\begin{aligned}
\mathcal{H} &= \sum_k \hbar\omega_k(\hat{a}_k^\dagger\hat{a}_k + 1/2) \\
\omega_k &= 2\sqrt{\kappa/m}\sin(ka/2)
\end{aligned} \tag{1.10}$$

with

$$\hat{a}_k = \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{x}_k + i\frac{\hat{p}_{-k}}{m\omega_k}\right), \quad \text{and} \quad \hat{a}_k^\dagger = \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{x}_{-k} - i\frac{\hat{p}_k}{m\omega_k}\right). \tag{1.11}$$

Notice the opposite momentum labels in $\hat{x}_k$ and $\hat{p}_{-k}$, and the relative signs of k between $\hat{a}$ and $\hat{a}^\dagger$. This is required to obtain the usual commutation relations for the raising and lowering operators;

$$[\hat{a}_k, \hat{a}_q^\dagger] = \delta_{k,q} \tag{1.12}$$

Checking the commutation relations

$$\begin{aligned}
[\hat{a}_k, \hat{a}_q^\dagger] &= \frac{m\sqrt{\omega_k\omega_q}}{2\hbar}\left[\left(\hat{x}_k + i\frac{\hat{p}_{-k}}{m\omega_k}\right), \left(\hat{x}_{-q} - i\frac{\hat{p}_q}{m\omega_q}\right)\right] \\
&= \frac{m\sqrt{\omega_k\omega_q}}{2\hbar}\left(\frac{i}{m\omega_k}\underbrace{[\hat{p}_{-k}, \hat{x}_{-q}]}_{=-i\hbar\delta_{k,q}} - \frac{i}{m\omega_q}\underbrace{[\hat{x}_k, \hat{p}_q]}_{=i\hbar\delta_{k,q}}\right) \\
&= \delta_{k,q}
\end{aligned}$$

Particle Interpretation/Fock Space:
Just as for the harmonic oscillator, armed with these tools we can describe the state of the harmonic chain in terms of the number of quanta — or occupation number n_k — of each mode k. A general state may be written

$$|\psi\rangle = |n_{q_1}, n_{q_2}, n_{q_3}...\rangle = \prod_q \frac{\left(\hat{a}_q^\dagger\right)^{n_q}}{\sqrt{n_q!}}|0\rangle,$$

where $|0\rangle$ is the vacuum state with no quanta in any mode. The collection of all such states with arbitrary occupations forms a space known as Foch space.

Observables:
One can evaluate the observable properties of the harmonic chain by first translating into $\hat{a}_k$ and $\hat{a}_k^\dagger$. For example, the mean squared displacement of a particle in the chain at finite temperature is given by

$$\begin{aligned}
\bar{x}^2 &= \frac{1}{N}\sum_n \langle\langle \hat{x}_n^2 \rangle\rangle \\
&\quad \text{Fourier transform - allows us to use the properties of independent k-modes} \\
&= \frac{1}{N}\sum_k \langle\langle \hat{x}_k \hat{x}_{-k} \rangle\rangle \\
&\quad \text{Express in terms of ladder operators} \\
&= \frac{1}{N}\sum_k \frac{\hbar}{2m\omega_k}\langle\langle (\hat{a}_k + \hat{a}_{-k}^\dagger)(\hat{a}_{-k} + \hat{a}_k^\dagger)\rangle\rangle \\
&= \frac{1}{N}\sum_k \frac{\hbar}{2m\omega_k}\langle\langle (\underbrace{\hat{a}_k\hat{a}_{-k}}_{=0} + \underbrace{\hat{a}_k\hat{a}_k^\dagger}_{=\hat{a}^\dagger\hat{a}+1=\hat{n}_k+1} + \underbrace{\hat{a}_{-k}^\dagger\hat{a}_{-k}}_{=\hat{n}_{-k}} + \underbrace{\hat{a}_{-k}^\dagger\hat{a}_k^\dagger}_{=0})\rangle\rangle \\
&= \frac{1}{N}\sum_k \frac{\hbar}{2m\omega_k}\left(\langle\langle \hat{n}_k \rangle\rangle + \langle\langle \hat{n}_k \rangle\rangle + 1\right) \\
&= \frac{1}{N}\sum_k \frac{\hbar}{m\omega_k}\left(\frac{1}{e^{\hbar\omega_k\beta}-1} + 1/2\right).
\end{aligned}$$

Zero-point Energy and Normal ordering:
Just as for the harmonic oscillator, the Hamiltonian for the harmonic chain has a constant term $\hbar\omega_k/2$ for each wavevector. This implies a minimum energy proportional to N,

$$\mathcal{H}_{\text{Zero-point}} = \sum_k \hbar\omega_k/2.$$

This energy cannot usually be extracted (except by changing boundary conditions *c.f.* the Casimir effect) and so is often ignored in field theory. For an infinite system the zero-point energy $\to \infty$. In the continuum limit, the situation is even more severe and the *energy density* $\to \infty$. This is the first infinity that we have encountered. Quantum field theory is plagued by them. To deal properly with all of the infinities that occur, one needs the renormalisation group. We will touch upon this towards the end of the first part of the course.

The infinite zero-point energy can be dealt with rather straightforwardly by *normal ordering*. The infinite zero-point energy arises from the form of the Hamiltonain $\mathcal{H} = \sum_k \hbar\omega_k(\hat{a}_k^\dagger\hat{a}_k + \hat{a}_k\hat{a}_k^\dagger)/2$, when we use the commutation relations to reorder the second term so that it can be written in terms of number operators. Similar infinities can arise from interaction terms — terms higher than quadratic order — in Hamiltonians. The trick to dealing with these is to find a consistent way to ignore them! Basically, we define the operation of normal ordering to consist of ordering the creation and annihilation operators so that the creation operators are on the left and the annihilation operators on the right:

$$: \hat{a}_k^\dagger\hat{a}_k + \hat{a}_k\hat{a}_k^\dagger := 2\hat{a}_k^\dagger\hat{a}_k \tag{1.13}$$

Applied to quadratic terms, normal ordering essentially ignores zero-point energy. Applied to interaction terms, it ignores self-interaction of particles that can lead to other unphysical divergences.

Problems:

Q1. What is the r.m.s. displacement of a mass in the harmonic chain in the groundstate?
Q2. What is the r.m.s. speed of a particle in the harmonic chain in the groundstate?
Q3. What are the r.m.s. displacement and speed at temperature T?
Q4. What is the heat capacity of the harmonic chain?

1.4 The Elastic String

Let us consider the limit in which the separation of masses in our chain becomes zero while maintaining a fixed length of chain L and mass density:

$$\begin{aligned}
&N \to \infty \\
&L = Na \text{ fixed} \\
&m \to 0 \text{ such that } \rho = m/a \text{ fixed} \\
&\kappa \to \infty \text{ such that } \tau = \kappa a \text{ fixed} \\
&n \to x/a \text{ position along string}, \quad x \in [-L/2, L/2] \\
&x_n \to \phi(x)|_{x=na} \text{ displacement field} \\
&p_n \to a\Pi_\phi(x)|_{x=na} \text{ momentum field} \\
&\lim_{a\to 0}\sum_n = \frac{1}{a}\int dx \\
&\lim_{a\to 0}(x_{n+1} - x_n) = a\partial_x\phi.
\end{aligned} \tag{1.14}$$

With these replacements, the *Hamiltonian and Commutations Relations* become

$$\begin{aligned}
\mathcal{H} &= \int dx \frac{1}{2}\left[\frac{1}{\rho}\hat{\Pi}_\phi^2 + \tau\left(\partial_x\hat{\phi}\right)^2\right] \\
\left[\hat{\phi}(x,t), \Pi_\phi(y,t)\right] &= i\hbar\delta(x-y)
\end{aligned} \tag{1.15}$$

This field theory is the same as that of the one-dimensional Klein-Gordon model of relativistic quantum particles. We shall see how the relativistic dispersion arises later. Notice

that the commutation relations are expressed at equal times, since the field operators — the displacement and momentum fields — are presented in the Heisenberg picture.

Heisenberg, Schrödinger and Dirac/Interaction Pictures:
In the Schrödinger picture of quantum mechanics, operators (such as position and momentum) are fixed and time-dependence is carried by the state or wavefunction. An alternative picture — due to Heisenberg — is to keep the state fixed in time and allow the operators to vary. The relationship between these two pictures can be understood by insisting that physical observables are unaffected by our notation.

In the Schrödinger picture $d_t|\psi\rangle = i\hat{\mathcal{H}}|\psi\rangle \Rightarrow |\psi(t)\rangle = e^{i\int dt\hat{\mathcal{H}}}|\psi(0)\rangle$. We can use this to deduce the time-dependence of the expectation of an operator $\hat{\Theta}$ as follows:

$$\langle\hat{\Theta}\rangle(t) = \langle\psi(t)|\hat{\Theta}_S|\psi(t)\rangle = \langle\psi(0)|\underbrace{e^{-i\int dt\hat{\mathcal{H}}}\hat{\Theta}_S e^{i\int dt\hat{\mathcal{H}}}}_{\hat{\Theta}_H}|\psi(0)\rangle$$

The subscripts S and H on $\hat{\Theta}$ indicate Schrödinger and Heisenberg versions respectively. Their relationship is $\hat{\Theta}_H = e^{-i\int dt\hat{\mathcal{H}}}\hat{\Theta}_S e^{i\int dt\hat{\mathcal{H}}}$. The equation of motion for $\hat{\Theta}_H$ can be deduced by taking a time derivative of this equation to be

$$d_t\hat{\Theta}_H = i[\hat{\Theta}_H, \hat{\mathcal{H}}]$$

The Interaction Picture is another alternative (that we will not use in this course) often used in field theory. This separates the Hamiltonian into *bare* and *interaction* parts, $\hat{\mathcal{H}}_0$ and $\hat{\mathcal{H}}_I$, respectively. The time dependence arising from the bare parts is carried by the operators and the additional time dependence arising from the interactions is carried by the states. This embodies the notion that interactions may cause particles/systems to change their states.

Fourier Transform (finite string):
As in the case of the chain, the elastic string is diagonalised by a Fourier transform. Applying the rules established above for the continuum limit, these are given by

$$\hat{\phi}(k,t) = \frac{1}{\sqrt{L}} \int dx e^{ikx} \hat{\phi}(x,t) \quad \text{and} \quad \hat{\Pi}_\phi(k,t) = \frac{1}{\sqrt{L}} \int dx e^{-ikx} \hat{\Pi}_\phi(x,t) \tag{1.16}$$

with $k = 2\pi n_k/L$ and n_k an integer in the range $[-\infty, \infty]$. The inverse transforms are

$$\hat{\phi}(x,t) = \frac{1}{\sqrt{L}} \sum_k e^{-ikx} \hat{\phi}(k,t) \quad \text{and} \quad \hat{\Pi}_\phi(x,t) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \hat{\Pi}_\phi(k,t). \tag{1.17}$$

The corresponding Fourier transformed commutation relations are given by

$$\left[\hat{\phi}(p,t), \hat{\Pi}_\phi(q,t)\right] = i\hbar\delta_{p,q} \tag{1.18}$$

The relationship between the forward and backwards transformations and the transformed commutation relations can be verified by using the summation/integral representation of the delta function

$$\begin{aligned} \frac{1}{L} \sum_{k=-\infty}^{\infty} e^{ik(x-y)} &= \delta(x-y) \\ \int_{-L/2}^{L/2} dx e^{-ix(q-p)} &= 2\pi\delta(p-q) = L\delta_{p,q}. \end{aligned} \tag{1.19}$$

As before, I use the slight abuse of notation $\delta_{p,q}$ to indicate δ_{n_p,n_q}, where $p = 2\pi n_p/L$.

Using these rules for the Fourier transformation of the Hamiltoiain can be written

$$\mathcal{H} = \frac{1}{\sqrt{L}} \sum_k \left[\frac{1}{2\rho} \hat{\Pi}_\phi(k) \hat{\Pi}_\phi(-k) + \frac{\kappa}{2} k^2 \hat{\phi}(k) \hat{\phi}(-k) \right].$$

Notice that the mode frequencies become $\omega = k\sqrt{\kappa/\rho}$ — *i.e.* a linear, relativistic dispersion with effective speed of light $\sqrt{\kappa/\rho}$.

Fourier Transform (infinite string):
In the case of the infinite chain, these transformations become

$$\hat{\phi}(k,t) = \int_{-\infty}^{\infty} dx e^{ikx} \hat{\phi}(x,t) \quad \text{and} \quad \hat{\Pi}_\phi(k,t) = \int_{-\infty}^{\infty} dx e^{-ikx} \hat{\Pi}_\phi(x,t) \tag{1.20}$$

The inverse transforms are

$$\hat{\phi}(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ikx} \hat{\phi}(k,t) \quad \text{and} \quad \hat{\Pi}_\phi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \hat{\Pi}_\phi(k,t). \tag{1.21}$$

The corresponding Fourier transformed commutation relations are given by

$$\left[\hat{\phi}(p,t), \hat{\Pi}_\phi(q,t)\right] = i\hbar\delta(p,q) \tag{1.22}$$

The relationship between the forward and backwards transformations and the transformed commutation relations can be verified by using the summation/integral representation of the delta function

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-y)} = \delta(x-y)$$
$$\int_{-\infty}^{\infty} dx e^{-ix(q-p)} = 2\pi\delta(p-q). \tag{1.23}$$

Notice that I have made a choice here about where I put the factors of 2π from the integral representation of the δ-function. The conventional physics choice is as above, so that wavevector integrals always come with a factor of $1/2\pi$.

The Hamiltonian takes the same relativistic form as the finite string, with the discrete summation over wavevectors becoming an integral;

$$\mathcal{H} = \int \frac{dk}{2\pi} \left[\frac{1}{2\rho} \hat{\Pi}_\phi(k) \hat{\Pi}_\phi(-k) + \frac{\kappa}{2} k^2 \hat{\phi}(k) \hat{\phi}(-k) \right].$$

Problems:

Q1. Verify the k-space commutation relations of the finite-length elastic string.
Q2. Verify the k-space Hamiltonian of the finite-length elastic string.
Q3. Verify the k-space commutation relations of the *infinite* elastic string.
Q4. Verify the k-space Hamiltonian of the *infinite* elastic string.

1.5 Canonical Quantization [Aside]

Some of you may be doing a quantum field theory course, where the idea of field operators is introduced by canonical quantization. This aside is given to show the connection between what we are doing here and that approach. It isn't an examinable part of the course, but hopefully will serve to give you greater insight about the connections between the things that you are learning.

