Week 0/ 1

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

0 Administrative affairs

(i) Office: AB1 - 014
Phone: 1213
Email: sebastian@iiserb.ac.in
Lecture hours: Slot X, Tue 10am L7, Wed, Thu 2pm L9, TA-Class and replacement slot Fri 2pm L11
Office hours: Tue 2-5 pm
webpage: http://home.iiserb.ac.in/∼sebastian/teaching.html

(ii) Literature: No Single Textbook

- Pethick and Smith, *"Bose-Einstein Condensation in Dilute Gases"* [**closest matching book**]
- R. Shankar, *"Principles of Q.M"*
- J.J. Sakurai, *"Modern Quantum Mechanics"*
- Negele and Orland, *"Quantum Many Particle Systems"*
- Petter and Walecka, *"Quantum Theory of Many Particle Systems"*
- L. Schiff, *"Quantum Mechanics"*
- Henrik Bruus, Flensberg, *"Introduction to Many Body Quantum Mechanics in Condensed Matter"*

There is no primary text-book. I collect material from wherever I find it best covered case-by-case.

(iii) Assessment:

- **Three scheduled Quizzes in the AIR studio with examineer: 15%** To supplement the exams, there will be three quizzes lasting one lecture hour, conducted using the examineer webpage . For quiz timings see webpage. These are "open notes" quizzes, so bring a copy of your notes. Quizzes will be simpler than exams, intended to encourage you to continuously keep on top of the material. **Make sure to bring an internet capable phone/tablet/laptop on the days of the quiz**, if you use online notes a **second** device for the notes. Please contact me if there is a problem with this. You also need some pen and paper for scrap notes on quiz days. There will also be a few, even easier ones that you can do from home over a few days.

- **Assignments: 15%** There will be about five assignments handed out with a two week deadline each. I expect you to form teams of 3-4 students and stick in these teams for the semester. Hand in only one solution per team. The TA is instructed to give full marks for *any serious attempt* at a given question of the assignment, even if the result is wrong. This is to discourage copying and encourage doing it yourself. Additionally however the TA is asked to deduct marks for messy presentation and blatant copying. These assignments are intended as your primary means of learning the essential course material, please do all of them diligently.
- **Numerics component of assignments:** Moderns science almost always necessitates the heavy use of computers. Most assignments will contain a numerics component, to be done using XMDS . I will provide a tool and template package that you have to only minorly edit. See notes on numerics assignments online.
- **Mid-Sem exam: 30%**
- **Final exam: 40%** The exams will try to test understanding of the essential *physics* concepts taught, not maths. For guidance regarding what are the most important concepts look at the quizzes and assignments. All exams will be designed to give a significant advantage to those students that solved all assignments by *themselves*.

Course outline

1) Motivation and Review: $\sim$ 1 week
   • Fields that require Many-Body QM, why degenerate gases?
   • Review essential pieces from single-particle QM

2) Quantum-many-body Formalism: $\sim$ 4-5 weeks
   • Second Quantisation, Bosons vs Fermions, quantum field operators, coherent states

3) Bose-Einstein Condensates (BECs): $\sim$ 4-5 weeks
   • Symmetry breaking/ mean field, Critical Temperature, Gross- Pitaevskii equation, Bogoliubov quasi-particles, Quantum field theory of BEC.

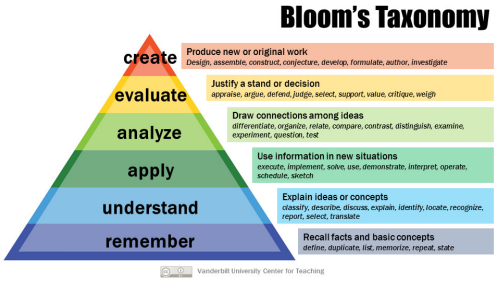
4) Degenerate Femi Gases $\sim$ 3-4 weeks
   • Fermi Surface, Degeneracy Pressure, Neutron stars, electron gas, pairing, superconductivity

5) *Online(?):* Quantum Simulators: $\sim$ 2-3 weeks
   • Analog and digital quantum Simulation, Bose-Hubbard model, BEC-BCS cross-over

Contents

[1] See Bruus and Flensberg

Learning objectives



left: Research on learning has classified possible targets in the pyramid on the left.

In terms of skills in the pyramid on the top, this course aims to foster levels 2 and 3 (understand, apply). This means also the exam will be designed to test these. In particular you should not be able to score a lot with only level 1 (remembering), since nowadays remembering is not that crucial thanks to the internet. After the course I would be grateful for feedback whether this course/exam design goal has been reached.

1 Motivation and Review

1.1 Quantum many-body theory and Quantum field theory (QFT)

Singe quantum particle can be described by a state $\varphi(\mathbf{x})$.

Many Particle Wavefunctions: are more complicated.

- We have to firstly take care of Bosonic/Fermionic Symmetries:

$$\psi\left(\mathbf{x}_1, \mathbf{x}_2\right) = \frac{1}{\sqrt{2}}\left[\varphi_1\left(\mathbf{x}_1\right)\varphi_2\left(\mathbf{x}_2\right) \pm \varphi_1\left(\mathbf{x}_2\right)\varphi_2\left(\mathbf{x}_1\right)\right] \tag{1.1}$$

- Then we often have to worry about particle creation or destruction $\psi(x_1) \leftrightarrow \psi(x_1, x_2) \leftrightarrow \psi(x_1, x_2, x_3) \leftrightarrow \cdots$
- Very helpful for this is Second Quantisation with creation and destruction operators: $\hat{a}, \hat{a}^\dagger$ (same algebra as Simple Harmonic oscillator ladder operators)
- The natural next step from there is Quantum field theory

$$\hat{\Psi}\left(\mathbf{x}\right) = \sum_n \underbrace{\varphi_n\left(\mathbf{x}\right)}_{\text{wave aspect}} \underbrace{\hat{a}_n}_{\text{particle aspect}} \tag{1.2}$$

  Where $\hat{\Psi}$ can be viewed as a type of destruction operator
- Compared to a classical field $\rightarrow$ now the field itself is quantised
- For $v \approx c$ we need to do relativistic Quantum Mechanics and then relativistic Quantum Field theory as used in elementary particle physics. We do not cover this, but will mention the Spin-Statistics theorem, which originates from there.
- Condensed matter physics provides lots of advanced QFT techniques, such as Greens-functions, Path-Integrals, Keldysh formalism or thermal field theory, we also do not require these.

1.2 Disciplines with many-body QM

Many sub-fields of physics require us to tackle many-body quantum mechanics.
• Atomic and Molecular Physics (many e^-)
• Chemistry (even more e^-)
• Nuclear Physics (many n,p)
• Particle Physics (several elementary particles, but usually more concerned with creation/ destruction/ conversion/ symmetries then with the number of particles)
• Condensed Matter Physics (10^{23} e^- or Quasiparticles like Spinon, Magnon, Plasmon etc.)

• Astrophysics (even more e^-/n)
Recently:
• Quantum Optics (many γ, usually non-interacting)
• Quantum Information (many 0,1)

1.3 Review

1.3.1 Single-particle States

In this course we will always assume the problem of a single particle to be solved, e.g with the

Time-independent Schrödinger equation (TISE)

$$\hat{H}_0|\varphi_n\rangle = E_n|\varphi_n\rangle. \tag{1.3}$$

- Where $\hat{H}_0$ is the single body Hamiltonian (depends on co-ordinates of just one particle)
- $|\,\varphi_n\,\rangle$ is the (typically) infinite single-particle basis. The φ_n are also called mode.
- E_n are single particle energies

Examples: We will require these to construct many-body theories later, so this is to set notation
(i) Free particles in Volume $\mathcal{V}$

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{h^2}{2m}\nabla^{\mathbf{2}} \qquad E_n = \frac{h^2k^2}{2m} = \frac{p^2}{2m} \tag{1.4}$$

$$|\psi_n\rangle \rightsquigarrow |\phi_k\rangle \quad = \quad \frac{1}{\sqrt{\mathcal{V}}}e^{i\mathbf{kx}} \tag{1.5}$$

where $\mathbf{k}$ is the wavenumber. Technically we have to distinguish continuous and discrete spectra, where the free particle is continuous, see books. We will always use a discrete notation for simplicity.

