Interacting Bosons

- Interaction operators in 2^{nd} quantization
- the Bose-Hubbard model
- Superfluidity
  - ↳ Bogoliubov's approach
  - ↳ Landau - Ginzburg's approach.

Two-body operators

In these notes we are going to take a first look at interacting systems of identical particles. Interactions are the reason behind most of the remarkable effects in condensed matter. But they are also much harder to treat. There are very few exactly soluble interacting problems, so most of the progress is usually based on approximations. We will see some of these in these notes.

A typical interacting Hamiltonian may look like

$$H = \sum_i \left\{ \frac{p_i^2}{2m} + U(x_i) \right\} + \frac{1}{2} \sum_{i \neq j} V(x_i, x_j) \qquad (1)$$

the first term is the non-interacting (free) Hamiltonian, where $U(x)$ is an external potential. The second term is a sum of 2-body interactions. Examples include the Coulomb repulsion

$$V(x_i - x_j) = \frac{e^2}{|x_i - x_j|} \qquad (2)$$

or a hard sphere interaction

$$V(x_i - x_j) = \begin{cases} V_0 & \text{if } |x_i - x_j| < a \\ 0 & \text{otherwise} \end{cases} \qquad (3)$$

Oh! I forgot to say: the factor of 1/2 in (1) is placed to avoid double counting.

We have learned how to write one-body terms in second quantization. For instance, the first term of Eq (1) may be written as

$$\mathcal{H}_1 = \int d^3x \, \psi^\dagger(x) \left[-\frac{\nabla^2}{2m} + U(x) \right] \psi(x) \qquad (4)$$

where $\psi(x)$ is the field operator. The last term makes sense:

$$U(x) \, \psi^\dagger(x) \psi(x) = (\text{potential } U) \times (\text{density of particles}).$$

If a certain region of space has a high density, in that region $U(x)$ would give a big contribution.

Following this intuition one may suspect that the 2-body interaction could be written as

$$V = \frac{1}{2} \int d^3x \, d^3y \; V(x, y) \, \psi^\dagger(x) \psi(x) \psi^\dagger(y) \psi(y) \qquad (\text{wrong}) \qquad (5)$$

This guess is almost correct; it just has one mistake: it contains a self-interaction, which is unphysical. What that means is that, if we define

$$|r\rangle = \psi^\dagger(r) |0\rangle \qquad (6)$$

which is a state with exactly one particle at position r, then $V|r\rangle \neq 0$. But it should be zero because a 2-body interaction should require 2 bodies!

To understand this matter further, let us manipulate (5) as follows. We use the commutation relations

$$[\psi(x), \psi^\dagger(y_1)]_\varepsilon = \psi(x)\psi^\dagger(y_1) - \varepsilon\,\psi^\dagger(y_1)\psi(x)$$
$$= \delta(x - y_1) \qquad (7)$$

where, recall, $\varepsilon = +1$ for Bosons and $\varepsilon = -1$ for Fermions.

We use this to write (5) as

$$V = \frac{1}{2}\int d^3x\, d^3y_1\; V(x, y_1)\, \psi^\dagger(x)\left[\delta(x-y_1) + \varepsilon\,\psi^\dagger(y_1)\psi(x)\right]\psi(y_1)$$

$$= \frac{1}{2}\int d^3x\; V(x, x)\, \psi^\dagger(x)\psi(x) +$$

$$+\frac{1}{2}\int d^3x\, d^3y_1\; V(x, y_1)\,\varepsilon\,\psi^\dagger(x)\psi^\dagger(y_1)\psi(x)\psi(y_1) \qquad (8)$$

A-HA! The first term is precisely the self-interaction, as it depends on $V(x, x)$. We can also tell that the second term is indeed a two-body interaction because it has $\psi(x)\psi(y_1)$ on the right. these are 2 annihilation operators, so whenever they act on a state with 0 or 1 particles (like (6)), it will give zero.

It turns out that, indeed, the correct way of writting down the second quantized version of a 2-body operator is by keeping only the second term in Eq (8).

there is still a ε there, which we can get rid by writing

$$\varepsilon\, \psi(x)\, \psi(y_1) = \psi(y_1)\, \psi(x)$$

then we finally get our pretty final result:

$$\boxed{\mathcal{V} = \frac{1}{2} \int d^3x\, d^3y_1\, v(x, y_1)\, \psi^\dagger(x)\, \psi^\dagger(y_1)\, \psi(y_1)\, \psi(x)} \qquad (9)$$

To read the order of the operations you must look at $\mathcal{V}$ backwards. So first you annihilate in x then you annihilate in y_1. Afterwards, you create in reverse order: first you create in y_1 then in x. there is an easy way to remember this: first you take off your shoes, then your socks. But when putting them back on, you put your socks first, then your shoes. For Bosons this order is irrelevant since $\psi(y_1)\psi(x) = \psi(x)\psi(y_1)$. But for Fermions, if you get the order wrong, you change the sign. this means you could turn a repulsive interaction into an attractive one! So be careful

This formula describes a sum of scattering events, where

Translation invariance and Fourier space

Two-body operators in other bases

We know how to change basis in second quantization: creation operators transform like kets. that is, if

$$|x\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|x\rangle \tag{10}$$

then

$$\psi^\dagger(x) = \sum_\alpha a_\alpha^\dagger \langle\alpha|x\rangle \tag{11}$$

Taking the adjoint:

$$\psi(x) = \sum_\alpha a_\alpha \langle x|\alpha\rangle \tag{12}$$

Substituting this in (9) we get

$$\hat{V} = \frac{1}{2}\int d^3x\, d^3y_1 \sum_{\alpha,\beta,\delta,\gamma} V(x,y_1)\, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \underbrace{\langle\alpha|x\rangle\langle\beta|y_1\rangle\langle y_1|\delta\rangle\langle x|\gamma\rangle}_{\langle\alpha,\beta|x,y_1\rangle\langle x,y_1|\gamma,\delta\rangle}$$

Now recall that $V(x,y_1)$ is actually the eigenvalue of the 2-body operator $\hat{V}$ in the $|x,y_1\rangle$ basis:

$$\hat{V}|x,y_1\rangle = V(x,y_1)\,|x,y_1\rangle$$

This means we can reverse the argument and write

$$V(x,y_1)\langle\alpha,\beta|x,y_1\rangle = \langle\alpha,\beta|\hat{V}|x,y_1\rangle$$

I get tired of q. I prefer to use k. So let me write

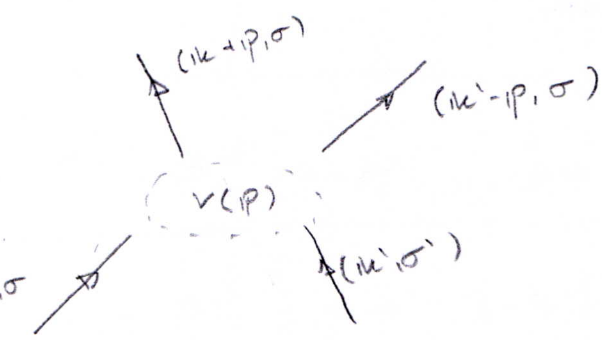
$$\boxed{V = \frac{1}{2\,\mathrm{vol}} \sum_{\substack{k\,k'\\ p}} v(p)\, a^{\dagger}_{k+p}\, a^{\dagger}_{k'-p}\, a_{k'}\, a_{k}} \tag{18}$$

Now we can interpret p as the momentum transferred during the scattering event. And $v(p)$ is the amplitude of transferring momentum p.

