Describing bosonic superfluids with particle conservation

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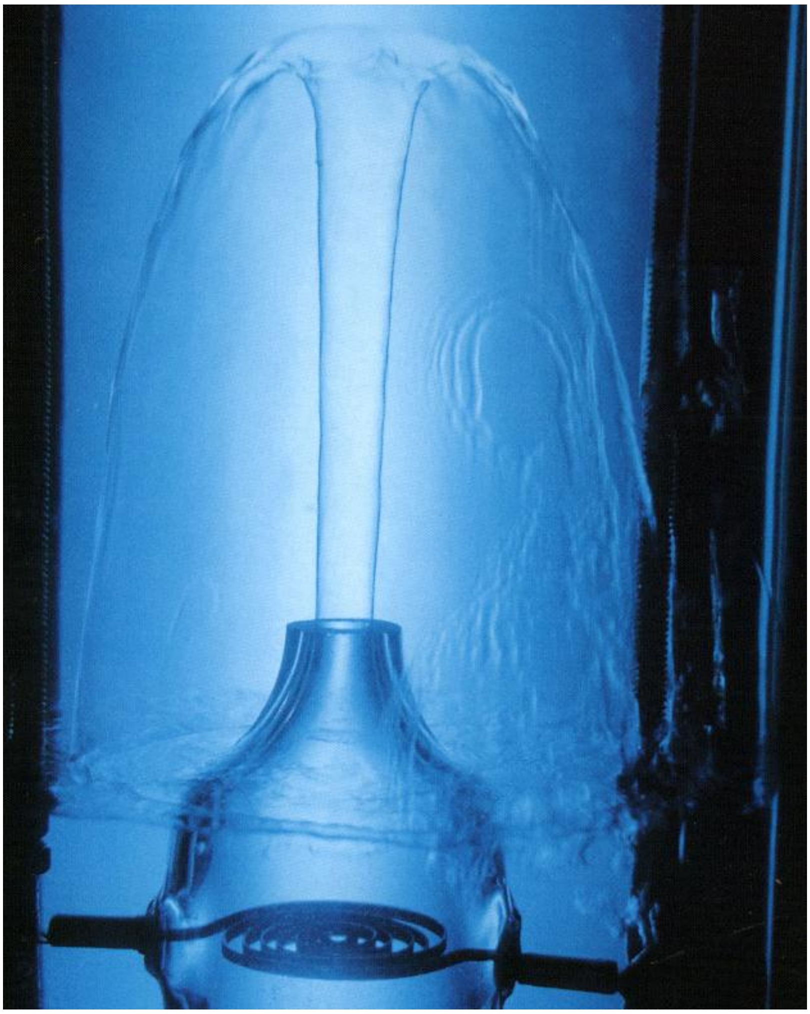

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COVER PHOTO: a fountain of superfluid Helium-4 will flow forever with a tiny amount of heating at the bottom (1) (2) (3).

1 Introduction

Over the past few decades, superconductivity has taken the world by storm. The promise of zero loss in electrical systems has led to hundreds of thousands of papers on the subject (4). Lesser known – and not nearly as world-changing – is superconductivity's little brother: superfluidity. Instead of having no resistance ('electrical friction') it is a liquid or gas with no viscosity ('fluidic friction'). This also produces some interesting effects, like superfluids crawling up walls by themselves (5) (6) and the creation of superfluid fountains (2) (3). Although superfluidity also has some practical applications[1], the main point of interest is fundamental understanding. And in this area, a fair few questions remain.

Descriptions of superfluidity and superconductivity on the most basic level are plagued with problems. In particular, the mainstream theory violates conservation of particles. That is to say, new particles spring into existence out of thin air and others suddenly disappear. This description is specifically created to exactly cancel out some tricky contributions to the energy. As the developers of the original BCS-theory for superconductivity point out, this isn't actually correct (7); but no one ever bothered to fix it. In subsequent years, it increasingly became 'the mainstream theory'. Because it worked well enough for most predictions, it was eventually left at that. However, any first year physics student can tell you that conservation laws are the building blocks of physics. Especially when you're looking at microscopic systems, particle conservation is a pretty big deal, since specific parts of your system may contain no more than one or two particles.

With all that in mind, we set out to see if there is a way to describe superfluids without violating conservation of particles. We use a simplified system based on superfluid spin-polarized atomic Hydrogen, which is believed to be essential for describing a number of physical systems, including neutron stars (8). The system is also roughly applicable to superfluid Helium-4, although our approximations are too restrictive to model it with high accuracy (9) (10) (11). Of course, if an exact calculation was doable, that would have been done a long time ago. So we are merely looking for an approximation that has less fundamental difficulties than the current one, while still being practical to calculate.

In section 2, we will describe the system in more detail and then go through the conventional approximation of its lowest lying states and their energies. We will take a look at some of the properties of both the system and the approximation, paying special attention to the violation of particle conservation.

In the next section, we will describe our method for a calculation that conserves the number of particles. Along the way, we introduce a set of operators that change the momentum of particles, instead of creating or annihilating them. We will see that these operators reduce to the conventional bosonic creation and annihilation operators when most particles are in the same state. We will apply this method to the original system to find its states and the associated energies. These results are then checked for consistency. To complete our overview, we summarize our results and look at the price we had to pay to guarantee particle conservation. Finally, we will briefly touch upon the possibilities for improving our method and other potential applications, in particular for superconductors.

Overall, this text will offer a solid alternative to the conventional description of superfluids and will provide you with the tools needed to use it.

1.1 Notes about notation

References to sources are numbered and placed in parentheses. You will find the complete references in chapter 5. Equations are numbered and placed in square brackets, as are references to them throughout the text. Operators are marked with a $\widehat{\ }$ above them. Complex conjugates are noted with a †. Commutators use the conventional notation of $[A, B] = AB - BA$.

Throughout the text you will find sidebars. These will refresh your memory on mathematical techniques or go into more detail about things mentioned in the text. None of the sidebars are essential to the main points being made, but each one explores a potentially interesting aspect of our system. Reading them is optional, but may help you put our findings into context.

[1] For example, superfluids can be used in gyroscopes (19) or as quantum solvents that allow particles to 'fly' frictionlessly, letting you research the properties of a molecular fluid as if it were a gas (20).

2 Describing a simplified superfluid

In the system below, we will be looking at a simplified and idealized bosonic superfluid (12) (13). The system consists of a very large collection of *N* identical spin-0 bosons with mass *m*. The particles are trapped in a large cube with sides *L* and periodic boundary conditions, giving rise to the quantized momentum spectrum

$$\vec{p} = \hbar\vec{q} \,:\, q_{x,y,z} = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \pm\frac{6\pi}{L}, \dots \,. \qquad [1]$$

We further assume that the temperature is sufficiently low for the particles to be almost exclusively in the lowest lying one-particle ground state. This means that for these low-energy N-particle states

$$n_{\vec{0}} = N - \sum_{\vec{q}\neq\vec{0}} n_{\vec{q}} \approx N \qquad [2]$$

$$\sum_{\vec{q}\neq\vec{0}} n_{\vec{q}} \ll N \,, \qquad [3]$$

which we will use repeatedly in our approximations. Here $n_{\vec{q}}$ is the number of particles with momentum $\vec{q}$, with $n_{\vec{0}}$ the number of particles in the one-particle ground state.

Neglecting particle interactions for the moment, we can write the Hamilton-operator of the system in the momentum representation as

$$\hat{H}_0 = \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m} \hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} \qquad [4]$$

with eigenvalues

$$E^{(0)} = \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m} n^{(0)}_{\vec{q}} \,, \qquad [5]$$

using the conventional definitions of the operators $\hat{a}$ and $\hat{a}^\dagger$ that annihilate and create particles respectively (14).[2] We then have as in [2] and [3]

$$\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}} = \hat{N} - \sum_{\vec{q}\neq\vec{0}} \hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} \approx \hat{N} \qquad [6]$$

$$\sum_{\vec{q}\neq\vec{0}} \hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} \ll \hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}} \approx \hat{N} \,, \qquad [7]$$

where the $\hat{N}$-operator counts the total number of particles. Once again, this is only true for very low-energy states. Note that with particle conservation, $\hat{N}$ goes to *N* when applied to our system, because the number of particles it counts is fixed at *N*.

But there actually is a weak repulsive interaction between the bosons – depending on the distance between the particles – which gives rise to the additional potential

$$\hat{V} = \frac{1}{2}\sum_{\vec{k},\vec{k'},\vec{q}} U(q)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}+\vec{q}}\hat{a}_{\vec{k}-\vec{q}} \,. \qquad [8]$$

Here $U(q)$ is the Fourier-transform of the spatial pair interaction per unit volume which depends on q (the absolute value of $\vec{q}$). This gives for our total Hamiltonian

$$\boxed{\begin{aligned}\hat{H} &= \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\left(\hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} + \hat{a}^\dagger_{-\vec{q}}\hat{a}_{-\vec{q}}\right) \\ &+ \frac{1}{2}\sum_{\vec{k},\vec{k'},\vec{q}} U(q)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}+\vec{q}}\hat{a}_{\vec{k}-\vec{q}} \,,\end{aligned}} \qquad [9]$$

where we have split the $\hat{H}_0$-component into two terms, for reasons that will become clear when we approximate $\hat{V}$.

Because the interaction is weak, we know that in the low-energy N-particle states almost all particles will remain in the one-particle ground state, meaning [2], [3], [6] and [7] still hold for low energies.

What is a?

In the rest of this text, we will use the creation and annihilation operators $\hat{a}^\dagger_{\vec{q}}$ and $\hat{a}_{\vec{q}}$ repeatedly. More than that, we will take knowledge of their use as a given. So if you are not intimately familiar with these operators, make sure to take a careful look at the quick overview below.

The annihilation operator $\hat{a}_{\vec{q}}$ removes a particle with momentum $\vec{q}$ from our system and picks up a counting factor along the way

$$\hat{a}_{\vec{q}}|\dots, n_{\vec{q}}, \dots\rangle = \sqrt{n_{\vec{q}}}|\dots, n_{\vec{q}} - 1, \dots\rangle \,, \qquad [10]$$

where the $n_{\vec{q}}$ in the ket represents the number of particles with momentum $\vec{q}$ in our system. Similarly, $\hat{a}^\dagger_{\vec{q}}$ adds a particle

$$\hat{a}^\dagger_{\vec{q}}|\dots, n_{\vec{q}}, \dots\rangle = \sqrt{n_{\vec{q}} + 1}|\dots, n_{\vec{q}} + 1, \dots\rangle \,. \qquad [11]$$

This also explains the form of our $\hat{N}$-operator. After all, applying $\hat{a}_{\vec{q}}$ and $\hat{a}^\dagger_{\vec{q}}$ to our system successively, gives

$$\begin{aligned}\hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}}|\dots, n_{\vec{q}}, \dots\rangle &= \hat{a}^\dagger_{\vec{q}}\sqrt{n_{\vec{q}}}|\dots, n_{\vec{q}} - 1, \dots\rangle \\ &= n_{\vec{q}}|\dots, n_{\vec{q}}, \dots\rangle \,.\end{aligned} \qquad [12]$$

This means we count the number of particles with momentum $\vec{q}$ while leaving the system itself unchanged. So when we apply $\hat{N}$, we find

$$\begin{aligned}\hat{N}|\dots, n_{\vec{q}}, \dots\rangle &= \sum_{\vec{q}} \hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}}\,|\dots, n_{\vec{q}}, \dots\rangle \\ &= N|\dots, n_{\vec{q}}, \dots\rangle \,.\end{aligned} \qquad [13]$$

[2] If you're fuzzy on those definitions, take a look at the 'What is a?' sidebar for a quick refresher.

