Notes on Lewenstein, Sanpera, and Ahufinger’s *Ultracold atoms in optical lattices: Simulating quantum many-body systems*

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**Ch 2. Some condensed matter**

Much of this chapter is familiar. However, there are some new ideas about low-dimensional systems that I didn’t know beforehand.

**BEC**

Here are some things I didn’t know about BEC before, or different ways to think about it. Consider a non-interacting Bose gas, such that the only thing generating the BEC is the quantum statistics.

- There is no Bose condensation in low dimensions. This follows because the total number of excited particles can be calculated as

\[
N_{\text{excited}} = \int_{\epsilon} n(\epsilon) \frac{e^{-\beta(\epsilon-\mu)}}{1 - e^{-\beta(\epsilon-\mu)}}.
\]

Here, the integral excludes the ground state. For \( T > 0 \), the integral diverges in \( d = 1, 2 \) and converges in \( d = 3 \). Therefore, there is no BEC in low dimensions at finite temperature.

In fact, at \( T = 0 \) the BEC can exist in \( d = 2 \) but not in \( d = 1 \), due to phase fluctuations. We can explain this using Kosterlitz-Thouless theory, which obviously is about vortices and exists only in \( d = 2 \) (see later subsection). In these cases, we say the “BEC transition is demoted to a BKT transition.”

- The dimension of the trap potential controls whether there is condensation. This is because the trap potential \( V(\mathbf{x}) \) changes the chemical potential \( \mu(\mathbf{x}) \).

In ultracold atoms, we will usually work with harmonic traps

\[
V(\mathbf{x}) \sim \mathbf{x}^2,
\]

but the dimension of \( \mathbf{x} \) depends on the dimensionality of our system. In this case, the density of states goes like

\[
n(\epsilon) \sim \epsilon^{d(1+s^{-1})-1}
\]
and we find that now, we can make BEC in $d = 1$ if we have weak interactions and in $d = 2$ without any interactions. The way to think about it is that the original integral in $d = 2$ (without the trap) was logarithmically divergent, which is as close as we can get to convergent. Therefore, if we use a harmonic trap, it pushes the integral “over the edge” and makes it converge.

- **Bogoliubov–de Gennes approach** to BEC: There are several ways of thinking about BEC (say, in high dimensions). One way is as a thermal phase transition – if I decrease the temperature, then some of the atoms will condense. Another way is as a quantum phase transition – given that $T = 0$, we can increase the number of particles (i.e. increase the chemical potential, $\mu$) until the BEC appears.

Let us use the QPT description with the field theory approach. This is BdG method. Our Hamiltonian contains the chemical potential $\mu$ as a parameter:

$$\mathcal{H} = \int_x \frac{1}{2m} |\nabla \phi|^2 - \mu \phi^\dagger \phi + \frac{g}{2} \phi^\dagger \phi^\dagger \phi \phi.$$ 

We are assuming a point interaction. There is a minus sign on the chemical potential term because the higher the chemical potential, the more particles we expect. Now, introduce quantum fluctuations

$$\phi = \Phi + \delta \phi.$$ 

Here, $\Phi \in \mathbb{C}$ is a classical expectation (not an operator) and $\delta \phi$ is a quantum operator which satisfies canonical commutations. The equation of motion is the stationary Gross-Pitaevskii equation

$$\mu \Phi = -\frac{1}{2m} \nabla^2 \Phi + g \Phi^* \Phi \Phi.$$ 

Since $\Phi = \langle \phi \rangle$ is an expectation, this is the equation of motion for the condensate. It is a kind of Schrodinger equation.

- Path-integral derivation of the time-dependent Gross-Pitaevskii equation: Obviously this follows from the path integral

$$Z = \int \mathcal{D}[\phi, \phi^*] e^{\phi^\dagger (i\partial_t \phi) - \mathcal{H}}.$$ 

The G-P equation follows from semiclassical approximation, or stationary-point approximation.

**Phase fluctuations at low energy**

At low energies, the *most important fluctuations are the Goldstone modes*, which are the *phase fluctuations*. We can see this, for example, in the context of BEC. There is a symmetry breaking for $\mu > 0$, in the sense that for $\mu > 0$ the ground state is

$$\Phi = \langle \phi \rangle = \sqrt{\frac{\mu}{g}} e^{i\theta}$$
where $\theta$ is arbitrary. $\theta$, of course, is the Goldstone mode. It’s not hard to see, for example from the path-integral formulation or Gross-Pitaevskii equation, that the Goldstone mode obeys a gapless phonon dispersion relation

$$\ddot{\theta} = -\frac{\mu}{m} \nabla \theta \implies \omega = uk, u = \sqrt{\frac{\mu}{m} g \rho_0}.$$ 

This holds in any dimension and reminds of the $U(1)$ kind of $XY$-model.

### 1D systems

Mermin-Wagner theorem says that phase fluctuations destroy order in $d \leq 2$. What this means is that

$$\lim_{x,t \to \infty} \langle \phi^\dagger(x,t)\phi(0,0) \rangle = 0 \text{ in } d \leq 2.$$ 

First we will say mathematically why this is true. Then we will say what this has to do with the phase fluctuations, i.e. the Goldstone mode.

- **Mathematical reason:** The mathematical reason why long-range order is destroyed in $d \leq 2$ has to do with the comparison of kinetic energy to the dimensionality of space. Let us define

$$G(x,t) = \langle \phi^\dagger(x,t)\phi(0,0) \rangle \text{ and } \tilde{G}(p,\omega) = \langle \phi^\dagger(k,\omega)\phi(k,\omega) \rangle.$$ 

Then we have

$$\tilde{G}(p,\omega) \sim \frac{1}{\omega^2 - u^2k^2} \implies G(x,t) = \int_{k,\omega} e^{ikx - \omega t} e^{i\theta(x,t)} e^{-i\theta(0,0)}.$$ 

This diverges due to the dimensionality of the $k$-integral (and also the $\omega$-integral, but often people are interested only in static properties, so in that case there would be no $\omega$-integral).

- **Physical reason:** What does this have to do with the phase fluctuations? In the symmetry-broken phase, this is very easy to see:

$$\langle \phi^\dagger(x,t)\phi(0,0) \rangle = \rho_0 (e^{-i\theta(x,t)} e^{i\theta(0,0)}) \to \rho_0 e^{-\frac{1}{2} i [\theta(x,t) - \theta(0,0)]^2},$$ 

and the last step holds (approximately) for a quadratic Hamiltonian.

(Since amplitude fluctuations are ignored, we are in fact looking at a transverse correlation function.) We shall prove later on that for any collection of Gaussian distributed variables,

$$\langle \exp(a\theta) \rangle = \exp\left(\frac{a^2}{2} \langle \theta^2 \rangle \right).$$

A system in which there is an order parameter, but the order parameter has no long-range correlation, is called a quasi-condensate. The density is constant but the phase experiences significant fluctuations. For a system of large length $L$, the result is

$$G_\theta(x,t) = -i \langle \hat{T}(\theta(x,t)\theta(0,0)) \rangle = \frac{ig}{4\pi \hbar u} \log \left( \frac{4\pi^2 x^2 - u^2 t^2 + i0^+}{L^2} \right).$$ 

From this, we can extract a phase coherence length $L_\theta$. The regime of BEC can still be obtained in $d = 1$, but only if $L_\theta \geq L$. 

3
2D systems

We will see in the two-dimensional systems that there is no long-range order for \( T > 0 \). However, there can be quasi-long-range order, in which the correlations fall off like a power law; this is called the Berezinskii-Kosterlitz-Thouless (BKT) phase. Let us study these phenomena in the context of the Bose gas.