If we also have spin in the game, but $\hat{v}$ is spin independent, then Eq (18) changes simply as

$$\boxed{V = \frac{1}{2\,\mathrm{vol}} \sum_{\substack{k\,k'\,p\\ \sigma\,\sigma'}} v(p)\, a^{\dagger}_{k+p,\sigma}\, a^{\dagger}_{k'-p,\sigma'}\, a_{k'\sigma'}\, a_{k\sigma}} \tag{19}$$

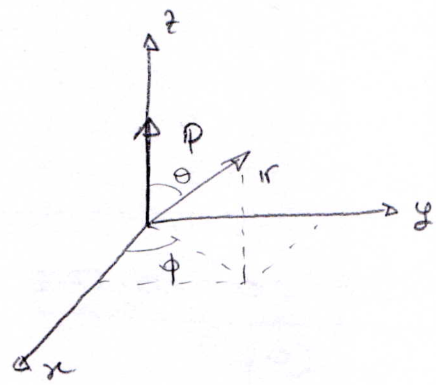
which we can draw as



Fourier representation of Coulomb and hard sphere interactions

We have seen the importance of the Fourier transform $v(\mathbf{p})$ in Eq (16). Now let us compute it for the Coulomb and hard-sphere interactions in (2) and (3).

First, assume only that $v(\mathbf{r})$ depends only on $r = |\mathbf{r}|$. Then choose the orientation of the $\mathbf{r}$ axis in such a way that $\mathbf{p}$ is in the z direction



then $\mathbf{p} \cdot \mathbf{r} = pr\cos\theta$ and we get

$$v(\mathbf{p}) = \int d^3\mathbf{r}\, v(\mathbf{r})\, e^{-i\mathbf{p}\cdot\mathbf{r}}$$

$$= \int dr\, d\phi\, d(\cos\theta)\, r^2 v(r)\, e^{-irp\cos\theta}$$

$$= 2\pi \int_0^\infty dr\, r^2 \int_0^\pi d(\cos\theta)\, e^{-ipr\cos\theta}$$

$$= 2\pi \int_0^\infty dr\, r^2 v(r) \frac{e^{-ipr} - e^{ipr}}{-ipr}$$

$$= \frac{4\pi}{p} \int_0^\infty dr\, v(r)\, r \sin pr$$

Thus, if $v(\mathbf{r})$ depends only on $r = |\mathbf{r}|$, we get

$$\boxed{v(p) = \frac{4\pi}{p} \int_0^\infty dr \, r\, v(r) \sin pr} \tag{20}$$

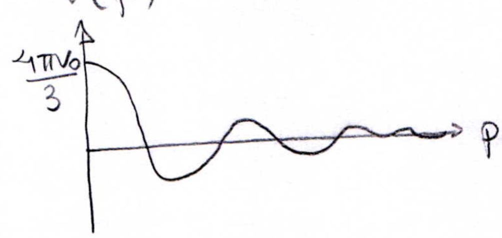
which, note, only depends on $p = |\mathbf{p}|$.
Now we specialize this, first to the hard sphere potential in Eq (3). In this case we get

$$v(p) = \frac{4\pi}{p} v_0 \int_0^a dr \, r \sin p r$$

or

$$\boxed{v(p) = 4\pi a^3 v_0 \left[\frac{\sin(ap) - ap\cos(ap)}{(ap)^3} \right]} \tag{21}$$

This looks like:



when $pa \ll 1$ a Taylor series expansion gives

$$\boxed{v(p) \simeq \frac{4\pi a^3}{3} v_0} \tag{22}$$

the first term is the volume of the particle.

Next we do the same for the coulomb potential

$$V(r) = \frac{e^2}{r}$$

However, if we do this naively, we will get into trouble. the coulomb potential falls down too slowly, which will give us trouble with the integral.

Instead, we will consider the <u>dressed coulomb potential</u>, or <u>Yokawa potential</u>

$$V(r) = \frac{e^2}{r} e^{-\mu r} \tag{23}$$

By the end of the calculation we can set $\mu = 0$.

Using Eq (20) we get

$$V(p) = \frac{4\pi e^2}{p} \int_0^\infty dr \; e^{-\mu r} \sin pr$$

$$= \frac{4\pi e^2}{p} \frac{1}{2i} \int_0^\infty dr \left[e^{-(\mu - ip)r} - e^{-(\mu + ip)r} \right]$$

$$= \frac{4\pi e^2}{p} \frac{1}{2i} \left\{ \frac{1}{\mu - ip} - \frac{1}{\mu + ip} \right\}$$

$$= \frac{4\pi e^2}{p} \frac{1}{2i} \left\{ \frac{2iP}{\mu^2 + p^2} \right\}$$

Thus

$$\boxed{V(p) = \frac{4\pi e^2}{p^2 + \mu^2}} \qquad (24)$$

We can now take $\mu \to 0$. Then $V(p)$ will be well behaved, except at $p = 0$.

The Bose-Hubbard model

The Hubbard model describes interacting Fermions in a lattice. It is the basis of our understanding of itinerant ferromagnetism and many other effects in condensed matter. we will get to it later on in the course.

The Bose-Hubbard model is the Bosonic cousin of the "Fermi-Hubbard" model and it is much easier to treat. It is defined on a lattice with sites $1, \dots, M$, each described by an operator a_i, the Hamiltonian is

$$H = \sum_i \left\{ \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right\} - J \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) \tag{25}$$

Let me explain: $\sum_i (-\mu) \hat{n}_i = -\mu \hat{N}$ is the chemical potential term. the last term is the tight-binding guy, with hopping between nearest neighbors. Finally, the first term is a on-site repulsion:

$$\frac{U}{2} n_i (n_i - 1) = \begin{cases} 0 & \text{if } n_i = 0 \\ 0 & \text{if } n_i = 1 \\ U & \text{if } n_i = 2 \\ 3U & \text{if } n_i = 3 \\ \vdots & \end{cases} \tag{26}$$

If there are less than 2 particles in a site, this term does not contribute. For 2 particles there is a repulsion $U > 0$. For 3 particles, the repulsion is $3U$ because there are 3 pairs of particles, and so on.

Note also that

$$\hat{n}_i(\hat{n}_i - 1) = a_i^\dagger a_i (a_i^\dagger a_i - 1)$$
$$= a_i^\dagger (a_i a_i^\dagger) a_i - a_i^\dagger a_i$$
$$= a_i^\dagger (1 + a_i^\dagger a_i) a_i - a_i^\dagger a_i$$

Thus

$$\hat{n}_i(\hat{n}_i - 1) = a_i^\dagger a_i^\dagger a_i a_i \qquad (27)$$

This has the form (9), with all creation operators to the left.