A final point to note is that our operators do not always commute. Instead they obey the following bosonic commutation relations:

$$\begin{aligned} \left[\hat{a}^\dagger_{\vec{q}}, \hat{a}^\dagger_{\vec{k}}\right] &= 0 \\ \left[\hat{a}_{\vec{q}}, \hat{a}_{\vec{k}}\right] &= 0 \\ \left[\hat{a}_{\vec{q}}, \hat{a}^\dagger_{\vec{k}\neq\vec{q}}\right] &= 0 \\ \left[\hat{a}_{\vec{q}}, \hat{a}^\dagger_{\vec{q}}\right] &= \hat{1} \end{aligned} \qquad [14]$$

2.1 Conventional approximation

The conventional approximation uses three steps to find the lowest lying states and associated energies of the system (12) (13).

For the first step, approximations [6] and [7] are used to remove the suppressed contributions to $\hat{V}$. For the second step, $\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{0}}$ and $\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}$ are approximated as being roughly equal to N, violating conservation of particle number. For the final step, we apply a Bogoliubov transformation to diagonalize $\hat{H}$ in terms of pairs of quasi-particle number operators (15) (16) (17).

2.1.1 Removing suppressed contributions to V

Because in our system almost all particles are in the one-particle ground state, the contributions from $\hat{a}_{\vec{0}}$-like terms will be much larger than from $\hat{a}_{\vec{q}\neq\vec{0}}$-like terms. After all, the creation and annihilation operators give rise to $\sqrt{n_{\vec{q}}}$-like terms. While the occupation of the one-particle ground state guarantees $\mathcal{O}\left(\sqrt{N}\right)$ terms from $\hat{a}_{\vec{0}}$ and $\hat{a}^\dagger_{\vec{0}}$, the much lower occupation of the excited one-particle states (as quantified in equation [3]) guarantees terms much smaller than $\sqrt{N}$ from $\hat{a}_{\vec{q}\neq\vec{0}}$-like terms. In particular, the separate terms of the sums in $\hat{V}$ can be broken up into progressively smaller parts by the number of $\hat{a}_{\vec{0}}$-like terms. This leads to a leading order term

$$\hat{V}^{(0)} = \frac{1}{2}U(0)\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\,, \qquad [15]$$

a number of second order corrections

$$\begin{aligned} \hat{V}^{(2)} &= \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} \\ &+ \frac{1}{2}\sum_{\vec{k'}\neq\vec{0}} U(k')\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{0}}\hat{a}_{\vec{k'}} \\ &+ \frac{1}{2}\sum_{\vec{k'}\neq\vec{0}} U(0)\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}}\hat{a}_{\vec{0}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0}} U(0)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{k}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0}} U(k)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{k}}\hat{a}_{\vec{0}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0}} U(k)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{-\vec{k}}\hat{a}_{\vec{0}}\hat{a}_{\vec{0}} \\ &= \sum_{\vec{q}\neq\vec{0}} U(0)\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} \\ &+ \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\left(\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}^\dagger_{\vec{q}}\hat{a}^\dagger_{-\vec{q}}\right) \\ &+ \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{0}}\left(\hat{a}^\dagger_{\vec{q}}\hat{a}_{\vec{q}} + \hat{a}^\dagger_{-\vec{q}}\hat{a}_{-\vec{q}}\right)\,, \end{aligned} \qquad [16]$$

a number of third order corrections

$$\begin{aligned} \hat{V}^{(3)} &= \frac{1}{2}\sum_{\vec{k'}\neq\vec{0},\vec{q}\neq\vec{0},\vec{k'}+\vec{q}\neq\vec{0}} U(q)\hat{a}^\dagger_{\vec{0}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}+\vec{q}}\hat{a}_{-\vec{q}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0},\vec{q}\neq\vec{0},\vec{k}-\vec{q}\neq\vec{0}} U(q)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{0}}\hat{a}_{\vec{q}}\hat{a}_{\vec{k}-\vec{q}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0},\vec{k'}\neq\vec{0},\vec{k}+\vec{k'}\neq\vec{0}} U(k')\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{0}}\hat{a}_{\vec{k}+\vec{k'}} \\ &+ \frac{1}{2}\sum_{\vec{k}\neq\vec{0},\vec{k'}\neq\vec{0},\vec{k'}+\vec{k}\neq\vec{0}} U(k)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}+\vec{k}}\hat{a}_{\vec{0}}\,, \end{aligned} \qquad [17]$$

and one fourth order sum

$$\hat{V}^{(4)} = \frac{1}{2}\sum_{\substack{\vec{k}\neq\vec{0},\vec{k'}\neq\vec{0},\\ \vec{q}\neq\vec{k}\text{ nor }-\vec{k'}}} U(q)\hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k'}}\hat{a}_{\vec{k'}+\vec{q}}\hat{a}_{\vec{k}-\vec{q}}\,. \qquad [18]$$

Note that conservation of momentum guarantees that there are no first order corrections $\hat{V}^{(1)}$ with three $\hat{a}_{\vec{0}}$-like terms.

Since $\hat{V}$ is small to begin with, and [15] is correct to second order, it is tempting to simply use [15] as our value for $\hat{V}$. This would then lead us to approximate our new energy levels as simply having increased by a roughly constant amount determined by the one-particle ground state occupation. However, although this would give us a good approximation of the *total energy* of the system, the errors in the energy of the one-particle excited states might still be significant and we are just as interested in these one-particle excited states as in the one-particle ground state.

After all, their occupation may be lower, but all interactions in our material involve a one-particle excited state as well. On top of that, the differences between the N-particle ground state and the low-energy N-particle excited states – which determine the superfluid properties of our system – is wholly dependent on the properties of our excited states as well. Therefore, an approximation that ignores these states will not do, no matter how well it approximates the total energy of the system. This means we will need to take into account the contributions from [16] as well, but we will still neglect the higher order terms from [17] and [18], leading to

$$\begin{aligned}\hat{V} \approx & \frac{1}{2}U(0)\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}\hat{a}_{\vec{0}} + \sum_{\vec{q}\neq\vec{0}} U(0)\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\left(\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{q}}^\dagger\right) \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}\left(\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{q}}\right) .\end{aligned} \qquad [19]$$

Finally, we use the exact equivalence from [6] to rewrite this, filling in the value of $\hat{N} = N$ and throwing out the fourth order sums that appear. (We can safely do this because they are significantly smaller than the terms we already neglected before.)

$$\boxed{\begin{aligned}\hat{V} \approx & \frac{N(N-1)U(0)}{2} \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\left(\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{q}}^\dagger\right) \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)N\left(\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{q}}\right) .\end{aligned}} \qquad [20]$$

Since the number of particles is still conserved in this approximation, it can safely be applied as part of an alternative method, so it will be our starting point in section 3.[3]

2.1.2 Approximating pairs of equal operators in V

This second part of the approximation is based on the idea that an approximation similar to the one for $\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}$ can be used for $\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger$ and $\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}$. Since these pairs only appear in a second order term in $\hat{V}$, even a rough approximation would be sufficient. Since the constant factor from applying any pair of creation or annihilation operators to a state is similar if the associated occupation is sufficiently high – as is the case for our one-particle ground state – we use the approximation

$$\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger \approx \hat{a}_{\vec{0}}\hat{a}_{\vec{0}} \approx N , \qquad [21]$$

where for simplicity we ignore phase factors of $e^{\pm 2i\varphi_0}$ that can be shown to cancel in the final approximation (13) (18).

The value of this constant factor is a good approximation, since the neglected terms are of fourth order. However, the effect on the state of the system is also completely neglected. Namely, we neglect the addition or removal of two particles, violating particle-number conservation. This is the problem we will look to solve by means of an alternative solution in section 3.

But for now, simply plugging [21] into [20] gives

$$\begin{aligned}\hat{V} \approx & \frac{N(N-1)U(0)}{2} + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q) * \\ & * \left(\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{q}} + \hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{q}}^\dagger\right) ,\end{aligned} \qquad [22]$$

so that we find for our approximated total Hamiltonian

$$\begin{aligned}\hat{H} \approx & \frac{N(N-1)U(0)}{2} \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \left(\frac{\hbar^2\vec{q}^2}{2m} + NU(q)\right)\left(\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{q}}\right) \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{q}}^\dagger\right) .\end{aligned} \qquad [23]$$

2.1.3 The Bogoliubov transformation

Equation [23] is fairly compact and only has pairs of operators. But ideally we would like to find a diagonalized form that lets us count occupations of states. In other words, it should only include operator pairs of the form $\hat{a}^\dagger\hat{a}$, like in the first term.

We cannot use any of the tricks for large numbers from §2.1.1 and §2.1.2, because for $\hat{a}_{\vec{q}\neq\vec{0}}$ the occupation is not large enough – in fact, many one-particle excited states may be empty. However, we can exploit the symmetric occurrence of $\vec{q}$ and $-\vec{q}$ in $\hat{H}$ to find a form that lets us count the occupation of states.[4] There is a general Bogoliubov transformation specifically for such operator pairs (15) (16) (17) (18):

$$\begin{aligned} & E\left(\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_2^\dagger\hat{a}_2\right) + \Delta\left(\hat{a}_1\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2^\dagger\right) \\ & = \sqrt{E^2 - \Delta^2}\left(\hat{c}_1^\dagger\hat{c}_1 + \hat{c}_2^\dagger\hat{c}_2 + \hat{1}\right) - E\hat{1}\end{aligned} \qquad [24]$$

for $E, \Delta \in \mathbb{R}$ and $E > |\Delta|$, where

$$\begin{aligned}\hat{c}_1 \equiv u\hat{a}_1 + v\hat{a}_2^\dagger, \quad \hat{c}_1^\dagger = u\hat{a}_1^\dagger + v\hat{a}_2 \\ \hat{c}_2 \equiv u\hat{a}_2 + v\hat{a}_1^\dagger, \quad \hat{c}_2^\dagger = u\hat{a}_2^\dagger + v\hat{a}_1 ,\end{aligned} \qquad [25]$$

are bosonic annihilation and creation operators for quasi-particles. They adhere to all rules for normal annihilation and creation operators, in particular the bosonic commuta-

[3] Actually, we will find that we don't need to throw out *all* the fourth order sums that appear when rewriting [19] for our method in section 3, but we will get to that there.

[4] For anyone who was still wondering about the reason why we split $\hat{H}_0$ into two terms back in equation [9], this is it.

tion relations. This is guaranteed by the carefully chosen values

$$u \equiv \frac{1}{2}\left(\frac{E+\Delta}{E-\Delta}\right)^{1/4} + \frac{1}{2}\left(\frac{E+\Delta}{E-\Delta}\right)^{-1/4}$$
$$v \equiv \frac{1}{2}\left(\frac{E+\Delta}{E-\Delta}\right)^{1/4} - \frac{1}{2}\left(\frac{E+\Delta}{E-\Delta}\right)^{-1/4} , \qquad [26]$$

also guaranteeing that $u, v \in \mathbb{R}$.