- 2D systems can support a BEC, but only at \( T = 0 \). Our conclusion will be

\[
\langle \theta(x,0) - \theta(0,0) \rangle^2 \sim \log \left( \frac{x}{\xi} \right) \implies \langle \phi^\dagger(x,0)\phi(0,0) \rangle \sim \left( \frac{x}{\xi} \right)^{1/n\lambda^2},
\]

where \( \xi = \frac{\hbar}{\sqrt{mp}} \). To understand this, consider the Bogoliubov-de Gennes equations for the fluctuations. Introducing some coupling \( g_{2D} = \frac{4\pi\hbar^2a}{m} \), we find

\[
i\partial_t \delta\phi = \left( -\frac{\nabla^2}{2m} + 2g_{2D}n_0 - \mu \right) \delta\phi + g_{2D}\Phi_0^2 \delta\phi^\dagger.
\]

Why did we need to introduce this particular coupling? The reason is it is convenient to describe some of the scattering properties off a general potential, but with the easier-to-handle \( \delta \)-function potential:

\[
V(r - r') = \frac{4\pi\hbar^2a}{m} \delta(r - r') = g\delta(r - r')
\]

has s-wave scattering length \( a \). Negative scattering length corresponds to attractive potential and positive scattering length corresponds to repulsive potential. We can use this because for ultracold atoms, the de Boglie wavelength is much longer than the effective length of the true interaction (which may be dipole-dipole, for example) and hence the interatomic potential can be approximated to be a contact potential, see [https://web.pa.msu.edu/people/mmoore/Lect18_DeltaScatterer.pdf](https://web.pa.msu.edu/people/mmoore/Lect18_DeltaScatterer.pdf). I can also argue for this on heuristic grounds. I claim that the \( \delta \)-function potential has another lengthscale associated with it; let us call it \( a \). If \( V(x) = g\delta(x) \), then dimensional analysis gives

\[
g = \frac{\hbar^2a}{ma} \implies a = \frac{\hbar^2}{mg}.
\]

A way to understand this is to argue

\[
[g] = [E][L]^d \text{ and } E \sim \frac{\hbar^2}{ma^2} \implies g \sim \frac{\hbar^2a}{m}
\]

in \( d = 3 \).

I guess another way I can imagine it is to consider a finite spherical well, \( V = 0 \) for \( r > a \) and \( V = V_0 \) for \( r < a \). Then the s-wave scattering length for small incoming momentum is (see [http://hitoshi.berkeley.edu/221B/scattering3.pdf](http://hitoshi.berkeley.edu/221B/scattering3.pdf))

\[
a_0 \sim a \left[ \frac{\tanh Ka}{Ka} - 1 \right] \text{ where } K^2 = \frac{2mV_0}{\hbar^2}.
\]
To get the intuition, I want to see what happens when I drive the radius $a$ to very small (approximating $\delta$-function) and increase the depth of the well, while preserving the scattering length. If $Ka$ is small, then Taylor series expansion gives

$$a_0 \sim a \left[ 1 - \frac{1}{3} (Ka)^2 + \cdots - 1 \right] \sim -K^2 a^3 \sim \frac{mV_0}{\hbar^2} a^3,$$

so this tells us something important about the scattering behavior. $a^3$ is like a volume, so we need to keep the integral of the potential over the scattering volume constant to have a constant $s$-scattering length. Interesting.

This is solved for the phase and density fluctuations. We can assume to a good approximation that the density fluctuations vanish and focus on the phase fluctuations, for which the solution is

$$\theta(x, t) = -i \sqrt{\frac{m\mu}{2V\hbar n}} \sum_k \frac{1}{\sqrt{k}} a_k e^{i(kx-\epsilon_k t)} + \text{h.c.}$$

and the energy is $\epsilon_k = uk$. We can use this solution explicitly to find the fluctuations of the phase:

$$\frac{1}{2} \langle (\theta(x, 0) - \theta(0, 0))^2 \rangle = \frac{m\mu}{V\hbar n} \sum_k 1 - \cos(kx) \frac{(n_k + \frac{1}{2})}{k}.$$

Here, $n_k$ is the occupation of the Bogoliubov-de Gennes mode of wavevector $k$, which is a quasiparticle mode; this is approximated for low-energy modes (i.e. the important ones) as

$$n_k \sim \frac{kT}{uk}.$$  

We see that for $T = 0$, $n_k = 0$ for all $k \neq 0$. For $T = 0$, the integral will behave kind of like

$$\int_0^\infty dk k \times \frac{1 - \cos(kx)}{k},$$

which for $k \to 0$ goes to zero and has to be regularized for $k \to \infty$, for which it approaches a constant. Anyway, this tends to a constant for $x \to \infty$. For $T > 0$ it will be kind of like

$$I(x) = \int_0^{\xi^{-1}} dk k \times \frac{1 - \cos(kx)}{k^2} + \int_{\xi^{-1}}^\infty (not \ as \ important \ \cdots) \sim \log(\frac{x}{\xi}).$$

Here, $\xi = \frac{\hbar}{\sqrt{m\mu}}$ is the healing length which tells us about the number of particles, and we performed the integral by noticing that $\nabla^2 I(x) \sim \delta(x)$, which implies that we should get Coulomb potential in 2D (a logarithm). Clearly, this reflects the logarithmic nature of the Kosterlitz-Thouless vortices, which interact with each other via 2D Coulomb potential. Anyway, the first integral ($T = 0$) has no divergence (and goes to a constant) while the second integral has a gentle logarithmic divergence in the IR.

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**Ch 3. Ultracold gases in optical lattices**

The optical lattice trapping of cold atoms can engineer systems to simulate things like Bloch oscillations, Landau-Zener tunneling, Josephson tunneling, etc. Here, we get our first exposure to ultracold atoms and optical lattices. We will make contact with experiment and see what people can control in the lattice systems.
Optical trapping of atoms

The basic tools to generate ultracold lattice gases are the **optical potentials**. If the field frequency is not close to resonance, it does not cause any real transition, but merely an oscillating dipole moment:

$$\mathbf{d}(\mathbf{r}, \omega_L) = \alpha(\omega_L) \mathbf{E}(\mathbf{r}, \omega_L)$$

Above, $\omega_L$ is the laser frequency and $\alpha$ is a matrix.

The polarizability $\alpha$ depends on how close $\omega_L$ is to the resonance frequencies $\omega_i$. If $\omega_L$ is much closer to one resonance $\omega_1$ than to the others $\omega_2,\omega_3,\ldots$, then the polarizability goes like

$$\alpha(\omega_L) \sim \frac{1}{\omega_L - \omega_1} := \frac{1}{\Delta}.$$ 

If the laser has pure frequency, then the energy shift looks like Stark effect

$$\Delta E(\mathbf{r}, t) = \mathbf{d} \cdot \mathbf{E} = -2\text{Re} \mathbf{E}^*(\mathbf{r}, t)\alpha(\omega_L)\mathbf{E}(\mathbf{r}, t).$$

Since one $\mathbf{E}$ is conjugated, the $e^{-i\omegaLt}$ time-dependence gets cancelled out, and the time-variation of $\Delta E$ is slow. We need to conjugate one of the $\mathbf{E}$ fields because otherwise the time-average of the potential would be zero everywhere, which doesn’t make sense. Actually I think $\Delta E(\mathbf{r}, t)$ is itself a time average. If we think about it without the complex phases, then

$$\mathbf{E}(\mathbf{r}, t) = E_0 \cos(k \cdot r - \omega_L t) \implies \Delta E(\mathbf{r}, t) = \alpha(\omega_L)|E_0|^2 \cos^2(k \cdot r - \omega_L t).$$

If polarizability is isotropic, then we just get the laser beam intensity $I$:

$$\Delta E(\mathbf{r}, t) = -2\text{Re}(\alpha)I(\mathbf{r}, t).$$

Note that the time-dependence of $\mathbf{E}(\mathbf{r}, t)$ is *fast* while the time-dependence of $I(\mathbf{r}, t)$ is *slow*.