(ii) Spin - $\frac{1}{2}$ states

$$\hat{H}_0 = \frac{\Delta E}{2}\hat{\sigma}_3 \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad E_{\uparrow\downarrow} = \pm\frac{\Delta E}{2} \tag{1.6}$$

The basis are spin-up and spin-down states $|\varphi_{\uparrow,\downarrow}\rangle$, specifically $|\varphi_\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cong |\uparrow\rangle$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix} \cong |\downarrow\rangle$

Example cont.: (iii) Simple Harmonic oscillator states (3D), with Hamiltonian

$$H_0 = \frac{\mathbf{p^2}}{2m} + \frac{1}{2}m\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) \tag{1.7}$$

3D Harmonic oscillator Quantum states

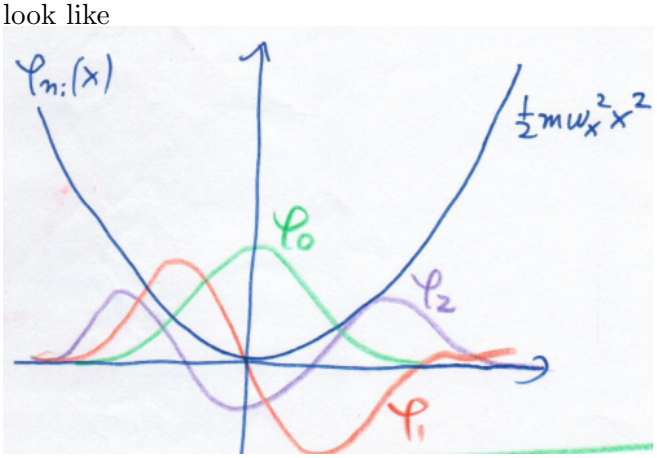
$$|\varphi_{\mathbf{n}}\rangle = |\varphi_{n_x n_y n_z}\rangle = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z) \qquad (= |\varphi_{\mathbf{n}}(\mathbf{x})\rangle) \tag{1.8}$$

$$\varphi_{n_i}(x_i) = \frac{1}{\sqrt{2^{n_i}(n_i)!\sqrt{\pi}\sigma_i}} e^{-\frac{x^2}{2\sigma^2}} H_{n_i}\left(\frac{x_i}{\sigma_i}\right) \tag{1.9}$$

where $x_i \in \{x, y, z\}$, and $H_n(x)$ are Hermite polynomials. The oscillator widths in the three directions are $\sigma_i = \sqrt{\hbar/(m\omega_i)}$. Energies:

$$E_n = \hbar\omega_x(n_x + \frac{1}{2}) + \hbar\omega_y(n_y + \frac{1}{2}) + \hbar\omega_z(n_z + \frac{1}{2}). \tag{1.10}$$

The 3D eigenstates thus factor into the 1D eigenstates which you know, and which look like



left: Sketch of 1D harmonic oscillator potential and the first few eigenstates

(iv) Other examples: from PHY 303/304: particle in a 1D/2D/3D box potential, Single electron in a Hydrogen atom...

Going back to the 1D oscillator, we recall the

Ladder-Operators (1D)

Lowering operator
$$\hat{b} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p} \tag{1.11}$$

Raising operator
$$\hat{b}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p} \tag{1.12}$$

We can show that $[\hat{b}, \hat{b}^\dagger]$=1 (from $[\mathbf{x}, \mathbf{p}] = i\hbar$)
New Hamiltonian using ladder operators (from 1D version of (1.7)).

$$\hat{H}_0 = \hbar\omega \left(\hat{b}^\dagger \hat{b} + \frac{1}{2} \right) \tag{1.13}$$

We can now show (e.g. in Shankar≅ pg. 204) the

Function of Raising and Lowering Operators

$$\hat{b}|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle \qquad \hat{b}|\varphi_0\rangle = 0, \tag{1.14}$$

$$\hat{b}^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle, \tag{1.15}$$

and define the phonon number Operator: $\hat{N} = \hat{b}^\dagger \hat{b}$ and $\hat{N}|\varphi_n\rangle = n|\varphi_n\rangle$.

- These properties follow solely from the commutation relation $\left[\hat{b}, \hat{b}^\dagger\right]$=1 , and hence we would not need to know the position space representation (1.9).

1.3.2 Single Particle Density Matrices

Quantum mechanics allows superpositions of two "opposite" states, e.g. $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Classically we can already have random probability distributions of opposite states e.g. P(↑) = 50%, P(↓) = 50% (let ↑↓ be"head/tail" for a flipped coin here). The quantum superposition is a stronger statement, since it involves complex phases. However we require some mathematics to describe both sources of randomness simultaneously, since e.g. experiments might involve both. The mathematics is provided by the concept of the

Density Matrix/ operator

$$\hat{\rho} = \sum_{nm} \rho_{nm} |\varphi_n\rangle\langle\varphi_m|, \tag{1.16}$$

where $|\varphi_n\rangle$ is a chosen single particle basis as in section 1.3.1.

Density Matrix Properties

- For a pure quantum state: $\hat{\rho} = |\psi\rangle\langle\psi|$. So the statement "my system is in state $|\,\psi\,\rangle$" is equivalent to saying "my system has a density matrix $|\psi\rangle\langle\psi|$".
- For a fully classical (mixed) state: $\rho_{nm} = 0$ for $n \neq m$
- Then $\hat{\rho} = \sum_n p_n |\varphi_n\rangle\langle\varphi_n|$ where p_n is the probability to be in state n.

- the expectation value of observable $\hat{O}$ is now $\mathrm{Tr}[\hat{O}\hat{\rho}]$, where $\mathrm{Tr}[...]$ denotes the trace, so the sum of diagonal elements.
- $\hat{\rho}$ is Hermitian, for pure states $\hat{\rho}^2 = \hat{\rho}$, always $\mathrm{Tr}[\hat{\rho}] = 1$
- We can define the purity P as $P = \mathrm{Tr}[\hat{\rho}^2]$, then

$$P = 1 \qquad \text{for pure states} \tag{1.17}$$
$$P < 1 \qquad \text{for mixed states} \tag{1.18}$$

See your favourite QM book, the online notes for PHY435 "Decoherence and open quantum systems" and related literature on my webpage for a more detailed discussion of density matrices (in this order).

Time-Evolution of states involving density matrices is via the von-Neumann equation

$$i\hbar \frac{\partial}{\partial t}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right] \tag{1.19}$$

Examples:
Single spin-$\frac{1}{2}$ (see (ii) earlier)
(i) Let its quantum state be $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. The corresponding density matrix is $\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)$.
We can write this in Matrix form

$$\underline{\underline{\rho}} = \begin{array}{c} \begin{matrix} |\uparrow\rangle & |\downarrow\rangle \end{matrix} \\ \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{matrix} |\uparrow\rangle \\ |\downarrow\rangle \end{matrix} \end{array} \tag{1.20}$$

(ii) If we had a classical mixture instead (50 % $\uparrow$, 50% $\downarrow$), we would write $\hat{\rho} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)$, which becomes

$$\underline{\underline{\rho}} = \begin{array}{c} \begin{matrix} |\uparrow\rangle & |\downarrow\rangle \end{matrix} \\ \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{matrix} |\uparrow\rangle \\ |\downarrow\rangle \end{matrix} \end{array} \tag{1.21}$$

Diagonal Elements are called populations or probabilities. $\rho_{nn} \cong$ probability to find system in state n. **Off-diagonal Elements** are called coherences, where $\rho_{12} \cong$ indicates the amount of coherence between state 1 and 2, this is $= 0$ classically.

- Note that in both examples above, the probability for $\uparrow$ and $\downarrow$ is 50% each.
- **Distinction**: However we can discriminate the coherent superpositions from the classical

mixtures through the appearance of interference terms in certain observables, for example:

$$\langle\hat{\sigma}_x\rangle = \begin{cases} \langle\psi|\hat{\sigma}_x|\psi\rangle = \frac{\hbar}{2}, & \text{for case (i), pure} \\ \mathrm{Tr}\left[\hat{\rho}\hat{\sigma}_x\right] = \mathrm{Tr}\begin{bmatrix} 0 & \frac{\hbar}{2\sqrt{2}} \\ \frac{\hbar}{2\sqrt{2}} & 0 \end{bmatrix} = 0, & \text{for case (ii), mixed} \end{cases} \tag{1.22}$$

1.3.3 Many Particle States

The generalisation of section 1.3.1 to many particles is to add one co-ordinate per particle:

Many-body TISE (general case)

$$\hat{H}(\mathbf{x}_1, ..., \mathbf{x}_n, \hat{\mathbf{p}}_1, ..., \hat{\mathbf{p}}_n)\psi_k(\mathbf{x}_1, ..., \mathbf{x}_2) = E_k\psi_k(\mathbf{x}_1, ..., \mathbf{x}_n) \tag{1.23}$$

- Typically very high dimensional PDE (e.g. already 9D for 3 particles in 3-dimensions.)
- Often too high dimensional to deal with it directly → We learn techniques to sometimes deal with this problem in this lecture.
- k is an index numbering the eigenstate, as in single particle QM. But now the state is a many-body state. Often it makes sense to de-compose it into a collection of e.g. single particle indices, such as $k \equiv \{n_1, n_2, \cdots n_N\}$, see next dotpoint.
- We can always write many body states in terms of single-body ones, but the decomposition might be complicated:

$$\psi_k(\mathbf{x}_1, ...\mathbf{x}_N) = \sum_{n_1,...,n_N} c_{k;n_1,n_2,...n_N}\varphi_{n_1}(\mathbf{x}_1)\varphi_{n_2}(\mathbf{x}_2)...\varphi_{n_N}(\mathbf{x}_N). \tag{1.24}$$

Orthogonality: Many body states as products of single particle basis are orthogonal, whenever any of the constituents differ, they inherit their orthogonality properties from the single particle states:

$$\begin{aligned} &\langle\varphi_{n_1}|\langle\varphi_{n_2}||\varphi_{n_1'}\rangle|\varphi_{n_2'}\rangle = \\ &\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \;\; \varphi^*_{n_1}(\mathbf{x}_1)\varphi^*_{n_2}(\mathbf{x}_2)\varphi_{n_1'}(\mathbf{x}_1)\varphi_{n_2'}(\mathbf{x}_2) \\ &= \left(\int d^3\mathbf{x}_1 \;\; \varphi^*_{n_1}(\mathbf{x}_1)\varphi_{n_1'}(\mathbf{x}_1)\right)\left(\int d^3\mathbf{x}_2 \;\; \varphi^*_{n_2}(\mathbf{x}_2)\varphi_{n_2'}(\mathbf{x}_2)\right) = \delta_{n_1 n_1'}\delta_{n_2 n_2'}. \end{aligned} \tag{1.25}$$

1.3.4 Entanglement

The generic many body states (1.24) can be classified as follows

Separable states: A many body state is called separable, if it can be written as a product of states for each particle:

$$\psi_{sep}\left(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\right) = \prod_{i=1}^{N} \phi_{n_i}\left(\mathbf{x}_i\right) \tag{1.26}$$

All states that are not separable are called entangled.