For our Hamiltonian in [23] we then have for each term in the sum over $\vec{q}$

$$E = \frac{1}{2}\left(\frac{\hbar^2 \vec{q}^2}{2m} + NU(q)\right)$$
$$\Delta = \frac{NU(q)}{2} \qquad [27]$$
$$\sqrt{E^2 - \Delta^2} = \frac{\hbar^2 \vec{q}^2}{4m}\sqrt{1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}} \equiv \frac{\epsilon_{\vec{q}}}{2} .$$

Thus the Hamiltonian can be written as

$$\hat{H} = \frac{N(N-1)U(0)}{2} - \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left[\frac{\hbar^2 \vec{q}^2}{2m} + NU(q)\right] + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left[\epsilon_{\vec{q}}\left(\hat{c}_{\vec{q}}^\dagger \hat{c}_{\vec{q}} + \hat{c}_{-\vec{q}}^\dagger \hat{c}_{-\vec{q}} + \hat{1}\right)\right] ,$$

resulting in

$$\boxed{\hat{H} = \frac{N(N-1)U(0)}{2} + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\epsilon_{\vec{q}} - \frac{\hbar^2 \vec{q}^2}{2m} - NU(q)\right) + \sum_{\vec{q}\neq\vec{0}} \epsilon_{\vec{q}} \hat{c}_{\vec{q}}^\dagger \hat{c}_{\vec{q}} .} \qquad [28]$$

From the general form of equations [25] and [26] it follows that for our system

$$\hat{c}_{\vec{q}} \equiv u_{\vec{q}} \hat{a}_{\vec{q}} + v_{\vec{q}} \hat{a}_{-\vec{q}}^\dagger, \quad \hat{c}_{\vec{q}}^\dagger = u_{\vec{q}} \hat{a}_{\vec{q}}^\dagger + v_{\vec{q}} \hat{a}_{-\vec{q}} , \qquad [29]$$

specified by

$$u_{\vec{q}} \equiv \frac{1}{2}\left(1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}\right)^{1/4} + \frac{1}{2}\left(1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}\right)^{-1/4}$$
$$v_{\vec{q}} \equiv \frac{1}{2}\left(1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}\right)^{1/4} - \frac{1}{2}\left(1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}\right)^{-1/4} . \qquad [30]$$

Basically, this is it. The first two terms of $\hat{H}$ describe the new N-particle ground state energy. We then have quasi-particles with energies $\epsilon_{\vec{q}}$ that are created and annihilated by $\hat{c}_{\vec{q}}^\dagger$ and $\hat{c}_{\vec{q}}$ respectively. These new quasi-particle operators can be described in terms of our original operators – and thus our original particles – as needed.

The only nagging issue is that little violation of particle-number conservation in the second part of the approximation.

3 The particle conservation method

As mentioned in the previous section, a good starting point for applying a method with particle conservation is equation [20]:

$$\begin{aligned}\hat{V} \approx & \frac{N(N-1)U(0)}{2} \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\left(\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{-\vec{q}}^{\dagger}\right) \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)N\left(\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^{\dagger}\hat{a}_{-\vec{q}}\right) .\end{aligned}$$

All approximations up to that point are simple, particle conservation still holds, and the problem is clearly isolated: the troubling terms in this equation are $\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}}$ and $\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{-\vec{q}}^{\dagger}$. The most obvious way to make these terms more pleasant, is to somehow transform them into terms of two operators instead of four. Once we get our Hamiltonian into that form, we have a wide array of tools at our disposal for simplifying it further.

We know that we cannot simply replace creation or annihilation operators with fixed numbers as is done in the conventional approximation, because that would break particle conservation. But we may still be able to compactify the tricky terms into sets of two operators, by introducing a pair operator $\hat{b}_{\vec{q}} \propto \hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{q}}$. To be more exact, we will define:

$$\boxed{\hat{b}_{\vec{q}\neq\vec{0}} \equiv \frac{\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{q}}}{\sqrt{N}} \Rightarrow \hat{b}_{\vec{q}\neq\vec{0}}^{\dagger} = \frac{\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{0}}}{\sqrt{N}} .} \quad [31]$$

Writing the troubling parts of our potential in terms of $\hat{b}$ would plainly reduce them to terms of only two operators. The structure of $\hat{b}$ also seems similar enough to that of $\hat{a}$ to believe that many of their properties could be the same. On top of that, $\hat{b}$ looks promising from a physical point of view, as expanded on in the 'What is b?' sidebar.

As nice as 'looks promising' sounds though, it doesn't mean much without a solid mathematical basis. In particular, two major questions remain. Firstly, does the $\hat{b}_{\vec{q}}$-operator exhibit the required bosonic behavior? Secondly, can the $\hat{b}_{\vec{q}}$-operator be applied to the complete Hamiltonian of our system, without creating all kinds of extra complications?

We will start by discussing the first question in §3.1 and §3.2. Once we have set up our general toolbox there, we will apply it to our Hamiltonian to answer our second question in §3.3. The three final paragraphs of this section will be used to check and reflect on our results.

What is b?
Suddenly, out of nowhere, we introduce some operator $\hat{b}$. But why would this be a useful operator? And what is its physical meaning? What does $\hat{b}_{\vec{q}}$ actually *do*?

We mainly have two criteria when building an operator. First, we want one that's as close as possible to $\hat{a}_{\vec{q}}$. We don't want to change the way our system works any more than we have to; we just want to correct one tiny problem. Second, we want it to be an operator that guarantees particle conservation.

In short, we are looking for a way to make sure one particle is created for every one that is annihilated – and vice versa – but in a way that hardly impacts our system. And that's where $\hat{a}_{\vec{0}}^{\dagger}$ comes in: adding one particle to the ground state causes only a tiny change to our system. That is after all what the conventional approximation is based on. So defining $\hat{b}$ is simply a matter of starting with the original $\hat{a}_{\vec{q}}$ and adding a term $\hat{a}_{\vec{0}}^{\dagger}$ to guarantee particle conservation. The $\frac{1}{\sqrt{N}}$ roughly normalizes $\hat{a}_{\vec{0}}^{\dagger}$, since there are about N particles in the ground state.

So now that we know how we got to $\hat{b}_{\vec{q}}$, what does it actually do? The answer is surprisingly simple: $\hat{b}_{\vec{q}}$ changes the momentum of a single particle. To be exact, it drops a particle from the $\vec{q}$-state to the ground state. Similarly, $\hat{b}_{\vec{q}}^{\dagger}$ takes a particle from the ground state and gives it a momentum $\vec{q}$.

However, because of the massive number of particles in the ground state and their low energy, we hardly notice there being one more or less of those. So what we would actually see is a particle with momentum $\vec{q}$ appearing or disappearing, without noticing the tiny change in the ground state. This makes $\hat{b}_{\vec{q}}$ act a lot like the original $\hat{a}_{\vec{q}}$.

Note that this change of particle momentum is what we intuitively expect a weak added potential to cause: it doesn't 'create' or 'annihilate' any particles, it simply moves them to a different energy state.

Finally, an added bonus of this physical picture of $\hat{b}_{\vec{q}}$ is that it is immediately obvious that no matter what combination of $\hat{b}$'s we use, particle number is always conserved. After all, $\hat{b}$ doesn't actually make any new particles, it only shifts the existing ones around a bit.

3.1 Commutation relations

We want to know if our $\hat{b}$-operator exhibits the same bosonic behavior as $\hat{a}$. In other words: does it conform to the same bosonic commutation relations? Let's answer this question in a slightly more general way than that of our particular system.

Consider some system with a large collection of *N* identical bosons and a number of one-particle states they can be in. We label one of these states as the 'base' state. This means particles in that state can be created or annihilated using operators $\hat{a}_{\vec{b}}^{\dagger}$ and $\hat{a}_{\vec{b}}$.[5] We can then define an operator $\hat{b}$ as in [31]

$$\hat{b}_{\vec{q}\neq\vec{b}} \equiv \frac{\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}}{\sqrt{N}} \Rightarrow \hat{b}_{\vec{q}\neq\vec{b}}^{\dagger} = \frac{\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}}}{\sqrt{N}} \,. \qquad [32]$$

Note that we do not define $\hat{b}_{\vec{b}}$, since we do not need it for our purposes, and it leads to a number of complications discussed in the 'What is b_b?' sidebar. We will assume for any $\hat{b}_{\vec{q}}$ that $\vec{q} \neq \vec{b}$ unless explicitly noted.

If we then look at the commutation relations for $\hat{b}$, we find

$$\begin{aligned}\left[\hat{b}_{\vec{q}}^{\dagger}, \hat{b}_{\vec{k}}^{\dagger}\right] &= \frac{1}{N}\left(\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}}\right) \\ &= 0 = \left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{k}}\right]\end{aligned} \qquad [33]$$

because all $\hat{a}$-operators involved commute. It gets more interesting when we look at

$$\begin{aligned}\left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{k}\neq\vec{q}}^{\dagger}\right] &= \frac{1}{N}\left(\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\right) \\ &= \frac{1}{N}\left(\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{q}} - \hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{q}}\right) \\ &= -\frac{\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{q}}}{N} \,.\end{aligned} \qquad [34]$$

This should be zero for a bosonic operator, but it clearly is not, unless there happen to be no particles with momentum $\vec{q}$ in the system we apply it to. For our last identity we find

$$\begin{aligned}\left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{q}}^{\dagger}\right] &= \frac{1}{N}\left(\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\right) \\ &= \frac{1}{N}\left(\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{b}}\hat{a}_{\vec{q}} - \hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{q}}\right) \\ &= \frac{1}{N}\left(\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{q}}\hat{a}_{\vec{b}} - \hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{q}}\right) \\ &= \frac{\hat{a}_{\vec{b}}^{\dagger}\hat{a}_{\vec{b}} - \hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{q}}}{N} = \frac{\hat{n}_{\vec{b}} - \hat{n}_{\vec{q}}}{N} \,.\end{aligned} \qquad [35]$$

This commutator should be equal to one, but once again it is not. Except in the specific case where we apply it to a system with all *N* particles in the 'base' state.

We can only conclude that in general, $\hat{b}$ is not a good bosonic operator and cannot be used.

3.2 The single state limit

The operator $\hat{b}$ may not be a good bosonic annihilation operator in general, but it can still be salvaged for a more specific set of systems. So let us look at the limit where almost all particles are in the 'base' state, analogous to equations [2] and [3] for our superfluid

$$n_{\vec{b}} \approx N \qquad [36]$$

$$\sum_{\vec{q}\neq\vec{b}} n_{\vec{q}} \ll N \,. \qquad [37]$$

If we now apply the commutator from [34] to our system

$$\begin{aligned}&\left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{k}\neq\vec{q}}^{\dagger}\right]\left|\dots, n_{\vec{q}}, \dots, n_{\vec{k}}, \dots\right\rangle \\ &= -\frac{\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{q}}}{N}\left|\dots, n_{\vec{q}}, \dots, n_{\vec{k}}, \dots\right\rangle \\ &= -\frac{\sqrt{n_{\vec{q}}\left(n_{\vec{k}}+1\right)}}{N}\left|\dots, n_{\vec{q}}-1, \dots, n_{\vec{k}}+1, \dots\right\rangle ,\end{aligned} \qquad [38]$$

with the prefactor being negligible since we know from [37] that $n_{\vec{q}} \ll N$ and $n_{\vec{k}} \ll N \Rightarrow n_{\vec{k}} + 1 \ll N$. So the contribution from this commutator may be small enough to safely neglect when applied to a system where equations [36] and [37] hold.[6]

For the commutator from [35], we get

$$\begin{aligned}\left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{q}}^{\dagger}\right]\left|\dots, n_{\vec{q}}, \dots\right\rangle &= \frac{\hat{n}_{\vec{b}} - \hat{n}_{\vec{q}}}{N}\left|\dots, n_{\vec{q}}, \dots\right\rangle \\ &= \frac{n_{\vec{b}} - n_{\vec{q}}}{N}\left|\dots, n_{\vec{q}}, \dots\right\rangle \\ &\approx \left|\dots, n_{\vec{q}}, \dots\right\rangle\end{aligned} \qquad [39]$$

from [36] and [37]. So it is now almost equal to 1.