Single harmonic Oscillator
The classical Lagrangian for the harmonic oscillator is given by

$$\mathcal{L} = \frac{m\dot{x}^2}{2} - \frac{1}{2}m\omega^2 x^2/2$$

and from it we can obtain the both the momentum conjugate to x — $p_x = \partial\mathcal{L}/\partial\dot{x}$ and the Hamiltonian

$$\mathcal{H} = \dot{x}p_x - \mathcal{L} = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

Canonical quantization imposes commutation relations between conjugate fields — in this case the position and momentum;

$$[\hat{x}, \hat{p}] = i\hbar.$$

Quantum Elastic Rope
For the quantum elastic rope, the Lagrangian is given by

$$\mathcal{L} = \int dx \left(\frac{1}{2}\rho\dot{\phi}(x)^2 - \frac{1}{2}\kappa(\partial_x\phi(x))^2\right)$$

from which w obtain the conjugate momentum $\Pi_\phi(x,t) = \delta\mathcal{L}/\delta\dot{\phi}(x,t) = \rho\dot{\phi}(x,t)$ and Hamiltonian

$$\mathcal{H} = \int dx\dot{\phi}\Pi_\phi - \mathcal{L} = \int dx \left(\frac{1}{2\rho}\Pi_\phi^2 - \frac{1}{2}\kappa(\partial_x\phi(x))^2\right)$$

Quantization involves imposing canonical commutation relations

$$\left[\hat{\phi}(x,t), \hat{\Pi}_\phi(y,t)\right] = i\hbar\delta(x-y)$$

.

Complex Quantum Elastic Rope
The displacement field in the cases above was chosen to be along the chain/rope. In fact, the model of transverse fluctuations takes precisely the same form. If we allow for transverse fluctuations in both transverse directions of the rope, we can encode this by allowing the real-space displacement field $\phi(x,t)$ to be complex — the real and imaginary parts describing the different components of the transverse displacement. The Langrangian in this case is precisely that obtained for the Klein-Gordon field;

$$\mathcal{L} = \int dx \left(\frac{1}{2}\rho\dot{\bar{\phi}}(x)\dot{\phi}(x) - \frac{1}{2}\kappa(\partial_x\bar{\phi}(x))(\partial_x\phi(x))\right) \tag{1.24}$$

from which w obtain the conjugate momentum $\Pi_\phi(x,t) = \delta\mathcal{L}/\delta\dot{\phi}(x,t) = \rho\dot{\bar{\phi}}(x,t)$ and $\bar{\Pi}_{\bar{\phi}} = \delta\mathcal{L}/\delta\dot{\bar{\phi}}(x,t) = \rho\dot{\phi}(x,t)$ and Hamiltonian

$$\mathcal{H} = \int dx \left(\dot{\phi}\Pi_\phi + \dot{\bar{\phi}}\bar{\Pi}_\phi\right) - \mathcal{L} = \int dx \left[\frac{1}{2\rho}\bar{\Pi}_\phi\Pi_\phi - \frac{1}{2}\kappa(\partial_x\bar{\phi}(x))(\partial_x\phi(x))\right]$$

Quantization involves imposing canonical commutation relations

$$\left[\hat{\phi}(x,t), \hat{\Pi}_\phi(y,t)\right] = i\hbar\delta(x-y).$$

Of course, in the case of the elastic rope, the fields that we are quantizing correspond to displacements and momenta and we are simply imposing the commutation relations $[\hat{x},\hat{p}] = i\hbar$. In the case of the Klein-Gordon model, the situation is somewhat different. The Euler-Lagrange equations arising from Eq.(1.24) are the Klein-Gordon equation, $\ddot{\phi} - d_x^2\phi = 0$. This is a relativistic analogue of the Schrödinger equation obtained from energy conservation, where first quantization (changing x and p to operators and imposing $[\hat{x},\hat{p}] = i\hbar$) has been used already identifying the energy with a derivative with respect to time and the momentum with a derivative with respect to position. Changing the Klein-Gordon field into a field operator is therefore a *second* quantization step. The insight is that one of the quanta of this field operator will have a wavefunction that obeys the Klein-Gordon equation. This is at first a difficult concept to appreciate. In the next section we shall see how the idea of second quantization can be alternatively introduced as a book keeping tool to keep track of many-body wavefunctions. This effectively leads to the same construction as obtained by this second quantization trick, and essentially provides a justification for it.

Chapter 2

Second Quantization

In the first chapter, we saw how creation and annihilation operators are a very convenient way of ealing with systems of many harmonic oscillators — armed with their commutation relations, we can calculate observable properties without ever having to write down a wavefunction. The idea of second quantization — and field theory in general — is to use this machinary to study many-body quantum systems[1]. The essence is to interpret the creation of a quantum of energy by the operation of $\hat{a}^\dagger$ as the creation of a particle of a quantum matter field;

$\hat{a}^\dagger_{\mathbf{k}}$ – Creates a particle with momentum $\mathbf{k}$ i.e. in a plane wave state
$\hat{a}^\dagger_{\mathbf{x}}$ – Creates a particle at the point $\mathbf{x}$ i.e. in a delta-function wavefunction state at $\mathbf{x}$.

2.1 Identical particles/Many-particle states

Many-body quantum mechanics in general — and theoretical condensed matter in particular — is concerned with the collective quantum behaviour of many identical quantum particles (for example electrons or phonons in a solid). In this chapter, we will review the formalism required to describe such systems. Consider a classical system of N identical particles. This might have a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i,j>i} V(x_i - x_j) + \sum_{i=1}^{N} U(x_i).$$

This is (first) quantized by taking the position and momentum variables to be operators satisfying commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{i,j},$$

where i and j are particle labels.

Solution for Non-interacting, Distinguishable Particles
When $V(x_i - x_j) \equiv 0$ and the particles are distinguishable, the Schrödinger equation is

[1]For relativistic systems — such as particles described by the Klein-Gordon equation — it is essential, since the energy density and hence particle number depend upon the inertial frame of reference.

separable. The solution is a product of single-particle solutions;

$$\begin{aligned}\psi(x_1, x_2, ...x_N) &= \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2) \; ... \; \psi_{\alpha_N}(x_N)e^{-iEt/\hbar} \\ &\quad \psi_\alpha(x) \;\; \text{single particle state with energy } E_\alpha \\ &\quad E = E_{\alpha_1} + E_{\alpha_2} \; ... \; E_{\alpha_N} \;\; \text{total energy} \end{aligned} \tag{2.1}$$

Identical Particles and Exchange
Invariance of observable properties under the exchange of indistinguishable particles places important constraints upon the wavefunction. Let us define the permutation operator as follows: $\hat{P}_{ij}$ permutes particles i and j so that

$$\hat{P}_{ij}\psi(x_1, \; ... \; x_i \; ... \; x_j \; ... \; x_n) = \psi(x_1, \; ... \; x_j \; ... \; x_i \; ... \; x_n).$$

For indistinguishable particles, $\hat{P}_{ij}$ should not change the results of measurements, *i.e.* expectations of operators are the same. Let us consider explicitly the expectation of an operator $\hat{\Theta}$ and the action of $\hat{P}_{ij}$ upon it.

$$\begin{aligned} & \langle\psi|\hat{\Theta}|\psi\rangle \;\; \text{invariant under } |\psi\rangle \rightarrow e^{i\Phi}|\psi\rangle \\ & \hat{P}_{ij}\hat{P}_{ji} = 1 \\ \Rightarrow \quad & \hat{P}_{ij}\psi(x_1, \; ... \; x_i \; ... \; x_j \; ... \; x_n) = \pm\psi(x_1, \; ... \; x_j \; ... \; x_i \; ... \; x_n) \\ & + \;\; \text{Bosons} \\ & - \;\; \text{Fermions} \end{aligned}$$

We will see presently the effects that this has upon our construction of many-particle wavefunctions.

2.2 Many-particle Basis States

In order to describe our many body system, we require a suitable set of basis states that satisfy the symmetry or anti-symmetry identified above. Let us start with a complete, orthonormal set of single-particle basis states, $\psi_\alpha(x)$. From these, we can construct a many particle state as follows:

$$\psi(x_1, \quad , x_N) = \mathcal{N}\sum_P (\pm)^P \psi_{\alpha_1}(x_1) \; ... \; \psi_{\alpha_N}(x_N) \tag{2.2}$$

$$\begin{aligned} & (\pm) \;\; \text{for bosons/fermions} \\ & P = \text{order of permutation} \\ & \{\alpha_1, \alpha_2, \; ... \; \alpha_N\} \;\; \text{some permutation of state labels} \\ & \mathcal{N} \;\; \text{Normalization} \end{aligned} \tag{2.3}$$

Note that here we sum over ALL permutations. Some other texts (such as that of Prof Chalker) sum over distinct permutations — *i.e.* if some of the labels are the same then swapping them isn't counted. Permutations are divided into even and odd depending upon the number of pairwise swaps that are required to perform them. An even number gives an even permutation and an odd number gives an odd permutation.

Normalization

$$1 = \int d\mathbf{x}_i \, ... d\mathbf{x}_N |\psi(\mathbf{x}_1, \, ... \, \mathbf{x}_N)|^2 \tag{2.4}$$

$$= |\mathcal{N}|^2 \sum_{P_\alpha} \sum_{P_\beta} (\pm)^{P_\alpha + P_\beta} \underbrace{\int d\mathbf{x}_1 \psi^*_{\alpha_1}(\mathbf{x}_1)\psi_{\beta_1}(\mathbf{x}_1)}_{=\delta_{\alpha_1,\beta_1}} \; ... \; \underbrace{\int d\mathbf{x}_N \psi^*_{\alpha_N}(\mathbf{x}_N)\psi_{\beta_N}(\mathbf{x}_N)}_{=\delta_{\alpha_N,\beta_N}} \tag{2.5}$$

$$= |\mathcal{N}|^2 \sum_{P_\alpha} (\pm)^{2P_\alpha} = |\mathcal{N}|^2 N! \tag{2.6}$$

From which we deduce that $\mathcal{N} = \frac{1}{\sqrt{N!}}$.
NB in the case where permutations are restricted to distinct permutations, the sum over permutations is different and the the result is $1 = |\mathcal{N}|^2 N!/(n_1! n_2! ...)$, where n_i is the number of times that a distinct single particle state ψ_{α_i} appears in the state. $n_i!$ gives the permutations of these.

Slater Determinants and Permantents
The wavefunction for fermions may be written in the following form:

$$\psi(\mathbf{x}_1 \quad \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{\alpha_1}(\mathbf{x}_1) & ... & ... & \psi_{\alpha_1}(\mathbf{x}_N) \\ \psi_{\alpha_2}(\mathbf{x}_1) & ... & ... & ... \\ ... & ... & ... & ... \\ \psi_{\alpha_N}(\mathbf{x}_1) & ... & ... & \psi_{\alpha_N}(\mathbf{x}_N) \end{vmatrix}. \tag{2.7}$$

The minus signs $(-)^P$ required for fermions are taken care of by the minus signs coming from the determinant. Note that the determinant is zero if any two or more of the single-particle states are the same. The determinant — known as a *Slater determinant* — therefore properly encodes the Pauli principle. An ordering convention is needed to fix the overall sign of the wavefunction. For bosons, we may construct a similar representation in terms of a permanent. This is essentially the same object as a determinant but without the minus signs.

2.3 Occupation Numbers and Fock Space

The states that we identified as many-particle basis states can be specified completely by the number of particles in each single-particle basis state. These are usually denoted

$$|n_1, n_2, \, ...\rangle,$$

where n_i is the number of quanta/particles in the state i. n_i takes values $0, 1$ for fermions and values $0, 1, 2, \, ..., \infty$ for bosons. This notation assumes: i. a particular identification of single-particle states. In condensed matter, we typically use either momentum or plane wave states, or an orthonormal set of states constructed from orbitals on particular atoms, *i.e* position states (known as Wanier states); ii. that the states are appropriately symmetrized or anti-symmetrized for bosons or fermions, respectively.

Fock Space: is the set of states with all possible combinations of the occupation numbers.

The Vacuum State: is the state in which none of the particle states are occupied. It is written as $|0\rangle$ and normalized $\langle 0|0\rangle = 1$.

Comparison with the Harmonic Oscillator:
This structure is very similar to that of the eigenstates of the harmonic oscillator and harmonic chain considered previously. In the case of the harmonic chain, for example, a generic eigenstate could be written $|n_{k_1}, n_{k_2}, \ ...\rangle$ describing a state with n_{k_i} quanta in the k_i^{th} wavevector mode. These modes are bosons and are given the name phonons when applied to vibrational modes of a crystal lattice. We have been using Fock space all along to describe the harmonic oscillator and its derivatives.

2.4 Creation and Annihilation Operators

Since the structure of Fock space discussed above is so reminiscent of of the state space of the harmonic oscillator, it is natural to expect that we can also find operators that are the analogue of the ladder/creation and annihilation operators. These operators will allow us to navigate Fock space and, moreover, to calculate properties of our many-body system without ever having to write down its wavefunction.

The basic notion is to identify creation operators $\hat{c}_a^\dagger$ that create a particle in the single-particle state $|\psi_a\rangle$. We will then manipulate the resulting states to determine the properties of the operators $\hat{c}_a^\dagger$. A many-particle state can be constructed from the action of many such operators,

$$\hat{c}_{a_1}^\dagger \ ... \ \hat{c}_{a_N}^\dagger |0\rangle = (n_1! n_2! \ ...)^{1/2} |n_1, n_2, \ ...\rangle. \tag{2.8}$$

This corresponds to a state described by the real-space, many-body wavefunction

$$\psi(\mathbf{x}_1, \ ...\mathbf{x}_N) = \langle \mathbf{x}_1, \ ...|(\hat{c}_1^\dagger)^{n_1} \ ... \ (\hat{c}_N^\dagger)^{n_N}|0\rangle = \frac{1}{\sqrt{N!}} \sum_P (\pm 1)^P \psi_{a_1}(\mathbf{x}_1) \ ... \ \psi_{a_N}(\mathbf{x}_N) \tag{2.9}$$

Hermitian Conjugation and Annihilation of the Vacuum
By definition, annihilation operators are given by the Hermitian conjugate of the creation operators. Their action on the vacuum is as follows:

$$\hat{c}_q^\dagger |0\rangle = 0 \quad \text{and} \quad \langle 0|\hat{c}_a^\dagger = 0.$$

Proof As for the harmonic oscillator

$$\begin{aligned}
& \hat{c}_a^\dagger|0\rangle \quad \text{state with one particle in} |\psi_a\rangle \\
& \text{Normalization} \;\Rightarrow\; \langle 0|\hat{c}_a\hat{c}_a^\dagger|0\rangle = 1 \\
\Rightarrow\quad & \langle 0| = \langle 0|\hat{c}_a\hat{c}_a^\dagger \quad \text{and} \quad |0\rangle = \hat{c}_a\hat{c}_a^\dagger|0\rangle \\
& \text{General state } |\phi\rangle \text{ other than the vacuum} \\
\Rightarrow\quad & \hat{c}_a^\dagger|\phi\rangle \text{ has more than one particle} \\
\Rightarrow\quad & \langle 0|\hat{c}_a\hat{c}_a^\dagger|\phi\rangle = 0 \\
\Rightarrow\quad & |0\rangle = \hat{c}_a(\hat{c}_a^\dagger|0\rangle) = \hat{c}_a|n_a = 1\rangle \\
\text{Also}\quad & \langle 0|\hat{c}_a^\dagger|\phi\rangle = 0 = \langle\phi|\hat{c}_a|0\rangle \\
\Rightarrow\quad & \langle 0|\hat{c}_a^\dagger = \hat{c}_a|0\rangle = 0
\end{aligned}$$