We reparameterize this in terms of a **detuning parameter** $\Delta := \omega_L - \omega_0$, where

$$V(\mathbf{r}) \propto \frac{I(\mathbf{r})}{\Delta}.$$ 

**Red-detuning**, where $\Delta < 0$, is when the atoms are attracted to the regions of high intensity. **Blue-detuning**, where $\Delta > 0$, is when the atoms are attracted to the regions of low intensity. To reduce heating caused by inelastic scattering, a large $|\Delta|$ is required. This is because

We can add two or more laser fields and create a standing wave. It makes a spatially periodic potential due to the interference pattern,

$$V(\mathbf{r}) = V_0 \sin^2(k \cdot r).$$

Sometimes, we express the potential depth $V_0$ in terms of the **recoil energy** $E_R = \frac{k^2}{2m}$ of the atoms, where $k = 2\pi/\lambda$ and $\lambda$ is the wavelength of lasers which form the standing wave.
Controlling parameters in cold optical lattices

What can we control in the ultracold lattice gases?

- Lattice geometry and dimension of the lattice: We can just change the direction and number of the laser beams. Easy.

- Elimination of phonons: Optical lattices are not “physical” things holding the atoms in place, so they do not support phonons. However, if the lattice is formed in an optical cavity, atom-light coupling may shift the cavity resonance and there can be “phonon-like” excitations. It leads to superfluid-Mott insulator crossover.

- Tunneling: The hopping parameter can be controlled well using pure tunneling, laser-assisted coherent transition, and lattice tilting (acceleration) techniques.

- On-site interactions: The scattering lengths (and hence the strengths) of on-site interactions can be modified using Feshbach resonances.

- Spin-dependent optical lattices: Given two counterpropagating laser beams with linear polarization forming a certain angle (the lin-lin configuration), atoms with different spin can experience different lattice potentials.

- Temperature: Typical critical temperatures of ultracold BEC are like 50 nK. When you get to 10 or less nK, it is cutting very close to the current experimental limit.

Mathieu equation

The solution of the single-particle Hamiltonian in 1D lattice with potential

\[ V(x) = \frac{V_0}{2E_R}(1 - \cos(2kx)) \]

is called the solution to **Mathieu equation**. The solution looks like this:
Many-body models

The canonical many-body model is the two-body interaction model

$$\mathcal{H} = \int \Psi^\dagger (\frac{-\nabla^2}{2m} + V_{\text{ext}}) \Psi + \frac{1}{2} \int_{\mathbf{r},\mathbf{r}'} \Psi^\dagger \Psi^\dagger V(\mathbf{r} - \mathbf{r}') \Psi \Psi'. $$

Usually, the optical gases are weakly-interacting. To make them strongly interacting, all you do is decrease the hopping parameter and leave the two-body interactions fixed. Then the hopping can be of the same order as the interaction.

Ch 4. Quantum simulators of condensed matter

Here is the question: what kinds of condensed matter systems can we mimic with the ultracold atoms in lattices? We should define what is meant by a quantum simulator. Feynman (1986) had a famous paper which pointed out that it might be possible to find a simpler, more experimentally accessible system to mimic a quantum system of interest, in the sense that classical simulations would be too expensive.

The modern idea of quantum simulators in ultracold lattice gases is that the quantum simulator does not really represent the true system, but it represents a simplified model of the true system. For example, if we think that superconductivity in the cuprates is described by 2D Hubbard model, then we can model 2D Hubbard model in the cold lattice. The quantum simulator, of course, is useful only if the classical simulator (i.e. a computer) cannot handle it.
Simulations of Hubbard model

Suppose we have multiple species $\alpha$ of bosons and multiple species $\beta$ of fermions. The lattice sites are labelled by $i$, and the most general Hubbard-type Hamiltonian we can realize with the cold atoms (assuming lowest band occupation only) is

$$\mathcal{H} = \mathcal{H}_{\text{hop}} + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{int-hop}} + \mathcal{H}_{\text{pot}} + \mathcal{H}_{\text{Rabi}}.$$

Here are some general notes about all these different terms.

- **Interaction term**: the dominant part is the on-site interaction. However, sometimes interaction between different sites, $V(i, j)$, is included.

- **Interaction-assisted hopping (int-hop)**: This is an interesting term. It looks like

  $$b_{i\alpha}^\dagger b_{j\beta}^\dagger b_{j\beta'} b_{i\alpha'}.$$

  Or, the important part is

  $$b_{i\alpha}^\dagger b_{j\beta}^\dagger b_{j\beta}.$$

  What this means is that initially, two particles were on site $j$. Then, they interact and one of them hops to site $i$. Apparently it is important for studying electrons and holes and are used in “hole superconductivity.”

- $\mathcal{H}_{\text{pot}}$ is the potential due to the lattice. $\mathcal{H}_{\text{Rabi}}$ describes an on-site transition achieved with a laser; it can look like

  $$\Omega_{\alpha\beta} b_{i\alpha}^\dagger b_{i\beta}.$$

  Here, $\alpha$ and $\beta$ are different states of the boson.

Spin models

Hubbard models can reduce to spin models in certain limits. Many of these limits are accessible with cold atoms. For example, if bosonic atoms can only occupy $2S + 1$ different states in a lattice site, then generally people can exploit the symmetry and break it to a spin symmetry for pseudo-spin $S$.

Ch 5. Bose-Hubbard models

We review methods to solve Bose-Hubbard model: Bogoliubov method, strong coupling expansion, mean-field and perturbative mean-field, Gutzwiller method, exact diagonalization, quantum Monte Carlo, semiclassical phase space method, and 1D methods: Jordan-Wigner transformation, Bethe ansatz, bozonization.

Let us take our Hubbard Hamiltonian to be the following:

$$\mathcal{H} = - \sum_{(ij)} t(b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i.$$
The phase diagram of the Hubbard model in $t$ and $U$ displays the Mott-insulator lobes which describe the transition between Mott insulator and superfluid states.

For weak interactions $U/t \ll 1$, the Bogoliubov mean-field approach can describe the excitation spectrum; however, it fails to describe the transition boundary to the insulating phase, in which the interaction cannot be assumed to be small. In this regime, called the strong-interaction limit $U/t \gg 1$, tunneling is treated as a perturbation, and the boundaries of the Mott insulator-superfluid transition can be calculated with high accuracy by going to high order in the expansion.

$t \gg U$: Bogoliubov theory

Suppose the lattice is in $d$ dimensions and has $M$ sites. There are $N$ total particles on the lattice, of which $N_0$ are in the BEC condensate, and we are at $T = 0$. With no interactions, clearly all of the particles would be in the ground state and we would have a perfect condensate. When interactions are turned on, atoms gradually start to leave the condensate.

Let’s go to momentum space. The result is

$$
\mathcal{H} = \sum_k (-\epsilon(k) - \mu) a_k^\dagger a_k + \frac{U}{2M} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2,k_3+k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}.
$$

To solve this problem, we make the Bogoliubov approximation

$$
\langle a_0 \rangle = \langle a_0^\dagger \rangle = \sqrt{N_0}
$$

and write $a_0 = \sqrt{N_0} + \delta a_0$. Let me ask the same question again – why can we replace $\langle a_0 \rangle = \sqrt{N_0}$ and not have to include arbitrary phase $\langle a_0 \rangle = \sqrt{N_0} e^{i\theta}$?