Now let us analyze the GS of the Hamiltonian (25) in the limits $J \to 0$ and $U \to 0$. If $J \to 0$ we get

$$H = \sum_i \left\{ \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\} \qquad (28)$$

This Hamiltonian depends only on $\hat{n}_i$, so it is already diagonal in the Fock basis. It's eigenvalues are

$$\mathcal{E} = \sum_i E(n_i) \qquad (29)$$

$$E(n_i) = \frac{U}{2} n_i(n_i - 1) - \mu n_i \qquad (30)$$

The ground-state is obtained by finding the occupation n_0 which minimizes $E(n)$. Well, this is a bit weird because n_0 is discrete. Let's make a table:

$\frac{\mu}{U} = 0$:

n	0	1	2
$\frac{E(n)}{U}$	0	0	1

$\rightsquigarrow n_0 = 0$

$\frac{\mu}{U} = 0.5$

n	0	1	2
$\frac{E(n)}{U}$	0	$-1/2$	0

$\rightsquigarrow n_0 = 1$

$\frac{\mu}{U} = 1.1$

n	0	1	2	3
$\frac{E(n)}{U}$	0	-1.1	-1.2	-0.3

$\rightsquigarrow n_0 = 2.$

We see that n_0 is always the integer right above $\frac{\mu}{U}$:

$$n_0\left(\frac{\mu}{U}\right) = \begin{cases} 0 & \frac{\mu}{U} < 0 \\ 1 & 0 \leq \frac{\mu}{U} < 1 \\ 2 & 1 \leq \frac{\mu}{U} < 2 \\ \vdots & \end{cases} \tag{31}$$

this is the occupation which minimizes the energy $E(n)$.

The GS of (28) will then be the Fock state

$$\boxed{|gs\rangle = |n_0, n_0, \dots\rangle = \bigotimes_i |n_0(\mu/U)\rangle} \tag{32}$$

and the corresponding energy will be

$$\mathcal{E}_{gs} = M\, E(n_0) \tag{33}$$

where M is the number of sites in the lattice.

the number of particles will be a function of μ:

$$N(\mu) = \langle \hat{N} \rangle = M\, n_0(\mu/U) \qquad (34)$$

We call

$$\frac{N(\mu)}{M} = n_0(\mu/U) \qquad (35)$$

the <u>filling</u> of the system. It is the <u>number of particles per site</u>

The GS of (28) therefore corresponds to all particles <u>fully localized</u> and homogeneously distributed through their respective sites. This is called a <u>Mott insulator</u>. It is an insulator because there is <u>no mobility</u>. But it is not a regular insulator, where the particles don't move because of the ionic potential. It is an insulator because to move means to increase the occupation of a given site, which causes a big repulsion.

In fact, we can define the excitation above the GS as the action of moving one particle to a neighboring site. Consider initially two sites with energy

$$E(n_0) + E(n_0) = 2\,\frac{U}{2}\, n_0(n_0-1) - 2\mu n_0$$

Now move one particle from one site to the other. The energy will change to

$$E(n_0+1) + E(n_0-1) = \frac{U}{2}(n_0+1)n_0 - \mu(n_0+1) +$$

$$+ \frac{U}{2}(n_0-1)(n_0-2) - \mu(n_0-1)$$

$$= 2\frac{U}{2}\left[n_0(n_0-1)+1\right] - 2\mu n_0$$

The energy difference is therefore

$$\boxed{\Delta E = U} \tag{36}$$

This is the energy cost for moving one particle out of the ground state. It therefore corresponds to the energy gap for creating an excitation. The Mott Insulator is thus a gapped phase.

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Next let us go back to (25) and assume $U=0$. Then we get

$$H = -\mu\hat{N} - J\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) \tag{37}$$

This is simply a tight-binding Hamiltonian. We can digonalize it by moving to Fourier space as

$$a_i^\dagger = \frac{1}{\sqrt{M}}\sum_{k} e^{i k\cdot R_i} c_k^\dagger \tag{38}$$

We've already done this problem before, but let's do it again.

For concreteness, I will assume a square lattice ($d=2$)

$$\mathcal{H} = -\mu\hat{N} - J\sum_i \Big[a^\dagger(\mathbb{R}_i)a(\mathbb{R}_i+\hat{x}) + a^\dagger(\mathbb{R}_i)a(\mathbb{R}_i-\hat{x}) + a^\dagger(\mathbb{R}_i)a(\mathbb{R}_i+\hat{y}) + a^\dagger(\mathbb{R}_i)a(\mathbb{R}_i-\hat{y})\Big]$$

Using (38) then gives

$$\sum_i a^\dagger(\mathbb{R}_i)a(\mathbb{R}_i+\hat{x}) = \frac{1}{N}\sum_i\sum_{\mathbb{k},\mathbb{q}} e^{i(\mathbb{k}-\mathbb{q})\cdot\mathbb{R}_i}\, e^{-iq_x a}\, c_{\mathbb{k}}^\dagger c_{\mathbb{q}}$$

$$= \sum_{\mathbb{k}} e^{-ik_x a} c_{\mathbb{k}}^\dagger c_{\mathbb{k}}$$

Doing the same for all other terms, we find

$$\mathcal{H} = -\mu\hat{N} - 2J\sum_{\mathbb{k}}\Big[e^{-ik_x a} + e^{ik_x a} + e^{-ik_y a} + e^{ik_y a}\Big] c_{\mathbb{k}}^\dagger c_{\mathbb{k}}$$

or

$$\mathcal{H} = \sum_{\mathbb{k}} (\epsilon_{\mathbb{k}} - \mu)\, c_{\mathbb{k}}^\dagger c_{\mathbb{k}} \tag{39}$$

where

$$\epsilon_{\mathbb{k}} = -J\big[\cos k_x a + \cos k_y a\big] \tag{40}$$

Thus, when $U=0$ the eigenstates will be completely <u>delocalized</u>. This is the <u>superfluid phase</u>.

The GS will correspond to having all particles in the $\mathbf{k}=0$ state. But now we are working on the Grand-canonical ensemble so the number of particles is allowed to fluctuate. That is, the ground state can be written as

$$|\psi\rangle = \sum_{M=0}^{\infty} \psi_M \frac{(c_0^\dagger)^M}{\sqrt{M!}} |0\rangle \qquad (41)$$

this is a superposition of states with different numbers of particles. All we do is fix the average number:

$$\langle \hat{N} \rangle = \sum_{\mathbf{k}} \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = \langle c_0^\dagger c_0 \rangle = N \qquad (42)$$

where I used the fact that only $\mathbf{k}=0$ is occupied. Using (41) then gives

$$\langle \hat{N} \rangle = \sum_{M=0}^{\infty} M \, |\psi_M|^2 = N \qquad (43)$$

Other than this and normalization $(\sum_M |\psi_M|^2 = 1)$, the coefficients ψ_M are arbitrary.

But N is very large so we expect ψ_M to be highly peaked around N. The natural choice is to assume that (41) is actually a <u>coherent state</u>, $\psi_M = \psi^M/\sqrt{M!}$

$$\boxed{|\psi\rangle = \sum_{M=0}^{\infty} \psi^M \frac{(c_0^\dagger)^M}{M!} |0\rangle} \qquad (44)$$

It is a property of coherent states that

$$c_0 |\psi\rangle = \psi |\psi\rangle \tag{45}$$

Thus

$$\langle c_0^\dagger c_0 \rangle = \langle \psi | c_0^\dagger c_0 | \psi \rangle = |\psi|^2 = N$$

that is

$$|\psi|^2 = N \tag{46}$$

the magnitude of ψ is therefore the number of particles. But ψ may in general be complex, so we write

$$\psi = \sqrt{N}\, e^{i\phi} \tag{47}$$

where ϕ is an arbitrary phase. This is the <u>order parameter</u> of the superfluid phase.

$$\psi = \langle a_i \rangle \begin{cases} = 0 & \text{Mott Insulator} \\ \neq 0 & \text{Superfluid} \end{cases} \tag{48}$$

Mean-field approximation

When both U and J are non-zero, it is not possible to diagonalize H [Eq (25)] exactly. So instead, we do a mean-field approximation. We already seen that when $J/U \gg 1$ the system will tend to a coherent state, where $\langle a_i \rangle \neq 0$.