Commutation and Anti-commutation
Considering the action of the permutation operator on a two-particle state, we have

$$\hat{c}_a^\dagger\hat{c}_b^\dagger|0\rangle = \pm\hat{c}_b^\dagger\hat{c}_a^\dagger|0\rangle$$

for bosons and fermions, respectively. This implies that

$$\left[\hat{c}_a^\dagger, \hat{c}_b^\dagger\right] = 0 = \hat{c}_a^\dagger\hat{c}_b^\dagger - \hat{c}_b^\dagger\hat{c}_a^\dagger \quad \text{Bosons} \tag{2.10}$$

$$\left\{\hat{c}_a^\dagger, \hat{c}_b^\dagger\right\} = 0 = \hat{c}_a^\dagger\hat{c}_b^\dagger + \hat{c}_b^\dagger\hat{c}_a^\dagger \quad \text{Fermions} \tag{2.11}$$

and (after Hermitian conjugation)

$$[\hat{c}_a, \hat{c}_b] = 0 \quad \text{Bosons} \tag{2.12}$$

$$\{\hat{c}_a, \hat{c}_b\} = 0 \quad \text{Fermions} \tag{2.13}$$

In order to reproduce the values of inner products of our general multi-particle state, Eq.(2.9), we must take[2]

$$\left[\hat{c}_a, \hat{c}_b^\dagger\right] = \delta_{ab} \quad \text{Bosons} \tag{2.14}$$

$$\left\{\hat{c}_a, \hat{c}_b^\dagger\right\} = \delta_{ab} \quad \text{Fermions} \tag{2.15}$$

Number Operators The action of the creation operators on Fock space is determined by the normalization of Eq.(2.8), which implies

$$\hat{c}_l^\dagger|n_1, n_2, \ \ldots\ n_l, \ \ldots\rangle = (\pm)^{n_1 + \ \ldots + n_{l-1}}\sqrt{n_l + 1}|n_1, n_2, \ \ldots\ n_l + 1, \ \ldots\rangle$$

The negative signs in the fermionic case come from commuting $\hat{c}_l^\dagger$ through all of the creation operators to the left. Note also that for fermions $(\hat{c}_l^\dagger)^2 = 0$ which implies that the right

[2]For example, consider the norm of the state $|n_1\rangle = \hat{c}_1^\dagger|0\rangle$. This is given by $1 = \langle n_1|n_2\rangle = \langle 0|\hat{c}_1\hat{c}_1^\dagger|0\rangle = \pm\langle 0|\hat{c}_1^\dagger\hat{c}_1|0\rangle + \langle 0|0\rangle$.

hand side of the above expression is zero when $n_l = 1$. The action of the annihilation operators can be considered similarly and we find

$$\hat{c}_l|n_1, n_2, \ ... \ n_l, \ ...\rangle = (\pm)^{n_1 + \ ... + n_{l-1}}\sqrt{n_l}|n_1, n_2, \ ... \ n_l - 1, \ ...\rangle$$

This is zero for both bosons and fermions if $n_l = 0$. That is, $\hat{c}_l$ annihilates a state proportional to the vacuum of the orbital l.

From these results, we deduce that

$$\hat{c}_l^\dagger \hat{c}_l|n_1, n_2, \ ... \ n_l, \ ...\rangle = n_l|n_1, n_2, \ ... \ n_l, \ ...\rangle.$$

2.5 Transformation Between Bases

It is often useful to address different physical questions with reference to different single particle bases (such as the position and momentum bases). We need then to understand how to transform our creation and annihilation operators between such bases. We have already seen an example of this for the harmonic chain. Let us think about this more generally for a moment.

2.5.1 The Transformation

Consider two orthonormal sets of basis functions $\{|\chi_a\rangle\}$ and $\{|\psi_a\rangle\}$. The transformation between them is acheived as follows[3]:

$$|\chi_a\rangle = \sum_b U_{ab}|\psi_b\rangle \tag{2.16}$$

$$U_{ab} = \langle\psi_b|\chi_a\rangle \tag{2.17}$$

The transformation is unitary ($UU^\dagger = 1$), as can be seen from the following simple calculation:

$$U_{ab}U^\dagger_{bc} = \sum_b \langle\psi_b|\chi_a\rangle(\langle\psi_b|\chi_c\rangle)^\dagger = \sum_b \langle\chi_c \underbrace{|\psi_b\rangle\langle\psi_b|}_{1} \chi_a\rangle = \langle\chi_c|\chi_a\rangle = \delta_{ac}.$$

Next, let us determine the corresponding transformation rule for the creation and annihilation operators.

$$\begin{aligned} \hat{c}_a^\dagger &\text{ creates a particle in } |\psi_a\rangle, \\ \hat{d}_a^\dagger &\text{ creates a particle in } |\chi_a\rangle. \end{aligned}$$

From the relationship between the orbitals, (2.17), we deduce that

$$\hat{d}_a^\dagger = \sum_b U_{ab}\hat{c}_b^\dagger \text{ and by Hermitian conjugation } \hat{d}_a = \sum_b \hat{c}_b(U^\dagger)_{ba} \tag{2.18}$$

[3]NB. the transformation matrix used here is the transpose of that used by Prof Chalker in his notes

2.5.2 Transforming (Anti-)Commutation Relations

Both commutation and anticommutation relations are preserved by this transformation[4]

Bosonic Commutation Relations:

$$\left[\hat{d}_a, \hat{d}_b^\dagger\right] = \sum_{cd} \left[\hat{c}_c (U^\dagger)_{ca}, U_{bd}\hat{d}_d^\dagger\right] = \sum_{cd} U_{bd}(U^\dagger)_{ca} \underbrace{\left[\hat{c}_c, \hat{c}_d^\dagger\right]}_{=\delta_{cd}} = \sum_c U_{bc}(U^\dagger)_{ca} = \delta_{ab}$$

Fermionic Anti-Commutation Relations:

$$\left\{\hat{d}_a, \hat{d}_b^\dagger\right\} = \sum_{cd} \left\{\hat{c}_c (U^\dagger)_{ca}, U_{bd}\hat{d}_d^\dagger\right\} = \sum_{cd} U_{bd}(U^\dagger)_{ca} \underbrace{\left\{\hat{c}_c, \hat{c}_d^\dagger\right\}}_{=\delta_{cd}} = \sum_c U_{bc}(U^\dagger)_{ca} = \delta_{ab}$$

The invariance of the commutations relations between position and wavevector basis that we noted in the case of the harmonic chain is just a special case of the invariance under general unitary transformations noted here.

2.5.3 Transforming Between x- and p-Bases

The position and momentum basis are often the most convenient for the calculation of physical observables in translationally invariant systems. It turns out that the transformation of states between these bases is simply a Fourier transform. The commutation relations $[\hat{x}, \hat{p}] = i\hbar$ imply that the momentum operator is given by $i\hbar\partial_{\mathbf{x}}$ in real space [5] and the following overlap between position and momentum eigenstates:

$$\langle \mathbf{x}|\mathbf{k}\rangle = \frac{e^{i\mathbf{x}.\mathbf{k}}}{\sqrt{2\pi\hbar}} = U_{\mathbf{k},\mathbf{x}}.$$

Using (2.18) the transformation from a position space creation operator to a momentum space one is given by

$$\hat{d}_{\mathbf{k}}^\dagger = \int d\mathbf{k} \frac{e^{-i\mathbf{x}.\mathbf{k}}}{\sqrt{2\pi\hbar}}\, \hat{c}_{\mathbf{x}}^\dagger.$$

The condition that the transformation be unitary simply reduces to the integral representation of the δ-function;

$$\int d\mathbf{x} U_{\mathbf{k},\mathbf{x}} U_{\mathbf{x},\mathbf{q}}^\dagger = \int d\mathbf{x} \frac{e^{i(\mathbf{k}-\mathbf{q}).\mathbf{x}}}{2\pi\hbar} = \delta(\mathbf{k}-\mathbf{q})/\hbar.$$

[4] An alternative notation uses $[A,B]_- = [A,B]$ and $[A,B]_+ = \{A,B\}$. Using this the equations look identical with the usual $\pm$ indicating where bosonic and fermionic versions differ

[5] and that the position operator is given by $-i\hbar\partial_{\mathbf{k}}$ in momentum space

Normalization of Momentum States and Fourier Transform Conventions
Fourier transformations and transformations between position and momentum bases have various factors of 2π (and $\hbar$) flying around. The easiest way to remember these is to keep a factor of $1/(2\pi\hbar)$ for each momentum in the measure.

Discrete:

$$\hat{c}^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{x}} e^{-i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{x}} \quad \hat{c}^\dagger_{\mathbf{x}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{k}} \quad \mathbf{x} = a(n_x, n_y, n_z) \quad \mathbf{k} = 2\pi(l, m, n)/a$$

Continuous, Finite Length:

$$\hat{c}^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{V}} \int d\mathbf{x} e^{-i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{x}} \quad \hat{c}^\dagger_{\mathbf{x}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{k}} \quad \mathbf{k} = 2\pi(l, m, n)/a$$

Continuous, Infinite Length:

$$\hat{c}^\dagger_{\mathbf{k}} = \int d\mathbf{x} e^{-i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{x}} \quad \hat{c}^\dagger_{\mathbf{x}} = \int \frac{d\mathbf{k}}{2\pi\hbar} e^{i\mathbf{k}.\mathbf{x}}\, \hat{c}^\dagger_{\mathbf{k}}$$

The astute will notice a slight difference compared with the previous page. This is because momentum states can be defined with 2 different normalizations. On the previous page

$$\langle \mathbf{x}|\mathbf{x}\rangle = V \quad \text{and} \quad \langle \mathbf{k}|\mathbf{k}\rangle = \frac{V}{2\pi\hbar}$$

whereas on this page we have used

$$\langle \mathbf{x}|\mathbf{x}\rangle = V \quad \text{and} \quad \langle \mathbf{k}|\mathbf{k}\rangle = V.$$

The point is that one cannot really talk about a plane wave state for a single particle as the prefactor would go to zero (the probability density would be spread out uniformly over the whole of space). Instead, one defines the state to have a certain density of particles per unit volume and one must decide what that density is.

2.6 Single- and Two-Particle Operators

2.6.1 Single-Particle Operators

We are going to build up gradually to a way of writing general single particle operators in a second quantised form - *i.e.* in terms of creation and annihilation operators.

Kinetic Energy
The classical kinetic energy for a collection of N particles takes the form

$$\mathcal{H}_{KE} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m_i}$$

i.e. the sum of the kinetic energy of each particle. The way in which we write this in second quantized form is to use the number operator in the momentum basis to count the number of particles with each momentum;

$$\hat{\mathcal{H}}_{KE} = \sum_{\mathbf{k}} \frac{(\hbar\mathbf{k})^2}{2m} \hat{n}_{\mathbf{k}}.$$

The expectation of this in a momentum Fock state $|n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ ...\rangle$ reduces to

$$\begin{aligned}
\langle \hat{\mathcal{H}}_{KE} \rangle &= \sum_{\mathbf{k}} \langle n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ ...| \underbrace{\frac{(\hbar\mathbf{k})^2}{2m} \hat{n}_{\mathbf{k}} |n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ ...\rangle}_{\text{when } \mathbf{k}=\mathbf{k}_i \Rightarrow \hat{n}_{\mathbf{k}}|n_{\mathbf{k}}\rangle = n_{\mathbf{k}}|n_{\mathbf{k}}\rangle} \\
&= \sum_{i,1}^{N} \frac{(\hbar\mathbf{k}_i)^2}{2m} n_{\mathbf{k}_i} \langle n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ ...|n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ ...\rangle \\
&= \sum_{i=1}^{N} \frac{(\hbar\mathbf{k}_i)^2}{2m} n_{\mathbf{k}_i}
\end{aligned}$$

General Case:
In general, an operator $\hat{\Theta}$ can be expressed in second quantized form by using the number operator in the eigenbasis of $\hat{\Theta}$.

Assume $\hat{\Theta}$ has eigenstates $|\psi_\alpha\rangle$ and eigenvalues Θ_α such that

$$\hat{\Theta}|\psi_\alpha\rangle = \Theta_\alpha|\psi_\alpha\rangle, \quad \text{or} \quad \Theta_\alpha = \langle\psi_\alpha|\hat{\Theta}|\psi_\alpha\rangle.$$

The first quantized expectation for an N particle system is given by

$$\langle\hat{\Theta}\rangle = \sum_{i=1}^{N} \Theta_{\alpha_i}.$$

Following the same procedure as for the kinetic energy, this can be written

$$\hat{\Theta} = \sum_{\alpha} \Theta_\alpha \hat{n}_\alpha = \sum_{\alpha} \Theta_\alpha \hat{c}_\alpha^\dagger \hat{c}_\alpha.$$

General Case in Arbitrary Basis:
Of course, we may wish to write our operator $\hat{\Theta}$ in a basis other than its eigenbasis. Using creation and annihilation operators in an arbitrary basis, it can be written as

$$\hat{\Theta} = \sum_{ab} \langle\psi_a|\hat{\Theta}|\psi_b\rangle \hat{c}_a^\dagger \hat{c}_b. \tag{2.19}$$

This can be shown as follows:

- Relate bases by $U_{\alpha a} = \langle \psi_a | \psi_\alpha \rangle$, which implies $\hat{c}^\dagger_\alpha = U_{\alpha b} \hat{c}^\dagger_b$ and $\hat{c}_\alpha = U^\dagger_{b\alpha} \hat{c}_b$ from our definition in Eq.(2.18) or alternatively $\hat{c}^\dagger_a = U^\dagger_{a\alpha} \hat{c}^\dagger_\alpha$ and $\hat{c}_a = \hat{c}_\alpha U_{\alpha a}$.