Now we keep only the quadratic terms and we can diagonalize via Bogoliubov transformation. The effective diagonalized Hamiltonian becomes

$$
\mathcal{H} = -\frac{U N_0 N_0}{2} + \frac{1}{2} \sum_k (\omega_k + \epsilon_k - 2dt - Un_0) + \sum_k \omega_k c_k^\dagger c_k
$$

and the dispersion is

$$
\omega_k^2 = (2dt - \epsilon_k)^2 + 2Un_0(2dt - \epsilon_k).
$$

We can very clearly see the effect of the dimensionality, $d$. The excitation spectrum is gapless in the thermodynamic limit, i.e. $M,N \to \infty$ with $N/M$ constant. Since $\omega_k \to 0$ as $k \to 0$, the energy of a single excitation can be arbitrarily small and we cannot describe the Mott insulators, for which the excitations must be gapped.

At $T = 0$, there are no excitations in the system, and the ground state is Bogoliubov vacuum $c_k |\Omega\rangle = 0$, where $c_k$ is the Bogoliubov operator. At finite temperature, $\langle c_k^\dagger c_k \rangle = n_B(\omega_k)$, where $n_B$ is the Bose-Einstein distribution. However, we can only do this for $N - N_0 \ll N$.

$U \gg t$: strong coupling expansion

The strong coupling expansion is an expansion in the small parameter $t/U$. We just divide everything by $U$, which gives

$$
\mathcal{H} = U \left[ \mathcal{H}_0 + \frac{t}{U} \mathcal{H}_1 \right],
$$

where
\[
H_0 = \sum_i \left(\frac{1}{2}n_i(n_i - 1) - \frac{\mu}{U}n_i \right) \text{ and } H_1 = \sum_{\langle ij \rangle} (-b_i^\dagger b_j - b_j^\dagger b_i).
\]

How can we determine the phase boundaries of the MI-SF transition? We require that, at the phase boundary (i.e. separated by the addition or subtraction of a single particle), there is zero difference in energy between the two phases (i.e. at the same number of particles, the two phases give the same energy). To do this, we need to know what the Mott insulator and superfluid ground states are! They are given by

\[
|\text{MI}(n_0)\rangle = \prod_{i=1}^M \frac{1}{\sqrt{n_0}} (b_i^\dagger)^n_0 |0\rangle,
\]

\[
|\text{SF}(n_0 + 1)\rangle = \frac{1}{\sqrt{M(n_0 + 1)}} \sum_{i=1}^M b_i^\dagger |\text{MI}(n_0)\rangle,
\]

\[
|\text{SF}(n_0 - 1)\rangle = \frac{1}{\sqrt{M(n_0)}} \sum_{i=1}^M b_i |\text{MI}(n_0)\rangle.
\]

I think these superfluid states look kind of funny. There is nothing that apparent in them to suggest they are “superfluid,” or, you know, actually condensed in the sense of BEC. You can, however, argue there is a condensate based on the fact that

\[
\langle b_i \rangle_{\text{SF}} \neq 0.
\]

In this sense, the superfluid state is a superposition of many quantum states in a sense that the Mott insulator is not. I think we just use them to get the symmetrized state which is just a little different from the Mott insulating state.

The procedure goes as follows: these are the states, but to calculate their energy we need to do perturbation theory to very high order in \(t/U\). So, for example, the energy of the Mott-insulator phase with \(n_0\) particles per site, to \(\mathcal{O}(t^2)\), is

\[
E_{\text{ground}}(n_0) = \left[NUn_0(n_0 - 1)/2 - \mu n_0 \right] - N\frac{t^2}{U}n_0(n_0 + 1).
\]

**Perturbative mean-field approach**

The mean-field approach is fun and easy. The idea is to introduce the superfluid order parameter

\[
\langle b_i \rangle = \phi_i
\]

and see when \(\phi_i\) disappears, to lowest order. This will give us an approximation for the MI-SF phase boundary. We approximate

\[
b_i^\dagger b_j \approx \phi(b_j + b_j^\dagger) - \phi^2
\]

so this describes either the Mott phase (\(\phi = 0\)), the deep superfluid phase (where this approximation is valid for \(\phi \neq 0\)) but not really the phase boundary. However, we will use it as an
approximation to the phase boundary. The Hamiltonian is now completely local because of the decoupling of the hopping term:

\[ H = \sum_i \left[ \frac{U}{2} n_i(n_i - 1) - \mu n_i - 2tz\phi(b_i^* + b_i) + 2tz|\phi|^2 \right]. \]

If \( t \) is small, we take

\[ v(t) = -2tz\phi(b_i^* + b_i) \]

to be the perturbation. The result for the energy is

\[ E_0/N = \frac{U}{2} n(n - 1) - \mu n + 2tzr\phi^2 \]

where

\[ r = \frac{2zt(U + \mu)}{U^2n(n - 1) - \mu U(2n - 1) + \mu^2 + 1}. \]

If \( r > 0 \), the energy is minimized for \( \phi = 0 \), so this is the Mott phase. If \( r < 0 \), the energy is minimized for \( \phi \neq 0 \), so this is the superfluid phase. Therefore, \( r = 0 \) gives an approximation for the superfluid boundary

\[ \frac{t}{U} = -\frac{n(n - 1) - \frac{\mu}{U}(2n - 1) + (\mu/U)^2}{2z(1 + \mu/U)}. \]

Check this math.

Gutzwiller approach

There is another approach called Gutzwiller mean-field approach, which works for both statics and dynamics. It is based on approximating the many-body wavefunction with a product over single-site contributions, and then using variational theory on the probability amplitudes. Let us see how this works.

Let \( |n\rangle_i \) denote the Fock state of \( n \) atoms in the \( i \) site, \( n_{\text{max}} \) be a maximum number of atoms in a site (to constrain the number of variational parameters), and \( f_{ni} \) be a (complex) amplitude (or variational parameter) describing the probability of having \( n \) atoms in the \( i \) lattice site. We take the variational state

\[ |\Psi\rangle = \prod_i \sum_{n=0}^{n_{\text{max}}} f_{ni} |n\rangle_i. \]

Obviously this can describe a superfluid because there is a superposition of lots of different states with different particle number, so the variational state \( |\Psi\rangle \) can support a nonzero superfluid order parameter. In fact,

\[ \phi_i = \sum_n \sqrt{n + 1} f_{ni}^* f_{n+1,i}. \]

It can also describe Mott-insulator if the number of atoms in a site is fixed. Then \( f_{ni} = \delta_{n,n_0} \) and the above pairwise product vanishes.

Gutzwiller method does not account for correlations between sites (which is what I was wondering about when I first saw it; compare to Eugene’s recent paper which is about using non-Gaussian states to introduce correlations). Since correlations are stronger in low dimensions, Gutzwiller
approach only works in high dimensions (usually 3 or more). Actually, let’s clear up what we mean by “correlations.” What we mean is the following:

\[ \langle \Psi | b_i \dagger b_j | \Psi \rangle = \langle \Psi | b_i \dagger | \Psi \rangle \langle \Psi | b_j | \Psi \rangle \text{ for } i \neq j. \]

If the expectations are factorizable, the variational manifold does not account for correlations.