- Less stringently, we can also talk about many-body states being separable or entangled with respect to two (or few) sub-systems A and B of the many-body Hilbertspace.

Examples: Separable:

$$|\psi\rangle = |\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \tag{1.27}$$

$$|\psi\rangle = \frac{1}{2}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes \left(|\uparrow\rangle + |\downarrow\rangle\right) = \frac{1}{2}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \tag{1.28}$$

$$\psi\left(x_1, x_2\right) = \frac{1}{\sqrt{\mathcal{V}}} e^{ik_1 x_1} \mathcal{N} \exp\left[-\frac{x_2^2}{2\sigma^2}\right] \tag{1.29}$$

Entangled:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right) \tag{1.30}$$

$$\psi\left(x_1, x_2\right) = \mathcal{N} \exp\left[-\frac{\left(x_1 - x_2\right)^2}{2\sigma_\perp^2} - \frac{\left(x_1 + x_2\right)^2}{2\sigma_\parallel^2}\right] \tag{1.31}$$

• In an entangled state (for two systems A,B) if we measure state A we typically know also about B.
• Entanglement also implies classical correlations, but it is much more than that (keywords: EPR paradox, Bell-theorem).
• The definition gets a bit more complicated for mixed states ($\hat{\rho}$).

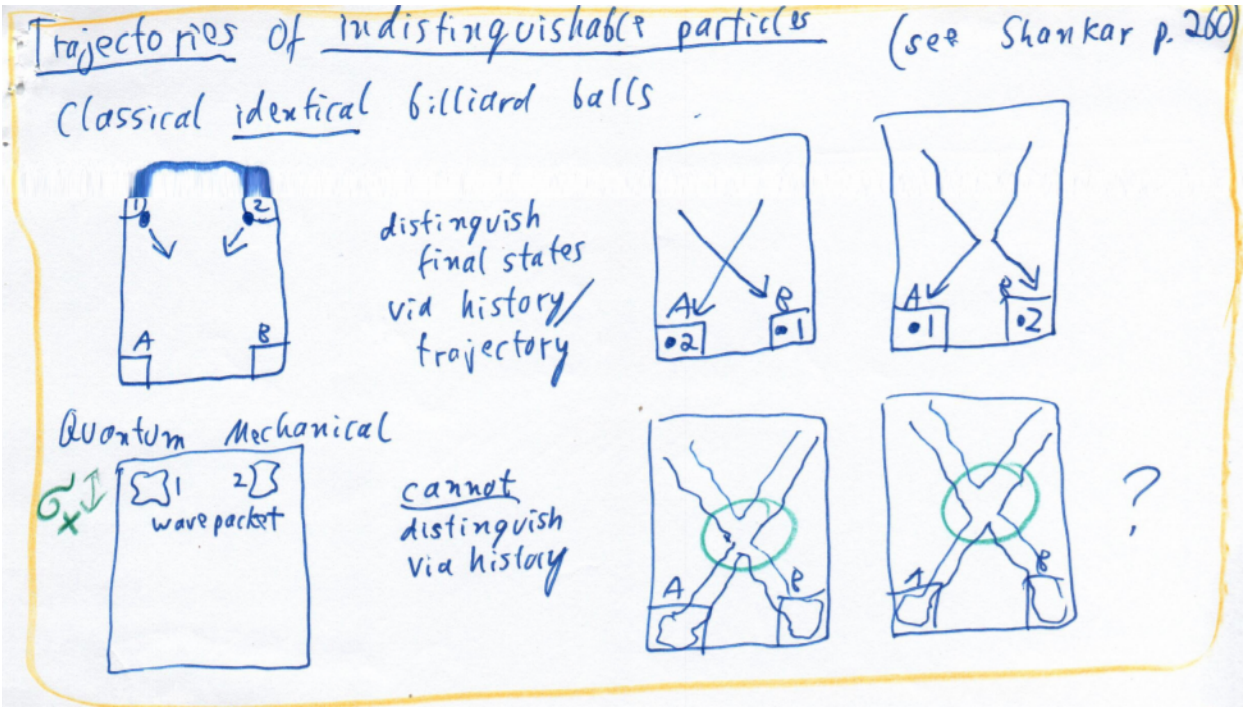
1.3.5 Indistinguishable Particles

So far we have implicitly treated our many particles as distinguishable. For example the state (1.29) implies, "particle 1 is in a momentum eigenstate with momentum $\hbar k_1$, and particle two has a Gaussian wavefunction with width σ". However:

- A statement like, "Particle 1 is in state n_1 and Particle 2 is in state n_2" makes sense if the particles are distinguishable (say $1 = e^-$ (electron), $2 = p$ (proton), $3 = \gamma$ (photon)).

- For indistinguishable particles, the uncertainty relation forces us to abandon the labels "Particle 1", "Particle 2" etc. (See box for "trajectories" below).

- This implies that mathematically, the state $\psi(\mathbf{x}_a, \mathbf{x}_b)$ must be equivalent to $\psi(\mathbf{x}_b, \mathbf{x}_a)$.



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Since the overall phase or sign of a wave-function does not matter, "being equivalent" still allows for

Identical particle exchange symmetry

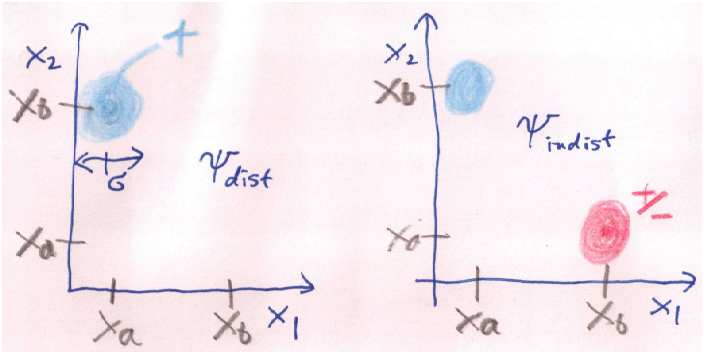
$$\psi(x_a, x_b) = \pm\psi(x_b, x_a) \tag{1.32}$$

$\oplus$ = Bosons=Symmetric under exchange of any two indistinguishable particles
$\ominus$ = Fermions= Anti-symmetric under exchange of any two indistinguishable particles.

- The most important consequence of this is the Pauli exclusion principle: **Two indistinguishable Fermions cannot be in the same single particle state**. *Proof: Try to write a contradicting state down.*

- The need for special treatment of indistinguishable particles comes from the green encircled region in the above figure i.e when the matter waves overlap.
  If this never happens, particles can be tracked and (anti-)symmetrization is irrelevant (we can still do it, but it makes no difference to the math)
  Example: One e^- inside you and another on the moon (see example next page and also Shankar p.273) .

Example: Relevance of many-body symmetries:
Consider two particles with a Gaussian 1D wave-function, one centered at x_a the other at x_b, with width σ each. We want to compare distinguishable particles with non-symmetrized wavefunction $\psi_{\text{dist}}(x_1, x_2) = \varphi_a(x_1)\varphi_b(x_2) \equiv \mathcal{N}^2 \exp\left[-(x_1 - x_a)^2/(2\sigma^2)\right] \exp\left[-(x_2 - x_b)^2/(2\sigma^2)\right]$ with indistinguishable particles, where we (anti-)symmetrized the wave function $\psi_{\text{indist}}(x_1, x_2) = [\varphi_a(x_1)\varphi_b(x_2) \pm \varphi_b(x_1)\varphi_a(x_2)]/\sqrt{2}$. $\mathcal{N}$ *is a normalisation factor.* Let us distinguish two cases:
case (i) $\sigma \ll |x_a - x_b|$, i.e. x_1 within you, x_2 on the moon.
Let us first draw the two wave-functions in a many-body coordinate system:



left: Non-symmetrised and symmetrised wave functions for case (i). (blue) $\psi > 0$, (red) $\psi < 0$, (white) $\psi \approx 0$.

Now consider the expectation value of any observable $\hat{O}$. For simplicity we assume $\hat{O}$ contains no derivatives.

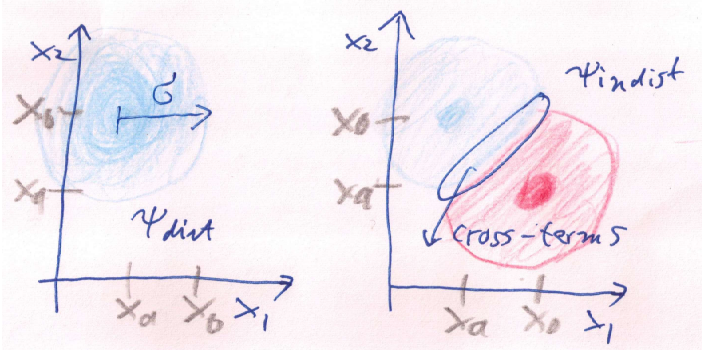
$$\langle \hat{O} \rangle = \int dx_1 dx_2 \ \psi^*(x_1, x_2) \hat{O} \, \psi(x_1, x_2)$$

$$\begin{cases} = \int dx_1 \int dx_2 \ |\varphi_a(x_1)|^2 |\varphi_b(x_2)|^2 \hat{O}, & \text{for } \psi_{\text{dist}} \\ = \int dx_1 \int dx_2 \left(|\varphi_a(x_1)|^2 |\varphi_b(x_2)|^2 \pm \frac{1}{2} \underbrace{[\varphi_a^*(x_1)\varphi_b(x_1)\varphi_b^*(x_2)\varphi_b(x_2)]}_{\approx 0} + \text{c.c.} \right) \hat{O}, & \text{for } \psi_{\text{indist}} \end{cases} \tag{1.33}$$

- In the second line we used that we can rename $x_1 \leftrightarrow x_2$ in the integration.
- The term in square brackets vanishes because the overlap of the Gaussians near x_a and x_b is essentially zero.