The small errors in equations [38] and [39] make sense when looking at our definition of $\hat{b}$: We use $\sqrt{N}$ to normalize $\hat{b}$, rather than $\sqrt{n_{\vec{b}}}$.[7] So if we drop one particle to the base state and then raise one from the base state with $\hat{b}_{\vec{k}}^{\dagger}\hat{b}_{\vec{q}}$, the number of particles counted in the base state will be higher than when we apply the operators in reversed order ($\hat{b}_{\vec{q}}\hat{b}_{\vec{k}}^{\dagger}$). However, the normalizing factor does not change, leading to the non-zero terms in our commu-

[5] Note that in general this 'base' state need not be the ground state. However, if you are only interested in our specific system, feel free to read $\vec{0}$ wherever $\vec{b}$ appears.

[6] In §3.3 we will see that for our superfluid the errors are of about the same size as the fourth order corrections from equation [18] that we neglected earlier.

[7] We would love to use $n_{\vec{b}}$, but its value changes when we change the system, making it a function of our operators and states instead of a constant.

tators. Because of the same normalization problem, we need the approximation from [36] to set $n_{\vec{b}}$ equal to *N*.

In short, for this single state limit all our corrections are small and well-understood. So if our system and our operators are well-behaved, we can say

$$\left[\hat{b}_{\vec{q}}, \hat{b}^{\dagger}_{\vec{k}\neq\vec{q}}\right] \ll \hat{1}$$
$$\left[\hat{b}_{\vec{q}}, \hat{b}^{\dagger}_{\vec{q}}\right] \approx \hat{1}\,, \qquad [40]$$

making $\hat{b}$ approximately bosonic.

What is b$_b$?

In §3.1 we quickly brushed off $\hat{b}_{\vec{b}}$ as something we do not need for our purposes. Although we will see that is true, wouldn't it nevertheless make sense to define $\hat{b}_{\vec{b}}$ consistently and be done with it? Just so we have a proper operator? As we will see, that is easier said than done.

Definition 1
We could define $\hat{b}_{\vec{b}}$ in the exact same way as we did for the other $\hat{b}$-states

$$\hat{b}_{\vec{b}} \equiv \frac{\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{b}}}{\sqrt{N}} = \hat{b}^{\dagger}_{\vec{b}}\,. \qquad [41]$$

Then, since $\hat{b}_{\vec{b}} = \hat{b}^{\dagger}_{\vec{b}}$, it immediately follows that

$$\left[\hat{b}_{\vec{b}}, \hat{b}^{\dagger}_{\vec{b}}\right] = 0\,. \qquad [42]$$

This makes sense from a physical perspective: an operator that changes the momentum of a particle from the momentum in the base state to… the momentum in that same base state, basically does nothing. So it had better not matter which 'nothing' we do first. Or to put it another way: $\hat{b}_{\vec{b}}$ differs by just a constant from the counting operator $\hat{n}_{\vec{b}}$, which leaves our system unchanged. With this definition though, we lose our bosonic commutation relations. This ground state operator is no longer like our bosonic $\hat{a}_{\vec{0}}$ at all!

But wait, it gets worse. When we look at the other commutators, we find

$$\left[\hat{b}_{\vec{b}}, \hat{b}^{\dagger}_{\vec{q}}\right] = \frac{1}{N}\left(\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{b}}\hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{b}} - \hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{b}}\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{b}}\right) = -\frac{\hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{b}}}{N} \qquad [43]$$

$$\left[\hat{b}_{\vec{b}}, \hat{b}_{\vec{q}}\right] = \frac{1}{N}\left(\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{b}}\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{q}} - \hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{q}}\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{b}}\right) = \frac{\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{q}}}{N}\,. \qquad [44]$$

Unlike the small terms we found for the other commutators of $\hat{b}$, the terms from equations [43] and [44] cannot simply be brushed aside in the single state limit. Since the occupation of our $\vec{b}$-states is so large, these terms are at best $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$ rather than $\mathcal{O}\left(\frac{1}{N}\right)$. Though these terms could arguably still be neglected, it is far from an elegant solution and our errors are suddenly a lot larger.

Definition 2
A somewhat more heavy-handed approach would be to simply define

$$\hat{b}_{\vec{b}} \equiv \hat{1} = \hat{b}^{\dagger}_{\vec{b}}\,.$$

After all, as we mentioned for the first definition, we know from physical considerations what $\hat{b}_{\vec{b}}$ *should* do: nothing at all. You might expect some constant factor in front of $\hat{1}$, but remember that we originally used the factor of $\frac{1}{\sqrt{N}}$ in our definition of $\hat{b}$ specifically to normalize it. Well, there's no better normalization than setting our operator to $\hat{1}$ by definition.

This solves all our problems with non-zero commutators – since everything commutes with the unit operator – and it makes physical sense. But it still leaves the problem of $\left[\hat{b}_{\vec{b}}, \hat{b}^{\dagger}_{\vec{b}}\right]$ being zero. In other words, this definition may be cleaner, but it's still not bosonic.

On top of that, this definition cannot be used to compactify sets of four $\hat{a}$-operators into more workable sets of two $\hat{b}$s. One of the main uses for a definition of $\hat{b}_{\vec{b}}$ would be to also compactify terms with three or four factors of $\hat{a}_{\vec{b}}$ into sets of two. But we cannot do anything with those terms in this definition. In fact, it would not even be possible to write them in terms of $\hat{b}$.

Definition 3
If our operator isn't close enough to our original $\hat{a}_{\vec{b}}$, we could always fall back on

$$\hat{b}_{\vec{b}} \equiv \hat{a}_{\vec{b}}, \quad \hat{b}^{\dagger}_{\vec{b}} = \hat{a}^{\dagger}_{\vec{b}}\,. \qquad [45]$$

This of course means we get our first commutator

$$\left[\hat{b}_{\vec{b}}, \hat{b}^{\dagger}_{\vec{b}}\right] = \left[\hat{a}_{\vec{b}}, \hat{a}^{\dagger}_{\vec{b}}\right] = \hat{1} \qquad [46]$$

exactly as we want it to be. We even find the proper

$$\left[\hat{b}_{\vec{b}}, \hat{b}^{\dagger}_{\vec{q}}\right] = \frac{1}{\sqrt{N}}\left(\hat{a}_{\vec{b}}\hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{b}} - \hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{b}}\hat{a}_{\vec{b}}\right) = 0\,. \qquad [47]$$

But we have no such luck with our final commutator

$$\left[\hat{b}_{\vec{b}}, \hat{b}_{\vec{q}}\right] = \frac{1}{\sqrt{N}}\left(\hat{a}_{\vec{b}}\hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{q}} - \hat{a}^{\dagger}_{\vec{b}}\hat{a}_{\vec{q}}\hat{a}_{\vec{b}}\right) = \frac{\hat{a}_{\vec{q}}}{\sqrt{N}} \qquad [48]$$

which gives at least an $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$ error, just like our first definition.

A second problem is the fact that this $\hat{b}_{\vec{b}}$ no longer has the built in particle conservation which we constructed $\hat{b}$ for to begin with. If we're not careful with this definition, our approximations may end up breaking particle conservation all over again.

And finally, this third definition has the same problem as the second one, although to a lesser extend: it cannot be used to compactify terms with three or four $\hat{a}_{\vec{0}}$s. Although unlike in the second definition, here we could at least write them in terms of $\hat{b}$, if not in only two terms.

In conclusion

Although there are some potentially usable definitions for the 'base' state of $\hat{b}$, they all have problems and none of them fit neatly into our system. It is a good thing then that we don't need a base state for our applications, because that avoids a whole lot of unnecessary complications.

3.3 Application to the simplified superfluid

We have found the answer to our first question: the $\hat{b}_{\vec{q}}$-operator exhibits the required bosonic behavior if our system has a single one-particle state that contains most particles. That is of course the case for our superfluid, where the ground state plays that role. One caveat was that things need to be 'well-behaved' for this to be true. In particular, approximating the commutation relations by throwing out higher order terms only works if the lower order terms don't cancel.

That leads us to our second question: can we rewrite our entire Hamiltonian in terms of $\hat{b}$ without running into problems? We will rewrite $\hat{V}$ and $\hat{H}_0$, giving us an expression for $\hat{H}$ in terms of $\hat{b}$. We then apply a Bogoliubov transformation to $\hat{H}$, leading to a tentative final form for $\hat{H}$. In the next section, we will check these results for consistency. So if you think we're going a bit too fast in §3.3.2, don't worry, we'll do a double-check in §3.4.

3.3.1 Rewriting the Hamiltonian

Rewriting $\hat{V}$ in terms of $\hat{b}$ turns out to be extremely easy. That is, if we use a slightly more exact approximation of the $U(q)$ part of equation [19]. Rather than replacing $\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}^\dagger$ with N, we switch the order to $\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}$ and neglect the fourth order correction the commutator leaves, to find

$$\begin{aligned}\hat{V} \approx{}& \frac{N(N-1)U(0)}{2} \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\left(\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{0}}^\dagger\hat{a}_{\vec{q}}\hat{a}_{-\vec{q}} + \hat{a}_{\vec{0}}\hat{a}_{\vec{0}}\hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{q}}^\dagger\right) \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}} U(q)\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}^\dagger\left(\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{q}}\right) \\ ={}& \frac{N(N-1)U(0)}{2} \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{b}_{\vec{q}}\hat{b}_{-\vec{q}} + \hat{b}_{\vec{q}}^\dagger\hat{b}_{-\vec{q}}^\dagger\right) \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{b}_{\vec{q}}^\dagger\hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right).\end{aligned} \quad [49]$$

Unfortunately, $\hat{H}_0$ (as given in equation [4]) is not in the right form to transform. But that can be solved by multiplying by 1

$$\begin{aligned}\hat{H}_0 &= \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}} \\ &= \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}}\frac{\hat{N}}{N} \\ &= \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\frac{\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}}\hat{a}_{\vec{0}}\hat{a}_{\vec{0}}^\dagger}{N} \\ &\quad -\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\frac{\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}}}{N} \\ &\quad +\sum_{\vec{q}\neq\vec{0},\vec{k}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\frac{\hat{a}_{\vec{q}}^\dagger\hat{a}_{\vec{q}}\hat{a}_{\vec{k}}^\dagger\hat{a}_{\vec{k}}}{N}\end{aligned} \quad [50]$$

where we have used the exact equivalence from equation [6] and switched $\hat{a}_{\vec{0}}$ and $\hat{a}_{\vec{0}}^\dagger$ to get our expression into the correct form for a transformation to $\hat{b}$.