**Dynamical Gutzwiller approach**

This is one kind of dynamical mean field theory. We allow the Gutzwiller amplitudes to vary in time and begin with the Schrödinger equation

\[ \langle \Psi | i\partial_t - \mathcal{H} | \Psi \rangle = 0. \]

This gives the equations of motion for the Gutzwiller amplitudes check this

\[ i\partial_t f_{ni} = \frac{U}{2} n(n-1)f_{ni} - \mu n - t(\bar{\phi}_i^* \sqrt{n+1}f_{n+1,i} + \bar{\phi}_i \sqrt{n}f_{n-1,i}) \]

where \( \bar{\phi}_i = \sum_{\langle j \rangle} \phi_j \), where \( \langle j \rangle \) is next to \( i \). The equation can be solved in real or imaginary time, where it is supposed to converge to the ground state of the system.

**1D methods**

1D methods are prominent because 1D makes some things easier. In particular, let’s think about fermionic Luttinger liquid and bosonization.

We expect the interesting physics to occur close to the surface of the Fermi sea, so define the fermions by left \( L \) and right \( R \), and by the wavevector \( k \) relative to \( k_F \). Then, the Luttinger model is

\[ \mathcal{H} = \sum_k -c_F(k)L^\dagger(k)L(k) + c_F(k)R^\dagger(k)R(k) + \frac{1}{L} \sum_{k_1,k_2,q} V(q)L^\dagger(k_1 - q)R^\dagger(k_2 + q)R(k_2)L(k_1). \]

Now, we are going to do something crazy: rewrite the Hamiltonian in terms of (bosonic) density operators. This is an elementary example of **bosonization**. Introduce density

\[ \rho_{L,R}(q) = \sum_k (L, R)^\dagger(k + q)(L, R)(k). \]

We claim these are (almost) good bosonic operators which satisfy the canonical commutations. Let us check this:

\[ [\rho_R(-q), \rho_R(q')] = \sum_{k=k_F-q}^{k_F} R^\dagger(k + q - q')R(k) \approx \frac{qL}{2\pi} \delta(q - q'), \]

where we used the **Luttinger-Tomonaga approximation**, which is similar to the RPA approximation (see my notes). Therefore, we define

\[ b^\dagger_q = \rho_R(q)\sqrt{2\pi/qL}, c^\dagger_{-q} = \rho_L(-q)\sqrt{2\pi/qL}. \]
The bosonic operators take a particle from state \( k \) and put it into state \( k + q \), etc. Hamiltonian is rewritten

\[
\mathcal{H} = \sum_{q>0} q c_F(b_q^+ b_q + c_{-q}^+ c_{-q}) + \frac{1}{2\pi} \sum_{q>0} (V(q) c_{-q}^+ b_q^+ + V(q)^* b_q c_{-q}).
\]

We use only \( q > 0 \) because \( b \) is for things moving to the right \((q > 0)\) and \( c \) is for things moving to the left \((q < 0)\). Thus, the problem has been reduced (in a good approximation) to an exactly solvable system of interacting bosonic harmonic oscillators.

**Bethe ansatz**

Bethe ansatz is an analytical method for finding exact eigenstates and eigenvalues of some strongly correlated 1D models (although sometimes it has to be complemented with numerical analysis). By appropriately exploiting the symmetries involved in the Hamiltonian it is possible to diagonalize the Hamiltonian exactly.

Let us examine Bethe’s original problem. Consider a 1D line of electrons with uniform next-neighbor interactions, which is mapped to spin-\( \frac{1}{2} \) Heisenberg model:

\[
\mathcal{H} = -J \sum_{i=1}^{N} \sigma_i \cdot \sigma_{i+1}.
\]

Bethe ansatz describes how to parametrize the eigenvectors.

Calling \( \sigma^+_i = \sum_i \sigma_i^z \), it’s easy to see that \([\mathcal{H}, \sigma^+_i] = 0 \). We can rewrite the Hamiltonian as

\[
\mathcal{H} = -J \sum_i \frac{1}{2}(\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) + \sigma_i^z \sigma_{i+1}^z.
\]

Due to the translational symmetry, and the fact that the total spin \( \sigma^+_T \) can label the states, it seems that we should construct the states as “Bloch” wavefunctions with fixed total z-spin, \( \sigma^+_T \).

We label the eigenstates with quantum number \( N/2 - r \), where \( r \) is the number of “flipped” spins (assuming we start with all the spins pointing up). So the eigenstate labeled with \( N/2 \) is just

\[
|N/2\rangle = |\uparrow, \cdots, \uparrow\rangle.
\]

The next set of eigenstates are dependent on momenta: the symmetrized linear combinations where \( k = 2\pi m/N \),

\[
|N/2 - 1, k\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn} \sigma_n^- |\uparrow, \cdots, \uparrow\rangle.
\]

The rest of the states follow in a generalization of the above procedure, which is called **Bethe ansatz**. Let us define

\[
|n_1, n_2, \cdots, n_r\rangle = \sigma_{n_1}^- \sigma_{n_2}^- \cdots \sigma_{n_r}^- |\uparrow, \cdots, \uparrow\rangle.
\]

In the case where \( r = 1 \), we took a linear combination of the z-basis vectors; in other words we took

\[
|N/2 - 1, k\rangle = \sum_n a_k(n) |n\rangle
\]
and determined the coefficients $a_k(n)$ based on the eigenvalue equation $\mathcal{H}|\psi\rangle = E|\psi\rangle$. Let us generalize this to $r = 2$,

$$|N/2 - 1, k_1, k_2\rangle = \sum_{1 \leq n_1 < n_2 \leq N} a_{k_1,k_2}(n_1, n_2)|n_1, n_2\rangle.$$ 

Since there are $\binom{N}{2}$ choices of $|n_1, n_2\rangle$, there are also $\binom{N}{2}$ eigenstates in $k$-space (preserve the dimension of Hilbert space). These are characterized by pairs of Bethe quantum numbers and you can show the allowed coefficients are

$$a_{k_1,k_2}(n_1, n_2) = e^{i(k_1 n_1 + k_2 n_2 + \theta_{12}/2)} + e^{i(k_1 n_2 + k_2 n_1 + \theta_{21}/2)}$$

where $\theta_{12} = -\theta_{21} = \theta$, $2 \cot \frac{\theta}{2} = \cot \frac{k_1}{2} - \cot \frac{k_2}{2}$. Generally, Bethe ansatz for an unrestricted number of flipped spins, $r$, is

$$|\psi\rangle = \sum_{1 \leq n_1 \leq \cdots \leq n_r \leq N} a_{k_1,\cdots,k_r}(n_1, \cdots, n_r)|n_1, \cdots, n_r\rangle.$$ 

The method is fermionic because it assumes the occupations are either 0 or 1 (spin up or down). However, it can be applied as an approximation to bosonic systems as well, if the occupations of the lattice sites are small (i.e. not larger than 2), and still gives some good predictions.

**Ch 6. Fermi-Hubbard, Fermi-Bose-Hubbard models**

This chapter presents various methods specific for fermionic systems and Fermi–Bose mixtures. It starts by discussing a lattice version of the BCS theory and then reviews BCS-BEC crossover theory for trapped Fermi gases close to the Feshbach resonance. The chapter analyses Fermi Hubbard models in the strongly correlated regime and t-J limit, and introduces the Gutzwiller projection method and the slave boson approach. It discusses in detail, in particular in the context of Fermi-Bose mixtures, effective low energy Hamiltonians and their derivation.

**BCS-BEC crossover**

The text derives regular BCS theory on a lattice; just as a reminder, the order parameter in BCS theory is the expectation of making a Cooper pair,

$$\Delta_i = U \langle f_{i\downarrow} f_{i\uparrow} \rangle \implies \Delta_i = \Delta,$$

if the lattice is translationally invariant.

Ultracold atomic Fermi gases allow us to study one of the fundamental problems of many-body physics – a two-component attractive Fermi gas with extremely strong interactions, which is possible because we can tune the effective interactions using a Feshbach resonance (which we will describe shortly).

