Chapter 5

Second quantization

Learning goals

- Why do we need Fermions and Bosons?
- What is second quantization?
- How do we find second quantized operators given first quantized expressions?

The proper treatment of symmetries help us tremendously in the understanding of problems in physics (and chemistry). In particular in quantum mechanics we use the machinery of representation theory frequently in order to organize the Hilbert space in a way that simplifies our problems at hand.
For a many-particle system of *identical particles*, and this is what we usually deal with in the field of quantum gases, the symmetry under permutations of the particles is especially important. In this chapter we learn how to efficiently use states that are living in a well defined irreducible representation of the symmetric group S_N. This is the content of the formalism called "second quantization".

5.1 Symmetrized states

For a system of N identical particles the Hamiltonian depends on the coordinates of all particles, however, owing to their indistinguishability the Hamiltonian can not change if we interchange the coordinates of two (or any number of) particles

$$H = H(1, 2, \dots, i, \dots, j, \dots, N-1, N) = H(1, 2, \dots, j, \dots, i, \dots, N-1, N), \tag{5.1}$$

where the numbers $1, 2, \dots$ are shorthand for the coordinates (including spin, etc) of particle number $1, 2, \dots$. Equation (5.1) defines a *symmetry* of the Hamiltonian. More formally, the group of all permutations of N elements is called the symmetric group S_N. Knowing the abstract symmetry group S_N we are now seeking how this group acts on the wave functions, i.e., we are looking for a representation.[1]
The natural way to construct such a representation is given by considering the many-particle wave function $\psi(1, 2, \dots)$

$$P_{ij}\psi(1, 2, \dots, i, \dots, j, \dots, N-1, N) = \psi(1, 2, \dots, j, \dots, i, \dots, N-1, N) \tag{5.2}$$

[1] Recall that a representation $\mathcal{R}$ is a map from a group G to the linear maps U in some vector space V

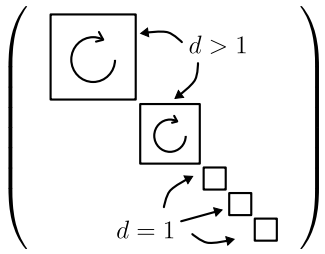
$$\begin{aligned} \mathcal{R} : G &\to GL(V) \\ g &\mapsto U(g), \end{aligned}$$

such that $U(g \circ h) = U(g)U(h)$, where $g, h \in G$.

Any permutation can be written as $P = \prod_{ij} P_{ij}$ and they all have the property $P_{ij}^2 = \mathbb{1}$ and hence the eigenvalues of P are ± 1 as can be seen from

$$P_{ij}^2\psi = P_{ij}\lambda\psi = \lambda^2\psi \stackrel{!}{=} \psi \qquad \Rightarrow \qquad \lambda = \pm 1. \tag{5.3}$$

Equation (5.2) defines a representation of S_N on the space of the N-particle wave functions. Let us recall the definition of an irreducible representation: It defines a subspace of the Hilbert space, which under the operation of any element g of the group G, transforms onto itself. If we represent the Hilbert space as a vector and the action of any $U(g)$ on it as a matrix it means that they separate into individual blocks: It turns out that the symmetric group has irreducible



representations of any dimensions d. However, two classes of *one dimensional* representations take a special role: the symmetric and anti-symmetric wave functions

$$\begin{aligned} P_{ij}\psi_{s/a}(1,2,\ldots,i,\ldots,j,\ldots,N-1,N) = &\quad \psi_{s/a}(1,2,\ldots,j,\ldots,i,\ldots,N-1,N) \\ &= \pm\psi_{s/a}(1,2,\ldots,i,\ldots,j,\ldots,N-1,N). \end{aligned} \tag{5.4}$$

As is evident from this equation, the symmetric and anti-symmetric wave-function define a one-dimensional irreducible representation of S_N. It turns out that nature chose to let all[2] systems be realized in one of these two representations. This is remarkable as we know, e.g., that in the hydrogen atom all irreducible representations of $SO(3)$ are realized. We call particles that are symmetric under permutations *bosons* and those that are anti-symmetric *fermions*. We now need to find a formulation of our many-body theory that accounts for this fact and only deals with symmetrized or anti-symmetrized wave functions.
In principle we could use single particle states that we then properly symmetrize. In particular we can start from

$$|i_1,\ldots,i_N\rangle = |i_1\rangle_1 \otimes \cdots \otimes |i_N\rangle_N, \tag{5.5}$$

where $|\cdot\rangle_j$ denotes the j'th particle and i_j are the quantum numbers of the j'th particle. In order to describe a fermion or boson we would have to symmetrize this state

$$S_\pm|i_1,\ldots,i_N\rangle = \frac{1}{N!}\sum_P (\pm 1)^{\sigma_P} P|i_1,\ldots,i_N\rangle, \tag{5.6}$$

where the sum runs over all permutations P and σ_P is the sign of the permutation. This approach of first dealing with single particle states and then symmetrizing them bears several problems

1. It is rather cumbersome.
2. It is restricted to exactly N particle, i.e., does not allow for a system with particle number fluctuations.
3. It carries too much information.