- Substitute in general expression

$$\begin{aligned}
\hat{\Theta} &= \sum_{ab\alpha\beta} \langle \psi_a | \hat{\Theta} | \psi_b \rangle U^\dagger_{a\alpha} U_{\beta b} \hat{c}^\dagger_\alpha \hat{c}_\beta \\
&= \sum_{ab\alpha\beta} U^\dagger_{a\alpha} \langle \psi_a | \hat{\Theta} | \psi_b \rangle U_{\beta b} \hat{c}^\dagger_\alpha \hat{c}_\beta \\
&= \sum_{ab\alpha\beta} \underbrace{\langle \psi_\alpha | \psi_a \rangle \langle \psi_a |}_{\sum_a |\psi_a\rangle\langle\psi_a| = 1} \hat{\Theta} \underbrace{| \psi_b \rangle \langle \psi_b | \psi_\beta \rangle}_{\sum_b |\psi_b\rangle\langle\psi_b| = 1} \hat{c}^\dagger_\alpha \hat{c}_\beta \\
&= \sum_{\alpha\beta} \underbrace{\langle \psi_\alpha | \hat{\Theta} | \psi_\beta \rangle}_{\hat{\Theta}|\psi_\beta\rangle = \Theta_\beta |\psi_\beta\rangle} \hat{c}^\dagger_\alpha \hat{c}_\beta \\
&= \sum_{\alpha\beta} \Theta_\beta \underbrace{\langle \psi_\alpha | \psi_\beta \rangle}_{\delta_{\alpha\beta}} \hat{c}^\dagger_\alpha \hat{c}_\beta \\
&= \sum_\alpha \Theta_\alpha \hat{c}^\dagger_\alpha \hat{c}_\alpha
\end{aligned}$$

2.6.2 Two-Particle Operators

Two-body operators — such as the interaction potential — depend upon the coordinates of a pair of particles. The first quantized form of the matrix elements of such an operator are given by

$$\Theta_{lmpq} = \int d\mathbf{x}_1 d\mathbf{x}_2 \psi^*_l(\mathbf{x}_1) \psi^*_m(\mathbf{x}_2) \Theta(\mathbf{x}_1, \mathbf{x}_2) \psi_p(\mathbf{x}_2) \psi_q(\mathbf{x}_1)$$

Using the properly (anti) symmetrized wavefunctions for (fermions) bosons, the expectation values of $\hat{\Theta}$ are

$$\begin{aligned}
\langle \hat{\Theta} \rangle &= \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{1}{\sqrt{2}} \left(\psi^*_l(\mathbf{x}_1) \psi^*_m(\mathbf{x}_2) \pm \psi^*_l(\mathbf{x}_2) \psi^*_m(\mathbf{x}_1) \right) \\
&\qquad \times \left(\Theta(\mathbf{x}_1, \mathbf{x}_2) + \Theta(\mathbf{x}_2, \mathbf{x}_1) \right) \frac{1}{\sqrt{2}} \left(\psi_p(\mathbf{x}_2) \psi_q(\mathbf{x}_1) \pm \psi_p(\mathbf{x}_1) \psi_q(\mathbf{x}_2) \right) \\
&= (\Theta_{lmpq} + \Theta_{mlqp}) \pm (\Theta_{lmqp} + \Theta_{mlpq})
\end{aligned}$$

This same expression can be recovered from the second quantized form

$$\hat{\Theta} = \sum_{lmpq} \Theta_{lmpq} \hat{c}^\dagger_l \hat{c}^\dagger_m \hat{c}_p \hat{c}_q$$

Taking the expectation with the second quantized form of the same states

$$\langle \hat{\Theta} \rangle = \langle 0 | \hat{c}_l \hat{c}_m \hat{\Theta} \hat{c}^\dagger_p \hat{c}^\dagger_q | 0 \rangle = \sum_{abcd} \Theta_{abcd} \underbrace{\langle 0 | \hat{c}_l \hat{c}_m \hat{c}^\dagger_a \hat{c}^\dagger_b}_{(\delta_{lb}\delta_{am} \pm \delta_{al}\delta_{bm})} \underbrace{\hat{c}_c \hat{c}_d \hat{c}^\dagger_p \hat{c}^\dagger_q | 0 \rangle}_{(\delta_{dp}\delta_{cq} \pm \delta_{dq}\delta_{cp})} = (\Theta_{lmpq} + \Theta_{mlqp}) \pm (\Theta_{lmqp} + \Theta_{mlpq})$$

Origin of minus signs
The minus signs here arise for fermions as terms anticommute if they have different labels

$$\hat{c}_c\hat{c}_d\hat{c}_p^\dagger\hat{c}_q^\dagger|0\rangle = -\hat{c}_d\hat{c}_c\hat{c}_p^\dagger\hat{c}_q^\dagger|0\rangle = \hat{c}_d\hat{c}_p^\dagger\hat{c}_c\hat{c}_q^\dagger|0\rangle = \underbrace{\hat{c}_d\hat{c}_p^\dagger}_{\text{when } p=d\Rightarrow 1-\hat{c}_p^\dagger\hat{c}_p} \underbrace{\hat{c}_c\hat{c}_q^\dagger}_{\text{when } c=q\Rightarrow 1-\hat{c}_c^\dagger\hat{c}_c} |0\rangle$$

$$\hat{c}_c\hat{c}_d\hat{c}_p^\dagger\hat{c}_q^\dagger|0\rangle = -\hat{c}_c\hat{c}_p^\dagger\hat{c}_d\hat{c}_q^\dagger|0\rangle = -\underbrace{\hat{c}_c\hat{c}_p^\dagger}_{\text{when } p=c\Rightarrow 1-\hat{c}_p^\dagger\hat{c}_p} \underbrace{\hat{c}_d\hat{c}_q^\dagger}_{\text{when } d=q\Rightarrow 1-\hat{c}_d^\dagger\hat{c}_d} |0\rangle$$

2.7 Diagonalizing Quantum Hamiltonians

The aim in using second quantization techniques is to reduce the expectation values that we are interested in — as far as possible — to number operators. As we saw in the case of the harmonic oscillator, it is then a simple matter to calculate the physical properties. Single particle operators can always be written in this form. Higher order many-particle operators can be expanded in terms of single-particle operators using mean-field theory and perturbative extensions (not part of this course).

2.7.1 Unitary transformations

Hamiltonians that conserve particle number can always be written

$$\hat{\mathcal{H}} = \sum_{ij} \mathcal{H}_{ij}\hat{a}_i^\dagger\hat{a}_j.$$

For $\hat{\mathcal{H}}$ to be Hermitian, $\mathcal{H}_{ij}$ must be a Hermitian matrix, implying i. that it has real eigenvalues and ii. that it can be diagonalized by a unitary transformation to a new basis. Let $\hat{\alpha}_i^\dagger = U_{ij}\hat{a}_j^\dagger$ be a creation operator in such a basis $\Rightarrow\ \hat{a}_j^\dagger = U_{ji}^\dagger\hat{\alpha}_i^\dagger$. Substituting into $\hat{\mathcal{H}}$,

$$\hat{\mathcal{H}} \;=\; \sum_{ij}\mathcal{H}_{ij}\hat{a}_i^\dagger\hat{a}_j = \sum_{ijkl}\mathcal{H}_{ij}U_{ik}\hat{\alpha}_k^\dagger\hat{\alpha}_l U_{lj}^\dagger = \sum_{kl}\underbrace{\left(\sum_{ij}\mathcal{H}_{ij}U_{ik}U_{lj}^\dagger\right)}_{(U^T\mathcal{H}U^*)_{kl}-\text{diagonal}}\hat{\alpha}_k^\dagger\hat{\alpha}_l = \sum_l \epsilon_l\hat{\alpha}_l^\dagger\hat{\alpha}_l$$

Solving a problem defined by a particular $\hat{\mathcal{H}}$ amounts to finding the unitary rotation that diagonalizes it. As we saw for the harmonic chain, often a Fourier transform forms one part of this. In the following, we will see a number of example where there is a residual diagonalization required - often of just a 2×2 or 4×4 matrix.

2.7.2 Bogoliubov Transformation

There are lots of physical systems for which a mean-field treatment leads to terms in the Hamiltonian that are bilinear in creation or annihilation operators;

$$\mathcal{H} = \epsilon_1 \hat{c}_1^\dagger \hat{c}_1 + \epsilon_2 \hat{c}_2^\dagger \hat{c}_2 + \lambda \hat{c}_1^\dagger \hat{c}_2^\dagger + \lambda^* \hat{c}_1 \hat{c}_2.$$

These terms are present in Bose condensates (the subject of the next chapter), superfluids, superconductors and anti-ferromagnets (a topic touched upon in Chapter 4). A Hamiltonian with such terms does not preserve particle number — the groundstate is a superposition of different numbers of particles, which occurs physically by the system exchanging particles with the condensate or environment. A unitary transformation cannot be used to diagonalize these Hamiltonians. Instead, one must use a Bogoliubov transformation. This takes a slightly different form for bosons and fermions. The procedure is very similar in the two cases with some additional negative signs in the latter case.

Bosonic Bogoliubov
The bosonic form of the Bogoliubov transformation is used for example for Bose condensates and anti-ferromagnets. After a Fourier transform, the Hamiltonian takes the following form (usually with additional momentum dependence of each term that we suppress here):

$$\hat{\mathcal{H}} = \epsilon(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + \lambda(\hat{c}_1^\dagger \hat{c}_2^\dagger + \hat{c}_2 \hat{c}_1).$$

This is diagonalized by a transformation of the form

$$\hat{c}_1^\dagger = u\hat{d}_1^\dagger + v\hat{d}_2, \quad \hat{c}_2^\dagger = u\hat{d}_2^\dagger + v\hat{d}_1. \tag{2.20}$$

There are various ways of going through the algebra to show this and to fix the coefficients of u and v in terms of ϵ and λ. Here is the way that I always do it

- Introduce a matrix form

$$\hat{\mathcal{H}} = \frac{1}{2}\left(\hat{c}_1^\dagger, \hat{c}_2, \hat{c}_2^\dagger, \hat{c}_1\right) \begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & \epsilon & 0 & 0 \\ 0 & 0 & \epsilon & \lambda \\ 0 & 0 & \lambda & \epsilon \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \\ \hat{c}_2 \\ \hat{c}_1^\dagger \end{pmatrix} - \epsilon \tag{2.21}$$

  The $-\epsilon$ term arises because the $\hat{c}\hat{c}^\dagger$ terms are in the opposite order in half of the terms as written in this matrix form.

- The Bogoliubov transformation can be written in the form

$$\underbrace{\begin{pmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \\ \hat{c}_2 \\ \hat{c}_1^\dagger \end{pmatrix}}_{\hat{c}} = \underbrace{\begin{pmatrix} u & v & 0 & 0 \\ v & u & 0 & 0 \\ 0 & 0 & u & v \\ 0 & 0 & v & u \end{pmatrix}}_{M} \underbrace{\begin{pmatrix} \hat{d}_1 \\ \hat{d}_2^\dagger \\ \hat{d}_2 \\ \hat{d}_1^\dagger \end{pmatrix}}_{\hat{d}} \tag{2.22}$$

  The spinors $\hat{c}$ and $\hat{d}$ on the left hand right hand sides are referred to as Nambu spinors

- Preserving the commutation relation (which, remember, happens automatically with unitary transformations) requires

$$\begin{aligned}
[\hat{c}_1, \hat{c}_1^\dagger] &= [u\hat{d}_1 + v\hat{d}_2^\dagger, u\hat{d}_1^\dagger + +v\hat{d}_2] \\
&= u^2 \underbrace{[\hat{d}_1, \hat{d}_1^\dagger]}_{=1} + uv \underbrace{[\hat{d}_1, \hat{d}_2]}_{=0} + uv \underbrace{[\hat{d}_2^\dagger, \hat{d}_1^\dagger]}_{=0} - v^2 \underbrace{[\hat{d}_2, \hat{d}_2^\dagger]}_{=1} \\
&= u^2 - v^2 \\
&= 1
\end{aligned}$$

- Using $u^2 - v^2 = 1$ we can identify the inverse of M as

$$M^{-1} = \begin{pmatrix} u & -v & 0 & 0 \\ -v & u & 0 & 0 \\ 0 & 0 & u & -v \\ 0 & 0 & -v & u \end{pmatrix}$$

  so that we can write the transformation, using the Nambu spinor notation, as

$$\hat{c} = M\hat{d}, \;\; \hat{c}^\dagger = \hat{d}^\dagger M \;\; \Leftrightarrow \;\; \hat{d} = M^{-1}\hat{c} \;\; \hat{d}^\dagger = \hat{c}^\dagger M^{-1}$$

- Next we insert resolutions of the identities $MM^{-1} = 1$ and $M^{-1}M = 1$ between the spinors and the Hamiltonian matrix as follows:

$$\hat{\mathcal{H}} = \frac{1}{2} \underbrace{\hat{c}^\dagger M^{-1}}_{\hat{d}^\dagger} \underbrace{M \begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & \epsilon & 0 & 0 \\ 0 & 0 & \epsilon & \lambda \\ 0 & 0 & \lambda & \epsilon \end{pmatrix} M}_{H'} \underbrace{M^{-1}\hat{c}}_{\hat{d}} - \epsilon$$

- The final task is to write out the components of H' and choose u and v so that the off-diagonal elements are zero. We only need to focus on the 2×2 block

$$\begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & \epsilon \end{pmatrix} \begin{pmatrix} u & v \\ v & u \end{pmatrix} = \begin{pmatrix} \epsilon[u^2 + v^2] + 2\lambda uv & 2\epsilon uv + \lambda[u^2 + v^2] \\ 2\epsilon uv + \lambda[u^2 + v^2] & \epsilon[u^2 + v^2] + 2\lambda uv \end{pmatrix}$$

- This can be solved by identifying $u = \cosh\theta$ and $v = \sinh\theta$ (so that $u^2 - v^2 = 1$) and using the double angle formula for $\sinh\theta$ and $\cosh\theta$ to get $u^2 + v^2 = \cosh 2\theta$ and $2uv = \sinh 2\theta$. Finally setting $-\lambda/\epsilon = \tanh 2\theta$, we obtain

$$\begin{aligned}
\mathcal{H} &= \tilde{\epsilon}\left(\hat{d}_1^\dagger \hat{d}_1 + \hat{d}_2^\dagger \hat{d}_2\right) - \epsilon + \tilde{\epsilon} \\
\tilde{\epsilon} &= \sqrt{\epsilon^2 - \lambda^2}
\end{aligned}$$

Fermionic Bogoliubov

This is used for example for superconductivity and superfluidity of fermions (*e.g.* in ^3He). The steps are very similar to those for bosons, but crucially, negative signs from the anti-commutation of fermionic operators changes things somewhat. The Hamiltonian takes the same form as before, with the following Nambu spinor representation:

$$\hat{\mathcal{H}} = \frac{1}{2}\left(\hat{c}_1^\dagger, \hat{c}_2, \hat{c}_2^\dagger, \hat{c}_1\right)\begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon & -\lambda \\ 0 & 0 & -\lambda & -\epsilon \end{pmatrix}\begin{pmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \\ \hat{c}_2 \\ \hat{c}_1^\dagger \end{pmatrix} + \epsilon$$

The opposite signs obtained for fermions are highlighted in red. These arise directly from the commutation relations, *e.g.* $\lambda\hat{c}_1\hat{c}_2 = -\lambda\hat{c}_2\hat{c}_1$ leads to the opposite sign for some of the λ terms. Similarly $\epsilon\hat{c}_1^\dagger\hat{c}_1 = \epsilon(1-\hat{c}_1\hat{c}_1^\dagger)$ leads to a $+\epsilon$ rather than $-\epsilon$ at the end.

- This is diagonalised by a Bogoliubov transformation of the form

$$\begin{pmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \\ \hat{c}_2 \\ \hat{c}_1^\dagger \end{pmatrix} = \begin{pmatrix} u & v & 0 & 0 \\ -v & u & 0 & 0 \\ 0 & 0 & u & -v \\ 0 & 0 & v & u \end{pmatrix}\begin{pmatrix} \hat{d}_1 \\ \hat{d}_2^\dagger \\ \hat{d}_2 \\ \hat{d}_1^\dagger \end{pmatrix} \tag{2.23}$$

  The manipulations from here are rather similar

- The anti-commutation relations must be preserved by the fermionic Bogoliubov transformation. This implies that

$$\{\hat{c}_1^\dagger, \hat{c}_1\} = \{u\hat{d}_1^\dagger + v\hat{d}_2, u\hat{d}_1 + v\hat{d}_2^\dagger\} = u^2\{\hat{d}_1^\dagger, \hat{d}\} + v^2\{\hat{d}_2, \hat{d}_2^\dagger\} = u^2 + v^2 = 1,$$

  which suggests taking $u = \cos\theta$ and $v = \sin\theta$.