We thus see that in this case, both approaches give the same result.

case (ii) $\sigma \sim |x_a - x_b|$, e.g. two electrons in an atom



left: Non-symmetrised and symmetrised wave functions for case (ii). Legend as above.

In this case the argument above no longer works, so the extra terms matter and can be crucial. In particular the overall integration for the expectation value depends on the sign $\pm$, so differs for Bosons and Fermions.

Week 2

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

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2 Quantum Many-Body Formalism

2.1 Second Quantisation

In principle we could work out most of many-body quantum mechanics using (anti-) symmetrized wave functions such as Eq. (1.32). We could generalise that expression to more particles using the

(Anti-) Symmetrization Operator

$$\hat{P}_{\{\frac{B}{F}\}}\psi\left(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,,,\mathbf{x}_N\right)=\mathcal{N}\sum_{\mathcal{P}}\xi^{\mathcal{P}}\psi\left(\mathbf{x}_{\mathcal{P}(1)},\mathbf{x}_{\mathcal{P}(2)},...,\mathbf{x}_{\mathcal{P}(N)}\right) \tag{2.1}$$

$\xi=-1$ (for Fermions) or $\xi=+1$ (for Bosons),
$\mathcal{P}=$ Permutation of $\{1,2,...,N\}$, (e.g. $\{1,3,2,4,...,N\}$),
$\xi^P \leftarrow \xi$ to the power of parity of permutation.
The normalisation factor is $\mathcal{N}=1/\sqrt{N!\prod_k n_k!}$, where the $\prod$ part is 1 for Fermions.

In practice, such a formalism gets cumbersome quickly. Discouraging example: Write the bosonic states for three particles in three states A, B, C. The only meaningful information in an (anti-) symmetrized many-body wave function is how many particles (not "which") are in which single-particle basis states ϕ_n. We thus introduce:

(Occupation) Number representation

$$|\,\mathbf{N}\,\rangle=|\,N_0,N_1,...,\rangle, \tag{2.2}$$

which denotes a state where N_0 particles are in state $|\,\phi_0\,\rangle$, N_1 particles are in state $|\,\phi_1\,\rangle$ etc. The vector[a] $\mathbf{N}=[N_0,N_1,N_2,\dots]^T$ just groups all these numbers. The space of all $\{|\,N_0,...\,\rangle\}$ is called the Fock Space.

[a] The superscript ^{T} means "transposed", turning the row I write into a column vector.

- Correct (anti-) symmetrisation is automatically implied in these states

Example (Bosons): If we explicitly write the Fock state in terms of single particles states in the position representation, we get:

$$\langle\, \mathbf{x} \,|\, 2100... \,\rangle = \frac{1}{\sqrt{3}}[\phi_0(\mathbf{x_1})\phi_\mathbf{0}(\mathbf{x_2})\phi_\mathbf{1}(\mathbf{x_3}) + \phi_\mathbf{0}(\mathbf{x_1})\phi_\mathbf{0}(\mathbf{x_3})\phi_\mathbf{1}(\mathbf{x_2}) + \phi_\mathbf{0}(\mathbf{x_2})\phi_\mathbf{0}(\mathbf{x_3})\phi_\mathbf{1}(\mathbf{x_1})]$$

We also define one special number state, the vacuum, which has no particles in any state

$$|\, 0 \,\rangle = |\, 0...0 \,\rangle. \tag{2.3}$$

Now define

Creation and Destruction Operators

creation operator for Bosons:
$$a_n^\dagger |\, N_0 N_1 ... \,\rangle = \sqrt{N_n + 1}\, |\, N_0 N_1 ... (N_n + 1) ... \,\rangle \tag{2.4}$$

annihilation operator for Bosons:
$$a_n |\, N_0 N_1 ... \,\rangle = \sqrt{N_n}\, |\, N_0 N_1 ... (N_n - 1) ... \,\rangle \tag{2.5}$$

creation operator for Fermions:
$$a_n^\dagger |\, N_0 N_1 ... \,\rangle = (-1)^{\sum_{k<n} N_k} (1 - N_n) |\, N_0 N_1 ... (N_n + 1) ... \,\rangle \tag{2.6}$$

annihilation operator for Fermions:
$$a_n |\, N_0 N_1 ... \,\rangle = (-1)^{\sum_{k<n} N_k} N_n |\, N_0 N_1 ... (N_n - 1) ... \,\rangle \tag{2.7}$$

- The last two relations already incorporate the Pauli inclusion principle on the level of the operators.
- The sign factors appearing for Fermions take care of the fact that a state that is anti-symmetric under exchange of particles $\mathbf{x_1} \leftrightarrow \mathbf{x_2}$, such as $\langle\, \mathbf{x} \,|\, 11 \,\rangle = \frac{1}{2}\big(\phi_a(\mathbf{x_1})\phi_\mathbf{b}(\mathbf{x_2}) - \phi_\mathbf{b}(\mathbf{x_1})\phi_\mathbf{a}(\mathbf{x_2})\big)$, then is also automatically anti-symmetric under exchange of state labels $a \leftrightarrow b$.

From these definitions, we can show

Commutation Relations

$$\begin{aligned} &[\hat{a}_i, \hat{a}_j] = 0, \quad [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} && \text{(Bosons)} \\ &\{\hat{a}_i, \hat{a}_j\} = 0, \quad \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0, \quad \{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij} && \text{(Fermions)} \end{aligned} \tag{2.8}$$

- To proof these, apply both sides to a general "test" Fock state.
- We used the

  Anti-Commutator: $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

- For Bosons this is inspired by the S.H.O ladder operators (1.12) for harmonic oscillator states. They share the commutator algebra with bosonic many-body creation operators.
- Using operatrs $\hat{a}^\dagger$, we can span the entire Fock space:

$$|\, N_0 N_1 N_2 ... \,\rangle = \frac{(\hat{a}_0^\dagger)^{N_0}(\hat{a}_1^\dagger)^{N_1}(\hat{a}_2^\dagger)^{N_2}...|\, 0 \,\rangle}{\sqrt{N_0! N_1! N_2! ...}} \tag{2.9}$$

- Fock-states obey orthonormality

$$\langle\, N_0' N_1' N_2' ... \,|\, N_0 N_1 N_2 ... \,\rangle = \delta_{N_0 N_0'} \delta_{N_1 N_1'} \delta_{N_2 N_2'} ...$$

By combining operators from above, we can define the

Particle number operator

$$\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k, \tag{2.10}$$

which fulfills $\hat{N}_k |\, \mathbf{N} \,\rangle = N_k |\, \mathbf{N} \,\rangle$.

- Thus Fock states are eigenstates of all the number operators $\hat{N}_k$, with the number of particles in single particle state $|\, \varphi_k \,\rangle$ as eigenvalues.
- We finally can define the total number operator

$$\hat{N} = \sum_k \hat{N}_k \tag{2.11}$$

2.1.1 N-Body Operators

Second quantisation now means to re-write everything in terms of creation and destruction operators

Consider a generic 2-body Hamiltonian (in the first quantised form), e.g.

$$\hat{H} = -\frac{\hbar^2}{2m}(\boldsymbol{\nabla}_{x_1}^2 + \boldsymbol{\nabla}_{x_2}^2) + V(\mathbf{x}_1) + V(\mathbf{x}_2) + U(\mathbf{x}_1, \mathbf{x}_2) \tag{2.12}$$

where $\boldsymbol{\nabla}_{x_1}^2$ and $\boldsymbol{\nabla}_{x_2}^2$ are kinetic energies of particle 1,2. V($\mathbf{x}_1$), V($\mathbf{x}_2$) are some external potentials (e.g. harmonic trap, gravity), and U($\mathbf{x}_1$, $\mathbf{x}_2$) is an interaction potential.
We can distinguish here:

Operator types
Single-body Operators (e.g. kinetic energy, potential energy), that are a sum of identical replica acting on each particle:

$$\hat{O}_1 = \sum_k \hat{o}^{(k)}, \text{ where } \hat{o}^{(k)} \text{ acts on a particle k.} \tag{2.13}$$

and a Two-body operator (Interaction potential), that contains both $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$, $\hat{O}_2 = \sum_{kl} \hat{o}^{(kl)}$.

- More generally, there can be N-body operators for any N, but typically the two above are sufficient.
- It is possible to express any first quantised Hamiltonian such as Eq. (2.12) in second quantised form, i.e. using $\hat{a}$, $\hat{a}^\dagger$. To see how, we need to realize:

Equality of operators: Operators $\hat{O}$ are maps in Hilbert Space $\implies$ they are identical if all matrix-elements such as $\langle \phi_A | \hat{O} | \phi_B \rangle$, for all states A and B, are the same.