The solution to this problem is called "second quantization".

[2]There are notable exceptions to this rule!

5.2 Second quantization

Instead of using single particle states we switch to what we call "occupation number" states

$$S_{\pm}|i_1,\ldots,i_N\rangle = |n_1,n_2,\ldots\rangle_{\pm}. \tag{5.7}$$

Here n_i keep track of how many particles are residing in state i and the $\pm$ on the ket indicates whether we deal with bosons or fermions. The total number of particles is given by

$$N = \sum_i n_i. \tag{5.8}$$

There are two important properties of these occupation states that follow directly from the single-particle states (we skip the $\pm$ on the ket for now):

$$\text{1.)} \quad \langle n_1,n_2,\ldots|n_1',n_2',\ldots\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots. \tag{5.9}$$

$$\text{2.)} \quad \sum_{n_1,n_2,\ldots} |n_1,n_2,\ldots\rangle\langle n_1,n_2,\ldots| = \mathbb{1}. \tag{5.10}$$

The space of all occupation number states *for all particle numbers* N is called *Fock* space.
Having this basis of properly symmetrized states at hand we would like to express all operators in it. A convenient way of doing so is by introducing creation and annihilation operators

$$\hat{a}_i^\dagger|\ldots,n_i,\ldots\rangle = \sqrt{n_i+1}|\ldots,n_i+1,\ldots\rangle, \tag{5.11}$$

$$\hat{a}_i|\ldots,n_i+1,\ldots\rangle = \sqrt{n_i+1}|\ldots,n_i,\ldots\rangle, \tag{5.12}$$

where the second line follows from the first (proof!). Making sure we keep the symmetrization of the occupation states consistent we immediately arrive at (proof!)

$$[\hat{a}_i,\hat{a}_j] = \hat{a}_i\hat{a}_j - \hat{a}_j\hat{a}_i = [\hat{a}_i^\dagger,\hat{a}_j^\dagger] = 0, \quad [\hat{a}_i,\hat{a}_j^\dagger] = \delta_{ij} \qquad \text{for bosons,} \tag{5.13}$$

$$\{\hat{a}_i,\hat{a}_j\} = \hat{a}_i\hat{a}_j + \hat{a}_j\hat{a}_i = \{\hat{a}_i^\dagger,\hat{a}_j^\dagger\} = 0, \quad \{\hat{a}_i,\hat{a}_j^\dagger\} = \delta_{ij} \qquad \text{for fermions.} \tag{5.14}$$

A direct consequence of $\{\hat{a}_i^\dagger,\hat{a}_i^\dagger\} = 2\hat{a}_i^\dagger\hat{a}_i^\dagger = 0$ is the Pauli principle that states that no single particle state can be occupied by more than one fermion.

5.2.1 Single particle operators

Let us now start to make use of these operators to express single particle operators in Fock space. We begin with the simplest, the occupation number operator

$$\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i \tag{5.15}$$

as $\hat{a}_i^\dagger\hat{a}_i|\ldots,n_i,\ldots\rangle = a_i^\dagger\sqrt{n_i}|\ldots,n_i-1,\ldots\rangle = n_i|\ldots,n_i,\ldots\rangle$. From this point on we can construct all operators by operator identities: If we know the matrix elements of the operators in single (or two-particle) states, we can construct the second quantized operator with the help of $\hat{n}_i$.
For example, the total particle number is given by

$$\hat{N} = \sum_i \hat{n}_i = \sum_i \hat{a}_i^\dagger\hat{a}_i. \tag{5.16}$$

Given that every state i is an eigenstate of the single particle Hamiltonian H to eigenvalue ϵ_i we can write

$$\hat{H} = \sum_i \epsilon_i\hat{a}_i^\dagger\hat{a}_i. \tag{5.17}$$

More generally, any single particle operator $\hat{T}$

$$\langle i|\hat{T}|j\rangle = t_{ij} \;\Rightarrow\; \hat{T} = \sum_{i,j} t_{ij}|i\rangle\langle j| = \sum_{ij} t_{ij}\hat{a}_i^\dagger\hat{a}_j. \tag{5.18}$$

5.2.2 Two particle operators

The same procedure using operator identities can be used for two-particle operators $V(\mathbf{r}, \mathbf{r}')$. Given the wave functions in state i, $\phi_i(\mathbf{r})$, we write

$$\hat{V} = \sum_{i,j,k,l} v_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \,, \tag{5.19}$$

where

$$v_{ijkl} = \int d\mathbf{r} d\mathbf{r}' \, \phi_i^*(\mathbf{r}) \phi_j^*(\mathbf{r}') V(\mathbf{r}, (\mathbf{r}') \phi_k(\mathbf{r}) \phi_l(\mathbf{r}'). \tag{5.20}$$