Let us write

$$a_i = \psi + (a_i - \psi) \tag{49}$$

where $\psi = \langle a_i \rangle$. We substitute this into the tight-binding form

$$a_i^\dagger a_j = [\psi^* + (a_i^\dagger - \psi^*)][\psi + (a_j - \psi)]$$

$$= |\psi|^2 + \psi^*(a_j - \psi) + \psi(a_i^\dagger - \psi^*) + \underbrace{(a_i^\dagger - \psi^*)(a_j - \psi)}_{\text{Assume is small and neglect}}$$

Thus, we approximate

$$a_i^\dagger a_j \simeq -|\psi|^2 + \psi^* a_j + \psi a_i^\dagger \tag{50}$$

Maybe it's clearer to write the hopping term as

$$-J \sum_i \sum_{j \in \Gamma_i} a_i^\dagger a_j$$

where Γ_i is the neighborhood of i. Then we get

$$-J \sum_i \sum_{j \in \Gamma_i} \left[-|\psi|^2 + \psi^* a_j + \psi a_i^\dagger \right]$$

Now: $\sum_{j \in \Gamma_i} (1) = 2d$ since the neighborhood consists of $2d$ sites. Thus

$$J |\psi|^2 \sum_i \sum_{j \in \Gamma_i} 1 = 2d J M |\psi|^2$$

$$-J \psi \sum_i \sum_{j \in \Gamma_i} a_i^\dagger = -2dJ\psi \sum_i a_i^\dagger$$

For the a_j guy, we exchange the labels $i \leftrightarrow j$. Then we get

$$-J \psi^* \sum_i \sum_{j \in \Gamma_i} a_j = -J \psi^* \sum_j a_j = -J \psi^* \sum_i a_i$$

whence, the hopping term is approximated by

$$-J\sum_i \sum_{j\in\Gamma_i} a_i^\dagger a_j \simeq 2dJM|\psi|^2 - 4J\sum_i (\psi a_i^\dagger + \psi^* a_i)$$

Going back now to the full Hamiltonian (25), we get

$$\mathcal{H} = \sum_i \left\{ \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\} + 2dJM|\psi|^2$$
$$- 2dJ\sum_i (\psi a_i^\dagger + \psi^* a_i)$$

But note that we may write this as

$$\mathcal{H} = \sum_i \mathcal{H}_i \qquad (51)$$

where

$$\boxed{\mathcal{H}_i = \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i + 2dJ|\psi|^2 - 2dJ(\psi a_i^\dagger + \psi^* a_i)} \qquad (52)$$

This Hamiltonian involves only a_i operators. It is therefore a sum of single-site Hamiltonians. Mean-field has therefore reduced the problem to a sum of independent Hamiltonians.

We want to find the ground-state of $\mathcal{H}$. But since the $\mathcal{H}_i$ are all independent and identical, it is equivalent if we diagonalize just the single-particle Hamiltonian

$$\boxed{H = \frac{U}{2} \hat{n}(\hat{n}-1) - \mu \hat{n} + g|\psi|^2 - g(\psi a^\dagger + \psi^* a)} \qquad (53)$$

where $g = 2dJ$. This is the Hamiltonian of a weird-looking Harmonic oscillator. We can diagonalize it numerically quite easily (see accompanying Mathematica notebook).

We can also find the phase boundary analytically, as follows. Let us assume that ψ is small. This will be true if we are in the SF phase, but very close to the MI phase. Then we separate (53) as

$$H = H_0 + V$$

$$H_0 = \frac{U}{2} \hat{n}(\hat{n}-1) - \mu \hat{n} + \underbrace{g|\psi|^2}_{\text{Just a constant}} \qquad (54)$$

$$V = -g(\psi a^\dagger + \psi^* a)$$

we know the GS of H_0. It is simply $|m_0\rangle$, where m_0 is given in (31). the GS energy is then

$$E_0(m_0) = \frac{U}{2} m_0 (m_0 - 1) - \mu m_0 + g|\psi|^2 \qquad (55)$$

Now we treat V like a perturbation. According to perturbation theory, the correction to the eigenvector will be

$$|m_0'\rangle = |m_0\rangle + \sum_{m \neq m_0} \frac{|m\rangle\langle m|V|m_0\rangle}{E_0(m_0) - E_0(m)} \qquad (56)$$

well:

$$V|m_0\rangle = -g\left(\psi a^\dagger |m_0\rangle + \psi^* a |m_0\rangle\right)$$
$$= -g\left\{\psi\sqrt{m_0+1}\,|m_0+1\rangle + \psi^*\sqrt{m_0}\,|m_0-1\rangle\right\}$$

thus

$$|m_0'\rangle = |m_0\rangle - g\left\{\frac{\psi\sqrt{m_0+1}\,|m_0+1\rangle}{E_0(m_0) - E_0(m_0+1)} + \frac{\psi^*\sqrt{m_0}\,|m_0-1\rangle}{E_0(m_0) - E_0(m_0-1)}\right\}$$

Using (30) we get

$$E_0(M_0) - E_0(M_0+1) = -(UM_0 - \mu)$$

$$E_0(M_0) - E_0(M_0-1) = -[\mu - U(M_0-1)]$$

Thus

$$\boxed{|M_0'\rangle = |M_0\rangle + g\left\{ \frac{\phi\sqrt{M_0+1}\,|M_0+1\rangle}{UM_0-\mu} \quad \frac{\phi^*\sqrt{M_0}\,|M_0-1\rangle}{\mu - U(M_0-1)} \right.} \qquad (57)$$

Now that we have the eigenvector of the perturbed GS, we may compute

$$\langle a\rangle = \langle M_0'|\,a\,|M_0'\rangle$$

$$= \langle M_0'| \left\{ \sqrt{M_0}\,|M_0-1\rangle + \frac{g\phi\sqrt{M_0+1}}{UM_0-\mu}\sqrt{M_0+1}\,|M_0\rangle + \frac{g\phi^*\sqrt{M_0}}{\mu-U(M_0-1)}\sqrt{M_0-2}\,|M_0-2\rangle \right\}$$

when we enter with $\langle M_0'|$, only a few terms will survive

$$\langle m_0' | a | m_0' \rangle = \left[\frac{g \psi^* \sqrt{m_0}}{\mu - U(m_0 - 1)} \right]^* \sqrt{m_0} \langle m_0 - 1 | m_0 - 1 \rangle$$

$$+ \frac{g \psi (m_0 + 1)}{U m_0 - \mu} \langle m_0 | m_0 \rangle$$

or, simplifying,

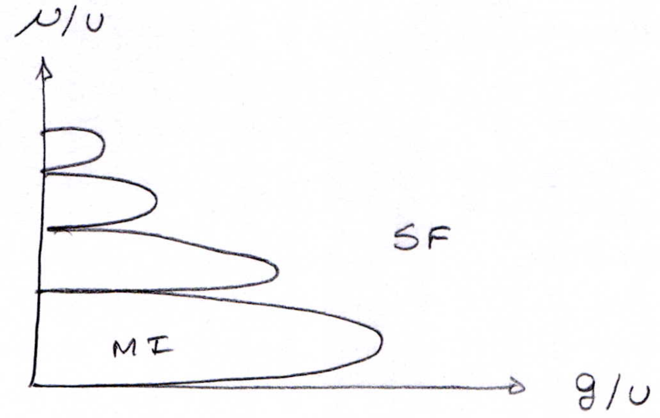
$$\boxed{\langle m_0' | a | m_0' \rangle = g \psi \left\{ \frac{m_0}{\mu - U(m_0 - 1)} + \frac{m_0 + 1}{U m_0 - \mu} \right\}} \qquad (58)$$

But $\langle m_0' | a | m_0' \rangle = \psi$, since from the start we have defined ψ as $\langle a \rangle$. Thus the ψ cancels on both sides of (58) and we are left with

$$\boxed{\frac{m_0}{\mu - U(m_0 - 1)} + \frac{m_0 + 1}{U m_0 - \mu} = \frac{1}{g}} \qquad (59)$$

This is an implicit equation for U, μ and g. It is the equation determining the phase boundary between the MI and CDW phases.