2.2 Second Quantised Hamiltonian

Let us assume $\hat{H} = \hat{A} + \hat{B}$, where $\hat{A} = \sum_k \hat{\mathcal{A}}^k$ is a single-body and $\hat{B} = \sum_{kl} \hat{\mathcal{B}}^{kl}$ a two-body operator. This results in

Second-Quantised Hamiltonian

$$\hat{H} = \sum_{nm} A_{nm} \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} B_{nm,lk} \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_l \hat{a}_k \tag{2.14}$$

$$\begin{aligned} &\text{with single-body matrix-elements: } A_{nm} = \langle \phi_n | \hat{\mathcal{A}} | \phi_m \rangle, \\ &\text{and two-body matrix-elements: } B_{nm,lk} = \langle \phi_n \phi_m | \hat{\mathcal{B}} | \phi_l \phi_k \rangle. \end{aligned} \tag{2.15}$$

Example: Consider N identical particles in a 1-D harmonic trap, interacting with $U(\mathbf{x}_1, \mathbf{x}_2) = U_0 \exp(\frac{-|\mathbf{x}_1 - \mathbf{x}_2|^2}{2\eta^2})$. First quantised Hamiltonian:

$$\hat{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla^2_{\mathbf{x}_k} + V(\mathbf{x}_k) \right) + \frac{1}{2} \sum_{k,l=1}^{N} U(\mathbf{x}_k, \mathbf{x}_l) \tag{2.16}$$

$V(\mathbf{x}_k) = \frac{1}{2} m\omega^2 \mathbf{x}_k^2$. We want to use the Harmonic oscillator basis (1.9) to define our $\hat{a}, \hat{a}^\dagger$. In the notation used for Eq. (2.15):

$$\hat{\mathcal{A}} = -\frac{\hbar^2}{2m} \nabla^{\mathbf{2}}_{\mathbf{x}} + V(\hat{\mathbf{x}}) = \hat{H}_{0,osc},$$
$$\hat{\mathcal{B}} = U(\hat{\mathbf{x}}, \hat{\mathbf{y}}).$$

Thus,

$$\mathcal{A}_{nm} = \langle\, \phi_n \,|H_{0,osc}|\, \phi_m \,\rangle = E_m \langle\, \phi_n \,|\, \phi_m \,\rangle = \delta_{nm} E_m, \cdots \tag{2.17}$$

Example continued:
...and

$$\begin{aligned} \mathcal{B}_{nm,lk} &= \langle\, \phi_n \phi_m \,|\hat{B}|\, \phi_l \phi_k \,\rangle \\ &= \int d^3\mathbf{x} \int d^3\mathbf{y}\ \ \phi_n^*(\mathbf{x}) \phi_m^*(\mathbf{y}) \frac{U(\mathbf{x}, \mathbf{y})}{2} \phi_n(\mathbf{x}) \phi_m(\mathbf{y}) \end{aligned}$$

The latter expression is quite complicated, involving many oscillator states and the Gaussian interaction potential, but can in principle be evaluated, at the very least numerically.
Hence, for the 1D case for simplicity:

$$\hat{H} = \sum_{n} \hbar\omega (n + \frac{1}{2}) \hat{a}_n^\dagger \hat{a}_n + \sum_{nmlk} B_{nm,lk} \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_l \hat{a}_k \tag{2.18}$$

Exercise: For $2 \leq N \leq 3$, explicitly confirm that the matrix elements of operators Eq. (2.16) and Eq. (2.18) are the same between a few pairs of Fock-states Eq. (2.2).

In the same manner, any first quantized many-body Hamiltonian can be converted to second quantized form for any choice of single-particle basis.

2.2.1 Basis Changes

We can always change the single particle basis underlying our second quantisation with a unitary transformation

$$|\,\phi_l\,\rangle = \sum_m u_{lm} |\,w_m\,\rangle \quad u_{lm} = \langle\, w_m \,|\, \phi_l \,\rangle \tag{2.19}$$

Define one set of operators for each, e.g.

$$\langle\, x\,|\hat{a}_n^\dagger|\,0\,\rangle = \phi_n(x) \quad \langle\, x\,|\hat{c}_n^\dagger|\,0\,\rangle = w_n(x)$$

We can show the following

Basis Transformation for Second-Quantised Operators

$$\hat{a}_l^\dagger = \sum_m u_{lm}\hat{c}_m^\dagger \tag{2.20}$$
$$\implies \hat{a} = \sum_m u_{lm}^* \hat{c}_m$$

Example: Let us rewrite the Hamiltonian Eq. (2.18) in the previous example 1.13 in the momentum basis. Hence we have a continuous form of the transformation Eq. (2.19):

$$\phi_l(x) = \int u_l(k) e^{ikx} dk \qquad \text{since } \langle\, x\,|\,W(k)\,\rangle = \exp[ikx]$$
$$u_l(k) = \frac{1}{2\pi}\int e^{-ikx}\phi_l(x)dx = \tilde{\phi}_l(k) \quad \leftarrow \quad \text{(Momentum space oscillator eigenfunction)}$$

i.e: $u_{lm} \to u_l(k)$ [m-index became continuous momentum "k" and $\sum_m \to \int dk$]
Hence we have $\hat{a}_l^\dagger = \int u_l(k)\hat{c}^\dagger(k)dk$. The single-body term of Eq. (2.18) becomes

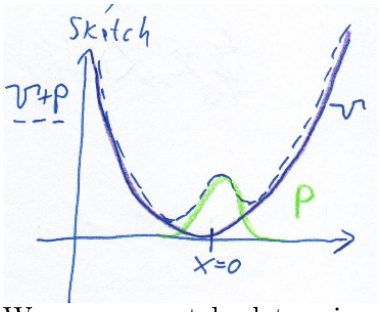
$$\sum_n \underbrace{\hbar\omega(n+\frac{1}{2})}_{=E_n}\hat{a}_n^\dagger\hat{a}_n = \sum_n E_n \int dk \int dk' u_n(k)u_n^*(k')\hat{c}^\dagger(k)\hat{c}(k')$$
$$= \int dk \int dk' h(k,k')\hat{c}^\dagger(k)\hat{c}(k')$$
$$h(k,k') = \sum_n E_n u_n(k)u_n^*(k')$$

This term describes the transitions between different momenta, as expected since momentum states are not eigenstates of the single-particle Hamiltonian $\hat{H}_{0,osc}$.

2.2.2 Application: Fermi Blocking vs Bose-Enhancement

Let us consider again N atoms in a harmonic trap, ignore interactions but add a small perturbing potential $P(x) = P_0 \exp\left(-\frac{x^2}{2\eta^2}\right)$. So Eq. (2.16) becomes

$$\hat{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_{x_k}^2 + V(x_k) + P(x_k) \right) \tag{2.21}$$



left: Sketch of trap and perturbing potential.

We can separately determine the contribution of P(x) to the single body operator and find

$$\hat{H} = [\sum_{n} E_n \hat{a}_n^\dagger \hat{a}_m + \sum_{nm} \kappa_{nm} \hat{a}_n^\dagger \hat{a}_m]$$
$$\kappa_{nm} = \int dx \ \phi_n^*(x) P(x) \phi_m(x) \tag{2.22}$$

In general, κ_{nm} may be non-zero for $n \neq m$, hence the perturbation induces transitions between oscillator states n, m.

Fermions:

top: What is the transition amplitude from $|\,A\,\rangle = |\,1,1,0,0,...\,\rangle \rightarrow |\,B\,\rangle = |\,2,0,0,0,...\,\rangle$ for Fermions? We consider the following matrix element of the Hamiltonian:

$$\langle\, B\,|\hat{H}|\,A\,\rangle = \langle\, 0\,|\hat{a}_0 \hat{a}_0 (\sum_{nm} \kappa_{nm} \hat{a}_n^\dagger \hat{a}_m) \hat{a}_0^\dagger \hat{a}_1 |\, 0\,\rangle = 0.$$

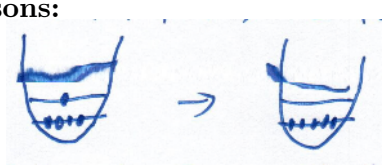
We can see that it must be zero in multiple ways:

1. $= 0$ from $\{\hat{a}_i, \hat{a}_j\} = 0$ in Eq. (2.8)
2. or $= \langle\, 1\,|\hat{a}_0 = [\hat{a}_0^\dagger|\, 1\,\rangle]^* = 0$ from Eq. (2.7)
3. or we say $\langle\, 2,0,0,...\,|$ for Fermions didn't make sense to begin with.

Either way, this demonstrates:

Fermi blocking: Fermionic particles cannot make a transition into a state already occupied by another particle.