We would like to neglect the second and third term in this expression of $\hat{H}_0$, so that we can write $\hat{H}_0$ in terms of $\hat{b}$. At first glance, they simply have two less $\hat{a}_{\vec{0}}$-like terms than the first term; just like the second order terms in $\hat{V}$ from equation [16] that we couldn't neglect. However, the reason we couldn't neglect our second order terms for $\hat{V}$ was that the leading terms only applied to the ground state. The second order terms in $\hat{V}$ *were* the leading order terms for excited states. However, that doesn't hold for $\hat{H}_0$, because it only describes excited states (the unperturbed one-particle ground state has zero energy). That means the second order terms in $\hat{H}_0$ are actually equivalent to the fourth order terms in $\hat{V}$ (from equation [18]) that could be neglected safely. That means we can neglect those terms, to find

$$\hat{H}_0 \approx \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\frac{\hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \hat{a}_{\vec{0}} \hat{a}_{\vec{0}}^\dagger}{N}$$
$$= \sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m} \hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} \qquad [51]$$
$$= \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{2m}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger \hat{b}_{-\vec{q}}\right).$$

You might still worry that while the terms we neglect are sufficiently small relative to $\hat{H}_0$, aren't they much larger than our corrections in $\hat{V}$? After all, wasn't our interaction weak, implying that $\hat{V}$ is small?

Luckily, our interaction being weak refers to the fact that the potential is not strong enough to excite the majority of our particles and that only 2-particle interactions need to be taken into account. It does not mean that our interaction is weak compared to $\hat{H}_0$. In fact, since we're looking at extremely low temperatures, almost all particles are in the zero-energy one-particle ground state without the added potential. That means $\hat{H}_0$ receives no contribution from the majority of our particles either and is thus also very small. In other words, the terms we neglect are tiny – about a factor of *N* smaller than the full Hamiltonian, which itself is small to begin with. But even so, they could potentially be larger than the corrections we've made to $\hat{V}$ so far, depending on the exact system. This is part of the 'price' we pay for our alternative approximation.

With these approximations, we can now write our complete Hamiltonian in terms of $\hat{b}$

$$\boxed{\begin{aligned}\hat{H} \approx{}& \frac{N(N-1)U(0)}{2} \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\frac{\hbar^2\vec{q}^2}{2m}+NU(q)\right)\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger \hat{b}_{-\vec{q}}\right) \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{b}_{\vec{q}} \hat{b}_{-\vec{q}} + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger\right).\end{aligned}} \qquad [52]$$

As those with an extraordinary memory will have seen, this looks extremely similar to equation [23], leaving us an obvious next step.

3.3.2 The Bogoliubov transformation revisited

Since we have a Hamiltonian of the same form as in [23] – albeit with a not-quite bosonic operator in place of $\hat{a}$ – we can also follow the same steps as used in §2.1.3. This would give us the final Hamiltonian

$$\boxed{\begin{aligned}\hat{H} ={}& \frac{N(N-1)U(0)}{2} \\ &+\frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\epsilon_{\vec{q}} - \frac{\hbar^2\vec{q}^2}{2m} - NU(q)\right) \\ &+\sum_{\vec{q}\neq\vec{0}} \epsilon_{\vec{q}} \hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}}\ ,\end{aligned}} \qquad [53]$$

with $\epsilon_{\vec{q}}$ defined exactly as in [27]

$$\epsilon_{\vec{q}} \equiv \frac{\hbar^2\vec{q}^2}{2m}\sqrt{1+\frac{4mNU(q)}{\hbar^2\vec{q}^2}} \qquad [54]$$

and

$$\hat{d}_{\vec{q}} \equiv u_{\vec{q}}\hat{b}_{\vec{q}} + v_{\vec{q}}\hat{b}_{-\vec{q}}^\dagger, \quad \hat{d}_{\vec{q}}^\dagger = u_{\vec{q}}\hat{b}_{\vec{q}}^\dagger + v_{\vec{q}}\hat{b}_{-\vec{q}}, \qquad [55]$$

where just like in equation [30]

$$\begin{aligned} u_{\vec{q}} &\equiv \frac{1}{2}\left(1+\frac{4mNU(q)}{\hbar^2\vec{q}^2}\right)^{1/4} + \frac{1}{2}\left(1+\frac{4mNU(q)}{\hbar^2\vec{q}^2}\right)^{-1/4} \\ v_{\vec{q}} &\equiv \frac{1}{2}\left(1+\frac{4mNU(q)}{\hbar^2\vec{q}^2}\right)^{1/4} - \frac{1}{2}\left(1+\frac{4mNU(q)}{\hbar^2\vec{q}^2}\right)^{-1/4} .\end{aligned} \qquad [56]$$

This would make our final description of the system basically the same as the one from the conventional approximation. The only difference being that our quasi-particles are now defined slightly differently, guaranteeing particle conservation.

3.4 Checking consistency

These results seem nice, but before we can celebrate, we once again have to answer the two questions we were faced with at the start of this chapter, but now for our latest transformation: First, did using this Bogoliubov transformation on our not-quite-bosonic $\hat{b}$s create any extra complications? Second, does the $\hat{d}$-operator still exhibit the required bosonic behavior?

3.4.1 The transformed Hamiltonian

To answer the first question, we have to determine if our 'guess' for the results of the Bogoliubov transformation in §3.3.2 is actually correct. The recognizable form and near-bosonic properties of $\hat{b}$ suggest that the transformation is close to exact. However, the Bogoliubov transformation relies on a number of terms cancelling, making even small errors risky if they do not cancel.

The most general way to check this would be to derive the Bogoliubov transformation rules again for an operator with a small non-bosonic component. As interesting as that might be though, we will content ourselves with checking if our 'guess' is correct. In other words, we will work out the transformed Hamiltonian from equation [53] and see if it reduces to the untransformed Hamiltonian from equation [52]. Of course there probably will be some corrections – $\hat{b}$ is not exactly bosonic after all – so the real question is if these corrections are small enough to neglect.

First, for ease of reading, let us define

$$x_{\vec{q}} \equiv \left(1 + \frac{4mNU(q)}{\hbar^2 \vec{q}^2}\right)^{1/4}, \qquad [57]$$

so that we can write

$$\begin{aligned} u_{\vec{q}} &= \frac{x_{\vec{q}}}{2} + \frac{x_{\vec{q}}^{-1}}{2} \\ v_{\vec{q}} &= \frac{x_{\vec{q}}}{2} - \frac{x_{\vec{q}}^{-1}}{2} \\ \epsilon_{\vec{q}} &= \frac{\hbar^2 \vec{q}^2 x_{\vec{q}}^2}{2m}, \end{aligned} \qquad [58]$$

based on the definitions for *u*, *v* and ϵ from [54] and [56].

With that notation established, let's take a look at $\hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}}$

$$\begin{aligned} &\hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}} = \left(u_{\vec{q}} \hat{b}_{\vec{q}}^\dagger + v_{\vec{q}} \hat{b}_{-\vec{q}}\right)\left(u_{\vec{q}} \hat{b}_{\vec{q}} + v_{\vec{q}} \hat{b}_{-\vec{q}}^\dagger\right) \\ &= u_{\vec{q}}^2 \hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + v_{\vec{q}}^2 \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger + u_{\vec{q}} v_{\vec{q}} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &= \left(\frac{x_{\vec{q}}^2}{4} + \frac{1}{2} + \frac{x_{\vec{q}}^{-2}}{4}\right) \hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} \\ &+ \left(\frac{x_{\vec{q}}^2}{4} - \frac{1}{2} + \frac{x_{\vec{q}}^{-2}}{4}\right) \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger \\ &+ \left(\frac{x_{\vec{q}}^2}{4} - \frac{x_{\vec{q}}^{-2}}{4}\right)\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &= \frac{1}{2}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} - \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger\right) \\ &+ \frac{x_{\vec{q}}^2}{4}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &+ \frac{x_{\vec{q}}^{-2}}{4}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right). \end{aligned} \qquad [59]$$

We can plug that result into the last term of our transformed Hamiltonian from equation [53]

$$\begin{aligned} &\sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}} = \sum_{\vec{q} \neq \vec{0}} \frac{\hbar^2 \vec{q}^2 x_{\vec{q}}^2}{2m} \hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}} \\ &= \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} - \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger\right) + \\ &\sum_{\vec{q} \neq \vec{0}} \frac{\hbar^2 \vec{q}^2 x_{\vec{q}}^4}{8m} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &+ \sum_{\vec{q} \neq \vec{0}} \frac{\hbar^2 \vec{q}^2}{8m} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right). \end{aligned} \qquad [60]$$

This gives us three terms. The first one can be rewritten to

$$\begin{aligned} &\frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} - \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger\right) \\ &= \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} - \hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} - \left[\hat{b}_{\vec{q}}, \hat{b}_{\vec{q}}^\dagger\right]\right) \\ &= -\frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \frac{\hat{n}_{\vec{0}} - \hat{n}_{\vec{q}}}{N} \\ &= -\frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \epsilon_{\vec{q}} \left(\hat{1} - \frac{\hat{N} - \hat{n}_{\vec{0}} + \hat{n}_{\vec{q}}}{N}\right), \end{aligned} \qquad [61]$$

where we have used the commutator from equation [35] and where the sum over $\vec{q}$ and the fact that $\epsilon_{-\vec{q}} = \epsilon_{\vec{q}}$ allowed us to rewrite the $\hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger$ term as $\hat{b}_{\vec{q}} \hat{b}_{\vec{q}}^\dagger$. The final result may seem needlessly complicated, but in this form it will partially cancel against other terms later.

The second term can be rewritten by working out $x_{\vec{q}}^4$

$$\begin{aligned} &\sum_{\vec{q} \neq \vec{0}} \frac{\hbar^2 \vec{q}^2 x_{\vec{q}}^4}{8m} \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &= \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \left(\frac{\hbar^2 \vec{q}^2}{4m} + NU(q)\right) * \\ &* \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}} \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &= \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \left(\frac{\hbar^2 \vec{q}^2}{4m} + NU(q)\right) * \\ &* \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger \hat{b}_{-\vec{q}} + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}} + \left[\hat{b}_{-\vec{q}}, \hat{b}_{-\vec{q}}^\dagger\right]\right) \\ &= \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \left(\frac{\hbar^2 \vec{q}^2}{4m} + NU(q)\right) * \\ &* \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger \hat{b}_{-\vec{q}} + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}} \hat{b}_{\vec{q}}\right) \\ &+ \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} \left(\frac{\hbar^2 \vec{q}^2}{4m} + NU(q)\right)\left(\hat{1} - \frac{\hat{N} - \hat{n}_{\vec{0}} + \hat{n}_{\vec{q}}}{N}\right). \end{aligned} \qquad [62]$$

Of course $\hat{n}_{\vec{q}}$ in the last expression was originally $\hat{n}_{-\vec{q}}$, but because we are summing over $\vec{q}$ and all other terms are independent of sign, $\hat{n}_{-\vec{q}}$ can be replaced by $\hat{n}_{\vec{q}}$ for the total sum.