The phase boundary will look like this



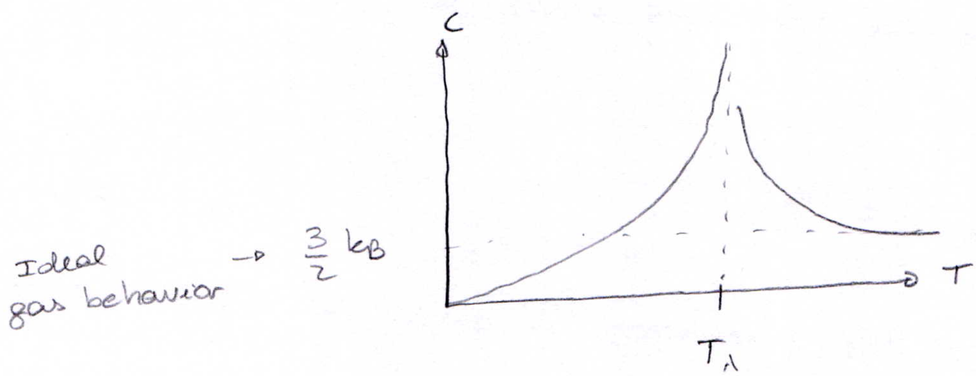
These are called <u>Mott lobes</u>

Superfluidity

Helium has 2 isotopes, ^4He (discovered in 1871) and ^3He (discovered only in 1939). Both have the remarkable property of remaining liquid even as $T \to 0$, unless high pressures are applied (25 atm for ^4He). This is a consequence of the weak interaction between the atoms.

However, at low temperatures, bove behave quite differently. ^3He has 2 p^+ and 1 n^0 and thus behaves as a spin 1/2 Fermion. ^4He, on the other hand, has 2 p^+ and 2 n^0 and thus behaves as a spin 0 Boson.

At $T_\lambda = 2.17$ K ^4He enters what is known as the He II or superfluid phase. This can be seen by analyzing the specific heat, which behaves like this:



This curve looks like the letter λ, so this is called the λ point

This property of $C(T)$ was already known by Onnes in 1908, (the first guy to liquify Helium).

In the superfluid phase Helium flows without viscosity. This was only discovered in 1938 by Kapitza, Allen and Misener. In the same year, Landau proposed that superfluidity was a form of Bose Einstein condensation. In fact, if we use the density of liquid Helium ($0.145 g/cm^3$) to estimate the BEC temperature, we find $3.14 K$, which is close to $T_\lambda = 2.17 K$.

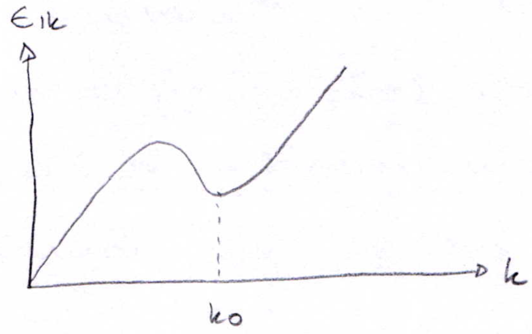
However, a superfluid and a BEC have one fundamental difference. Namely, in a superfluid the atoms interact. One evidence of this is that, at low temperatures, the specific heat behaves as $c \sim T^3$, which we know is the law for phonons. This means the superfluid must support acoustic waves, which can only exist if the atoms interact with each other.

This led Landau to suggest first that the excitations in a superfluid should therefore have a phonon-like dispersion relation

$$\epsilon_{k} \simeq c\,|k| \qquad (60)$$

If a body moves through the medium, it will excite phonons which propagate through the fluid.

But the actual dispersion relation can be measured by neutron scattering and looks like this



See Palevsky et. al.
PRL 112 (1958)

For low k indeed we find a linear dispersion. But as we approach a certain value

$$k_0 = (1.92 \pm 0.01) \times 10^8 \ cm^{-1} \tag{61}$$

the dispersion bends in a weird way. At the vicinity of k_0 it behaves like

$$\epsilon_k \simeq \Delta + \frac{\hbar^2 (k-k_0)^2}{2\sigma} \quad (k \sim k_0) \tag{62}$$

where $\frac{\Delta}{k_B} = (8.65 \pm 0.04) \ K$ and $\frac{\sigma}{m} = 0.16 \pm 0.01$

Thus, around k_0 we have a non-relativistic dispersion, with an effective mass that is smaller than the actual He mass.

Landau put forth a famous criterion to test whether something can be a superfluid.

Consider an object with mass M moving in the superfluid with momentum $\vec{P}$. It can loose energy by exciting a phonon. Let $\hbar k$ be the momentum of the phonon and ϵ_k it's corresponding energy. Then, momentum conservation implies

$$\vec{P}_i = \vec{P}_f + \hbar k$$

thus

$$\vec{P}_f = \vec{P}_i - \hbar k$$

Similarly, conservation of energy implies

$$\mathcal{E}_i = \frac{\vec{P}_i^{\,2}}{2M} = \frac{\vec{P}_f^{\,2}}{2M} + \epsilon_k = \mathcal{E}_f$$

Thus the phonon energy will be

$$\epsilon_k = \frac{\vec{P}_i^{\,2}}{2M} - \frac{(\vec{P}_i - \hbar k)^2}{2M}$$

$$= -\frac{\hbar^2 k^2}{2M} + \frac{\hbar}{M} \vec{P}_i \cdot k$$

Letting $\vec{v} = \frac{\vec{P}_i}{M}$ denote the initial velocity of the object we then get

$$\hbar\,(\vec{v} \cdot \mathbb{k}) = \epsilon_{\mathbb{k}} + \frac{\hbar^2 k^2}{2M} \geq \epsilon_{\mathbb{k}}$$

Since $vk \geq \vec{v} \cdot \mathbb{k}$ we may also write

$$\boxed{v \geq \frac{\epsilon_{\mathbb{k}}}{k}} \tag{63}$$

This is the required condition for the process of emitting a phonon to occur.

Now suppose $\epsilon_{\mathbb{k}} = ck$. Then we get

$$v \geq c = (239 \pm 5)\ m/s$$

objects moving slower than c will therefore not emit phonons. This is why they are superfluid.

If we had assumed that $\epsilon_k \approx k^2$ then $\frac{\epsilon_k}{k} \sim k$ and thus there would be no velocity threshold below which no phonons would be emitted. A superfluid therefore requires that, as $k \to 0$, the dispersion becomes linear.