Feshbach resonance in scattering of fermions is when fermions scatter from an “open” channel (where they are weakly coupled) to a “closed” channel (strongly coupled). The open channel represents an “unbound” state and the closed channel represents a bound state.
The Feshbach resonance is tuned by changing the energy of the bound state (in the closed channel) via an external magnetic field, $B$; the energy can pass through zero. The scattering length diverges with $B$ like

$$a_s(B) = a_{bg}(1 - \frac{B_w}{B - B_0}).$$

**BCS-BEC in two-channel model**

First let us describe what the BCS-BEC crossover is. The BCS state involves pairing in momentum-space, $\Delta \propto \sum_k \langle f_{-k\downarrow} f_{k\uparrow} \rangle$. The BEC involves a condensate of bound pairs in real space, and the crossover occurs by increasing the attraction from weak (BEC) to strong (BCS). There is a change in the sign of the scattering length. In the picture below, BCS is on the RHS and BEC is on the LHS.

![Diagram](image)

To see how this could occur, consider a theory of **resonant Fermi superfluidity**, with resonant referring to the Feshbach resonance. Suppose $\psi_\sigma$ represents the fermions and that two fermions can come together and make a bound state $\psi_B$. Then the Hamiltonian could look like

$$\mathcal{H} = \int r \sum_\sigma \hat{\psi}_\sigma^\dagger \left( -\frac{\nabla^2}{2m} \psi_\sigma + \psi_B^\dagger (-\frac{\nabla^2}{4m} + \nu) \psi_B + g(\psi_B^\dagger \psi_\uparrow^\dagger \psi_\downarrow + \text{h.c.}) \right).$$

The energy $\nu$ is called the **detuning** with respect to the open channel continuum. It is supposed to be small near resonance. We call the different $\psi_\sigma(r, t)$ the **hyperfine states** due to possible splitting of the degeneracy.

In the regime of low energies and densities, this model can be recast as an effective Hamiltonian for the “free” particles in the same way that we derive the $2 \rightarrow 2$ effective Coulomb interaction from the three-particle interaction of QED. The result is

$$\mathcal{H} = \sum_{k\sigma} (\epsilon_k - \mu) \hat{\psi}_k^\dagger \psi_{k\sigma} + \frac{\lambda}{V} \sum_{kqp} \hat{\psi}_{k\uparrow}^\dagger \hat{\psi}_{p\downarrow}^\dagger \hat{\psi}_{k+q\downarrow} \hat{\psi}_{-q\uparrow}.$$

The interaction is **attractive**, $\lambda < 0$. Check this.
Well, that was easy – now we have an energy which is basically ready for BCS procedure. Note
that in the regular BCS theory, the interactions must also be (at least weakly) attractive. If they
are repulsive, the only solution of gap equation is $\Delta = 0$. For attractive interactions, no matter
how small, there is a nonzero solution for $\Delta$ in the region $0 < \mu < 4td$, where $t$ is the hopping
parameter. In the original BCS theory, the attractive interactions are described by $U$ (which
presumably has to do with the phonons and also the “effective charge screening” that Eugene
talked about, in which a moving electron leaves a region of excess positive charge). In this theory
of resonant effective interaction, the attractive interaction has to do with????

It turns out that we can relate the BCS interaction $U$ with the Feshbach effective interaction $\lambda$.
It is

$$ \frac{1}{U} = \frac{1}{\lambda} + \frac{1}{V} \sum_k \frac{1}{2\epsilon_k} $$

where $V$ is volume of Wannier function in the lattice site, and the sum is cut off by the inverse
lattice constant.

We can obtain a mean-field description of the BCS-BEC model by taking the expectation of
Hamiltonian with BCS wavefunction, assuming a gap $\Delta$ and chemical potential $\mu$, and then
finding $\Delta$ and $\mu$ self-consistently. The result is

$$ E = -\frac{m}{4\pi a_s} \Delta^2 + \int \left( \xi_k - E_k + \frac{\Delta^2}{2\epsilon_k} \right). $$

Here, $E_k = \sqrt{\xi_k^2 + \Delta^2}$ and $\xi_k = \epsilon_k - \mu$.

is of weakly-correlated pairs of fermions; the BEC regime is of diatomic molecules in the atomic
Fermi gas.

**Summary of Hubbard and $t - J$ models**

Hubbard model is the hopping model with on-site interactions. $t - J$ model is applicable for large
on-site repulsive interactions. In this case, all sites are either singly occupied or not occupied at
all, and we can recast the interaction part of the Hamiltonian in an effective spin kind of thing:

$$ \mathcal{H} = \sum_{\langle ij \rangle} t_{ij} f^\dagger_{i\sigma} f_{j\sigma} + J \sum_{\langle ij \rangle} S_i \cdot S_j. $$

Here, we have $S_i = \frac{1}{2} f^\dagger_{i\alpha} \sigma_{\alpha\beta} f_{i\beta}$ which describes flipping a spin, basically.

Unfortunately all of the systematic computational methods fail to simulate this model in the
regions of interest. (1) Quantum Monte Carlo methods suffer from the fermion sign problem (2)
high-$T$ expansions fail due to calculational complexity (3) tensor network methods are inefficient.

Let’s study the **slave boson method**, just to learn what it is.

**Slave boson approach**

Slave boson method was originally developed for the Kondo problem and for heavy fermion com-
ounds, where electron’s effective mass is thousands of times larger than its free mass. Let’s use
it to study $t - J$ model.

The main idea of the slave-boson method is to introduce an additional auxiliary bosonic and fermionic field so that the single-particle-per-site constraint can be realized automatically. The advantage, as we shall see below, is that the slave-boson approach opens the way towards novel kinds of mean-field theories in which one pairs auxiliary fermions or allows for condensation of auxiliary bosons.

Write the regular fermionic operators $f$ as the product of auxiliary boson and fermion operators $b$ and $c$.

$$f_{i\sigma} = \hat{c}_{i\sigma} \hat{b}_i.$$  

Also, we impose constraint

$$\hat{c}_{i\uparrow} \hat{c}_{i\downarrow} + \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + \hat{b}_i \hat{b}_i = 1.$$  

It’s not clear to me (1) why this can be done, or in what regime it can be done (2) why we should impose such a constraint on $c$ and $b$. For a review of slave boson method see [https://www.cond-mat.de/events/correl15/manuscripts/fresard.pdf](https://www.cond-mat.de/events/correl15/manuscripts/fresard.pdf)

Apparently, slave-boson approach allows us to rewrite the Heisenberg effective spin interaction in terms of only the $c$ operators,

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{4} \left[ c_{i\sigma} c_{j\sigma} (\hat{c}_{i\uparrow} \hat{c}_{j\uparrow} - \hat{c}_{i\downarrow} \hat{c}_{j\downarrow}) (\hat{c}_{i\uparrow} - \hat{c}_{i\downarrow}) - \hat{c}_{i\alpha} \hat{c}_{i\alpha} \right].$$  

I’m pretty sure this is due to the normalization identity above. Since we have this form, we can construct a new kind of mean-field theory in which there is pairing of the auxiliary fermions. Obviously this is possible, but I’m not sure how this is an improvement over the original theory. We define the following order parameters:

$$\chi_{ij} = \sum_{\sigma} \langle \hat{c}_{i\sigma} \hat{c}_{j\sigma} \rangle, \Delta_{ij} = \langle \hat{c}_{i\uparrow} \hat{c}_{j\downarrow} - \hat{c}_{i\downarrow} \hat{c}_{j\uparrow} \rangle, b = \langle \hat{b}_i \rangle.$$