- Clearly $M^{-1} = M^T$ allowing us to diagonalize the Hamiltonian as follows:

$$\hat{\mathcal{H}} = \frac{1}{2}\underbrace{\hat{c}^\dagger M}_{\hat{d}^\dagger}\underbrace{M^T\begin{pmatrix} \epsilon & \lambda & 0 & 0 \\ \lambda & -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon & -\lambda \\ 0 & 0 & -\lambda & -\epsilon \end{pmatrix}M}_{H'}\underbrace{M^{-1}\hat{c}}_{\hat{d}} + \epsilon$$

- As in the bosonic case, the final task is to write out the components of H' and choose u and v so that the off-diagonal elements are zero. We only need to focus on the 2×2 block

$$\begin{pmatrix} u & -v \\ v & u \end{pmatrix}\begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix}\begin{pmatrix} u & v \\ -v & u \end{pmatrix} = \begin{pmatrix} \epsilon[u^2-v^2]-2\lambda uv & 2\epsilon uv + \lambda[u^2-v^2] \\ 2\epsilon uv + \lambda[u^2-v^2] & -\epsilon[u^2-v^2] + 2\lambda uv \end{pmatrix}$$

  which leads to the conditions $\tan 2\theta = -\lambda/\epsilon$ and $\tilde{\epsilon} = \cos 2\theta\epsilon - \sin 2\theta\lambda = \sqrt{\epsilon^2+\lambda^2}$

- The resulting Hamiltonian is

$$\begin{aligned} \mathcal{H} &= \tilde{\epsilon}\left(\hat{d}_1^\dagger\hat{d}_1 + \hat{d}_2^\dagger\hat{d}_2\right) + \epsilon - \tilde{\epsilon} \\ \tilde{\epsilon} &= \sqrt{\epsilon^2+\lambda^2} \end{aligned}$$

Chapter 3

The Weakly-Interacting Bose Gas

Superfluidity was first observed in liquid helium below about 2.1K. Similar phenomena - at least the phenomenon of Bose condensation - have since been observed in ultra-cold atomic gases and quantum magnets. After the rather formal interlude of the previous chapter, we now poses the analytical tools to describe Bose condensation in detail.

3.1 The Hamiltonian

The Hamiltonian for the weakly interacting Bose gas contains a kinetic term describing the motion of non-relativistic bosons in free space and a point repulsion between them (*i.e* the particles excert no force upon one another until they are immediately adjacent and then they repel).

$$\mathcal{H} = \mathcal{H}_{KE} + \mathcal{H}_{int} = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \frac{U}{2V} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{p}} \hat{c}_{\mathbf{q}} \hat{c}_{\mathbf{k}+\mathbf{p}-\mathbf{q}}$$

To understand the form of the repulsive interaction, we first note that it can be written in first quantized form as

$$\mathcal{H}_{int} = \frac{U}{2} \sum_{i \neq j} \delta(\mathbf{x}_i - \mathbf{x}_j)$$

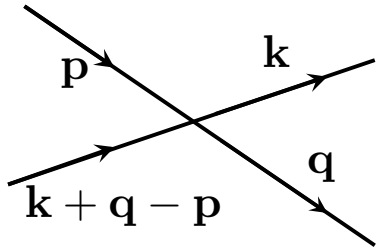
by which we imply that it is diagonal in the position basis and given by the product of the densities at two different points. In second quantized form, in the position basis, then we have

$$\mathcal{H}_{int} = \frac{U}{2} \int d\mathbf{x} d\mathbf{y}\ \delta(\mathbf{x} - \mathbf{y}) \hat{n}(\mathbf{x}) \hat{n}(\mathbf{y}),$$

where $\hat{n}(\mathbf{x}) = \hat{c}^\dagger_{\mathbf{x}}\hat{c}_{\mathbf{x}}$ is the number operator at the point $\mathbf{x}$. Substituting Fourier expansions for the position-basis creation and annihilation operators

$$\begin{aligned}
\mathcal{H}_{int} &= \frac{U}{2}\int d\mathbf{x}d\mathbf{y}\ \delta(\mathbf{x}-\mathbf{y})\int \frac{d\mathbf{k}}{(2\pi)^d}\frac{d\mathbf{p}}{(2\pi)^d}\frac{d\mathbf{q}}{(2\pi)^d}\frac{d\mathbf{l}}{(2\pi)^d}e^{i\mathbf{x}.(\mathbf{k}-\mathbf{p})+i\mathbf{y}.(\mathbf{q}-\mathbf{l})}\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{q}}\hat{c}_{\mathbf{l}} \\
&= \frac{U}{2}\int \frac{d\mathbf{k}}{(2\pi)^d}\frac{d\mathbf{p}}{(2\pi)^d}\frac{d\mathbf{q}}{(2\pi)^d}\frac{d\mathbf{l}}{(2\pi)^d}\underbrace{\int d\mathbf{x}e^{i\mathbf{x}.(\mathbf{k}-\mathbf{p}+\mathbf{q}-\mathbf{l})}}_{=(2\pi)^d\delta(\mathbf{k}-\mathbf{p}+\mathbf{q}-\mathbf{l})}\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{q}}\hat{c}_{\mathbf{l}} \\
&= \frac{U}{2}\int \frac{d\mathbf{k}}{(2\pi)^d}\frac{d\mathbf{p}}{(2\pi)^d}\frac{d\mathbf{q}}{(2\pi)^d}\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{q}}\hat{c}_{\mathbf{k}-\mathbf{p}+\mathbf{q}}
\end{aligned}$$

Notice that the momenta of the ingoing bosons that are annihilated matches that of the outgoing, created bosons. This can be represented by a Feynman diagram:



3.2 Mean Field Theory

At the end of Chapter 2, we learnt how to diagonalize a quadratic, second quantized Hamiltonian. In the present case, however, the interaction is quartic in creation and annihilation operators. Based upon our knowledge of the non-interacting Bose gas, we can develop a leading-order approximation that reduces the Hamiltonian to quadratic form.

Non-interacting Bose Gas: All particles in $\mathbf{k} = 0$ state.

Interacting Bose Gas:
Assume macroscopic occupation of the $\mathbf{k} = 0$ state; $\langle\hat{c}^\dagger_0\hat{c}_0\rangle = N_0$. A number of steps follow from this

- Replace $\hat{c}_0$ by a c-number (commuting number rather than operator) $\hat{c}_o \to \sqrt{N_0}$.
- Expand $\mathcal{H}$ in powers of N_0

$$\mathcal{H}_{int} = \frac{UN_0^2}{2V} + \frac{UN_0}{2V}\sum_{\mathbf{k}\neq 0}\left(4\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}} + \hat{c}^\dagger_{\mathbf{k}}\hat{c}^\dagger_{-\mathbf{k}} + \hat{c}_{\mathbf{k}}\hat{c}_{-\mathbf{k}}\right) + O(1)$$

- The total number of particles N can be expressed as

$$N = N_0 + \sum_{\mathbf{k}\neq 0}\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}}$$

- Substitute back and retain quadratic terms

$$\mathcal{H}_{int} = \frac{UN^2}{2V} + \frac{UN}{2V}\sum_{\mathbf{k}\neq 0}\left(2\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}} + \hat{c}^\dagger_{\mathbf{k}}\hat{c}^\dagger_{-\mathbf{k}} + \hat{c}_{\mathbf{k}}\hat{c}_{-\mathbf{k}}\right)$$

- Adding to the non-interacting part of the Hamiltonian

$$\mathcal{H} = V\frac{U\rho^2}{2} + \sum_{\mathbf{k}\neq 0}\left[\left(\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right)\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}} + \frac{U\rho}{2}(\hat{c}^\dagger_{\mathbf{k}}\hat{c}^\dagger_{-\mathbf{k}} + \hat{c}_{\mathbf{k}}\hat{c}_{-\mathbf{k}})\right] \tag{3.1}$$

- This has precisely the same form as the Hamiltonian considered in 2.7.2. It can be diagonalised with a Bogoliubov transformation resulting in a diagonal Hamiltonian

$$\begin{aligned}\mathcal{H} &= {\sum_{\mathbf{k}\neq 0}}' \left[\epsilon_{\mathbf{k}}(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}^\dagger_{-\mathbf{k}}\hat{\alpha}_{-\mathbf{k}}) + \epsilon_{\mathbf{k}} - \frac{\hbar^2\mathbf{k}^2}{2m}\right], \\ \epsilon_{\mathbf{k}} &= \left[\left(\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right)^2 - (U\rho)^2\right]^{1/2}\end{aligned} \tag{3.2}$$

  where $\sum'$ indicates that the summation be carried out wit $k_x > 0$ say and the point $\mathbf{k} = 0$ excluded.

3.3 Landau's Critical Superfluid Velocity

The dispersion of excitation found above has different behaviour at large and small momenta;

$$\begin{aligned}\epsilon_{\mathbf{k}} &\sim \frac{\hbar^2\mathbf{k}^2}{2m} \qquad \text{large } |\mathbf{k}| \quad \left(\text{such that } \frac{\hbar^2\mathbf{k}^2}{2m} >> U\rho\right) \\ &\sim \sqrt{\frac{U\rho}{m}}|\mathbf{k}| \quad \text{small } |\mathbf{k}|\end{aligned}$$

The latter dependence at low $|\mathbf{k}|$ is responsible for the superfluid properties as can be seen by the following argument due to Landau:

Consider a superfluid of total mass M and velocity $\mathbf{v}$. The only way that friction can arise is by exciting some of the $\mathbf{k} \neq 0$ modes that we have revealed above. Suppose producing one such mode reduces the bulk velocity to $\mathbf{v} - \Delta\mathbf{v}$.

Conservation of Momentum:

$$M\mathbf{v} = M\mathbf{v} - M\Delta\mathbf{v} + \hbar\mathbf{k}$$

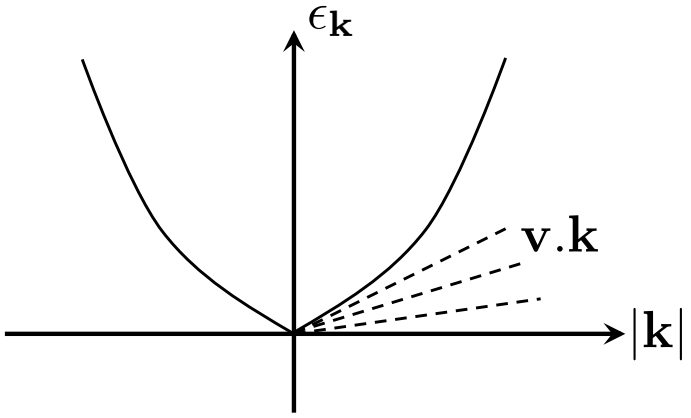
Conservation of Energy:

$$\frac{1}{2}M\mathbf{v}^2 = \frac{1}{2}M(\mathbf{v} - \Delta\mathbf{v})^2 + \epsilon_{\mathbf{k}}$$

Together which imply

$$\hbar\mathbf{k}.\mathbf{v} = \epsilon_{\mathbf{k}}$$

The quantity $\mathbf{v}.\mathbf{k}$ takes different values depending upon the relative direction of $\mathbf{v}$ and $\mathbf{k}$ and is maximum for $\mathbf{k}$ parallel to $\mathbf{v}$.



If $|\mathbf{v}| < \epsilon_{\mathbf{k}}/(\hbar|\mathbf{k}|$ for all $\mathbf{k}$, then no bosons are excited and there is no friction. This implies a critical velocity for superfluid flow

$$v_c = \min_{\mathbf{k}} \left(\frac{\epsilon_{\mathbf{k}}}{\hbar|\mathbf{k}|} \right). \tag{3.3}$$

From our previous results $\epsilon_{\mathbf{k}} \approx \sqrt{U\rho/m}\hbar\mathbf{k}$ so that the critical velocity is given by

$$v_c = \sqrt{\frac{U\rho}{m}}.$$

The finite interaction crucially changes the properties of the Bose system allowing the possibility of superfluidity.

3.4 Superfluid Fraction

The Hamiltonian is diagonalized by a Bogoliubov transformation from the original Base operators $\hat{c}_{\mathbf{k}}$ to new ones $\hat{\alpha}_{\mathbf{k}}$ with dispersion $\epsilon_{\mathbf{k}}$ given by Eq.(3.2). Since the Hamiltonian for the latter is diagonal, we can easily write an expression for the occupation of these modes at finite temperature in terms of the Bose distribution function

$$\langle \hat{\alpha}^\dagger_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} \rangle = n_B(\epsilon_{\mathbf{k}}) = \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} - 1}.$$

This can be used to calculate thermodynamic properties of the Bose gas, such as the superfluid density;

$$\rho_0 = \rho - \sum_{\mathbf{k}\neq 0} \langle \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} \rangle. \tag{3.4}$$

The trick is to use the form of the Bogoliubov transformation to write the expectation in Eq.(3.4) in terms of the $\hat{\alpha}$ operators. The solution to this is the subject of one of the problem sets.

Chapter 4

Quantum Magnets

In this chapter, we will use the language of second quantization to discuss properties of quantum magnets — magnets in which atoms in a lattice have unpaired electron spins that may interact with the spins on other sites. We will focus upon insulating magnets in which the electrons that carry the spins are fixed in a give atomic orbital, as opposed to itinerant, where they would be free to hop around.

Despite the apparent simplicity of this set up, the collective quantum behaviour of such systems is incredibly rich. Just about every phenomenon of modern quantum physics is revealed by these systems — they provide the first example of topology in quantum physics (through the Haldane conjecture that we will discuss later) and a magnetic model (due to Kitaev) is the basis of some of the most widely studied quantum error correcting codes. The prototypical model of this behaviour is deceptively simple. The complications are all down to emergent collective behaviour.

4.1 The Heisenberg model

The Heisenberg model is the simplest model of quantum magnetic behaviour. Its Hamiltonian is given by

$$\hat{\mathcal{H}} = \sum_{\langle ij \rangle} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \tag{4.1}$$

where i, j are the sites of some lattice, it e.g. 2d sqare or triangular, 3d cubic *etc.* $\langle i, j \rangle$ indicates a sum over neighbouring sites. J_{ij} are exchange interactions between 2 spins on the sites i and j. Negative couplings favour parallel spins and ferromagnetic ordering, positive couplings favour anti-ferromagnetic couplings.