5.3 Basis transformations

Basis transformations can be readily imported from the first quantized language

$$|\lambda\rangle = \sum_i \langle i|\lambda\rangle |i\rangle \quad \Rightarrow \quad \hat{a}_\lambda^\dagger = \sum_i \langle i|\lambda\rangle \hat{a}_i^\dagger. \tag{5.21}$$

While any orthonormal basis leads to an equally valid description of a system, one basis is rather generic as many operators find a natural definition in it: the site basis $|\mathbf{r}\rangle$:

$$\langle \mathbf{r}|i\rangle = \phi_i(\mathbf{r}) \qquad |\mathbf{r}\rangle : \quad \text{particle localized at } \mathbf{r}. \tag{5.22}$$

Creation and annihilation operators in this particular basis get a special name: *field operators*

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r}) a_i^\dagger. \tag{5.23}$$

5.4 Important operators

Before concluding this chapter we give a list of important operators in second quantized form using field operators.
The **kinetic energy**:

$$\hat{T} = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j = \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \int d\mathbf{r} \, \phi_i^*(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} \right] \phi_j(\mathbf{r}) = \frac{\hbar^2}{2m} \int d\mathbf{r} \, \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}). \tag{5.24}$$

The **potential energy**:

$$U = \int d\mathbf{r} \, U(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}). \tag{5.25}$$

Two particle **interactions**:

$$V = \int d\mathbf{r} d\mathbf{r}' \, \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}'). \tag{5.26}$$

And finally the **Hamiltonian** for particles interacting with a contact pseudo potential

$$H = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}) + U(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{4\pi a \hbar^2}{m} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]. \tag{5.27}$$

Chapter 6

Microscopic description of a Bose gas

Learning goals

- How does the excitation spectrum of a weakly interaction Bose gas look like?
- What justifies the Bogoliubov approximation?
- What is superfluid flow? When does it occur?
- What is "quantum depletion?

In Chap. 3 we learned how to include interactions between the particles in a Bose gas via the non-linear Schrödinger, or Gross Pitaevskii equation. Via the Gross-Pitaevskii equation we reduced the description of the many-body system to the problem of finding a single-particle wave function that is then occupied by *all* particles, i.e., we speak of "full condensation".
The restriction to full condensation essentially renders the problem classical as quantum fluctuations do not occur. In the present chapter we introduce a method to include such quantum fluctuations. Along the way we will find the excitation spectrum of the Bose gas. Moreover, we will be able to quantify to what extent interactions lead to deviations from full condensation, the so called "quantum depletion".

6.1 Bogoliubov approximation

Our starting point is the Hamiltonian of bosons interacting via a contact pseudo-potential

$$H = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} \nabla\hat{\psi}^\dagger(\mathbf{r}) \nabla\hat{\psi}(\mathbf{r}) + \frac{U_0}{2} \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \right]. \tag{6.1}$$

For simplicity we consider a uniform Bose gas ($U(\mathbf{r}) = 0$). Hence, we have a translationally invariant system and should therefore use momentum eigenstates[1]

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \hat{a}_{\mathbf{p}}, \qquad \hat{a}_{\mathbf{p}} = \frac{1}{\sqrt{V}} \int d\mathbf{r}\, e^{-i\mathbf{p}\cdot\mathbf{r}} \hat{\psi}(\mathbf{r}). \tag{6.2}$$

Note that the above transformation is unitary and just amounts to a change of basis. In particular, the commutation relations are preserved

$$[\hat{a}_{\mathbf{p}}, a_{\mathbf{p}'}] = [\hat{a}^\dagger_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}] = 0 \qquad \text{and} \qquad [\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}'}] = \delta_{\mathbf{p},\mathbf{p}'}. \tag{6.3}$$

In the new operators, the Hamiltonian reads

$$H = \sum_{\mathbf{p}} \frac{\hbar^2 p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{U_0}{V} \sum_{\mathbf{p},\mathbf{p}',\mathbf{q}} \hat{a}^\dagger_{\mathbf{p}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p}-\mathbf{q}} \hat{a}_{\mathbf{p}} \hat{a}_{\mathbf{p}'}. \tag{6.4}$$

[1] We remember that given a symmetry, it is profitable to go the the irreducible representations of this symmetry. The different momentum sectors are exactly these irreducible representations.