Bosons:



top: What is the transition amplitude from $|\,A'\,\rangle = |\,N,1,0,0,...\,\rangle \rightarrow |\,B'\,\rangle = |\,N+1,0,0,0,...\,\rangle$ for Bosons?
The corresponding matrix element to the one above is:

$$\langle\, B'\,|\hat{H}|\,A'\,\rangle = \langle\, N+1,0,0,..\,|\sum_{nm}\kappa_{nm}\hat{a}_n^\dagger\hat{a}_m|\,N,1,0,...\,\rangle$$
$$\overset{Eq.\ (2.4)-(2.5)}{=} \langle\, N+1,0,0,...\,|\kappa_{01}\sqrt{N+1}\times 1|\,N+1,0,0,...\,\rangle = \sqrt{N+1}\kappa_{01}$$

We see that there is

Bose-Enhancement: The quantum transition amplitude of a Boson into a single-body state already occupied by N other identical Bosons is enhanced by a factor $\sqrt{N+1}$

Week 3

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

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2.3 Quantum Fields

Let us expand our assembly of the second quantized Hamiltonian in (2.21) again

$$\hat{H} = \sum_{nm} \langle\, \varphi_n \,|\hat{\mathcal{A}}|\, \varphi_m \,\rangle \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} \langle\, \varphi_n \varphi_m \,|\hat{\mathcal{B}}|\, \varphi_l \varphi_k \,\rangle \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_l \hat{a}_k \tag{2.23}$$

Please refer again to section 2.1.1 for the definitions of $\hat{A}$, $\hat{\mathcal{A}}$, $\hat{B}$, $\hat{\mathcal{B}}$. Using the position space representation of $|\,\varphi_n\,\rangle$, this becomes

$$\hat{H} = \sum_{nm} \int dx\; \varphi_n^*(x) \hat{\mathcal{A}}(x) \varphi_m(x) \hat{a}_n^\dagger \hat{a}_m + \sum_{nmlk} \int dx \int dy\; \varphi_n^*(x) \varphi_m^*(y) \hat{\mathcal{B}}(x,y) \varphi_l(x) \varphi_k(y) \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_l \hat{a}_k \tag{2.24}$$

We now lump together the position space single particle basis functions $\varphi_n(x)$ and operators $\hat{a}_n$ into the

Field Operator

$$\hat{\Psi}(x) = \sum_n \varphi_n(x) \hat{a}_n \tag{2.25}$$

Using this notation, the Hamiltonian is

$$\hat{H} = \int dx\; \hat{\Psi}^\dagger(x) \hat{\mathcal{A}}(x) \hat{\Psi}(x) + \int dx \int dy\; \hat{\Psi}^\dagger(y) \hat{\Psi}^\dagger(x) \hat{\mathcal{B}}(x,y) \hat{\Psi}(x) \hat{\Psi}(y) \tag{2.26}$$

For the same case as (2.16) we have:

Hamiltonian for particles in a 1D harmonic trap (with interactions)

$$\hat{H} = \int dx\; \hat{\Psi}^\dagger(x) \underbrace{\left[-\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right]}_{\equiv \hat{H}_o} \hat{\Psi}(x) + \frac{1}{2} \int dx \int dy\; \hat{\Psi}^\dagger(y) \hat{\Psi}^\dagger(x) U(x-y) \hat{\Psi}(x) \hat{\Psi}(y) \tag{2.27}$$

- Field operator is also simply the annihilation operator for the position-basis. Think of it as annihilating a particle at position "x". To see this consider the state $|\,x\,\rangle = \hat{\Psi}^\dagger(x)|\,0\,\rangle = \sum_n \varphi_n(x)\hat{a}_n^\dagger|\,0\,\rangle$. If we now consider the overlapp of two of these states we have

$$\langle\, y\,|\,x\,\rangle = \langle\, 0\,|\sum_{nm}\varphi_m^*(y)\varphi_n(x)\hat{a}_m\hat{a}_n^\dagger|\,0\,\rangle. \tag{2.28}$$

  Using the orthogonality of Fock states, this reduces to $\langle\, y\,|\,x\,\rangle = \sum_n \varphi_n^*(y)\varphi_n(x) \overset{\text{see QM book}}{=} \delta(x-y)$. Since the states only overlap for $x = y$, they must be position eigenstates.

- All three descriptions (2.12), (2.14), (2.27) are fully equivalent, which is "best" depends on the problem.

- Using (2.8) and $\sum_n \varphi_n(x)\varphi_n^*(y) = \delta(x-y)$ we can show

Commutation relations for field operators

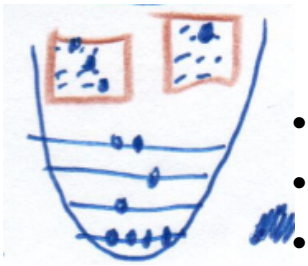
$$\begin{aligned} \text{Bosons}: \left[\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right] &= \delta(x-y), \qquad \left[\hat{\Psi}(x), \hat{\Psi}(y)\right] = 0 \\ \text{Fermions}: \left\{\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right\} &= \delta(x-y), \qquad \left\{\hat{\Psi}(x), \hat{\Psi}(y)\right\} = 0 \end{aligned} \tag{2.29}$$

2.3.1 Examples of Quantum Fields

Advantages/strengths of quantum field concept:

- Naturally deals with particle creation/anhilation and conversion. Different Fock-states (2.2) can be viewed as different excited states of the underlying the field.
- Formulated in time and space (t, **x**), quantum fields can naturally address spatial and temporal coherence properties (e.g. see chapter 3).
- Can conveniently formulate Lorentz-invariant (relativistic) theories and take care of causality.

Examples:
Example A: Harmonically trapped dilute Bose gas

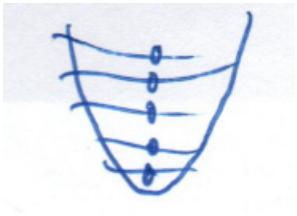


$$\hat{\Psi}(x) = \sum_n \underbrace{\varphi_n(x)}_{\text{SHO modes}} \hat{a}_n$$

- typically atom number conserved and non-relativistic
- Field operator useful to describe coherence and condensation.
- Atom number may fluctuate if part of the system external.

Examples cont:

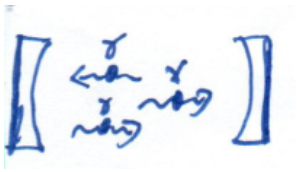
Example B: Harmonically trapped dilute Fermi gas.



We expect here that Fermi blocking or the Pauli exclusion principle play a crucial role. These first two examples are the sole focus of this lecture. The remaining ones are listed to provide links to other lectures.

Example C: Quantized light field / electric field in QED, Quantum Optics

$$\hat{\vec{E}}(\vec{r},t) = \sum_k \vec{\epsilon}_k \mathcal{E}_k \hat{a}_k e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{r}} + \text{H.c.}$$



where,

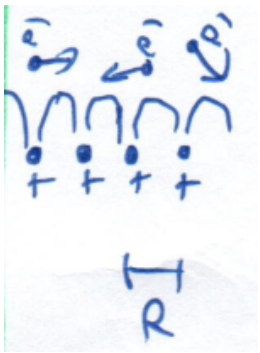
$\vec{\epsilon}_k$ - Polarization vector, $\mathcal{E}_k$ - Amplitude, $e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{r}}$ - Plane wave (Photon-mode)

Example D: Relativistic spin $\frac{1}{2}$ field (e.g. quarks/electrons)

$$\hat{\Psi}_\alpha(x) = \sum_{s=\pm\frac{1}{2}} \int \frac{d^3p}{(2\pi)^3 2p_0} \left(\underbrace{e^{-ipx} u_\alpha(p,s)\hat{a}(p,s)}_{\text{particle}} + \underbrace{e^{ipx} v_\alpha(p,s)\hat{a}^\dagger(p,s)}_{\text{anti-particle}} \right)$$

where α - spin index, x - 4-vector(t,$\mathbf{x}$), $u_\alpha(p,s)$ - Spinor

Example E: Non-relativistic electron gas in condensed-matter



$$\hat{\Psi}_\sigma(x) = \sum_n \int dk \;\; \hat{a}_{nk} \underbrace{u_{nk}(r)}_{\text{Bloch-function}} \underbrace{e^{ikx}}_{\text{plane-wave}} \underbrace{\chi_\sigma}_{\text{spin}}$$

where, n - Band index, $u_{nk}(r)$ - Bloch function with periodicity R

$$u_{nk}(r+R) = u_{nk}(r)$$

- Quantum fields are operators and thus on the same level as an Observable in single body quantum mechanics.
- A specific physical situation requires us in principle to specify also an underlying (many-body)

quantum state $|\,\psi\,\rangle$.

- With that we can then evaluate specific expectation values involving the quantum field.

Example: Interplay of quantum field and quantum state: Consider N Bosonic atoms in a 1D harmonic trap as in Example A above.
Using (2.10) and (2.25), we can show that the total number of atoms is:

$$N = \int dx \hat{\Psi}^\dagger(x)\hat{\Psi}(x). \tag{2.30}$$

This motivates viewing $\hat{\rho}(x) = \hat{\Psi}^\dagger(x)\hat{\Psi}(x)$ as operator for the density of atoms.
We shall see two sources of fluctuations for this density: One due to the underlying quantum state of the field, and one due to the discreteness of the individual atoms. To measure local density, we count atoms in a small region of size L as shown in the figure, to find the local number of atoms in this region

$$\hat{n}_{\rm loc}(x_0) = \int_{x_0}^{x_0+L} dx \hat{\Psi}^\dagger(x)\hat{\Psi}(x), \tag{2.31}$$

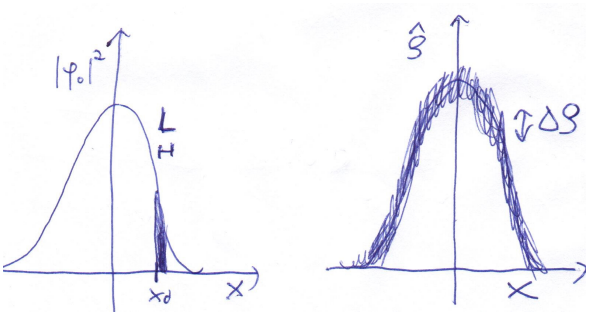
and then use $\hat{\rho} = n_{\rm loc}(x_0)/L$ to get a density. Let us define the local number uncertainty

$$\Delta n_{\rm loc}(x_0)^2 = \langle \hat{n}_{\rm loc}(x_0)^2\rangle - \langle \hat{n}_{\rm loc}(x_0)\rangle^2. \tag{2.32}$$

You should have seen similar expressions for e.g. position uncertainty ΔX in basic QM.