Commutation Relations: The spin operators obey commutation relations

$$\left[\hat{S}_i^\mu, \hat{S}_j^\nu\right] = i\hbar\epsilon^{\mu\nu\lambda}\hat{S}_i^\lambda\delta_{ij}$$

The consequences of these are not trivial and render the sate-space and dynamics considerably more complicated than that of bosons. Classically, spin/angular momentum is a vector of any length in any direction. Quantum mechanics restricts the length and direction:

Quantum Numbers: The total spin operator and its projection onto a particular axis (say the z-axis) form a commuting set of operators $\left[\hat{\mathbf{S}}^2, \hat{S}^z\right] = 0$ with which we may associate quantum numbers

$$\begin{aligned} \hat{\mathbf{S}}^2|S,m\rangle &= \hbar^2 S(S+1)|S,m\rangle \\ \hat{S}^z|S,m\rangle &= \hbar m|S,m\rangle \end{aligned} \tag{4.2}$$

where $m \in \{-S, -(S-1), ...S\}$ *i.e.* a tower of $2S+1$ states. As you will recall from previous quantum mecahnics courses, this can be derived by constructing ladder operators

$$\hat{S}^{\pm} + \hat{S}_x \pm i\hat{S}_y \tag{4.3}$$

that move states up and down this tower of states:

$$\begin{aligned} \hat{S}^{\pm}|S,m\rangle &= \hbar\sqrt{(S \mp m)(S \pm +1)}|S, m \pm 1\rangle \\ \hat{S}^{+}|S,S\rangle &= 0 \\ \hat{S}^{-}|S,-S\rangle &= 0 \end{aligned} \tag{4.4}$$

This algebra is actually very hard to deal with in general for systems of interacting spins. Notice, though, that the top and the bottom of the tower of states look rather like the bosonic state space. If the physics is such that these states dominate the behaviour, then we can make approximations that map our Hamiltonian based upon spin operators to one based upon bosonic operators.

Origin of the Heisenberg Model
Various different mechanisms collected together under the heading "exchange" contribute to the interaction between spins in the Heisenberg model

a) Direct Exchange:
This leads to anti-ferromagnetic coupling and ultimately has the same origin as Hund's rul in atoms (though it has the opposite effect). Consider two neighbouring sites:

 Symmetric spins
⇒ antisymmetric spatial wavefunction[a] ⇒ Node at $x_1 - x_2 = 0$ ⇒ Lower Coulomb

 anti-symmetric spins
⇒ symmetric spatial wavefunction ⇒ no node in wavefunction ⇒ Higher Coulomb
This is also called *potential exchange*, because it relies upon the difference in potential energy between 2 configurations.

b) Super/Kinetic Exchange:
This type of exchange is driven by virtual hopping between lattice sites. This spreads the electronic wavefunction and so lowers its kinetic energy.

 Symmetric spins
⇒ Pauli exclusion forbids double occupancy and there is no virtual hopping.

 anti-symmetric spins
⇒ Virtual hopping allowed ⇒ wavefunction spreads and lowers kinetic energy

[Anderson, PhyS. Rev. **79**, 350 (1950)]

[a] Electrons are fermions

4.2 Holstein-Primakoff transformation

The non-trivial commutation relations of the spin operators make them tricky to deal with. Bosonic operators are much easier and the Holstein-Primakoff transformation allows a way to swap between the two.

$$\begin{aligned} \hat{S}^z &= S - \hat{b}^\dagger \hat{b} \\ \hat{S}^+ &= \sqrt{2S}\left(1 - \frac{\hat{b}^\dagger \hat{b}}{2S}\right)^{1/2} \hat{b} \\ \hat{S}^- &= \sqrt{2S}\hat{b}^\dagger \left(1 - \frac{\hat{b}^\dagger \hat{b}}{2S}\right)^{1/2} \end{aligned} \tag{4.5}$$

One can easily check[1] that the bosonic commutation relations $[\hat{b}, \hat{b}^\dagger] = 1$ reproduce the spin commutation relations in the form $\left[\hat{S}^+, \hat{S}^-\right] = 2\hat{S}^z$. Identifying our boson operator per site of the lattice, the fact that spin operators on different sites commute is readily accommodated by the similar commutation of bosonic operators on different sites.

Approximate Form:
In the limit that the expectations of $\hat{S}^z$ on each site are near to S, there are very few excitations in the bosonic representation. In this case, the mapping may be reduced to

$$\begin{aligned} \hat{S}^z &= S - \hat{b}^\dagger \hat{b} \\ \hat{S}^+ &= \sqrt{2S}\hat{b} \\ \hat{S}^- &= \sqrt{2S}\hat{b}^\dagger \end{aligned} \tag{4.6}$$

which amounts to turning the bosonic tower of states upside down and matching it with the top of the tower of spin states. In physical situations in which only a few bosons are excited, *i.e.* $\langle \hat{b}^\dagger \hat{b} \rangle \ll 1$, the fact that the bosonic tower of states does not terminate does not show up. We shall see now how this approximation allows us to calculate certain properties of magnetic systems.

4.3 The Heisenberg ferromagnet

Consider an insultating magnet in which all of the nearest neighbour interactions are ferromagnetic, *i.e.* in which $J < 0$.

4.3.1 The Groundstate

The groundstate is such that all of the spins are aligned — say in the z-directions — so that $\hat{S}^z_{\mathbf{x}}|S, S\rangle = \hbar S|S, S\rangle$ on each site and

$$|\psi_{\text{Groundstate}}\rangle = \bigotimes_{\mathbf{x}} |S, S\rangle$$

This state is an eigenstate of the Heisenberg model. To see this, we write the Heisenberg model in the form

$$\hat{\mathcal{H}} = -J \sum_{\langle \mathbf{x},\mathbf{y} \rangle} \hat{\mathbf{S}}_{\mathbf{x}} \cdot \hat{\mathbf{S}}_{\mathbf{y}} = -J \sum_{\langle \mathbf{x},\mathbf{y} \rangle} \left[\hat{S}^z_{\mathbf{x}} \hat{S}^z_{\mathbf{y}} + (\hat{S}^+_{\mathbf{x}} \hat{S}^-_{\mathbf{y}} + \hat{S}^-_{\mathbf{x}} \hat{S}^+_{\mathbf{y}})/2 \right]$$

so that

$$\hat{\mathcal{H}}|\psi_{\text{Groundstate}}\rangle = -J \sum_{\langle \mathbf{x},\mathbf{y} \rangle} S^2 |\psi_{\text{Groundstate}}\rangle,$$

where we have used the fact that $\hat{S}^+|S, S\rangle = 0$.

[1] And you should!!

4.3.2 Excitations

Excitations about this groundstate can be found using the approximate form of the Holstein Primakoff transformation Eq(4.5), after which the Hamiltonian reduces to

$$\mathcal{H} = -J\sum_{\langle \mathbf{x},\mathbf{y}\rangle} S^2 - JS\sum_{\langle \mathbf{x},\mathbf{y}\rangle}\left(\hat{b}^\dagger_{\mathbf{x}}\hat{b}_{\mathbf{y}} + \hat{b}^\dagger_{\mathbf{y}}\hat{b}_{\mathbf{x}} - \hat{b}^\dagger_{\mathbf{x}}\hat{b}_{\mathbf{x}} - \hat{b}^\dagger_{\mathbf{y}}\hat{b}_{\mathbf{y}}\right)$$

and the groundstate $\bigotimes_{\mathbf{x}}|S,S\rangle$ becomes the vacumm state of the bosons $\bigotimes|0\rangle$.

Our task now is to diagonalize this Hamiltonian. Because the system is translationally invariant, the first step towards this (actually the only step in this case) is to Fourier transform. Let us do this for the simple cubic lattice, taking the Fourier transform relations

$$\hat{b}_{\mathbf{x}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}}\hat{b}_{\mathbf{k}} \quad \hat{b}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}}\hat{b}_{\mathbf{x}}$$

where N is the total number of sites in the lattice, $\mathbf{k} = 2\pi(n,m,l)/L$ with n,m and l integers and L the size of the lattice. With these definitions, we find

$$\begin{aligned}\mathcal{H} &= -\frac{1}{2}JS^2Nz - \frac{JS}{N}\sum_{\mathbf{x},\mathbf{d}}\sum_{\mathbf{k},\mathbf{q}} e^{i\mathbf{x}\cdot(\mathbf{k}-\mathbf{q})}[e^{i\mathbf{d}\cdot\mathbf{q}}-1]\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{q}} \\ &= -\frac{1}{2}JS^2Nz - \frac{JS}{N}\sum_{\mathbf{k}}\sum_{\mathbf{d}}[e^{i\mathbf{d}\cdot\mathbf{k}}-1]\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}}\end{aligned}$$

where $\mathbf{d}$ is the displacement between adjacent lattice sites and z is the coordination number of a site of the lattice. We may summarize this result in 3d as

$$\begin{aligned}\mathcal{H} &= \underbrace{-\frac{1}{2}JS^2Nz}_{\text{const}} + \sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}} \\ \epsilon_{\mathbf{k}} &= 2J\left[3-\cos(ak_x)-\cos(ak_y)-\cos(ak_z)\right].\end{aligned}$$

We have reduce our description of the excitations to that of a bosonic, harmonic osicllator-like mode. Notice that since the ferromagnet is an eigenstate of the Hamiltonian, there are no zero-point fluctuations. This is quite a special case. The bosonic modes have low energy dispersion

$$\epsilon_{\mathbf{k}} \sim JS\mathbf{k}^2.$$

These modes are gapless — their energy goes to zero as $|\mathbf{k}|$ does. This is because they are Goldstone modes; they arise because the spin rotational symmetry of the Hamiltonian is broken by the groundstate — it costs zero energy to rotate between these groundstates and this coresponds to precisely the $\mathbf{k}=0$ limit of the excitations described here. The fact that the dispersion is quadratic (and not linear as for phonons) as $|\mathbf{k}|\to 0$ is because time reversal symmetry is broken (remember that angular momentum and hence spin reverse sign under time-reversal).

4.3.3 Thermal Fluctuations

The breaking of rotational symmetry by the ferromagnetic state can be quantified by an order parameter - the magnetization. The free energy of the system may in fact be expanded as a function of this order parameter. This powerful technique — known as a Ginzburg-Landau expansion — can reveal key generic properties of thermodynamic phases and transitions between them. Here we shall satisfy ourselves by considering the effect of thermal fluctuations upon the magnetization of our system.

The magnetization per site (assuming polarization in the z-direction)is given by

$$M = \frac{1}{N}\sum_{\mathbf{x}} \langle S^z_{\mathbf{x}} \rangle.$$

Using the Holstein-Primakoff transformation, Eq.(4.5) this can be written in terms of the bosonic operators as

$$\begin{aligned} M &= \frac{1}{N}\sum_{\mathbf{x}} \langle S - \hat{b}^\dagger_{\mathbf{x}} \hat{b}_{\mathbf{x}} \rangle \\ &= S - \frac{1}{N^2}\sum_{\mathbf{x}}\sum_{\mathbf{k},\mathbf{q}} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{x}} \langle \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{q}} \rangle \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} \langle \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle, \end{aligned}$$

where we have also Fourier transformed as our Hamiltonian is diagonal in momentum space. This latter fact, combined with the fact that there are not a fixed number of bosons results in the expectation $\langle \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle$ begin given by the Bose distribution. The magnetisation is therefore given by

$$\begin{aligned} \Delta M &= \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} - 1} \\ &\quad \text{Taking the continuum limit} \\ &= \frac{1}{\Omega}\int_{BZ} d^d\mathbf{k} \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} - 1} \\ &\quad \Omega \quad \text{is the Brillouin zone volume, and} \quad \epsilon_{\mathbf{k}} \sim SJ\mathbf{k}^2 \\ &= T\int_0^{\sqrt{T/SJ}} \frac{k^{d-1}dk}{SJk^2} \\ &\sim \begin{cases} T\left[\frac{1}{k}\right]_0^{\sqrt{T/SJ}} & d=1 \\ T\left[\log[k]\right]_0^{\sqrt{T/SJ}} & d=2 \\ T\left[k\right]_0^{\sqrt{T/SJ}} & d=3 \end{cases} \end{aligned}$$

The integral diverges at low k — called an IR (infra-red) divergence — in one and two dimensions. It converges in three dimensions so that $\Delta M \sim T^{3/2}$. The divergence in $d = 1$ and 2 shows that fluctuations overwhelm antiferromagnetic order - an illustration of the *Mermin-Wagner* theorem that a continuous symmetry cannot be broken in $d \leq 2$ at finite temperature.

4.4 The Heisenberg Anti-ferromagnet

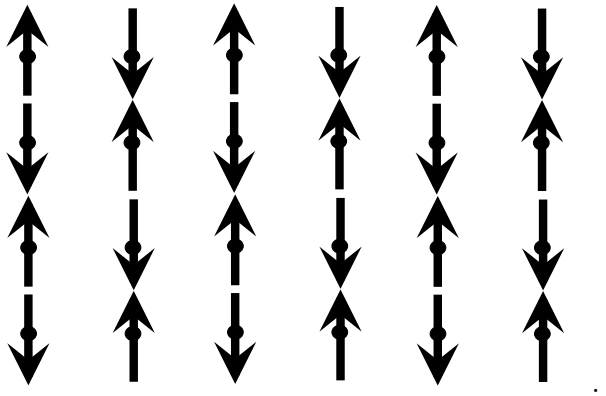
Next we shall consider the anti-ferromagnetic Heisenberg model on a bi-partite lattice

$$\mathcal{H} = J \sum_{\langle \mathbf{x},\mathbf{y} \rangle} \hat{\mathbf{S}}_{\mathbf{x}} \cdot \hat{\mathbf{S}}_{\mathbf{y}} = J \sum_{\langle \mathbf{x},\mathbf{y} \rangle} \left[\hat{S}^z_{\mathbf{x}} \hat{S}^z_{\mathbf{y}} + (\hat{S}^+_{\mathbf{x}} \hat{S}^-_{\mathbf{y}} + \hat{S}^-_{\mathbf{x}} \hat{S}^+_{\mathbf{y}})/2 \right]. \tag{4.7}$$

A bi-partite lattice is one whose sites can be divided into two sets such that sites on one set are only nearest neighbours in the other. The square, cubic and hypercubic lattice are examples.

4.4.1 The Néel state

At the classical level, the Hamiltonian is minimised when the spins on the different sub-lattices are anti-parallel. This is known as the Néel state. On the square lattice it takes the form



$$|\psi_{\text{Neél}}\rangle = \bigotimes_{\mathbf{x}} |S, \pm S\rangle,$$

where the two different signs occur for the different sub-lattices. Unlike the ferromagnet, this is not an eigenstate of the Hamiltonian. This is demonstrated by the action of the $\hat{S}^+_{\mathbf{x}} \hat{S}^-_{\mathbf{y}}$ terms. In the case of the ferromagnet, such terms always give zero as on one of the sites $\hat{S}^+ |S, S\rangle = 0$. In the anti-ferromagnetic case, however, such terms are not zero — they generate quantum fluctuations away from the classical Néel state.

4.4.2 Holstein-Primakoff transformation

To study these quantum fluctuations away from the Néel state we use the Holstein-Primakoff transformation. The transformation must be applied slightly differently on the two sub-lattices.