Bogoliubov's method

Let us consider a gas of Bosons in the language of second quantization. We take as our full Hamiltonian

$$\mathcal{H} = \sum_{k} \epsilon_k a_k^\dagger a_k + \frac{1}{2v_0} \sum_{\substack{k k' \\ p}} V(p)\, a_{k+p}^\dagger a_{k'-p}^\dagger a_{k'} a_k \qquad (64)$$

where v_0 is the volume. We will assume $V(p)$ is the hard sphere potential, Eqs (21) or (22),

Oops: $\epsilon_k = \frac{k^2}{2m}$

$$V(p) = 4\pi a^3 v_0 \left\{ \frac{\sin(ap) - ap\cos(ap)}{(ap)^3} \right\} \simeq \frac{4\pi a^3 v_0}{3} \qquad (65)$$

where I defined $g = \frac{4\pi a^3}{3} v_0$. This choice seems reasonable for He atoms.

The Hamiltonian (64) cannot be diagonalized exactly. Bogoliubov came up with the following idea to treat it approximately. If $V=0$ we know the system will be in a BEC state, where $a_{k=0}$ will be macroscopically occupied. We will therefore do a mean field approximation only for a_0. That is, we write

$$a_0 = \langle a_0 \rangle + (a_0 - \langle a_0 \rangle)$$

the first term is the average of a_0 and the second term are the fluctuations around the average

Bogoliubov's approximation consists in neglecting these fluctuations and writting

$$a_0 \simeq \langle a_0 \rangle = \sqrt{N_0} \tag{66}$$

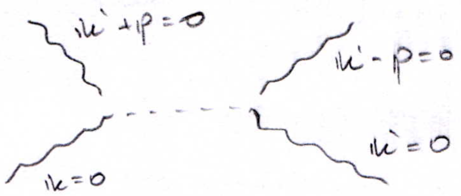
where N_0 is the number of particles in the condensate. We shall now sepparate $\mathcal{H}$ into terms involving $\mathbb{k}=0$ and terms involving $\mathbb{k}\neq 0$. First, the non-interacting part is sepparated as

$$\begin{aligned} \mathcal{H}_0 &= \overset{0}{\epsilon_0}\, a_0^\dagger a_0 + \sum_{\mathbb{k}\neq 0} \epsilon_{\mathbb{k}}\, a_{\mathbb{k}}^\dagger a_{\mathbb{k}} \\ &= \sum_{\mathbb{k}\neq 0} \epsilon_{\mathbb{k}}\, a_{\mathbb{k}}^\dagger a_{\mathbb{k}} \end{aligned} \tag{67}$$

Now, for the interaction part, we sepparate $\sum_{\mathbb{k}\mathbb{k}'\mathbb{p}}$ into terms having involving the zero momentum state. For instance, there is a term with $\mathbb{k}=\mathbb{k}'=\mathbb{p}=0$

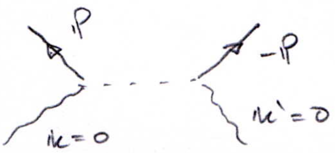
$$(0) \qquad \mathbb{k}=\mathbb{k}'=\mathbb{p}=0 : \qquad \frac{V(0)}{2\mathcal{V}_0}\, a_0^\dagger a_0^\dagger a_0 a_0 = \frac{V(0)}{2\mathcal{V}_0} N_0^2$$

this represents a scattering event fully inside the BEC



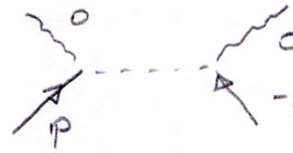
Now let us look at terms where two of $\mathbf{k}, \mathbf{k}', \mathbf{p}$ are zero, but one is non-zero. We have

(1) $\mathbf{k} = \mathbf{k}' = 0,\ \mathbf{p} \neq 0 : \quad \displaystyle\sum_{\mathbf{p}\neq 0} \frac{V(\mathbf{p})}{2\mathcal{V}_0} a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} \overbrace{a_0 a_0}^{N_0}$

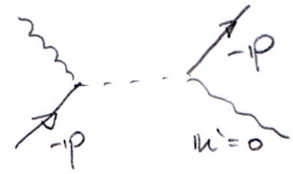


(2) $\mathbf{k} + \mathbf{p} = \mathbf{k}' - \mathbf{p} = 0 \quad : \quad \displaystyle\sum_{\mathbf{p}\neq 0} \frac{V(\mathbf{p})}{2\mathcal{V}_0} \underbrace{a_0^{\dagger} a_0^{\dagger}}_{N_0} a_{\mathbf{p}} a_{-\mathbf{p}}$

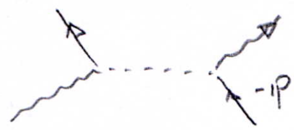
(so $\mathbf{k}' = -\mathbf{k} = \mathbf{p}$)



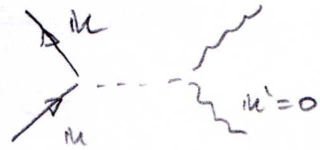
(3a) $\mathbf{k}' = 0;\ \mathbf{k} + \mathbf{p} = 0 : \quad \displaystyle\sum_{\mathbf{p}\neq 0} \frac{V(\mathbf{p})}{2\mathcal{V}_0} a_0^{\dagger} a_{-\mathbf{p}}^{\dagger} a_0 a_{-\mathbf{p}}$



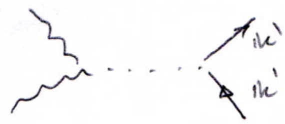
(3b) $\mathbf{k} = 0;\ \mathbf{k}' - \mathbf{p} = 0 : \quad \displaystyle\sum_{\mathbf{p}\neq 0} \frac{V(\mathbf{p})}{2\mathcal{V}_0} a_{\mathbf{p}}^{\dagger} a_0^{\dagger} a_{-\mathbf{p}} a_0$



(4a) $\mathbf{k}' = 0;\ \mathbf{p} = 0 : \quad \displaystyle\sum_{\mathbf{k}\neq 0} \frac{V(0)}{2\mathcal{V}_0} a_{\mathbf{k}}^{\dagger} a_0^{\dagger} a_0 a_{\mathbf{k}}$



(4b) $\mathbf{k} = 0;\ \mathbf{p} = 0 : \quad \displaystyle\sum_{\mathbf{k}'\neq 0} \frac{V(0)}{2\mathcal{V}_0} a_0^{\dagger} a_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} a_0$



Combining everything and substituting $a_0 = \sqrt{N_0}$, we get

$$\mathcal{H}_1 = \frac{V(0)}{2\mathcal{V}_0} N_0^2 + \sum_{\mathbf{p}\neq 0} \frac{V(\mathbf{p}) N_0}{2\mathcal{V}_0} \Big\{ a_{\mathbf{p}}^{\dagger} a_{-\mathbf{p}}^{\dagger} + a_{\mathbf{p}} a_{-\mathbf{p}} + a_{-\mathbf{p}}^{\dagger} a_{-\mathbf{p}} + a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \Big\} + \sum_{\mathbf{k}\neq 0} \frac{V(0) N_0}{2\mathcal{V}_0} 2 a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \tag{68}$$

Combining with $\mathcal{H}_0$ in (67) we then get

$$\mathcal{H} = \sum_{k \neq 0} \epsilon_k a_k^\dagger a_k + \frac{V(0)}{2\mathcal{V}_0} N_0^2 + \sum_{k \neq 0} \frac{V(0) N_0}{\mathcal{V}_0} a_k^\dagger a_k$$

$$+ \sum_{k \neq 0} \frac{V(k) N_0}{2 \mathcal{V}_0} \left\{ a_k^\dagger a_{-k}^\dagger + a_k a_{-k} + a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right\} \tag{69}$$

But we still have N_0 here, which we don't know what it is.