### Deriving effective Hamiltonian

The book has very nice treatment of how to systematically derive effective Hamiltonian using perturbation theory (i.e. degenerate perturbation theory, in which effective Hamiltonian only connects states which were originally degenerate). The explanation is really good and result is

$$\langle \alpha, i | \hat{H}_{\text{eff}} | \alpha, j \rangle = E_{\alpha i} \delta_{ij} + t(\alpha, i | \hat{H}_{\text{int}} | \alpha, j) \quad - \frac{\hbar^2}{2} \left( \langle \alpha, i | \hat{H}_{\text{int}} [\hat{Q}_{\alpha i} + \hat{Q}_{\alpha j}] \hat{H}_{\text{int}} | \alpha, j \rangle \right)$$  

The $Q$ operator is defined

$$Q_{\alpha i} = \sum_{k, \gamma \neq \alpha} |\gamma k\rangle \langle \gamma k| E_{\gamma k} - E_{\alpha i}.$$  

### Ch 7. Spinor atomic gases

**Spinor atomic gases** are those with atoms of nonzero internal angular momentum whose orientation in space is not externally constrained, i.e. by a nonzero external $\mathbf{B}$-field. Therefore, the
spinor degree of freedom corresponds to a manifold of degenerate states, kind of like a Dicke state. The total spin is something like
\[ F = I + L + S, \]
where \( I \) is the nuclear spin, \( L \) is the orbital angular momentum, and \( S \) is the spin. Thus, each ground-state manifold consists of all Zeeman states labelled by
\[ |F, m_F \rangle \text{ where } m_F = -F, \ldots, F. \]
If there is no magnetic field, typically \( F \) can change as well as \( m_F \).

**What are the spinor interactions?**

We would like to know how the spinor particles interact with each other. The dominant contribution will be the two-body short range \( s \)-wave interactions, but how does it couple to the spin?

We make the following symmetry arguments:

- Due to rotational symmetry, the interaction can depend only on total spin and not on orientation. I think this will be true only for the \( s \)-wave interactions, which obviously are spherically symmetric. This means that the interaction between \( |Fm_F \rangle \) and \( |F'm_{F'} \rangle \) has to be split up into different channels due to addition of angular momentum. Generally, we will get\[ |m_F - m_{F'}| \leq F_{\text{tot}} \leq F + F'. \]

- Collisions between two identical bosons must pick an even total spin, \( S = 0, \ldots, 2F - 2, 2F \). Collisions between two identical fermions must pick an odd total spin, \( S = 1, \ldots, 2F - 1 \). This is due to identical particle interchange. Generally if I have identical particles \( \psi_1, \psi_2 \) both of spin \( J \) and also some total spin \( S \), the identical particle interchange will cause me to pick up a phase factor
\[ \text{phase} = (-1)^{2J}(-1)^S. \]
The way to think about this is to analogize to spin-\( \frac{1}{2} \) particles. Consider “identical particles” 1 and 2. We write
\[ |\psi\rangle = \frac{1}{\sqrt{2}}(|1, 2\rangle - |2, 1\rangle) \]
and we have to have relative negative sign (antisymmetric combination) because \( |1, 2\rangle = -|2, 1\rangle \) due to the interchange. The relative negative sign is itself like an angular momentum with a certain symmetry, \( S = \frac{2n+1}{2} \).

On the other hand, for bosons if we wrote the same thing, then \( |1, 2\rangle = |2, 1\rangle \) and we would need the \( S = n \) “overall angular momentum” states.

**Contact potential**

The \( s \)-wave interaction in the case of a contact potential can therefore be written as a sum over the allowed “total” states, with projection operator \( \mathcal{P}_S \) picking out the total spin \( S \) out of the big sum...
you get from adding the individual atomic spins $\mathbf{F}, \mathbf{F}'$ together with Clebsch-Gordan coefficients. We add some couplings $g_S$ and the result is

$$V(r_1 - r_2) = \delta(r_1 - r_2) \sum_S g_S \mathcal{P}_S.$$  

For fermions, $S = 1, 3, \cdots, 2F - 1$ and for bosons, $S = 0, 2, \cdots, 2F$. Not all of the $S$ are used in the sum. For example, $S = 0$ can never be used unless the states we are adding have zero projection on $\hat{z}$-axis, $m + m' = 0$.

It is possible to rewrite this general form as a combination of the $\mathbf{F}_i$ operators, where $\mathbf{F}_i$ is a vector operator describing the spin of boson $i$, $i = 1, 2$. That is because generally

$$\mathbf{F}_1 \cdot \mathbf{F}_2 = \sum_S \lambda_S \mathcal{P}_S \quad \text{and} \quad (\mathbf{F}_1 \cdot \mathbf{F}_2)^n = \sum_S \lambda^n_S \mathcal{P}_S.$$  

This tells us that the variables $(\mathbf{F}_1 \cdot \mathbf{F}_2)^n$ and $\mathcal{P}_S$ are in the same vector space. Therefore, we can always write the interaction as a linear combination

$$V(r_1 - r_2) = \delta(r_1 - r_2) \sum_{n=0}^F \alpha_n (\mathbf{F}_1 \cdot \mathbf{F}_2)^n.$$  

Generally, $\alpha_n$ are linear combinations of the different interactions $g_S$. In the real world, we would have to have a potential smeared out over a finite range. I think this form is convenient so we don’t have to write like $|r_1 - r_2|^{\beta_S}$ again and again in the summation.

**Mean field treatment of spinor BEC**

Let us study Bose condensation of the spinor atomic gases. The complexity of the problem increases as $F$ increases; $F = 1$ was first detected in the $^{23}$Na optically trapped gas. Therefore, we will be studying the simplest mean-field theory ($F = 1$ for all atoms) in which the spinor description of the gas really matters.

We will take $\mathbf{F}$ to be the spin-1 matrices, since we are dealing with spin-1:

$$F_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad F_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$  

We have to use them because we have terms like $\mathbf{F}_1 \cdot \mathbf{F}_2$ in the energy, as we saw in the previous section. This is because, for example, $2\mathbf{F}_1 \cdot \mathbf{F}_2 = (\mathbf{F}_1 + \mathbf{F}_2)^2 - \mathbf{F}_1^2 - \mathbf{F}_2^2$ is rotationally-invariant. This is the only possibility if we are considering the s-wave interactions.

Let us take Hamiltonian

$$\mathcal{H} = \int \Psi_m^\dagger (-\frac{\nabla^2}{2m} + V_{\text{ext}}(r)) \Psi_m + \frac{c_0}{2} \Psi_m^\dagger \Psi_m \Psi_j^\dagger \Psi_j + \frac{c_2}{2} \Psi_m^\dagger F_{mj} \Psi_j \cdot (\Psi_k^\dagger F_{lk} \Psi_k).$$

We minimize the energy with fixed particle number by incorporating Lagrange multiplier:

$$\delta E = \delta \langle \mathcal{H} - \mu \mathcal{N} \rangle = 0.$$
Here, $\mu$ is chemical potential. If we want to investigate Bose condensation, we introduce an order parameter for each spin-polarization of the atomic gas,

$$\phi_m := \langle \Psi_m \rangle.$$

The order parameter is, in this case, a three-component vector. Let us decompose in terms of magnitude $\sqrt{n}$, which tells us about how large the Bose condensate is, and “direction” $\xi$, which tells us about whether the gas prefers to be in $S_z = -1, 0, 1$ phases. The result is the parametrization

$$\phi = \sqrt{n}\xi$$

and the energy can be written to leading order as

$$E_{F=1} = \int_r \left[ \frac{1}{2m} \left( (\nabla \sqrt{n})^2 + n(\nabla \xi)^2 \right) + (V_{\text{ext}}(r) - \mu)n(r) + \frac{n^2}{2} (c_0 + c_f \langle F \rangle^2) \right].$$

Here, we have written

$$V_{F=1}(r_1 - r_2) = \left( c_0 + c_2 F_1 \cdot F_2 \right) \delta(r_1 - r_2) \quad \text{and} \quad \langle F \rangle = \sum_{kl} \xi_k^* F_{kl} \xi_l.$$

The Hamiltonian is invariant under changes in $\xi$ through $U(1) \times SO(3)$ symmetry, $SO(3)$ for the orientation of spin-1 and $U(1)$ for the overall complex phase on the order parameter. The symmetry will get broken in the ground states below.