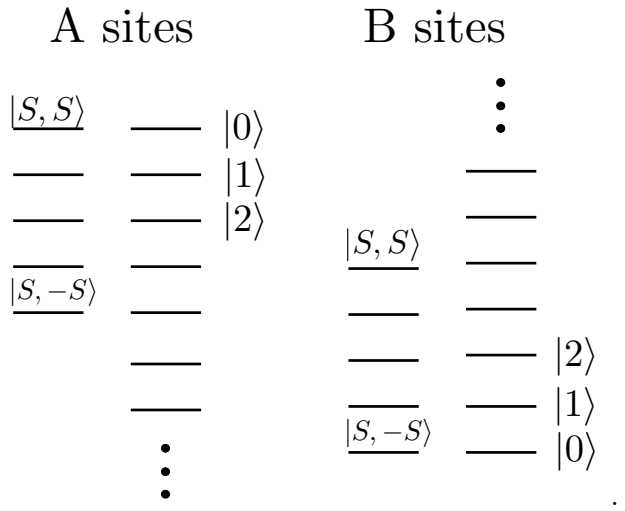
A sub-lattice $|S, S\rangle$:

$$\begin{aligned} \hat{S}^z &= S - \hat{a}^\dagger \hat{a} \\ \hat{S}^+ &= \sqrt{2S}\hat{a} \\ \hat{S}^- &= \sqrt{2S}\hat{a}^\dagger \end{aligned}$$

B sub-lattice $|S,S\rangle$:

$$\begin{aligned}\hat{S}^z &= \hat{a}^\dagger\hat{a} - S \\ \hat{S}^+ &= \sqrt{2S}\hat{a}^\dagger \\ \hat{S}^- &= \sqrt{2S}\hat{a}\end{aligned}$$

This amounts to matching the bosonic tower of states to the spin tower of states from the bottom up in one case and from the top down in the other:



Substituting these transformations into the Heisenberg Hamiltonian, we find

$$\mathcal{H} = -J\sum_{\langle \mathbf{x},\mathbf{y}\rangle} S^2 + JS\sum_{\langle \mathbf{x},\mathbf{y}\rangle}\left[\hat{a}^\dagger_{\mathbf{x}}\hat{a}_{\mathbf{x}} + \hat{a}^\dagger_{\mathbf{y}}\hat{a}_{\mathbf{y}} + \hat{a}^\dagger_{\mathbf{x}}\hat{a}^\dagger_{\mathbf{y}} + \hat{a}_{\mathbf{x}}\hat{a}_{\mathbf{y}}\right].$$

The easiest way to proceed now is to introduce a coordinate $\mathbf{z}$ that runs over all of the lattice sites and a coordinate $\mathbf{d}$ that runs over nearest neighbour vectors. With these, the Hamiltonian can be written

$$\mathcal{H} = -\frac{JS^2Nz}{2} + \frac{JS}{2}\sum_{\mathbf{z},\mathbf{d}}\left[2\hat{a}^\dagger_{\mathbf{z}}\hat{a}_{\mathbf{z}} + \hat{a}^\dagger_{\mathbf{z}}\hat{a}^\dagger_{\mathbf{z}+\mathbf{d}} + \hat{a}_{\mathbf{z}}\hat{a}_{\mathbf{z}+\mathbf{d}}\right],$$

which after Fourier transform becomes

$$\mathcal{H} = -\frac{JS^2Nz}{2} + \frac{JSz}{2}\sum_{\mathbf{k}}\left[\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}^\dagger_{-\mathbf{k}}\hat{a}_{-\mathbf{k}} + \gamma_{\mathbf{k}}\left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{-\mathbf{k}} + \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\right)\right],$$

where[2] $\gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\mathbf{d}}\cos(\mathbf{k}\cdot\mathbf{d})$. This may be written in matrix form as

$$\mathcal{H} = -\frac{JS(S+1)Nz}{2} + \frac{JSz}{2}\sum_{\mathbf{k}}\left(\hat{a}^\dagger_{\mathbf{k}}, \hat{a}_{-\mathbf{k}}\right)\begin{pmatrix}1 & \gamma_{\mathbf{k}}\\ \gamma_{\mathbf{k}} & 1\end{pmatrix}\begin{pmatrix}\hat{a}_{\mathbf{k}}\\ \hat{a}^\dagger_{-\mathbf{k}}\end{pmatrix}$$

[2]Note that since $\mathbf{d}$ takes pairs of values on the hypercubic lattice, $\gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\mathbf{d}} e^{i\mathbf{k}\cdot\mathbf{d}} = \frac{1}{z}\sum_{\mathbf{d}}\cos(\mathbf{k}\cdot\mathbf{d})$

An alternativ approach — used in John Chalker's notes, for example — is to rotate the spins on the B sub-lattice

$$S^z \to -S^z, \quad S^x \to -S^x, \quad S^y \to S^y$$

which preserves the commutation relations. The Hamiltonian then becomes

$$\mathcal{H} = -J \sum_{\langle \mathbf{xy} \rangle} \left[\hat{S}^z_{\mathbf{x}} \hat{S}^z_{\mathbf{y}} + (\hat{S}^+_{\mathbf{x}} \hat{S}^+_{\mathbf{y}} + \hat{S}^-_{\mathbf{x}} \hat{S}^-_{\mathbf{y}})/2 \right]$$

and the Holstein-Primakov transformation can be used in the same form for each sub-lattice.

4.4.3 Bogoliubov transformation

Evidently the Fourier transform alone is not enough to diagonalize the Hamiltonian. The anomalous terms such as $\hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}$ require us to use a Bogoliubov transfromation as developed in section 2.7.2. The result is.

$$\mathcal{H} = -\frac{1}{2} JS(S+1)Nz + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \left(\hat{\alpha}^\dagger_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + 1/2 \right)$$

with

$$\epsilon_{\mathbf{k}} = JSz\sqrt{1-\gamma^2_{\mathbf{k}}} \sim |\mathbf{k}| \quad \text{at small} \quad \mathbf{k}$$

and the Bogoliubov transformation given by

$$\begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}^\dagger_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{\alpha}_{\mathbf{k}} \\ \hat{\alpha}^\dagger_{-\mathbf{k}} \end{pmatrix} \qquad \begin{matrix} u_{\mathbf{k}} = \cosh(\theta_{\mathbf{k}}) \\ v_{\mathbf{k}} = -\sinh(\theta_{\mathbf{k}}) \end{matrix} \qquad \tanh(2\theta_{\mathbf{k}}) = -\gamma_{\mathbf{k}}$$

Notice that the low-frequency dispersion is linear, unlike the ferromagnet. This is because the Néel state does not break time-reversal symmetry in a macroscopic sense (time-reversal simply swaps the sublattices).

4.4.4 Fluctuations of the Antiferromagnet

As we have already noted, the classical Néel state is not an eigenstate of the anti-ferromagnetic Heisenberg model. This has several consequences. Firstly, it leads to a zero-point contribution to the energy. These zero-point fluctuations also reduce the sub-lattice magnetization even at zero temperature.

The average (staggered) magnetization per site is given by

$$S - \Delta S = S - \frac{1}{N} \sum_{\mathbf{z}} \langle \hat{a}^\dagger_{\mathbf{z}} \hat{a}_{\mathbf{z}} \rangle = S - \frac{1}{N} \sum_{\mathbf{k}} \langle \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} \rangle.$$

Since the Hamiltonian is diagonal in terms of $\hat{\alpha}$ and $\hat{\alpha}^\dagger$, we must re-write the magnetization in terms of them

$$\begin{aligned} S - \Delta S &= S - \frac{1}{N}\sum_{\mathbf{k}} \langle (u_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}_{-\mathbf{k}})(u_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{-\mathbf{k}})\rangle \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} \left(u^2_{\mathbf{k}}\langle \hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}\rangle + v^2_{\mathbf{k}}\langle \hat{\alpha}_{-\mathbf{k}}\hat{\alpha}^\dagger_{-\mathbf{k}}\rangle + u_{\mathbf{k}}v_{\mathbf{k}}(\underbrace{\langle \hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}^\dagger_{-\mathbf{k}}\rangle}_{=0} + \underbrace{\langle \hat{\alpha}_{-\mathbf{k}}\hat{\alpha}_{\mathbf{k}}\rangle}_{=0}) \right) \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} \left(u^2_{\mathbf{k}}\langle \hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}\rangle + v^2_{\mathbf{k}}\langle \hat{\alpha}^\dagger_{-\mathbf{k}}\hat{\alpha}_{-\mathbf{k}}\rangle + v^2_{\mathbf{k}} \right) \end{aligned}$$

At zero temperature, the number of bosons is zero. The constant, zero-point term is still present, however;

$$\begin{aligned} \Delta S &= \frac{1}{N}\sum_{\mathbf{k}} v^2_{\mathbf{k}} \\ &= \frac{1}{2\Omega}\int_{BZ} d\mathbf{k} \left[\frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}} - 1 \right] \\ &\quad \text{At small } |\mathbf{k}|, \;\; \gamma_{\mathbf{k}} \sim 1 - |\mathbf{k}|^2/z \\ &= \frac{1}{4z\Omega}\int dk\; k^{d-2} \end{aligned}$$

This integral is infra-red convergent for $d \geq 2$, but logarithmically divergent in $1d$ (it always converges in the ultra-violet because of the cut-off at the Brillouin zone edge). Cutting the integral explicitly with π/a at the Brillouin zone boundary and at π/L for a system of size L, we find

$$\Delta S \sim \frac{1}{2\pi}\int_{\pi/L}^{\pi/a} dk/k \sim \frac{1}{2\pi}\log(L/a).$$

The quantum fluctuations diverge as L increases such that the sublattice magnetization $\to 0$ when $S = \frac{1}{2\pi}\log(L/a)$. Rearranging, we may say that the lengthscale at which this occurs is given by $\xi \sim ae^{2\pi S}$ is approximately the correlation length in the one-dimensional system. This result also demonstrates that the effects of quantum fluctuations are most dramatic for small S.

4.4.5 Haldane's Conjecture

Whilst the analysis given above is qualitatively correct for half-integer spins, it misses some key physics for integer spins. The distinction was first realised by Duncan Haldane [Phys. Rev. Lett **50**, 1153 (1983)] who, by considering topological effects of quantum spins known as instantons, was able to argue that whilst 1/2 integer spin anti-ferromagnets are gapless, integer spin anti-ferromagnets have a gap to the first excitation above the groundstate. The following two sections consider briefly two different ways of studying the properties of integer and 1/2-integer spin chains. The details are not examinable *per se* (though one of the problems sets contains an example of the use of the Jordan-Wigner transformation).

4.4.6 Jordan-Wigner Transformation

A spin 1/2 has two states. Since fermionic creation and annihilation operators also have two states, it is tempting to try to construct a fermionic representation. It is natural to identify

$$\hat{S}^z_m = \hat{c}^\dagger_m \hat{c}_m - 1/2, \quad \text{with} \quad \hat{S}^+_m \propto \hat{c}^\dagger_m \quad \hat{S}^-_m \propto \hat{c}_m.$$

However, although on a given site everything works fine (for example $\{\hat{S}^+_m, \hat{S}^-_m\} = \{\hat{c}_m, \hat{c}^\dagger_m\} = 1$), there is a problem for pairs of spins on different sites. Spin operators at different sites *commute*, but fermion operators on different sites *anti-commute*.

This is fixed by the *Jordan-Wigner transformation:*[3]

$$\begin{aligned} \hat{S}^+_m &= \hat{c}^\dagger_m \prod_{l<m} (1 - 2\hat{n}_l) \\ \hat{S}^-_m &= \prod_{l<m} (1 - 2\hat{n}_l) \hat{c}_m \\ \hat{S}^z_m &= \hat{n}_m - 1/2 \end{aligned} \tag{4.8}$$

The strings, $\prod_{l<m}(1 - 2\hat{n}_l)$, lead to additional negative factors that cancel those from the anti-commutation of fermionic operators:

$$\begin{aligned} \hat{c}^\dagger_m (1 - 2\hat{n}_m) &= -(1 - 2\hat{n}_m)\hat{c}^\dagger_m \\ \hat{c}_m (1 - 2\hat{n}_m) &= -(1 - 2\hat{n}_m)\hat{c}_m \end{aligned}$$

These expressions can be checked by evaluating the expectation between two fermionic Fock states.

XY anti-ferromagnet
Let us apply this method to the Hamiltonian

$$\mathcal{H} = J \sum_n \left[\frac{1}{2} (\hat{S}^+_n \hat{S}^-_{n+1} + \hat{S}^-_m \hat{S}^+_{n+1}) + \Delta \hat{S}^z_n \hat{S}^z_{n+1} \right].$$

For $\Delta = 1$ this is the Heisenberg model, and for $\Delta = 0$ it is an XY model. It turns out that we can solve the problem in the latter case. Using the Jordan-Wigner transformation, the Hamiltonian reduces to

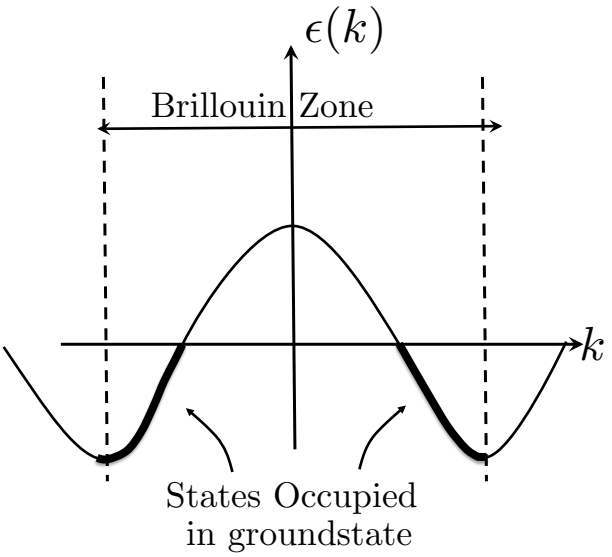
$$\mathcal{H} = \frac{J}{2} \sum_n \big[\underbrace{(\hat{c}^\dagger_n \hat{c}_{n+1} + \hat{c}^\dagger_{n+1} \hat{c}_n)}_{\text{fermionic hopping}} + \underbrace{2\Delta (\hat{c}^\dagger_n \hat{c}_n - 1/2)(\hat{c}^\dagger_{n+1} \hat{c}_{n+1} - 1/2)}_{\text{interaction}} \big]$$

For $\Delta = 0$ this reduces to a model of non-interacting fermions hopping along the 1d line. A Fourier transform completes the diagonalisation of the problem, giving

$$\mathcal{H} = \sum_k J \cos(ak) \hat{c}^\dagger_k \hat{c}_k$$

[3]NB: one may also write this as $\hat{S}^+_m = \hat{c}^\dagger_m \exp[i\pi \sum_{l<m}(1 - 2\hat{n}_l)$ and $\hat{S}^+_m = \exp[-i\pi \sum_{l<m}(1 - 2\hat{n}_l)\hat{c}_m$ as can be verified by considering the action on fermionic Fock states.

We have reduced the problem to one of non-interacting fermions with dispersion $\epsilon(k) = \cos(ak)$. Up to now, diagonalization has reduced our problems to non-interacting bosons whose groundstate consists of the absence of bosons. In the non-interacting fermion case, the groundstate is given by a filled fermi sea — fermion states with $\epsilon(k) < 0$ are occupied and those with $\epsilon(k) > 0$ are empty.