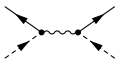
In its present form this Hamiltonian is still not tractable. While we want to investigate the influence of quantum fluctuations away from the Gross-Pitaevskii limit, we are still interested in a system that is condensed. Hence, the lowest energy single-particle states is supposed to be macroscopically occupied. Therefore we replace

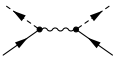
$$a_0^\dagger \to \sqrt{N_0} \qquad \text{and} \qquad a_0 \to \sqrt{N_0}. \tag{6.5}$$

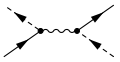
The expectation value of these operators should differ by $\sqrt{N_0+1}$ vs. $\sqrt{N_0}$. If $N_0 \gg 1$ we are on a good track even if N_0, the number of condensed atoms, is not $N_0 = N$. This replacement of one operator with a number is called the *Bogoliubov approximation*.
Let us now apply this approximation to the Hamiltonian (6.4). The first term is simple

$$\sum_{\mathbf{p}} \frac{\hbar^2 p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = 0\, \hat{a}_0^\dagger \hat{a}_0 + \sum_{\mathbf{p}}{}' \frac{\hbar^2 p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = \sum_{\mathbf{p}}{}' \frac{\hbar^2 p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}. \tag{6.6}$$

The prime on the sum indicates that we only sum over non-zero values of $\mathbf{p}$. As for the interactions we have to work a bit harder. First, momentum conservation imposes constraints on which terms we can retain after making the replacement $\hat{a}_0 \to \sqrt{N_0}$: Only an even number of $\hat{a}_{\mathbf{q}}$ operators are allowed. Moreover, the momentum labels must be such that the total momentum is conserved.
We use diagrams for illustration. Wavy lines indicate the scattering U_0. Arrows emanating from the dots correspond to $\hat{a}_{\mathbf{p}}^\dagger$ while inward pointing arrows indicate $\hat{a}_{\mathbf{p}}$. Every arrow also carries a momentum which we do not show explicitly. Finally, the dashed lines correspond to the condensate operators $\hat{a}_0^\dagger$ and a_0. Let us now try to collect all terms with two solid arrows:

1.) $\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger \hat{a}_0 \hat{a}_0$  $\longrightarrow N_0 \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger$,

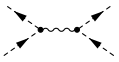
2.) $\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}}$  $\longrightarrow N_0 \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}}$,

3.) $\hat{a}_0^\dagger \hat{a}_{\mathbf{p}}^\dagger \hat{a}_0 \hat{a}_{\mathbf{p}}$ 

$\hat{a}_{\mathbf{p}}^\dagger \hat{a}_0^\dagger \hat{a}_{\mathbf{p}} \hat{a}_0$ ⋮

$\hat{a}_0^\dagger \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} \hat{a}_0$ ⋮

$\hat{a}_{\mathbf{p}}^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_{\mathbf{p}}$ ⋮ $\longrightarrow 4N_0 \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}$.

4.) $\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0$  $\longrightarrow N_0^2$

Collecting the terms in 1.) to 4.) together with Eq. (6.6) we find

$$H = \sum_{\mathbf{p}}{}' \frac{\hbar^2 p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{N_0^2 U_0}{V} + \frac{U_0 N_0}{V} \sum_{\mathbf{p}}{}' \left(4 \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} \right). \tag{6.7}$$

Remember that we wanted to investigate the quantum depletion, i.e, the possibility that $N_0 \neq N$. Therefore we need to replace N_0 in the above Hamiltonian via

$$\sum \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = \hat{a}_0^\dagger a_0 + \sum{}' \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = N \quad \Rightarrow \quad N_0 = N - \sum{}' a_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}. \tag{6.8}$$

We replace N_0 in (6.7) via this expression and collect again terms only up to quadratic order in $\hat{a}_{\mathbf{p}}$. We see that this amounts to replace $N_0 \to N$ in the last term. The term corresponding to the self interaction of the condensate becomes

$$\frac{N_0^2 U_0}{V} \to \frac{U_0}{V} N^2 - 2 \frac{N}{V} \sum_{\mathbf{p}}{}' \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}. \tag{6.9}$$

We obtain for the final Bogoliubov Hamiltonian

$$H = \frac{N^2 U_0}{2V} + \sum_{\mathbf{p}}{}' \frac{\hbar^2 p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + n U_0 \sum_{\mathbf{p}}{}' \left(2\hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} \right), \tag{6.10}$$

where $n = N/V$ is the full particle density. In the next section we try to find the eigenmodes of this Hamiltonian.

6.2 Bogoliubov transformation

When we want to identify the bosonic eigenmodes of a system we are seeking an expression for the Hamiltonian of the from

$$H = \sum_m \left(\epsilon_m \gamma^\dagger_m \gamma_m \right) + E_0 \qquad \text{with} \qquad [\gamma_m, \gamma^\dagger_n] = \delta_{nm}, \;\; [\gamma_m, \gamma_n] = [\gamma^\dagger_m, \gamma^\dagger_n] = 0 \tag{6.11}$$