All we know is $N = \langle \hat{N} \rangle$. Let us write

$$\hat{N} = N_0 + \sum_{k \neq 0} a_k^\dagger a_k \tag{70}$$

Then, in the second line of (69) we can replace N_0 by N since the correction would be something quartic in a's.

But in the first line of (69) we have the combination

$$\frac{V(0) N_0^2}{2\mathcal{V}_0} + \sum_{k \neq 0} \frac{V(0) N_0}{\mathcal{V}_0} a_k^\dagger a_k =$$

$$= \frac{V(0)}{2\mathcal{V}_0} \left\{ N_0^2 + 2 N_0 \sum_{k \neq 0} a_k^\dagger a_k \right\}$$

comparing with (70), we see that this is approximately

$$\hat{N}^2 = N_0^2 + 2 N_0 \sum_{k \neq 0} a_k^\dagger a_k + \underbrace{\left(\sum_{k \neq 0} a_k^\dagger a_k \right)^2}_{\text{small.}}$$

Thus we may approximate (69) by

$$\mathcal{H} = \mathcal{E}_0 + \sum_{k \neq 0} \epsilon_k a_k^{+} a_k +$$

$$+ \sum_{k \neq 0} \beta_k \left\{ a_k^{+} a_{-k}^{+} + a_k a_{-k} + a_k^{+} a_k + a_{-k}^{+} a_{-k} \right\}$$

where

$$\mathcal{E}_0 = \frac{V(0) N^2}{2 v_0} \tag{71}$$

$$\beta_k = \frac{V(k) N}{2 v_0} \tag{72}$$

Finally, we use the fact that $V(-k) = V(k)$ to write

$$\sum_{k \neq 0} \beta_k a_{-k}^{+} a_{-k} = \sum_{k \neq 0} \beta_k a_k^{+} a_k$$

we then finally arrive at

$$\boxed{\mathcal{H} = \mathcal{E}_0 + \sum_{k \neq 0} \left\{ (\epsilon_k + 2\beta_k) a_k^{+} a_k + \beta_k (a_k^{+} a_{-k}^{+} + a_k a_{-k}) \right\}} \tag{73}$$

which is the Bogoliubov Hamiltonian.

Eq (73) is not yet diagonal, as it mixes operators with k and $-k$. We can diagonalize it using the Bogoliubov transformation (Bogoliubov is everywhere!). We introduce new operators b_k and b_{-k} according to

$$b_k^{+} = u_k a_k^{+} - v_k a_{-k}$$

where u_k, v_k are constants. We assume $u_k = u_{-k}$ and $v_k = v_{-k}$. Moreover, we take them to be real. We may then write

$$\begin{pmatrix} b_k^{+} \\ b_{-k} \end{pmatrix} = \underbrace{\begin{pmatrix} u_k & -v_k \\ -v_k & u_k \end{pmatrix}}_{M} \begin{pmatrix} a_k^{+} \\ a_{-k} \end{pmatrix} \qquad (74)$$

Imposing that we must have $[b_k, b_k^{+}] = 1$ yields the constraint

$$u_k^2 - v_k^2 = 1 \qquad (75)$$

Thus, the matrix M in Eq (74) represents a <u>hyperbolic rotation</u>

$$u_k = \cosh \theta_k$$
$$v_k = \sinh \theta_k \qquad (76)$$

The inverse transformation is

$$\begin{pmatrix} a^{+}_{k} \\ a_{-k} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} b^{+}_{k} \\ b_{-k} \end{pmatrix} \tag{77}$$

The task now is to substitute this in (73) and see what happens. Let's do it term-by-term

$$a^{+}_{k} a_{k} = (u_k b^{+}_{k} + v_k b_{-k})(u_k b_k + v_k b^{+}_{-k})$$

$$= u_k^2 b^{+}_{k} b_k + v_k^2 b_{-k} b^{+}_{-k} + u_k v_k (b^{+}_{k} b^{+}_{-k} + b_{-k} b_k)$$

$$a^{+}_{k} a^{+}_{-k} = (u_k b^{+}_{k} + v_k b_{-k})(u_k b^{+}_{-k} + v_k b_k)$$

$$= u_k v_k (b^{+}_{k} b_k + b_{-k} b^{+}_{-k}) + u_k^2 b^{+}_{k} b^{+}_{-k} + v_k^2 b_{-k} b_k$$

$$a_k a_{-k} = (a^{+}_{k} a^{+}_{-k})^{+}$$

$$= u_k v_k (b^{+}_{k} b_k + b_{-k} b^{+}_{-k}) + u_k^2 b_{-k} b_k + v_k^2 b^{+}_{k} b^{+}_{-k}$$

Thus, (73) becomes

$$\mathcal{H} = \mathcal{E}_0 + \sum_{k\neq 0} \Big\{ \big[(\epsilon_k + 2\beta_k) u_k^2 + 2\beta_k u_k v_k \big] b^{+}_{k} b_k$$

$$+ \big[(\epsilon_k + 2\beta_k) v_k^2 + 2\beta_k u_k v_k \big] b_{-k} b^{+}_{-k}$$

$$+ \big[(\epsilon_k + 2\beta_k) u_k v_k + \beta_k (u_k^2 + v_k^2) \big] (b^{+}_{k} b^{+}_{-k} + b_{-k} b_k) \Big\}$$

(77)

We now choose u_k and v_k in such a way that makes $\mathcal{H}$ diagonal. This means we choose

$$(\epsilon_k + 2\beta_k) u_k v_k + \beta_k (u_k^2 + v_k^2) = 0 \qquad (78)$$

which will kill the last term in (77). We are assuming weak interactions, so we may take $\epsilon_k + 2\beta_k > 0$.* Then, if we write

$$(\epsilon_k + 2\beta_k) u_k v_k = -\beta_k (u_k^2 + v_k^2)$$

we see that $u_k v_k < 0$. We will need this later. Squaring both sides we get

$$(\epsilon_k + 2\beta_k)^2 u_k^2 v_k^2 = \beta_k^2 (u_k^2 + v_k^2)^2$$

But we also have $u_k^2 - v_k^2 = 1$ so

$$(\epsilon_k + 2\beta_k)^2 (1 - v_k^2) v_k^2 = \beta_k^2 (1 + 2 v_k^2)^2$$

$$(\epsilon_k + 2\beta_k)^2 (v_k^2 - v_k^4) = \beta_k^2 (1 + 4 v_k^2 + 4 v_k^4)$$

$$v_k^4 \left[(\epsilon_k + 2\beta_k)^2 - 4\beta_k^2 \right] + v_k^2 \left[(\epsilon_k + 2\beta_k)^2 - 4\beta_k^2 \right] + - \beta_k^2 = 0$$

* If we take $V(k) = g$ in (65) then this is also true. But if we take a general $V(k)$, then it may become negative. I have never seen anyone discuss what happens in this case.