Spin Correlations:
In the same way as the properties of a bosonic system or the fluctuations of the anti-ferromagnet after the Holstein-Primakoff transformation can be calculated by writing operators in terms of the bosons, so in the present case, we can calculate properties of the XY anti-ferromagnet by writing operators in terms of the fermion operators. Let us focus upon the correlations of the the z-component of spin in two different places[4].

$$\begin{aligned}\frac{1}{N}\sum_y \langle \hat{S}^z_y \hat{S}^z_{y+x}\rangle &= \frac{1}{N}\sum_{\mathbf{y}}\left(\langle \hat{c}^\dagger_y \hat{c}_y \hat{c}^\dagger_{y+x}\hat{c}_{y+x}\rangle - \frac{1}{2}\langle \hat{c}^\dagger_y \hat{c}_y + \hat{c}^\dagger_{y+x}\hat{c}_{y+x}\rangle + \frac{1}{4}\right) \\ &= \left(\frac{1}{N^2}\sum_{k_1,k_2,k_3,k_4}\langle \hat{c}^\dagger_{k_1}\hat{c}_{k_2}\hat{c}^\dagger_{k_3}\hat{c}_{k_4}\rangle e^{ix(k_4-k_1)}\delta(k_1-k_2+k_3-k_4) - \frac{1}{N}\underbrace{\sum_k \langle \hat{n}_k\rangle}_{N/2} + \frac{1}{4}\right)\end{aligned}$$

There are two sets of contributions to this correlator: i. $k_1 = k_2$ and $k_3 = k_4$ with both

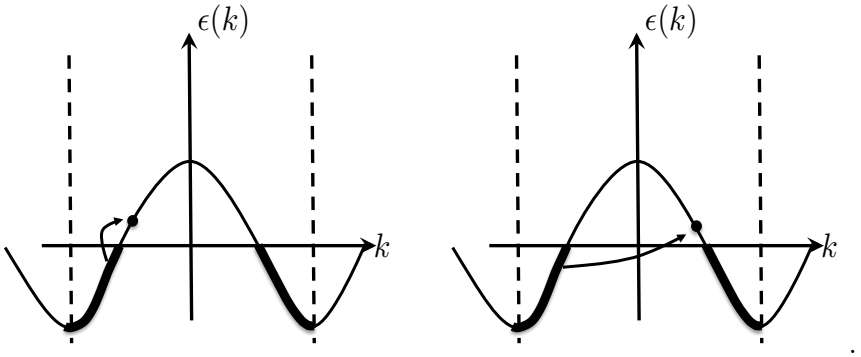
[4]Other correlators can be calculates, but involve strings between the points being correlated and so are a little more complicated

electronic states occupied - cancels $-1/4$. ii. $k_1 = k_4$ occupied $k_2 = k_3$ unoccupied

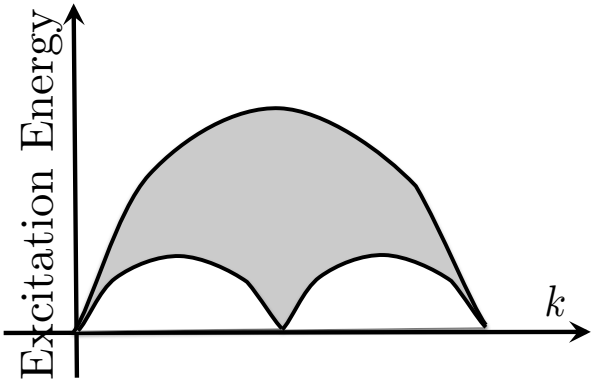
$$\begin{aligned}
\frac{1}{N}\sum_y \langle \hat{S}^z_y \hat{S}^z_{y+x}\rangle &= \frac{1}{N^2}\sum_{k_1,k_2} \underbrace{\langle \hat{c}^\dagger_{k_1}\hat{c}_{k_2}\hat{c}^\dagger_{k_2}\hat{c}_{k_1}\rangle}_{\langle \hat{c}^\dagger_{k_1}\hat{c}_{k_1}\rangle\langle \hat{c}^\dagger_{k_2}\hat{c}_{k_2}\rangle} e^{ix(k_2-k_1)} \\
&= \frac{1}{N^2}\sum_{k_1,k_2} n_F(k_1)\left(1-n_F(k_2)\right) e^{ix(k_2-k_1)} \\
&= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 n_F(k_1)\left(1-n_F(k_2)\right) e^{ix(k_2-k_1)} \\
&= +\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \left(1-n_F(k_2)\right) e^{ix(k_2-k_1)} \\
&\quad -\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \left(1-n_F(k_1)\right)\left(1-n_F(k_2)\right) e^{ix(k_2-k_1)} \\
&= +\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_1 e^{-ixk_1} \int_{-\pi/2}^{\pi/2} dk_2 e^{ixk_2} - \frac{1}{(2\pi)^2}\int_{-\pi/2}^{\pi/2} dk_1 e^{-ixk_1} \int_{-\pi/2}^{\pi/2} dk_2 e^{ixk_2} \\
&= +\frac{1}{(2\pi)^2}\underbrace{\int_{-\pi}^{\pi} dk_1 e^{-ixk_1}}_{=2\pi \text{when } x\to 0} \underbrace{\left[\frac{2\sin(x\pi/2)}{x}\right]}_{\approx 2\pi\delta(x)} - \frac{1}{(2\pi)^2}\left[\frac{2\sin(x\pi/2)}{x}\right]\left[\frac{2\sin(x\pi/2)}{x}\right] \\
&= \delta(x) - \frac{1}{\pi^2 x^2}\sin^2(\pi x/2a)
\end{aligned}$$

where we have used the zero temperature limit in the last step so that $n(k) = 1$ for $\pi/2 < k < \pi$ and $-\pi < k < -\pi/2$ and zero otherwise. The resulting power-law decay $1/x^2$ is very different from the Néel state.

Excitations:
The above calcuation shows that correlations in the groundstate of the 1d anti-ferromagnet are very different from the Néel state. The excitations are also very different from the spinwave excitations of the Néel state found in higher dimensions. The excitations at a given wavevector q involve exciting a fermion from an occupied state to an unoccupied state — *a particle-hole pair.*



For a given wavevector q the energy can be distributed in a range of ways between the particle and hole, giving a range of energies for each q.



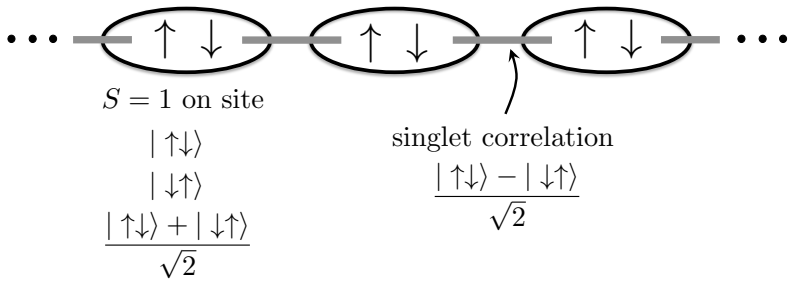
This characteristic dispersion of energy is very different from the sharply defined dispersion of spinwaves. It is frequently observed in neutron scattering experiments on one-dimensional magnets.

4.4.7 Integer Spin Case

In the above, we were able to discuss the properties of the spin 1/2 chain by considering the simplified, XY spin chain. Similarly, a simplified version of the spin 1 chain enables us to appreciate some of its properties. This is known as the AKLT (after Affleck, Kennedy, Lieb and Tasaki). The Hamiltonian is given by

$$\mathcal{H} = \sum_n \left[J_1 \hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1} + J_2 (\hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1})^2 \right]$$

and is solved by a cunning trick — the spin 1 on each site is considered to be constructed from the triplet sector of 2 spin 1/2. It turns out that the groundstate of this model can be constructed by putting two of these fractional spins on neighbouring sites into a singlet state. This can be illustrated schematically as



The gap to the first excitation above the groundstate can be understood as the energy required to break the singlet correlation between sites.

Notice that there are unpaired spins 1/2 at the ends of the chain. This is the first example of a topological edge state. The study of such states is an extremely active area of current research, in part because of their possible use in quantum information processing.

Chapter 5

The Renormalization Group

The ideas of thermodynamics — developed by the Victorians intent upon optimising steam engines — provide some of the most fundamental notions of science. Indeed, it is not too much of a stretch to argue that they form a meta-theory of physics. All of the developments of theoretical physics since this — quantum mechanics, special and general relativity, string theory, information theory *etc* — must obey the laws and constraints imposed by thermodynamics. The last piece of the story of thermodynamics was provided by a set of ideas known as the *renormalisation group*, first developed by Wilson and Fisher This is really a collection of methods that embody the question,

" How does the behaviour of a system change when viewed on different length or timescales?"

Addressing this allowed a complete classification of classical phase transitions and was essential in resolving the thorny issue of infinities in quantum field theory.

5.1 The 1d Classical Ising Model

In order to give a feel for the renormalization group, we will consider a simple model that can be solved exactly — the 1d Ising model. This is model of classical spins $\sigma_n = \pm 1$ whose Hamiltonian is given by

$$\mathcal{H} = \sum_n \left(-J\sigma_n\sigma_{n+1} - h\sigma_n \right). \tag{5.1}$$

For reasons that will become apparent in a moment, we consider N spins, where N is an integer power of 2. The partition function for this model (from which all physical observables can be calculated) is given by

$$\mathcal{Z} = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}. \tag{5.2}$$

The fundamental question of the renormalisation group is to ask how this model behaves on different length scales. In order to do this, as a first step, we will carry out the sum over

spins on every other site. Summing over spins on odd sites we find

$$\begin{aligned}
\mathcal{Z} &= \sum_{\{\sigma_n\}} e^{\beta\sum_n (J\sigma_n\sigma_{n+1}+h\sigma_n)} \\
&= \sum_{\{\sigma_{2m}\}}\sum_{\{\sigma_{2m+1}\}} \underbrace{e^{\beta h(\sigma_0+\sigma_N)/2}}_{\text{See note}} \exp\left[\beta\sum_m \left[J(\sigma_{2m}\sigma_{2m+1}+\sigma_{2m+1}\sigma_{2m+2})+h\sigma_{2m+1}+h(\sigma_{2m}+\sigma_{2m-2})/2\right]\right] \\
&= \sum_{\{\sigma_{2m}\}} e^{\beta h(\sigma_0+\sigma_N)/2} \ \ldots \ \begin{pmatrix} e^{\beta[J(\sigma_{2m}+\sigma_{2m+2})+h]} \\ + \\ e^{-\beta[J(\sigma_{2m}+\sigma_{2m+2})+h]} \end{pmatrix} e^{\beta h(\sigma_{2m}+\sigma_{2m+2})/2} \ \ldots
\end{aligned}$$

NB: the spins at the ends enter differently. We ignore this in what follows as we are interested in the thermodynamic limit. It turns out after summing over the odd spins, the partition function over the even spins takes the same form (up to an overall constant factor that doesnt change the physics) with modified constants.

We can find the modified constants as follows:

- Compare

$$Ce^{\beta'(J'\sigma_{2m}\sigma_{2m+2}+h(\sigma_{2m}+\sigma_{2m+2})/2)} = e^{\beta(h/2+J)(\sigma_{2m}+\sigma_{2m+2})+\beta h} + e^{\beta(h/2-J)(\sigma_{2m}+\sigma_{2m+2})-\beta h}$$

- This must be true for all σ_{2m} and σ_{2m+2}. Comparing explicit expressions for different values of σ_{2m} and σ_{2m+2}

$$\sigma_{2m} = \sigma_{2m+2} = 1 \qquad Ce^{\beta'(J'+h')} = e^{2\beta(J+h)} + e^{-2\beta J} \tag{5.3}$$
$$\sigma_{2m} = \sigma_{2m+2} = -1 \qquad Ce^{\beta'(J'-h')} = e^{-2\beta J} + e^{2\beta(J-h)} \tag{5.4}$$
$$\sigma_{2m} = -\sigma_{2m+2} = 1 \qquad Ce^{-\beta' J'} = e^{\beta h} + e^{-\beta h} \tag{5.5}$$

- Solving for C, $\beta' J'$ and $\beta' h'$

$$\begin{aligned}
(5.3)/(5.4) \qquad & e^{2\beta' h'} = \frac{e^{2\beta(J+h)} + e^{-2\beta J}}{e^{-2\beta J} + e^{2\beta(J-h)}} \\
(5.3)(5.4)/(5.5)^2 \qquad & e^{4\beta' h'} = \frac{\left(e^{2\beta(J+h)} + e^{-2\beta J}\right)\left(e^{-2\beta J} + e^{2\beta(J-h)}\right)}{\left(e^{\beta h} + e^{-\beta h}\right)^2} \\
(5.3)(5.4)(5.5)^2 \qquad & C^4 = \left(e^{2\beta(J+h)} + e^{-2\beta J}\right)\left(e^{-2\beta J} + e^{2\beta(J-h)}\right)\left(e^{\beta h} + e^{-\beta h}\right)^2
\end{aligned}$$

- Or alternatively, in terms of $x = e^{-4\beta J}$, $y = e^{-2\beta h}$ and $z = C^{-4}$

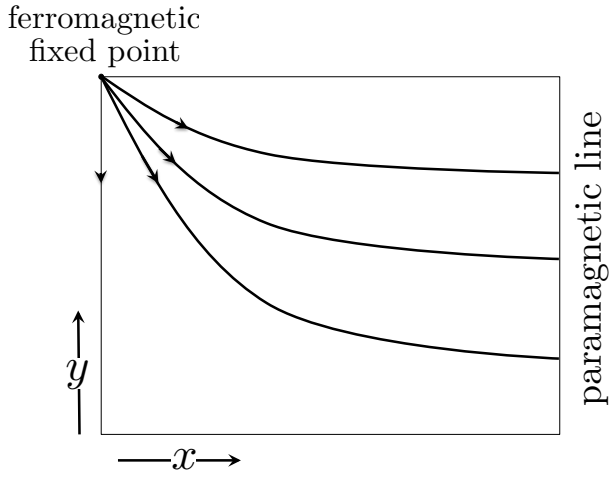
$$\begin{aligned}
x' &= \frac{x(1+y)^2}{(x+y)(1+xy)} \\
y' &= \frac{y(x+y)}{1+xy} \\
z' &= \frac{z^2 x y^2}{(x+y)(1+xy)(1+y)^2}
\end{aligned} \tag{5.6}$$

The equations (5.6) are known as the *RG flow equations*. They tell us how the parameters of the Hamiltonian change under our RG transformation (the particular transformation used here is known as decimation). Notice that in this case, the equations for x and y are independent of z so we can study the renormalization in the xy-plane only.

Fixed Points:
Fixed points are an important concept in using the renormalisation group. They represent sets of parameters or Hamiltonians that do not change under renormalisation. The physics is then said to be scale invariant and typically falls into classes of universal behaviour that are independent of minor short-distance variations in the starting Hamiltonian. To find the fixed points, we take $x = x'$ and $y = y'$. The solutions are

$$\begin{aligned} (x^*, y^*) &= (1, 0 \leq y^* \leq 1) \quad \text{line of fixed points with } T \to \infty \\ &= (0, 1) \qquad\qquad\quad \text{fixed point with } h = 0, \;\; T = 0 \\ &= (0, 0) \qquad\qquad\quad \text{fixed point with } h = \infty, \;\; T = 0 \end{aligned} \tag{5.7}$$

The flow to these fixed points can be represented diagrammatically as follows:



The results presented here were first derived in a seminal paper of Nelson and Fisher Ann Phys **91**, 226(1975).