Looking at Eq. (6.10) we see that it is not of this form due to the "anomalous" terms $\propto \hat{a}^\dagger \hat{a}^\dagger$. In order to bring (6.10) into the above form we apply a *Bogoliubov transformation*.[2] In order to do so it is convenient to introduce a matrix notation

$$H = \sum_{\mathbf{p}}{}'' \begin{pmatrix} \hat{a}_{\mathbf{p}} & \hat{a}^\dagger_{-\mathbf{p}} \end{pmatrix}^\dagger \begin{pmatrix} \frac{\hbar^2 p^2}{2m} + U_0 n & U_0 n \\ U_0 n & \frac{\hbar^2 p^2}{2m} + U_0 n \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{p}} \\ \hat{a}^\dagger_{-\mathbf{p}} \end{pmatrix} + \frac{N^2 U_0}{2V} + \sum_{\mathbf{p}}{}'' \frac{\hbar^2 p^2}{2m} \tag{6.12}$$

$$= \sum_{\mathbf{p}}{}'' \hat{\mathbf{a}}^\dagger_{\mathbf{p}} \, \mathsf{H}(\mathbf{p}) \, \hat{\mathbf{a}}_{\mathbf{p}} + \frac{N^2 U_0}{2V} + \sum_{\mathbf{p}}{}'' \frac{\hbar^2 p^2}{2m}, \tag{6.13}$$

where we introduce the notation Σ'' in which we only sum over positive values of $\mathbf{p}$ to avoid double-counting.
What do we profit from such a matrix notation? First, it is evident that the two entries of the vector $\hat{\mathbf{a}}_{\mathbf{p}}$ couple, owing to the off-diagonal matrix elements nU_0. This implies that to diagonalize the matrix $\mathsf{H}(\mathbf{p})$ we need to mix these two entries. However, such a mixing in its most trivial form would violate the commutation relations

$$[\hat{\gamma}_{\mathbf{p}}, \hat{\gamma}^\dagger_{\mathbf{p}}] = [\hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{-\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}} + \hat{a}_{-\mathbf{p}}] = [a_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}}] + [\hat{a}_{\mathbf{p}}, \hat{a}_{-\mathbf{p}}] + [\hat{a}^\dagger_{-\mathbf{p}}, \hat{a}^\dagger_{\mathbf{p}}] + [\hat{a}^\dagger_{-\mathbf{p}}, \hat{a}_{-\mathbf{p}}] = 1 - 1 = 0. \tag{6.14}$$

(Note, that only the commutator $[\hat{\gamma}_{\mathbf{p}}, \hat{\gamma}^\dagger_{\mathbf{p}}]$ is problematic, $[\hat{\gamma}^\dagger_{\mathbf{p}}, \hat{\gamma}^\dagger_{\mathbf{p}}]$ and $[\hat{\gamma}_{\mathbf{p}}, \hat{\gamma}_{\mathbf{p}}]$ don't introduce any problems.) This brings us to the second profit of this matrix formulation. We need a transformation

$$\hat{\mathbf{a}}_{\mathbf{p}} = \mathsf{M} \hat{\boldsymbol{\gamma}}_{\mathbf{p}} \tag{6.15}$$

such that $[\hat{\gamma}_{\mathbf{p}}, \hat{\gamma}^\dagger_{\mathbf{p}}] = 1$. It is straight forward to show that this is equivalent to demand M to be in the in the group $O(1,1)$[3]

$$\mathsf{M}^\dagger \Sigma \mathsf{M} \stackrel{!}{=} \Sigma \qquad \text{with} \qquad \Sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6.16}$$

Note that these are just Lorentz transformations with one spatial and one temporal direction.[4]

[2] This method was originally introduced by Holstein and Primakoff [Phys. Rev. B **58**, 1098 (1940)] for spin-waves but later rediscovered by Bogoliubov in the context of weakly interacting bosons [J. Phys. U.S.S.R. **11**, 23 (1947)].

[3] This discussion can be readily generalized to situations whith more bosonic flavors f. It only amounts to consider $SU(f,f)$ instead of $SU(1,1)$.

[4] For fermions, one would have to preserve $\Sigma = \mathbb{1}$. This is fulfilled by the standard unitary basis transformations and hence the requirement to enforce fermionic commutations when removing anomalous terms does not induce any constraints.

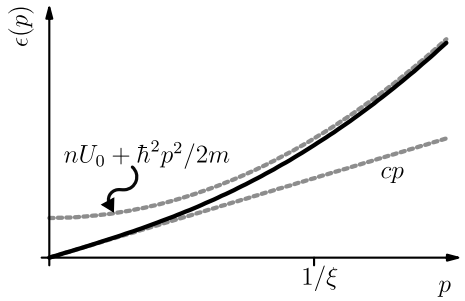


Figure 6.1: **Bogoliubov spectrum.** The energy as a function of momentum. In black the full dispersion. The dashed lines indicate the limiting behavior.