And finally, for the third term

$$\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{8m}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}\hat{b}_{-\vec{q}}^\dagger - \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{-\vec{q}}\hat{b}_{\vec{q}}\right)$$
$$= \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{4m} * \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}} - \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger - \hat{b}_{-\vec{q}}\hat{b}_{\vec{q}} + \left[\hat{b}_{-\vec{q}}, \hat{b}_{-\vec{q}}^\dagger\right]\right)$$
$$= \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{4m}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right) - \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{4m}\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}}\hat{b}_{\vec{q}}\right) + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} \frac{\hbar^2\vec{q}^2}{4m}\left(\hat{1} - \frac{\hat{N} - \hat{n}_{\vec{0}} + \hat{n}_{\vec{q}}}{N}\right), \quad [63]$$

where we have once again turned $\hat{n}_{-\vec{q}}$ into $\hat{n}_{\vec{q}}$.

These three terms neatly combine into

$$\sum_{\vec{q}\neq\vec{0}} \epsilon_{\vec{q}} \hat{d}_{\vec{q}}^\dagger \hat{d}_{\vec{q}} = \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\frac{\hbar^2\vec{q}^2}{2m} + NU(q) - \epsilon_{\vec{q}}\right)\left(\hat{1} - \frac{\hat{N} - \hat{n}_{\vec{0}} + \hat{n}_{\vec{q}}}{N}\right) + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\frac{\hbar^2\vec{q}^2}{2m} + NU(q)\right)\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right) + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger + \hat{b}_{-\vec{q}}\hat{b}_{\vec{q}}\right). \quad [64]$$

Finally, we put this result into the total transformed Hamiltonian from equation [53] to find

$$\hat{H} = \frac{N(N-1)U(0)}{2} + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\frac{\hbar^2\vec{q}^2}{2m} + NU(q)\right)\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right) + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}} NU(q)\left(\hat{b}_{\vec{q}}\hat{b}_{-\vec{q}} + \hat{b}_{\vec{q}}^\dagger \hat{b}_{-\vec{q}}^\dagger\right) + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\epsilon_{\vec{q}} - \frac{\hbar^2\vec{q}^2}{2m} - NU(q)\right)\left(\frac{\hat{N} - \hat{n}_{\vec{0}} + \hat{n}_{\vec{q}}}{N}\right) \quad [65]$$

where we have moved around our terms to show the similarity to the untransformed Hamiltonian from equation [52]. In fact, except for the last term, this is the exact form of the original Hamiltonian. So the only question left is: is that last term small?

We immediately recognize that the last fraction is small. Since equations [2] and [3] tell us that the terms in the numerator roughly cancel, that makes the fraction $\mathcal{O}\left(\frac{1}{N}\right)$. While $\left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right)$ from the second term in equation [65] is much larger: $\mathcal{O}(1)$.[8] That means we can safely neglect our final term with its tiny fraction, unless the first part of that final term is much *larger* than the first part of the second term.

Plainly, $\frac{\hbar^2\vec{q}^2}{2m}$ and $NU(q)$ in our final term are no larger than the *exact same* expressions in the second term. The size of $\epsilon_{\vec{q}}$ however, is not as clear. Could it be that $\epsilon_{\vec{q}}$ is much larger than the other expressions?

$$\epsilon_{\vec{q}} = \frac{\hbar^2\vec{q}^2}{2m}\sqrt{1 + \frac{4mNU(q)}{\hbar^2\vec{q}^2}} = \sqrt{\left(\frac{\hbar^2\vec{q}^2}{2m}\right)^2 + 2\frac{\hbar^2\vec{q}^2}{2m}NU(q)} \leq \sqrt{\left(\frac{\hbar^2\vec{q}^2}{2m}\right)^2 + 2\frac{\hbar^2\vec{q}^2}{2m}NU(q) + \left(NU(q)\right)^2} = \frac{\hbar^2\vec{q}^2}{2m} + NU(q)\,, \quad [66]$$

guaranteeing that $\epsilon_{\vec{q}}$ is no larger than the first part of our second term, which makes the second term $\mathcal{O}(N)$ times larger than the final term. This means the final term can indeed be neglected safely.

As we had hoped, we find that the error in our final result is no larger than the errors in the commutators of $\hat{b}$. In short, the Bogoliubov transformation leads to an accurate approximation of our original Hamiltonian that introduces no larger errors than previous steps.

3.4.2 Commutation relations for d

We needed $\hat{b}$ to be roughly bosonic, since it required a number of commutations of $\hat{b}$-terms to construct our final Hamiltonian. Strictly speaking, this is not the case for $\hat{d}$. In fact, we don't need any commutations to determine the energy levels of the quasi-particles that are created and annihilated by $\hat{d}$-operators. However, we are not just interested in the energy levels. We are looking for an operator that can describe the complete behavior of our system. So we need $\hat{d}$ to be roughly bosonic to be able to use it for anything beyond the most basic applications.

The check for the bosonic behavior of $\hat{d}$ is fairly straightforward, but it takes some work. We find for our first type of commutator

[8] The trivial case where our second term is not $\mathcal{O}(1)$ because all particles are in the ground state poses no problem, since that means our last term is also zero.

$$\begin{aligned}\left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{\vec{k}}^\dagger\right] &= u_{\vec{q}}u_{\vec{k}}\left[\hat{b}_{\vec{q}}^\dagger,\hat{b}_{\vec{k}}^\dagger\right] + u_{\vec{q}}v_{\vec{k}}\left[\hat{b}_{\vec{q}}^\dagger,\hat{b}_{-\vec{k}}\right] \\ &+v_{\vec{q}}u_{\vec{k}}\left[\hat{b}_{-\vec{q}},\hat{b}_{\vec{k}}^\dagger\right] + v_{\vec{q}}v_{\vec{k}}\left[\hat{b}_{-\vec{q}},\hat{b}_{-\vec{k}}\right] \\ &= u_{\vec{q}}v_{\vec{k}}\left[\hat{b}_{\vec{q}}^\dagger,\hat{b}_{-\vec{k}}\right] + v_{\vec{q}}u_{\vec{k}}\left[\hat{b}_{-\vec{q}},\hat{b}_{\vec{k}}^\dagger\right].\end{aligned} \quad [67]$$

Where the first and last term in the first equivalence are zero because of the commutators from equation [33].

If $\vec{k}=\vec{q}$:

$$\left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{\vec{q}}^\dagger\right] = 0\,. \quad [68]$$

If $\vec{k}=-\vec{q}$:

$$\begin{aligned}\left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{-\vec{q}}^\dagger\right] &= u_{\vec{q}}v_{\vec{q}}\left(\left[\hat{b}_{\vec{q}}^\dagger,\hat{b}_{\vec{q}}\right] + \left[\hat{b}_{-\vec{q}},\hat{b}_{-\vec{q}}^\dagger\right]\right) \\ &= u_{\vec{q}}v_{\vec{q}}\left(\frac{\hat{n}_{\vec{q}}-\hat{n}_{\vec{0}}}{N} + \frac{\hat{n}_{\vec{0}}-\hat{n}_{-\vec{q}}}{N}\right) \\ &= u_{\vec{q}}v_{\vec{q}}\frac{\hat{n}_{\vec{q}}-\hat{n}_{-\vec{q}}}{N},\end{aligned} \quad [69]$$

where we have used that $u_{\vec{q}}=u_{-\vec{q}}$ and $v_{\vec{q}}=v_{-\vec{q}}$, as well as the commutator from equation [35]. For other values of $\vec{k}$:

$$\left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{\vec{k}}^\dagger\right] = u_{\vec{q}}v_{\vec{k}}\frac{\hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{k}}}{N} - v_{\vec{q}}u_{\vec{k}}\frac{\hat{a}_{\vec{k}}^\dagger\hat{a}_{-\vec{q}}}{N}, \quad [70]$$

as follows from the commutator in equation [34].

Commutators of the form $\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{k}}\right]$ give analogous results, so that we only have one more type of commutator to consider

$$\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{k}}^\dagger\right] = u_{\vec{q}}u_{\vec{k}}\left[\hat{b}_{\vec{q}},\hat{b}_{\vec{k}}^\dagger\right] + v_{\vec{q}}v_{\vec{k}}\left[\hat{b}_{-\vec{q}}^\dagger,\hat{b}_{-\vec{k}}\right], \quad [71]$$

so that for $\vec{k}=\vec{q}$

$$\begin{aligned}\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{q}}^\dagger\right] &= u_{\vec{q}}^2\left[\hat{b}_{\vec{q}},\hat{b}_{\vec{q}}^\dagger\right] + v_{\vec{q}}^2\left[\hat{b}_{-\vec{q}}^\dagger,\hat{b}_{-\vec{q}}\right] \\ &= u_{\vec{q}}^2\frac{\hat{n}_{\vec{0}}-\hat{n}_{\vec{q}}}{N} - v_{\vec{q}}^2\frac{\hat{n}_{\vec{0}}-\hat{n}_{-\vec{q}}}{N} \\ &\approx u_{\vec{q}}^2 - v_{\vec{q}}^2 = 1\,.\end{aligned} \quad [72]$$

Here we have applied the conclusions we could draw from equation [39] to make our approximation. Let us also quickly clarify that last step. Using our definitions from equation [58], we know that

$$u_{\vec{q}}^2 - v_{\vec{q}}^2 = \frac{1}{4}\left(x_{\vec{q}}+\frac{1}{x_{\vec{q}}}\right)^2 - \frac{1}{4}\left(x_{\vec{q}}-\frac{1}{x_{\vec{q}}}\right)^2 = 1\,. \quad [73]$$

Continuing for $\vec{k}=-\vec{q}$

$$\begin{aligned}\left[\hat{d}_{\vec{q}},\hat{d}_{-\vec{q}}^\dagger\right] &= u_{\vec{q}}^2\left[\hat{b}_{\vec{q}},\hat{b}_{-\vec{q}}^\dagger\right] + v_{\vec{q}}^2\left[\hat{b}_{-\vec{q}}^\dagger,\hat{b}_{\vec{q}}\right] \\ &= \left(u_{\vec{q}}^2 - v_{\vec{q}}^2\right)\left[\hat{b}_{\vec{q}},\hat{b}_{-\vec{q}}^\dagger\right] \\ &= -\frac{\hat{a}_{-\vec{q}}^\dagger\hat{a}_{\vec{q}}}{N}.\end{aligned} \quad [74]$$

Finally, for other values of $\vec{k}$

$$\begin{aligned}\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{k}}^\dagger\right] &= u_{\vec{q}}u_{\vec{k}}\left[\hat{b}_{\vec{q}},\hat{b}_{\vec{k}}^\dagger\right] + v_{\vec{q}}v_{\vec{k}}\left[\hat{b}_{-\vec{q}}^\dagger,\hat{b}_{-\vec{k}}\right] \\ &= -u_{\vec{q}}u_{\vec{k}}\frac{\hat{a}_{\vec{k}}^\dagger\hat{a}_{\vec{q}}}{N} + v_{\vec{q}}v_{\vec{k}}\frac{\hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{k}}}{N}.\end{aligned} \quad [75]$$