Case (i): Quantum state $\psi = |\,N,0,0,0\cdots\rangle$, i.e. all N atoms are in the ground state. We can see a mean local number $\langle\hat{\rho}\rangle = Np_{\rm loc}$ and an uncertainty $\Delta n_{\rm loc}(x_0) = \sqrt{N(p_{\rm loc} - p_{\rm loc}^2)}$, where $p_{\rm loc} = \int_0^L du|\varphi_0(x_0+u)|^2$ is the single atom probability to be in the chosen region. The uncertainty arises because the density measurement is based on a finite sample number of atoms.
Case (ii): Quantum state $\psi = [|\,N-k,0,0,0\cdots\rangle + |\,N+k,0,0,0\cdots\rangle]/\sqrt{2}$ for $k < N$. Now the atom number itself is uncertain. We find again $\langle\hat{\rho}\rangle = Np_{\rm loc}$ but this time $\Delta n_{\rm loc}(x_0) = \sqrt{N(p_{\rm loc} - p_{\rm loc}^2) + k^2 p_{\rm loc}^2}$. Thus while we can have the same mean density, increasing k increases the density fluctuations. This now happens because of the quantum state itself.

Note that all the properties above changed based on quantum state.



- As we see later, often the detailed specification of the underlying quantum state can be avoided however, by simply postulating certain properties of expectation values of field operators, and then working with those.

2.3.2 Dynamics of quantum fields

Here the field operators are mainly a way to re-write the Hamiltonian. Much of the usual methodology of quantum mechanics can be applied as before.

E.g. Consider the Heisenberg picture[1] for the field operator in (2.27): $i\hbar\dot{\hat{\Psi}} = [\hat{\Psi}, \hat{H}]$:

Heisenberg equation for Field operator

$$i\hbar\dot{\hat{\Psi}}(x,t) = \hat{H}_0\hat{\Psi}(x,t) + \int d^3y\ \hat{\Psi}^\dagger(y,t)U(x-y)\hat{\Psi}(y,t)\hat{\Psi}(x,t) \tag{2.33}$$

- We have made use of the commutation relation (2.29).
- We shall begin exploring BEC from here in chapter 3.

Example: Non-interacting evolution of atom-field (thus the Hamiltonian is as in (2.16) but with $U = 0$)
Insert $\hat{\Psi}(x) = \sum_n \varphi_n(x)\hat{a}_n$ into (3.38).

$$i\hbar\sum_n \varphi_n(x)\dot{\hat{a}}_n = \hat{H}_0\left(\sum_n \varphi_n(x)\hat{a}_n\right) \tag{2.34}$$

$$= \sum_n \underbrace{\hat{H}_0\varphi_n(x)}_{=E_n\varphi_n(x)}\ \hat{a}_n \tag{2.35}$$

$$\tag{2.36}$$

Multiplying by $\int dx\varphi_m^*(x)$

$$i\hbar\dot{\hat{a}}_m = E_m\hat{a}_m \tag{2.37}$$

$$\implies \hat{a}_m(t) = \hat{a}(0)e^{-i\frac{E_m t}{\hbar}} \tag{2.38}$$

$$\implies \hat{\Psi}(x,t) = \sum_n \varphi_n(x)e^{-i\frac{E_n t}{\hbar}}\hat{a}(0) \tag{2.30b}$$

The number of cases where (2.30) can be solved is limited. But we also still have:

[1] If unfamiliar, please revise all three QM dynamical pictures (Schrödinger-, Heisenberg-, Interaction picture)

Time-evolution operator:

$$\hat{U}(t,t_0) = \mathcal{T}\left[\exp\left[-i\int_{t_0}^{t} dt' \hat{H}(t')\right]\right] \tag{2.39}$$

- Evolves a (many-body) quantum state in time

$$|\,\psi(t)\,\rangle = \hat{U}(t,t_0)|\,\psi(t_0)\,\rangle$$

- $\hat{H}$ & initial/final states can be written using field operators.
- We can move to the interaction picture to replace $\hat{H}(t')$ with some (weaker) interaction $\hat{V}$(t') in (2.31).
- Then expand exponential in a power series $\rightarrow$ time-dependent perturbation theory, Feynman diagrams (not here).

2.3.3 Observables and Green's functions[2]

1. As usual in QM, all physical observations related to a quantum field can be written as expectation value of an operator.
2. In 2.2.1 we showed of all operators can be expressed by creation-(destruction-) operator $\hat{a}^\dagger(\hat{a})$.
3. These in turn can all be expressed through field operators.

All up, a huge list of phenomena can be understood from correlation functions:

Green's function: Roughly of the form

$$G^{(n)}(x_1 t,...,x_n t|x_1' t',...,x_n' t') = \langle \hat{\Psi}^\dagger(x_n,' t'),...,\hat{\Psi}^\dagger(x_1,' t')\hat{\Psi}(x_n,t),...,\hat{\Psi}(x_1,t)\rangle \tag{2.40}$$

There are lots and lots of alternative definitions.

2.3.4 Spin-statistics theorem

This really belongs to the realm of relativistic quantum mechanics or particle physics, but we could not resist sketching it here. You know that:

[2] See Bruus and Flensberg

Spin-statistics theorem:

$$\begin{aligned} \text{Half-integer spin particles} &= \text{Fermions } (s = \frac{1}{2}, \frac{3}{2}, etc.) \\ \text{Integer spin particles} &= \text{Bosons } (s = 0, 1, 2, etc.) \end{aligned} \tag{2.41}$$

This follows necessarily from casuality and Lorentz invariance.

Rough sketch of the proof:

- Hamiltonian density $\hat{H} = \int d^4x \hat{\mathscr{H}}(x)$ (where $x = (t, \mathbf{x})$) must obey $\left[\hat{\mathscr{H}}(x), \hat{\mathscr{H}}(y)\right] = 0$ for $(x-y)^2 = c^2\Delta t^2 - \Delta x^2 < 0$. (A)
  (This means space-like seperated events cannot affect each other.)
- Quantum fields obey specific transformation laws under Lorentz-transformations Λ (4x4 matrix), depending on spin of the field.

$$U(\Lambda)\hat{\Psi}^\dagger(x)U^{-1}(\Lambda) = \hat{\Psi}^\dagger(\Lambda x) \qquad \text{(spin zero)}$$

$$U(\Lambda)\hat{\Psi}^\dagger_s(x)U^{-1}(\Lambda) = \sum_{s'} \underbrace{D_{ss'}(\Lambda^{-1})}_{\equiv\ representation\ matrix} \hat{\Psi}^\dagger_{s'}(\Lambda x) \qquad \text{(spin 1/2)}$$

- It turns out that (A) works out if

$$\left[\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right] = 0 \qquad \text{for } (x-y)^2 < 0 \qquad \text{(integer spin)}$$

$$\left\{\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\right\} = 0 \qquad \text{for } (x-y)^2 < 0 \qquad \text{(half-integer spin)}$$

2.3.5 Notation overview-I

We have introduced a lot of different but similar symbols for single vs many body states and operators. We will attempt to stick to the following notation:

Notation:

$\lvert w_n \rangle, \lvert \varphi_n \rangle, w_n(\mathbf{x}), \varphi_n(\mathbf{x})$	Single particle bases and their position representation.
$\lvert \psi \rangle$, $\psi(\mathbf{x}_1, \mathbf{x}_2, ...)$	Many-body state and its (1st quantized) position representation.
$\hat{\Psi}(\mathbf{x})$	Field operator
$\hat{b}, \hat{b}^\dagger$	Harmonic oscillator ladder operator.
$\hat{a}_n, \hat{a}^\dagger_n, \hat{c}_n, \hat{c}^\dagger_n$	Creation and anhilation operators for various bases $\lvert w_n \rangle, \lvert \varphi_n \rangle$

Week 4

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

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2.4 Coherent states

Coherent states are a very useful concept in many areas of quantum physics. We discuss two types, which are mathematically/algebraically identical but conceptually subtly different:

2.4.1 Coherent Harmonic Oscillator States

- Question: What is the "most classical" type of oscillation we can get in the quantum harmonic oscillator:
- Answer: Define

Coherent State

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \exp[\alpha \hat{b}^\dagger]|0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\varphi_n\rangle, \;\; \alpha \in \mathbb{C} \tag{2.42}$$

We can write this also as: $|\alpha\rangle = \mathrm{D}(\alpha)|0\rangle$, where $\mathrm{D}(\alpha) = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}}$ is the displacement operator.

- Here $\hat{b}^\dagger$ is a ladder operator from (1.12).
- Coherent states are not necessarily eigenstates of the harmonic oscillator Hamiltonian $\hat{H}_{SHO}$ in (1.13), since they have an uncertain energy/number of oscillator quanta.