Thus we get the equation

$$v_k^4 + v_k^2 - \frac{\beta_k^2}{E_k^2} = 0$$

where I define

$$\boxed{E_k = \sqrt{\epsilon_k^2 + 4\epsilon_k \beta_k}} \qquad (79)$$

the solution of this equation is

$$v_k^2 = -\frac{1}{2} \pm \frac{1}{2}\sqrt{1 - \frac{4\beta_k^2}{E_k^2}} = -\frac{1}{2} \pm \frac{1}{2}\sqrt{\frac{\epsilon_k^2 + 4\epsilon_k\beta_k + 4\beta_k^2}{E_k^2}}$$

we must take the positive solution because we chose v_k to be real. That is

$$\boxed{v_k^2 = \frac{1}{2}\left[\frac{\epsilon_k + 2\beta_k}{E_k} - 1\right]} \qquad (80)$$

Since $u_k^2 - v_k^2 = 1$, we then also get

$$\boxed{u_k^2 = \frac{1}{2}\left[\frac{\epsilon_k + 2\beta_k}{E_k} + 1\right]} \qquad (81)$$

Multiplying the two we get

$$u_k^2 v_k^2 = \frac{1}{4}\left\{\frac{(\epsilon_k + 2\beta_k)^2}{E_k^2} - 1\right\} = \frac{\beta_k^2}{E_k^2}$$

Now we need to remember that $u_k v_k < 0$. thus, taking the square root we get

$$\boxed{u_k v_k = -\frac{\beta_k}{E_k}} \tag{82}$$

with all these results, we can now go back to our Hamiltonian (77). we get

$$(\epsilon_k + 2\beta_k) u_k^2 + 2\beta_k u_k v_k = \frac{(\epsilon_k + 2\beta_k)}{2}\left[\frac{\epsilon_k + 2\beta_k}{E_k} + 1\right] - \frac{2\beta_k^2}{E_k}$$

$$= \frac{1}{2}\left\{\frac{(\epsilon_k + 2\beta_k)^2 - 4\beta_k^2}{E_k} + (\epsilon_k + 2\beta_k)\right.$$

$$= \frac{1}{2}\left\{\frac{\epsilon_k^2 + 4\epsilon_k\beta_k}{E_k} + (\epsilon_k + 2\beta_k)\right.$$

$$= \frac{1}{2}\left[E_k + (\epsilon_k + 2\beta_k)\right] \tag{83}$$

Similarly

$$(\epsilon_k + 2\beta_k)\, v_k^2 + 2\beta_k u_k v_k = \frac{1}{2}\left[E_k - (\epsilon_k + 2\beta_k)\right]$$

Thus, Eq (77) becomes

$$\mathcal{H} = \mathcal{E}_0 + \frac{1}{2}\sum_{k\neq 0}\Big\{\left[E_k + (\epsilon_k + 2\beta_k)\right] b_k^+ b_k +$$

$$+ \left[E_k - (\epsilon_k + 2\beta_k)\right] b_{-k} b_{-k}^+ \Big\}$$

Now we write $b_{-k} b_{-k}^+ = b_{-k}^+ b_{-k} + 1$. We also use the fact that $E_{-k} = E_k$ and similarly for ϵ_k, β_k. We then get

$$\mathcal{H} = \mathcal{E}_0 + \frac{1}{2}\sum_{k\neq 0}\left[E_k - (\epsilon_k + 2\beta_k)\right] +$$

$$+ \sum_{k\neq 0} E_k\, b_k^+ b_k$$

Finally, we define

$$\mathcal{E}_{gs} = \mathcal{E}_0 + \frac{1}{2}\sum_{k\neq 0}\left[E_k - (\epsilon_k + 2\beta_k)\right] \tag{84}$$

Then we may finally write the diagonal form of the Hamiltonian as

$$\boxed{\mathcal{H} = \mathcal{E}_{gs} + \sum_{\mathbf{k}\neq 0} E_k \, b^{+}_{\mathbf{k}} b_{\mathbf{k}}} \qquad (85)$$

this is the Hamiltonian of independent bosonic particles with dispersion relation

$$E_k = \sqrt{\epsilon_k^2 + 4\,\epsilon_k \beta_k}$$

$$= \sqrt{\left(\frac{k^2}{2m}\right)^2 + 4\,\frac{k^2}{2m}\,\frac{V(\mathbf{k})N}{2\mathcal{V}_0}} \qquad (86)$$

Define

$$c(\mathbf{k})^2 = \frac{2}{m}\,\frac{V(\mathbf{k})N}{2\mathcal{V}_0} \qquad (87)$$

Using (65) we get

$$c(\mathbf{k})^2 = \frac{N}{m\mathcal{V}_0}\,4\pi a^3 V_0 \left[\frac{\sin(ak) - (ak)\cos(ak)}{(ak)^3}\right]$$

Notice here the appearance of the parameter

$$\boxed{\eta = \frac{4\pi a^3}{3} \frac{N}{v_0}}$$

this is the ratio between the typical extent of the hard-sphere interaction, $\frac{4\pi a^3}{3}$, to the typical volume occupied by each atom, v_0/N: when η is large, the hard-sphere repulsion should become important.

We may then write

$$\boxed{c(k)^2 = \frac{32 V_0}{m} \left[\frac{\sin(ak) - (ak)\cos(ak)}{(ak)^3} \right]} \tag{88}$$

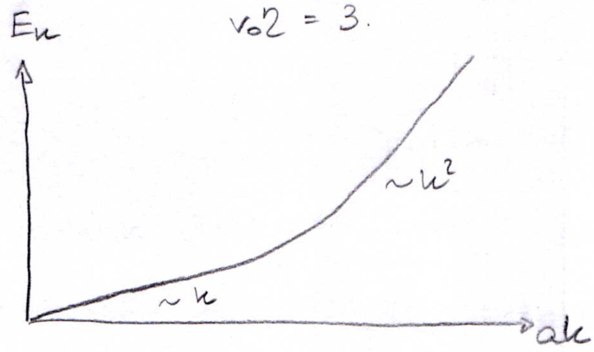
and, when $ak \ll 1$, this reduces to

$$c(k) \simeq \frac{2 V_0}{m} \tag{89}$$

the dispersion relation (86) then becomes

$$\boxed{E_k = \sqrt{\left(\frac{k^2}{2m}\right)^2 + c^2 k^2}} \tag{90}$$

A plot of E_k for different values of $2V_0$, with $m=1$, looks like this:

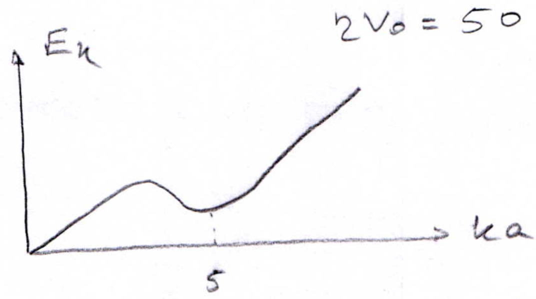


For low $2V_0$, the curve is linear for low k and quadratic for high k:

$$E_k \simeq \begin{cases} ck & \text{if } ka \ll 1 \\ \frac{k^2}{2m} & \text{if } ka \gg 1 \end{cases}$$

Thus, Bogoliubov's theory predict a phonon-like spectrum at low k. This is precisely the condition for the existence of superfluidity

If 2 is large the curve becomes



This is remarkably similar to the actual dispersion relation. I have never seen anyone discuss this and I don't know if it could be irrealistic. But I do find it curious.