To summarize, we find the following set of commutators

$$\begin{aligned}&1)\ \left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{\vec{q}}^\dagger\right] = 0 \\ &2)\ \left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{-\vec{q}}^\dagger\right] = u_{\vec{q}}v_{\vec{q}}\frac{\hat{n}_{\vec{q}}-\hat{n}_{-\vec{q}}}{N} \\ &3)\ \left[\hat{d}_{\vec{q}}^\dagger,\hat{d}_{\vec{k}\neq\pm\vec{q}}^\dagger\right] = u_{\vec{q}}v_{\vec{k}}\frac{\hat{a}_{\vec{q}}^\dagger\hat{a}_{-\vec{k}}}{N} - v_{\vec{q}}u_{\vec{k}}\frac{\hat{a}_{\vec{k}}^\dagger\hat{a}_{-\vec{q}}}{N} \\ &4)\ \left[\hat{d}_{\vec{q}},\hat{d}_{\vec{q}}^\dagger\right] = \frac{\hat{n}_{\vec{0}}}{N} - \frac{u_{\vec{q}}^2\hat{n}_{\vec{q}} - v_{\vec{q}}^2\hat{n}_{-\vec{q}}}{N} \\ &5)\ \left[\hat{d}_{\vec{q}},\hat{d}_{-\vec{q}}^\dagger\right] = -\frac{\hat{a}_{-\vec{q}}^\dagger\hat{a}_{\vec{q}}}{N} \\ &6)\ \left[\hat{d}_{\vec{q}},\hat{d}_{\vec{k}\neq\pm\vec{q}}^\dagger\right] = v_{\vec{q}}v_{\vec{k}}\frac{\hat{a}_{-\vec{q}}^\dagger\hat{a}_{-\vec{k}}}{N} - u_{\vec{q}}u_{\vec{k}}\frac{\hat{a}_{\vec{k}}^\dagger\hat{a}_{\vec{q}}}{N}.\end{aligned} \quad [76]$$

Commutators 1 is bosonic and commutator 5 gives a correction of the same form as the commutators for $\hat{b}$, meaning it is small enough to neglect in the same way.

Being able to neglect all the other terms though, depends on the size of *u* and *v*. Even our casual conclusion in equation [72] that commutator 4 is roughly equal to 1 hinges on that point. If *u* and *v* are each $O(1)$, all troubling commutator terms are much smaller than 1 and we can safely say $\hat{d}$ is roughly bosonic as well. However, we *cannot* say that, because *u* and *v* may be much larger than 1. As we can see from equation [56], if

$$NU(q) \gg \frac{\hbar^2\vec{q}^2}{4m}, \quad [77]$$

then *u* and *v* can become much larger than 1. In short, we cannot guarantee that our commutators will remain roughly bosonic.[9]

This brings us to the final price we have to pay for our approximation. While we have found a way to guarantee particle conservation, we have lost the bosonic behavior of our ‘particles’ in the process. Our only hope is that we can do the same thing that was done in the conventional approximation: Neglect the errors.

Let us take a look at the four troublesome terms from equation [76]: Commutators 2 and 3, the second term from commutator 4 and finally commutator 6.

$$\begin{aligned}\hat{d}_{\vec{q}}^\dagger\hat{d}_{-\vec{q}}^\dagger &= u_{\vec{q}}^2\hat{b}_{\vec{q}}^\dagger\hat{b}_{-\vec{q}}^\dagger + u_{\vec{q}}v_{\vec{q}}\left(\hat{b}_{\vec{q}}^\dagger\hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}\hat{b}_{-\vec{q}}^\dagger\right) \\ &\quad + v_{\vec{q}}^2\hat{b}_{-\vec{q}}\hat{b}_{\vec{q}} \\ &\geq u_{\vec{q}}v_{\vec{q}}\left(\hat{b}_{\vec{q}}^\dagger\hat{b}_{\vec{q}} + \hat{b}_{-\vec{q}}^\dagger\hat{b}_{-\vec{q}}\right),\end{aligned} \quad [78]$$

where we have used equations [55] and [35]. We have also used the fact that all our operators create positive terms when applied to a superfluid system. This allows us to order our operators as larger and smaller – although this is not technically a meaningful distinction. Then from [78]

[9] In fact, we could show that *u* and *v* will grow large for sufficiently large occupations of one-particle excited states. There the rough equality holds $u_{\vec{q}} \approx v_{\vec{q}} \sim \sqrt{n_{\vec{q}}}$. It would go too far to derive this equation here, but suffice it to say that our problem is more than just a mathematical oddity.

$$u_{\vec{q}}v_{\vec{q}}\left(\hat{b}_{\vec{q}}^{\dagger}\hat{b}_{\vec{q}}+\hat{b}_{-\vec{q}}^{\dagger}\hat{b}_{-\vec{q}}\right)\approx u_{\vec{q}}v_{\vec{q}}\left(\hat{n}_{\vec{q}}+\hat{n}_{-\vec{q}}\right) \\ \geq N\left[\hat{d}_{\vec{q}}^{\dagger},\hat{d}_{-\vec{q}}^{\dagger}\right], \qquad [79]$$

where besides the second commutator from equation [76], we have used equations [31] and [6], and we inserted $\hat{N}=N$. Similarly, for commutator 3

$$\hat{d}_{\vec{q}}^{\dagger}\hat{d}_{\vec{k}\neq\pm\vec{q}}^{\dagger}\geq u_{\vec{q}}v_{\vec{k}}\hat{b}_{\vec{q}}^{\dagger}\hat{b}_{-\vec{k}}+u_{\vec{k}}v_{\vec{q}}\hat{b}_{\vec{k}}^{\dagger}\hat{b}_{-\vec{q}} \\ \approx u_{\vec{q}}v_{\vec{k}}\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{-\vec{k}}+u_{\vec{k}}v_{\vec{q}}\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{-\vec{q}} \\ \geq N\left[\hat{d}_{\vec{q}}^{\dagger},\hat{d}_{\vec{k}\neq\pm\vec{q}}^{\dagger}\right], \qquad [80]$$

where we have also used equation [34]. We then look at the second term from commutator 4

$$\hat{d}_{\vec{q}}\hat{d}_{\vec{q}}^{\dagger}\geq u_{\vec{q}}^{2}\hat{b}_{\vec{q}}^{\dagger}\hat{b}_{\vec{q}}+v_{\vec{q}}^{2}\hat{b}_{-\vec{q}}^{\dagger}\hat{b}_{-\vec{q}} \\ \approx u_{\vec{q}}^{2}\hat{n}_{\vec{q}}+v_{\vec{q}}^{2}\hat{n}_{-\vec{q}} \\ \geq N\left(\frac{\hat{n}_{\vec{0}}}{N}-\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{q}}^{\dagger}\right]\right), \qquad [81]$$

using equation [35] again. Finally, for commutator 6

$$\hat{d}_{\vec{q}}\hat{d}_{\vec{k}\neq\pm\vec{q}}^{\dagger}\geq u_{\vec{q}}u_{\vec{k}}\hat{b}_{\vec{k}}^{\dagger}\hat{b}_{\vec{q}}+v_{\vec{q}}v_{\vec{k}}\hat{b}_{-\vec{q}}^{\dagger}\hat{b}_{-\vec{k}} \\ \approx u_{\vec{q}}u_{\vec{k}}\hat{a}_{\vec{k}}^{\dagger}\hat{a}_{\vec{q}}+v_{\vec{q}}v_{\vec{k}}\hat{a}_{-\vec{q}}^{\dagger}\hat{a}_{-\vec{k}} \\ \geq N\left[\hat{d}_{\vec{q}},\hat{d}_{\vec{k}\neq\pm\vec{q}}^{\dagger}\right], \qquad [82]$$

here using equation [34] once more.

What we see then is that every one of our commutators is at least a factor of *N* smaller than the products of the operators that feature in the commutator. This means that, unless there is an almost total cancellation of the leading terms, we will always be able to neglect the errors in the commutators. While they may not always be smaller than 1, they will be a factor of *N* smaller than our leading terms.

This leaves us with the same type of error that was found in the conventional approximation as discussed in §2.1.2: an error of one in *N* that seems insignificant, but that is nevertheless worrying because it violates one of the fundamental laws of physics. We have simply exchanged breaking conservation of particle number for changing the fundamental nature of the particles themselves.

We are unfortunately not able to resolve this issue. However, even with this flaw, our method has a number of distinct advantages over the conventional approximation. On top of that, while the obvious ways around our problem do not lead to complete solutions, they do highlight and build upon the advantages of this approximation. The details of these advantages are discussed in the sidebar ‘Observations on the d commutators’.

Observations on the d commutators

In §3.4.2, we considered the commutators of $\hat{d}$ from equation [76] closely enough to assure ourselves that the relative size of our errors was no larger than in the conventional approximation. However, there is more to consider when looking at these commutators. We will touch on three aspects here, without going into all the technical details and mathematical derivations. First, whether we can find values for the occupations of one-particle excited states for which our commutators are still roughly bosonic. Second, whether the commutators become bosonic when we assume spatial symmetry in occupation of one-particle states, i.e. $n_{\vec{q}}\approx n_{-\vec{q}}$. Third, if we could simply describe $\hat{d}^{\dagger}$ as creating ‘particles’ that are neither bosonic nor fermionic, so that we can simply take all the commutator terms into account.

The roughly bosonic zone

We can plainly see that our commutators from equation [76] are roughly bosonic when we assume that the involved one-particle excited states only have $\mathcal{O}(1)$ occupations. The factors of $\frac{1}{N}$ in these commutators will then guarantee that all errors are much smaller than 1.

When the occupations of our one-particle excited states are much larger than 1, this is not so plain, but we can use a number of approximations to simplify our system. Since we are only looking at orders of magnitude here, we can suffice with fairly rough approximations. In particular, we know that for these high values we can say $v_{\vec{q}}\sim\sqrt{n_{\vec{q}}}$. Then, since $\sqrt{n_{\vec{q}}}\gg 1$, we can see from equation [56] that $u_{\vec{q}}\approx v_{\vec{q}}$, because the equal first term $\frac{1}{2}\left(1+\frac{4mNU(q)}{\hbar^{2}\vec{q}^{2}}\right)^{1/4}$ in both *u* and *v* must dominate. So we can say that, for $\sqrt{n_{\vec{q}}}\gg 1$

$$u_{\vec{q}}\approx v_{\vec{q}}\sim\sqrt{n_{\vec{q}}}\,. \qquad [83]$$

If we apply our commutators from [76] to a system where the one-particle excited state occupations are high enough, they will all yield terms of a similar form. Using the first halves of commutators 2 and 3 as examples, we find terms

$$u_{\vec{q}}v_{\vec{q}}\frac{n_{\vec{q}}}{N}\sim\frac{n_{\vec{q}}^{2}}{N} \qquad [84]$$

and

$$u_{\vec{q}}v_{\vec{k}}\frac{\sqrt{n_{\vec{q}}+1}\sqrt{n_{-\vec{k}}}}{N}\sim\frac{n_{\vec{q}}\sqrt{n_{\vec{k}}n_{-\vec{k}}}}{N}, \qquad [85]$$

with similar terms for commutators 4 and 6. So we could guarantee that all our commutator terms are much smaller than 1 by requiring for the one-particle excited state occupations

$$n_{\vec{q}\neq\vec{0}} \ll \sqrt{N}\,. \qquad [86]$$

Our roughly bosonic zone extends to anywhere the condition from [86] holds. In fact, the only occupations that have to be sufficiently small are the ones actually involved in the commutations, meaning the roughly bosonic zone covers even more states. Even so, this is a much more stringent requirement than the original one from equation [3]. Nevertheless, it is still an improvement over the conventional approximation, which *always* breaks particle conservation by adding or removing two particles regardless of requirements.