The requirement of M to obey (6.16) complicates the diagonalization of (6.12) significantly. Without any conditions we know that we can diagonalize $\mathsf{H}(\mathbf{p})$ via a *unitary* transformation M, i.e., $\mathsf{D} = \mathsf{M}^\dagger \mathsf{H}(\mathbf{p})\mathsf{M}$, with D diagonal. In the present case we need to fall back to $\mathsf{D} = \mathsf{M}^{-1}\mathsf{H}(\mathbf{p})\mathsf{M}$. We have two ways to proceed. (i) Find a shortcut to the spectrum. (ii) Properly parametrize the group $SU(1,1)$ and find the actual transformation.
We start along the first path and write

$$\mathsf{M}^\dagger \Sigma \mathsf{M} = \Sigma \quad \Rightarrow \quad \mathsf{M}^{-1} = \Sigma \mathsf{M}^\dagger \Sigma. \tag{6.17}$$

Using this expression for the inverse of M we write for the diagonalization problem

$$\Sigma \mathsf{D} = \mathsf{M}^\dagger \Sigma \mathsf{H}(\mathbf{p})\mathsf{M}, \tag{6.18}$$

where all constraints on M have now already taken into account and we can diagonalize $\Sigma\mathsf{H}(\mathbf{p})$ without any further restrictions. We explicitly write

$$\Sigma \mathsf{H}(\mathbf{p}) = \begin{pmatrix} \frac{\hbar^2 p^2}{2m} + U_0 n & U_0 n \\ -U_0 n & -\frac{\hbar^2 p^2}{2m} - U_0 n \end{pmatrix} \qquad \Rightarrow \tag{6.19}$$

$$[\Sigma \mathsf{H}(\mathbf{p})]^2 = \begin{pmatrix} \left(\frac{\hbar^2 p^2}{2m} + U_0 n\right)^2 - (U_0 n)^2 & 0 \\ 0 & \left(\frac{\hbar^2 p^2}{2m} + U_0 n\right)^2 - (U_0 n)^2 \end{pmatrix} \tag{6.20}$$

With this simple trick of squaring the matrix $\Sigma\mathsf{H}(\mathbf{p})$ we immediately have access to the spectrum

$$\epsilon(\mathbf{p}) = \sqrt{\left(\frac{\hbar^2 p^2}{2m}\right)^2 + \frac{\hbar^2 p^2 n U_0}{m}} = \begin{cases} \sqrt{\frac{nU\hbar^2}{m}} p = cp & p \ll \sqrt{U_0 n/\hbar^2 m} \\ \frac{\hbar^2 p^2}{2m} + nU_0 & p \gg \sqrt{U_0 n/\hbar^2 m} \end{cases}. \tag{6.21}$$

The excitations are linearly dispersing sound modes at low momenta while for larger energies they are just free particles that feel a mean-field shift of nU_0. The point where this character changes is given by the inverse coherence length, see Fig. 6.1

$$\frac{1}{\xi} = \sqrt{\frac{U_0 n}{\hbar^2 m}}. \tag{6.22}$$

To find the eigenmodes we have to parametrize the transformation matrix M. From the lecture on special relativity we know that Lorentz boosts can be written with the help of hyperbolic functions

$$\mathsf{M} = \begin{pmatrix} \cosh(\chi) & \sinh(\chi) \\ \sinh(\chi) & \cosh(\chi) \end{pmatrix} \tag{6.23}$$

Inserting this into $\mathsf{M}^{-1}\mathsf{H}(\mathbf{p})\mathsf{M}$ and requiring off-diagonal terms to vanish we readily obtain

$$\chi = \frac{1}{2}\text{arctanh}\left(\frac{U_0 n}{\frac{\hbar^2 p^2}{2m} + U_0 n}\right). \tag{6.24}$$

We will regularly use the expressions $u_{\mathbf{p}} = \cosh^2(\chi)$ and $v_{\mathbf{p}} = \cosh^2(\chi)$. A vanishing $v_{\mathbf{p}}$ signals that the eigenstates are the bare bosons while for a finite $v_{\mathbf{p}}$ we deal with a collective excitation made of $\hat{a}_{\mathbf{p}}$ and $\hat{a}^\dagger_{\mathbf{p}}$. We conclude this section by writing the full diagonlized Hamiltonian

$$H = \underbrace{\frac{N^2 U_0}{2V}}_{\text{classical energy}} + \underbrace{\sum_{\mathbf{p}}{}' \epsilon(\mathbf{p})\hat{\gamma}^\dagger_{\mathbf{p}}\hat{\gamma}_{\mathbf{p}}}_{\text{quasi-particles}} - \underbrace{\sum_{\mathbf{p}}{}' \left(\frac{\hbar^2 p^2}{2m} + U_0 n - \epsilon(\mathbf{p})\right)}_{\text{quantum fluctuations}}. \tag{6.25}$$

6.3 Depletion

To calculate to what extent the quantum fluctuations in the weakly interacting Bose gas deplete the condensate we rewrite the number operator

$$\hat{N} = N_0 + \sum_{\mathbf{p}}{}' \hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} = \overbrace{N_0}^{\text{condensate}} + \underbrace{\sum_{\mathbf{p}}{}' v^2_{\mathbf{p}}}_{\text{quantum depletion}} + \overbrace{\sum_{\mathbf{p}}{}' \left(u^2_{\mathbf{p}} + v^2_{\mathbf{p}}\right)\hat{\gamma}^\dagger_{\mathbf{p}}\hat{\gamma}_{\mathbf{p}}}^{\text{(thermal) quasiparticles}}. \tag{6.26}$$

At zero temperature there are now quasiparticles present and the number of condensed particles N_0 is only reduced by quantum depletion $N = N_0 + N_{\text{qd}}$. We obtain

$$N_{\text{qd}} = \sum_{\mathbf{p}}{}' v^2_{\mathbf{p}} = \int \frac{d\mathbf{p}}{(2\pi)^3} v^2_{\mathbf{p}} = \frac{8}{3\sqrt{\pi}}\left(na^3\right)^{1/2}. \tag{6.27}$$

Hence, even at zero temperatures *not all particles are condensed*.