We need to find out under what conditions the order parameter $\phi$ is nonzero. This means there will be some kind of condensate. There can be quantum phase transition between different regimes, depending on the couplings. In the following, note that for a well-defined state $|\psi\rangle = |1, m\rangle$ the expectation of $F_x$ and $F_y$ is always zero,

$$\langle F_x \rangle_{\psi} = \langle F_y \rangle_{\psi} = 0 \implies \langle F \rangle^2 = \langle F_z \rangle_{\psi},$$

and this is because of Heisenberg uncertainty. However, $\langle F^2 \rangle_{\psi} \neq 0$.

- **Ferromagnetic phase:** In “ferromagnetic” phase, energy is minimized for $\langle F \rangle^2 = 1$. This happens if the couplings are tuned such that $c_2 < 0$.

  If $|\langle F \rangle| = 1$, then the ground state corresponds to all rotations of the state $|1, 1\rangle$ or equivalently $|1, -1\rangle$. We can say that

$$\xi_{\text{ferro}} = e^{i\phi} U \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

and the order parameter has symmetry $SO(3)$. That is because the $U(1)$ is redundant with part of the $SO(3)$,

$$\xi_F = e^{i\varphi} U \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = e^{i(\varphi-\gamma)} \begin{pmatrix} e^{-i\alpha \cos_2 (\beta/2)} \\ \sqrt{2}\cos (\beta/2) \sin (\beta/2) \\ e^{i\alpha \sin^2 (\beta/2)} \end{pmatrix}.$$
• Polar or “antiferromagnetic” phase: Energy minimized by demanding \( \langle F \rangle = 0 \). This occurs when \( c_2 > 0 \) and the symmetry group is \( U(1) \times S^2 \). Basically, you substitute \(
abla 0 \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \) into the above transformation and find that the angle \( \gamma \), which was originally part of the \( SO(3) \), drops out (i.e., has no effect).

In the spinor atomic gases, there is no notion of up-down-up-down classical alignment like we see in the antiferromagnets in metals. I think we just know that, you know, average order parameter \( m_z \) is zero so we call it antiferromagnet.

Here is a list of ground states and quantum phase transitions. The \( F = 2 \) case, is, of course, more complicated.

### Table 7.2 Classification of the ground-state spinors for \( F = 1 \) and \( F = 2 \).

<table>
<thead>
<tr>
<th>Phase</th>
<th>Conditions</th>
<th>Ground-state spinor</th>
<th>( \langle \vec{F} \rangle )</th>
<th>( \langle S^+ \rangle )</th>
<th>Atomic species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferromagnetic ( F = 1 )</td>
<td>( c_2 &lt; 0 )</td>
<td>((1, 0, 0))</td>
<td>( \neq 0 )</td>
<td>(-)</td>
<td>( ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>Polar ( c_2 &gt; 0 )</td>
<td></td>
<td>((0, 1, 0))</td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na} )</td>
</tr>
<tr>
<td>Ferromagnetic ( F = 2 )</td>
<td>( c_2 &lt; 0 )</td>
<td>((1, 0, 0, 0, 0))</td>
<td>( \neq 0 )</td>
<td>(0)</td>
<td>( ^{83}\text{Rb} )</td>
</tr>
<tr>
<td>( c_2 - c_1/20 &lt; 0 )</td>
<td>( (0, 0, 0, 0, 1))</td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>( c_1 &lt; 0 )</td>
<td>( (0, 0, 1, 0, 0))</td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>Polar ( c_2 - c_1/20 &gt; 0 )</td>
<td>((0, 1, 0, 1, 0)/\sqrt{2})</td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>( (1, 0, 0, 0, 1)/\sqrt{2})</td>
<td></td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>Cyclic ( c_1 &gt; 0 )</td>
<td>((1, 0, \sqrt{2}, 0, 1)/2)</td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
<tr>
<td>( c_2 &gt; 0 )</td>
<td>((1, 0, \sqrt{2}, 0, 1)/2)</td>
<td></td>
<td>(0)</td>
<td>(-)</td>
<td>( ^{23}\text{Na}, ^{87}\text{Rb} )</td>
</tr>
</tbody>
</table>

**Spin textures and topological defects**

Topological defects in scalar condensates correspond to singularities of the order parameter that cannot be adiabatically or smoothly eliminated. The vectorial nature of the order parameter of spinor condensates in general allows for more complex topological defects than in scalar condensates—for a review see Ueda and Kawaguchi (2010). These physical defects are described by homotopy groups of the order-parameter space.

Let us focus on topological defects in the spin-1 condensates.

**Vortices**

The superfluid velocity is \( v_s = \frac{\hbar}{m} \nabla \xi \). This makes sense because it is just expectation of momentum, and we don’t care about \( \sqrt{n} \) because that is *number* of particles, but not how quickly they travel. We can use this to compute superfluid velocity in ferromagnetic (F) and polar/antiferromagnetic (P) cases:

\[
\mathbf{v}_P = \frac{\hbar}{m} \nabla \phi, \quad \mathbf{v}_F = \frac{\hbar}{m} \left( \nabla (\phi - \gamma) - \cos \beta \cdot \nabla \alpha \right).
\]
Here, \((\alpha, \beta, \gamma)\) are the Euler angles describing \(SO(3)\) and \(\phi\) is the \(U(1)\) angle. There is a vortex if the particles go around in a circle, i.e. if

\[
\oint \mathbf{v} \cdot d\mathbf{r} \neq 0.
\]

So, this means there is nonzero angular momentum about an axis going through the vortex. This is a very rich subject and I think I will understand it more after I read different book.

**Bosonic spinor gases in optical lattices**

Why study the spinor gases? It can be a way of simulating magnetic quantum systems, where we can control all of the parameters! Compared to the scalar bosons, the spinor bosonic gases exhibit more complicated phase diagram on the Mott Insulator side of the phase diagram. The Bose-Hubbard energy for spin-1 particles is just

\[
\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} b_{i \sigma}^\dagger b_{j \sigma} + \frac{U}{2} \sum_i n_i (n_i - 1) + \frac{U}{2} \sum_i \left( S_i^2 - 2n_i \right) - \mu \sum_i n_i, \quad \text{where} \quad S_i = \sum_{\sigma \sigma'} b_{i \sigma}^\dagger F_{\sigma \sigma'} b_{i \sigma'}.
\]

Here, \(F = (F_x, F_y, F_z)\) are the usual spin-1 matrices.

If you think about the bosons on a particular site and decompose the total spin on site \(i\) as something like

\[
|S_{1i} m_i \rangle \oplus |S_{2i} m_i \rangle \oplus \cdots \oplus |S_{n_i} m_i \rangle
\]

where \(n_i\) is the number of particles on site \(i\), we claim that

\[
|S_{ij} m_i \rangle |n_i \rangle \neq 0 \implies S_{ij} + n_i \text{ is even}.
\]

Why?