Symmetry

One striking feature of all the troubling commutators in [76] is the symmetry in the terms we subtract from each other. This symmetry becomes even more striking when we only consider the situation with high one-particle excited state occupations where [83] holds. We could then, for example, compactify commutator 3 from [76] into

$$\left[\hat{d}^\dagger_{\vec{q}}, \hat{d}^\dagger_{\vec{k}\neq\pm\vec{q}}\right] \sim \frac{\sqrt{n_{\vec{q}}n_{\vec{k}}}}{N}\left(\hat{a}^\dagger_{\vec{q}}\hat{a}_{-\vec{k}} - \hat{a}^\dagger_{\vec{k}}\hat{a}_{-\vec{q}}\right). \qquad [87]$$

[10]

This in itself does not tell us anything if there is no relationship between the occupation of the $\vec{q}$-state and the $-\vec{q}$-state (nor the $\vec{k}$-state and $-\vec{k}$-state). However, we could assume that there is no preferred direction to the momentum of our particles. In that case, we would expect roughly the same amount of particles in either state. So wouldn't the commutator then cancel since $n_{\vec{q}} \approx n_{-\vec{q}}$ and thus applying $\hat{a}^\dagger_{\vec{q}}$ or $\hat{a}_{-\vec{q}}$ would give roughly the same particle count?

Unfortunately, 'roughly the same particle count' turns out to be very different from 'exactly the same particle count'. Specifically, if we assume our particles with momentum $|\vec{q}|$ are randomly distributed between $\vec{q}$ and $-\vec{q}$, we expect a normal distribution.[11] That means the uncertainty in the occupation of either state will be $\mathcal{O}\left(\sqrt{n_{\vec{q}}}\right)$. Meaning the difference between the occupations could be $\mathcal{O}\left(\sqrt{n_{\vec{q}}}\right)$ as well. So [87] could be of order

$$\frac{\sqrt{n_{\vec{q}}n_{\vec{k}}}}{N}\left(\sqrt{n_{\vec{k}}} + \sqrt{n_{\vec{q}}}\right) = \frac{n_{\vec{k}}\sqrt{n_{\vec{q}}} + n_{\vec{q}}\sqrt{n_{\vec{k}}}}{N}\,. \qquad [88]$$

And for this to be much smaller than one, we would still need the requirement

$$n_{\vec{q}\neq\vec{0}} \ll N^{\frac{2}{3}}\,. \qquad [89]$$

Unsurprisingly, looking at our other commutators yields similar results. So this approximation expands our roughly bosonic zone a bit. It can also show that our actual errors are significantly smaller than the upper limits given in equations [78] through [82]. However, at the end of the day, assuming this symmetry is not enough to guarantee bosonic behavior in all the states we are considering. In particular, it does not cover the lowest energy one-particle excited states, which usually have occupations $\mathcal{O}\left(N^{\frac{2}{3}}\right)$. (18)

As a final worrying thought, consider that in equation [88] we make the same mistake that is made in the conventional approximation: We ignore the fact that our creation and annihilation operators don't just count particles, but change the system itself as well. Admittedly, we still preserve particle conservation in this case and we only use this approximation on terms that are already small enough to neglect. However, this does go to show that having non-zero commutators makes for a very complicated system.

Non-bosonic 'particles'

That observation leads us neatly to our final idea: accepting these new quasi-particles created by $\hat{d}^\dagger$ as being neither bosonic nor fermionic. In that case, the non-zero commutators would simply be considered one of their physical features.

However, as simple as this idea seems, it brings with it a host of problems. First and foremost is the fact that none of our rules for bosons are guaranteed to work for our new particles. We do not know if they are governed by Bose-Einstein statistics; we do not know if they have integer spin; ironically, first principles do not even require that the number of these 'particles' is conserved. All those properties follow from the fact that what $\hat{d}^\dagger$ creates is approximately bosonic.

Second, even if we knew the properties of these new types of particles, working with them would still be hideously complex. Every commutation would complicate a calculation immensely and give rise to all kinds of additional terms. The simplest operations would take longer and become harder, while more complex calculations would become virtually impossible to do by hand.

However, the upshot of all this is not that we shouldn't

[10] We use the fact that [87] describes the leading term, as opposed to the term for the difference between *u* and *v*. A more thorough calculation would show that under our assumptions that term is smaller by roughly a factor of $\sqrt{n_{\vec{q}}} + \sqrt{n_{\vec{k}}}$.

[11] Technically, the particles are distributed among many more states with an equally large momentum (at least six, since our system has a six-sided symmetry in the $\vec{x}$, $-\vec{x}$, $\vec{y}$, $-\vec{y}$, $\vec{z}$ and $-\vec{z}$ directions).

consider our non-bosonic commutator terms, but that we *could* do it, if we really wanted to. This is one final advantage of our method over the conventional approximation: We know exactly what our errors are. If we are ever unsure whether neglecting the non-bosonic commutator terms is justified, we can choose to take them into account and compare the results. In those few cases where these tiny errors might have significant results, we can determine their exact significance.

So in the end, our method breaks a rule as fundamental as conservation of particles. But unlike the conventional approximation, it has a clearly defined zone where this fundamental rule still roughly holds and commutation relations are approximately bosonic. And even outside that zone there is a clear and unambiguous way to quantify the effect of an error and make sure it has not influenced the results.

3.5 Results

In the previous chapters, we have described a model of superfluid spin-polarized atomic Hydrogen. We looked at the conventional approximation of this system and found it to be flawed, because it breaks particle conservation. This led us to introduce the operator

$$\hat{b}_{\vec{q}\neq\vec{0}} \equiv \frac{\hat{a}_{\vec{0}}^{\dagger}\hat{a}_{\vec{q}}}{\sqrt{N}} \Rightarrow \hat{b}_{\vec{q}\neq\vec{0}}^{\dagger} = \frac{\hat{a}_{\vec{q}}^{\dagger}\hat{a}_{\vec{0}}}{\sqrt{N}} ,$$

which describes the dynamic parts of our system in terms of particles changing momentum instead of being created and annihilated.

Describing the Hamiltonian in terms of $\hat{b}$ led us to a description of our system that did not break particle conservation. However, we had to pay two prices for this. First, we were forced to approximate not just the interaction potential $\hat{V}$, but also the kinetic Hamiltonian $\hat{H}_0$. Second, unlike the original annihilation operator $\hat{a}$, both our $\hat{b}$-operator and the derived $\hat{d}$-operator, which is used to describe the particle content of the system, have a non-bosonic component.

Fortunately, we were able to show that both of these effects are small, are easily explained and do not lead to larger errors in our final results. This means we now have a solid alternative to the conventional approximation of these superfluids, leading to a final description of the system in terms of the Hamiltonian

$$\begin{aligned}\hat{H} = {} & \frac{N(N-1)U(0)}{2} \\ & + \frac{1}{2}\sum_{\vec{q}\neq\vec{0}}\left(\epsilon_{\vec{q}} - \frac{\hbar^2\vec{q}^2}{2m} - NU(q)\right) \\ & + \sum_{\vec{q}\neq\vec{0}} \epsilon_{\vec{q}}\hat{d}_{\vec{q}}^{\dagger}\hat{d}_{\vec{q}} \ .\end{aligned}$$

Although it trades breaking particle conservation for breaking bosonic commutation, this Hamiltonian is very similar to the one found in the conventional approximation. In fact, the energy spectrum described has the exact same form as in the conventional approximation. The last term similarly creates and annihilates quasi-particles with energy $\epsilon_{\vec{q}}$. The only difference is that our quasi-particles are of a slightly different nature than in the conventional approximation; the dynamic part of the system is now described as a collection of momentum changes for existing particles.

In short, we have shown that it is possible to calculate the properties of a superfluid system with particle conservation by describing it in terms of momentum changes rather than particle creation and annihilation.

3.6 Further research

Although our description of superfluid systems is fairly complete, three major questions still remain: how accurate is it, can this accuracy be improved and how widely applicable is our method? These are the questions we will quickly expand on below.

3.6.1 Testing the approximation accuracy

We already know that the conventional approximation of superfluids has withstood the test of time, so the question of how accurate our method is might more aptly be posed as: which method is the best, the conventional approximation or our new alternative? Although 'best' is obviously a subjective term, studying the properties of both methods further could teach us about the strengths and weaknesses of each.

In particular, we could create simulations of our system for different *N*, *L* and $U(q)$ to see how close the results are to those yielded by each approximation. Choosing a particular interaction strength $U(q)$ would determine enough about the system to make a simulation possible. The challenge of course is that the total number of particles *N* needs to be large enough for our approximations to be meaningful. On the other hand, it needs to be small enough that it can be simulated in a reasonable time. Finding a balance between the two that yields meaningful results is challenging, but becomes ever easier with increasing computing power.

3.6.2 Improving the approximation accuracy

Even more useful than ascertaining the accuracy of our approximation would be to actually improve upon it. Specifically, the introduction of $\hat{b}$ causes two types of errors. Decreasing either one would make our approximation more exact.

First of all there are the inherent errors caused by the $\hat{b}$-operator algebra being not-exactly bosonic. These errors seem to be unavoidable without radical changes. That said, there may be ways to decrease these errors or their effects by changing the definition of $\hat{b}$ slightly.

Secondly there are errors caused by the normalizing factor $\frac{1}{\sqrt{N}}$ in $\hat{b}$ not being the exact factor needed to normalize the creation or annihilation of a second particle.

As mentioned in §3.2, our approximation would actually be more accurate if we could use $n_{\vec{b}}$ instead of N for our normalizing factor. This is not trivial to do because $n_{\vec{b}}$ is not a constant, but it may still be possible. After all, we know exactly what we want our added term in $\hat{b}$ – as compared to $\hat{a}$ – to do: add or remove a particle from the ground state without adding a constant factor. So in a non-technical way, we already know what the normalizing factor should be. The question that remains is how to put this non-technical concept into a mathematical mold that actually works in our current system. This is a challenging task, but finding a way to do this could remove errors of this second kind completely.

3.6.3 Generalizing the approximation method

We have developed a solid technique for describing our system in terms of particle momentum changes. But while we have derived some simple properties of the core operator $\hat{b}$, we have looked at only enough for our specific purposes.

An interesting question could be if $\hat{b}$ is more widely applicable. What are its general properties? And how does it relate to the more conventional raising and lowering operators, which seem fairly similar? Most importantly: what other types of systems could be described more accurately or compactly using our new operator? Is it of more general use than just for these superfluids?

Specifically, applying a variation on our method to superconductors might offer an alternative to the conventional BCS-theory of superconductivity, which breaks particle conservation just like the conventional method for superfluids. (7)

4 Acknowledgements

There are some times when a research project is just perfect; times when everything runs smoothly and simply falls into place; times when you get so caught up in what you do that you're done before you know it.

This was not one of those times.

In fact, finishing this research and this text has been one of the longest and hardest processes of my life.

But even knowing I spent bouts of work spread over four years on a supposed six-month project, it always felt like a joy coming back to it. And the reason for that was undoubtedly my supervisor: Wim Beenakker.

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[12] The complimentary mug with "I'm ready to give it the full 30% today!" notwithstanding.

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