6.4 Bragg scattering

How can one measure the dispersion relation (6.21) derived above? One needs a way to perturb the system and observe its reaction to this perturbation. The framework to understand such a probe theoretically is given by linear response theory. Generically we are asking the question on how an observable $\hat{O}$ changes du to the application of a perturbation $\hat{M}$. Let us specify here the experimentally relevant example of Bragg scattering.

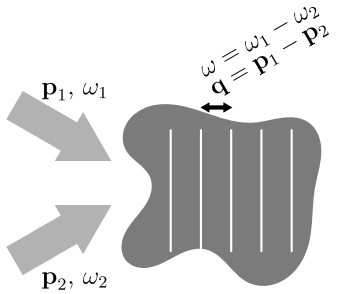


Figure 6.2: **Bragg scattering**.

In Bragg spectroscopy two laser beams at an angle and with a detuning ω are crossed onto the atomic cloud, cf. Fig. 6.2. Both laser beams are far detuned to any atomic transition so (approximately) no photon is absorbed. However, the atoms can scatter a photon from one beam into the other, thereby absorbing $\hbar\omega$ from the beams. Moreover, if the two beams are characterized by $\mathbf{p}_1$ and $\mathbf{p}_2$, the atomic cloud also takes up the momentum $\mathbf{q} = \mathbf{p}_1 - \mathbf{p}_2$. This process couples to the density of the atoms at momentum $\mathbf{q}$ and therefore

$$\hat{M} = \hat{\rho}_{\mathbf{q}} = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}+\mathbf{q}} a_{\mathbf{p}}. \tag{6.28}$$

If we take an absorption image after the excitation one again couples to the density, in particular also to its $\mathbf{q}$'th Fourier component, i.e., we also have $\hat{O} = \hat{\rho}_{-\mathbf{q}}$. Let us now go through the development of the linear response theory on this specific example.
For simplicity we consider an operator which has a vanishing expectation value in the ground state $0 = \langle 0|\delta\hat{\rho}_{\mathbf{q}}|0\rangle$ by subtracting $\delta\hat{\rho}_{\mathbf{q}} = \hat{\rho}_{\mathbf{q}} - \langle 0|\rho_{\mathbf{q}}|0\rangle$. When then write

$$H' = H + \delta H = H + F(t)\delta\hat{\rho}_{\mathbf{q}} \quad \Rightarrow \quad \langle\hat{\rho}_{-\mathbf{q}}(t)\rangle = \int dt'\, \chi(t-t')F(t'). \tag{6.29}$$

Our task is to find $\chi(t)$. We switch to the interaction representation with respect to the unperturbed Hamiltonian

$$\delta\tilde{\rho}_{-\mathbf{q}}(t) = e^{iHt/\hbar}\delta\hat{\rho}_{-\mathbf{q}}e^{-iHt/\hbar}. \tag{6.30}$$

Inserted into the expectation value we obtain

$$\langle\delta\hat{\rho}_{-\mathbf{q}}(t)\rangle = \langle 0|e^{i\delta Ht/\hbar}\,\delta\tilde{\rho}_{-\mathbf{q}}(t)\,e^{-i\delta Ht/\hbar}|0\rangle. \tag{6.31}$$

In linear response we are interested in the change in $\langle\delta\hat{\rho}_{\mathbf{q}}\rangle$ at vanishingly small perturbation and hence

$$\chi(t) = \frac{\partial}{\partial F}\bigg|_{F=0}\langle\delta\hat{\rho}_{\mathbf{q}}\rangle \quad \Rightarrow \quad \chi(t) = -\frac{i}{\hbar}\langle[\delta\tilde{\rho}_{-\mathbf{q}}(t), \delta\hat{\rho}_{\mathbf{q}}]\rangle. \tag{6.32}$$

The measured rate is then given by the dynamic structure factor

$$S(\mathbf{q},\omega) = -\mathrm{Im}\int dt\, e^{i\omega t}\chi(t) \tag{6.33}$$

We now proceed by inserting unities of the form $\mathbb{1} = \sum_m |m\rangle\langle m|$

$$\chi(t) = -\frac{i}{\hbar}\sum_m \langle 0|\delta\tilde{\rho}_{-\mathbf{q}}(t)|m\rangle\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle - \langle 0|\delta\hat{\rho}_{\mathbf{q}}|m\rangle\langle m|\delta\tilde{\rho}_{-\mathbf{q}}(t)|0\rangle \tag{6.34}$$

$$= -\frac{i}{\hbar}\sum_m \langle 0|e^{iHt/\hbar}\delta\hat{\rho}_{-\mathbf{q}}e^{-iHt/\hbar}|m\rangle\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle - \langle 0|\delta\hat{\rho}_{\mathbf{q}}|m\rangle\langle m|e^{iHt/\hbar}\delta\hat{\rho}_{-\mathbf{q}}e^{-iHt/\hbar}|0\rangle \tag{6.35}$$

$$= -\frac{i}{\hbar}\sum_m \langle 0|\delta\hat{\rho}_{-\mathbf{q}}|m\rangle\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle e^{i(\epsilon_m-\epsilon_0)t/\hbar} - \langle 0|\delta\hat{\rho}_{\mathbf{q}}|m\rangle\langle m|\delta\hat{\rho}_{-\mathbf{q}}|0\rangle e^{-i(\epsilon_m-\epsilon_0)t/\hbar} \tag{6.36}$$

$$= -\frac{i}{\hbar}\sum_m |\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle|^2\left(e^{i(\epsilon_m-\epsilon_0)t/\hbar} + e^{-i(\epsilon_m-\epsilon_0)t/\hbar}\right) \tag{6.37}$$

Taking the Fourier transform if this expression we obtain

$$\chi(\omega) = \int dt\,\chi(t)e^{i\omega t/\hbar - \eta|t|/\hbar} \quad \Rightarrow \tag{6.38}$$

$$S(\mathbf{q},\omega) = -\mathrm{Im}\sum_m |\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle|^2\left(\frac{1}{\omega-(\epsilon_m-\epsilon_0)+i\eta)} - \frac{1}{\omega+(\epsilon_m-\epsilon_0)+i\eta)}\right) \tag{6.39}$$

$$= 2\pi\sum_m |\langle m|\delta\hat{\rho}_{\mathbf{q}}|0\rangle|^2\delta\left[\omega-(\epsilon_m-\epsilon_0)\right]. \tag{6.40}$$

Let us now write the density operator in the basis of eigenstates

$$\delta\hat{\rho}_{\mathbf{q}} = \sum_{\mathbf{p}} \hat{a}^{\dagger}_{\mathbf{p}+\mathbf{q}}\hat{a}_{\mathbf{p}} - \langle 0|\hat{\rho}_{\mathbf{q}}|0\rangle \approx \sqrt{N_0}\left(\hat{a}^{\dagger}_{\mathbf{q}} + a_{-\mathbf{q}}\right) = \sqrt{N_0}(u_{\mathbf{q}} + v_{\mathbf{q}})\hat{\gamma}^{\dagger}_{\mathbf{q}}. \tag{6.41}$$

Here we only kept terms $\propto \sqrt{N_0}$ and those that lead to a non-vanishing matrix element between the ground- and excited states. We therefore find that we can indeed measure the excitation spectrum of a weakly interacting Bose bas via Bragg spectroscopy as the final expression for the dynamic structure factor reads

$$S(\mathbf{q},\omega) \approx N_0 \left(u_{\mathbf{q}} + v_{\mathbf{q}}\right)^2 \delta(\omega - \epsilon_{\mathbf{q}}). \tag{6.42}$$

6.5 Landau critical velocity

In the final section of this chapter we discuss an important experimental consequence of the shape of the excitation spectrum: superfluid flow. Superfluidity is the ability of a fluid to flow past obstacles without dissipating any energy. How is this possible? Imagine a scatterer inside a flowing fluid. This scatterer will breaks translational symmetry and has potentially the power to excite quasi-particles $\hat{\gamma}_{\mathbf{q}}$. The Landau critical velocity tells us under which conditions such excitations are indeed induced by an obstacle.
Let us compare energies. For this it is the most convenient to go to the co-moving frame with the liquid (with velocity $\mathbf{v}$). The energy is then given by

$$E_{\text{qp}} = E_0 + \epsilon(\mathbf{q}) - \mathbf{q}\cdot\mathbf{v} + \frac{1}{2}Nmv^2 \tag{6.43}$$

$$E_{\text{gs}} = E_0 + \frac{1}{2}Nmv^2 \tag{6.44}$$

The first (second) line describes the energy of the system in the co-moving frame in the presence (absence) of a quasi-particle excitation $\hat{\gamma}_{\mathbf{q}}$. It is evident that the system can lower its energy by exciting $\hat{\gamma}_{\mathbf{q}}$ if the velocity of the flow exceeds

$$v_{\text{crit}} = \min \frac{\epsilon_{\mathbf{q}}}{q}. \tag{6.45}$$

For our case this amounts to

$$v_{\text{crit}} = c = \sqrt{\frac{nU_0}{m}}. \tag{6.46}$$