Properties of coherent states

$$\hat{b}|\alpha\rangle = \alpha|\alpha\rangle, \qquad \hat{b}^\dagger|\alpha\rangle = \left(\frac{\partial}{\partial\alpha} + \frac{\alpha^*}{2}\right)|\alpha\rangle, \qquad \langle\alpha|\hat{b}^\dagger = \langle\alpha|\alpha^*, \tag{2.43}$$

$$\langle\alpha|\alpha'\rangle = \exp\left[\alpha^*\alpha' - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right] \text{ (Not orthogonal)}, \tag{2.44}$$

$$\langle\alpha|\alpha\rangle = 1, \tag{2.45}$$

$$\mathbb{I} = \frac{1}{\pi}\int d\alpha|\alpha\rangle\langle\alpha|. \tag{2.46}$$

- Coherent state is a right-eigenstate of destruction operator
- Two different coherent states are typically not orthogonal, unless $|\alpha - \alpha'|$ is very large (and even then only approxiately).

Proof of (2.43): Let $|\bar{\alpha}\rangle = e^{\frac{|\alpha|^2}{2}}|\alpha\rangle$

$$\begin{aligned}\hat{b}|\bar{\alpha}\rangle &= \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\hat{b}|\varphi_n\rangle = \sum_{n=1}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\sqrt{n}|\varphi_{n-1}\rangle \\ &\underset{n\longmapsto n+1}{=} \sum_{n=0}^{\infty}\frac{\alpha^{n+1}}{\sqrt{(n+1)!}}\sqrt{n+1}|\varphi_n\rangle = \alpha\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle = \alpha|\bar{\alpha}\rangle\end{aligned}$$

$$\begin{aligned}\hat{b}^\dagger|\bar{\alpha}\rangle &= \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\hat{b}^\dagger|\varphi_n\rangle = \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\sqrt{n+1}|\varphi_{n+1}\rangle \\ &= \sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\frac{1}{n+1}\frac{\partial}{\partial\alpha}\alpha^{n+1}\sqrt{n+1}|\varphi_{n+1}\rangle = \sum_{n=0}^{\infty}\frac{\partial}{\partial\alpha}\frac{\alpha^{n+1}}{\sqrt{(n+1)!}}|\varphi_{n+1}\rangle \\ &= \frac{\partial}{\partial\alpha}\sum_{n=1}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle = \frac{\partial}{\partial\alpha}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|\varphi_n\rangle = \frac{\partial}{\partial\alpha}|\bar{\alpha}\rangle\end{aligned}$$

(Rest follows from the product rule.)

Example: Oscillation of coherent state: What is the meaning of α? Let $\alpha_0 \in \mathbb{R}$
Convert the equation $\hat{b}|\alpha_0\rangle = \alpha_0|\alpha_0\rangle$ to the position basis:

$$\langle x|\hat{b}|\alpha_0\rangle = \alpha_0 \underbrace{\langle x|\alpha_0\rangle}_{\equiv\tilde{\alpha}_0(x)}$$

$$\xrightarrow[Eq.\ (1.12)]{\text{Using}} \quad \frac{\partial}{\partial x}\tilde{\alpha}_0(x) = \left(-\frac{m\omega}{\hbar}x + \sqrt{\frac{2m\omega}{\hbar}}\alpha_0\right)\tilde{\alpha}_0(x)$$

$$\xRightarrow[\text{DE}]{\text{Solve}} \quad \tilde{\alpha}_0(x) = C\ \exp\left[-\frac{(x-\alpha_0')^2}{2\sigma^2}\right],$$

where $\sigma = \sqrt{\frac{\hbar}{m\omega}}$ and $\alpha_0' = \sqrt{2}\sigma\alpha_0$. Thus the position space representation of a coherent state has a Gaussian shape, with center location governed by α_0'.
We now want to find the time evolution of the coherent state $|\,\alpha_0\,\rangle$. The latter is assembled from oscillator eigen states that obey:

$$\hat{H}_0|\varphi_n\rangle = E_n|\varphi_n\rangle, \quad E_n = \hbar\omega\left(n+\frac{1}{2}\right).$$

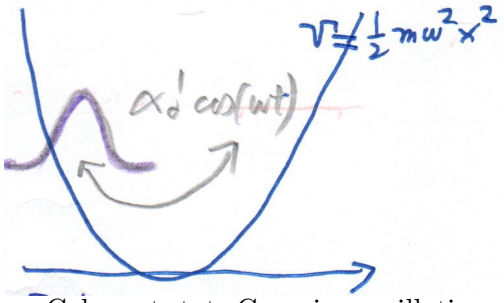
Since the Hamiltonian is time-independent, we can us the standard rules for time evolution to find

$$\begin{aligned}
\Rightarrow |\alpha(t)\rangle &= \sum_n \frac{\alpha_0^n}{\sqrt{n!}} e^{-i\omega(n+\frac{1}{2})t}|\varphi_n\rangle \\
&= \sum_n \frac{1}{\sqrt{n!}}(\alpha_0 e^{-i\omega t})^n e^{-i\frac{\omega}{2}t}|\varphi_n\rangle \\
&= e^{-i\frac{\omega}{2}t}|\alpha_0 e^{-i\omega t}\rangle.
\end{aligned}$$

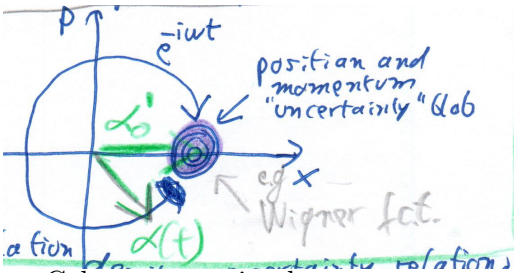
Can show after some fiddling:

$$|\tilde{\alpha}(x,t)|^2 = C'\exp\left[-\frac{(x-\alpha_0'\cos(\omega t))^2}{\sigma^2}\right]$$

.
We thus always have a ground-state shaped Gaussian oscillating in the potential with amplitude α_0'.



top: Coherent state Gaussian oscillating in a harmonic trap



top: Coherent state in phase space, represented by Wigner function (see below)

2.4.2 Wigner function

In the example above, bottom right, we also wanted to show a phase space representation of a quantum harmonic oscillator in a coherent state.

Classically we have the idea of phase-space (x, p). Quantum mechanically $\Delta x \Delta p \geq \hbar/2 \rightarrow$ particle cannot have a fixed phase-space coordinate. We can still represent a quantum state $\varphi(x)$ in phase-space, using the

Wigner distribution

$$W(x,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \varphi^*(x+y)\varphi(x-y)e^{2ipy/\hbar}dy \tag{2.47}$$

- Properties

$$\int_{-\infty}^{\infty} dp\, W(x,p) = |\varphi(x)|^2 \text{ (position-space distribution)},$$

$$\int_{-\infty}^{\infty} dx\, W(x,p) = |\tilde{\varphi}(p)|^2 \text{ (momentum-space distribution)}.$$

- $W(x,p)$ is a quasi-probability distribution (means we can get some expectation values by integrating over it, but it may have regions with $W(x,p) < 0$)
- The interpretation is that when drawing $W(x,p)$, non-zero regions show the location of a quantum-state in phase-space. This was used in the figure of the example above.

We can alternatively define the

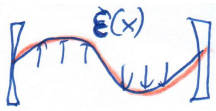
Wigner function from the number-state representation

$$\chi_W(\lambda, \lambda^*) = Tr\{\hat{\rho}e^{\lambda\hat{a}^\dagger - \lambda^*\hat{a}}\} \tag{2.48}$$

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2}\int d^2\lambda e^{-\lambda\alpha^* + \lambda^*\alpha}\chi_W(\lambda, \lambda^*) \tag{2.49}$$

- The above gives the same as (2.47) for harmonic oscillator ladder operators $\hat{a} \rightarrow \hat{b}$.
- It directly generalizes to Fock states (2.2), when $\hat{a}$ are many-body creation and destruction opertors.

Example, Laser:

Consider a single-mode photon field at frequency ω: 

$$\hat{H} = \hbar\omega \hat{a}^\dagger \hat{a}, \text{ just as for oscillator}$$

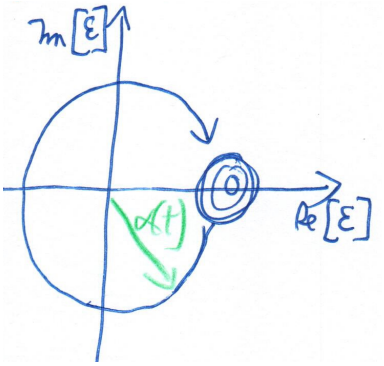
Electric field (c.f. Example C page 19)

$$\hat{E}(x,t) = \mathcal{E}(x,t)\hat{a} + h.c.$$

Taking expectation value in the coherent state $|\alpha(t)\rangle$, we can show (exercise)

$$\langle\alpha(t)|\hat{E}(x,t)|\alpha(t)\rangle = 2\,\mathfrak{Re}\{\mathcal{E}(x,t)\underbrace{\alpha_0 e^{-i\omega t}}_{\alpha(t)}\}$$

Thus here, the complex number $\alpha(t)$ characterizes amplitude and phase of the oscillating electric field.



2.4.3 Coherent many-body states

Due to identical properties of ladder $\hat{b}$ operators and $\hat{a}, \hat{c}$, we can equally define a

Many-body coherent state (Bosons):

$$|\alpha\rangle = \exp[\hat{a}_m^\dagger \alpha]|0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle, \alpha \in \mathbb{C} \tag{2.50}$$

where $|n\rangle$ is a Fock-state that represents the occupation of mode $|\phi_m\rangle$.

- this now describes a superposition of different occupation numbers (Fock-states) of single-body mode $|\varphi_m\rangle$

- all properties of (2.43)-(2.46) apply

We can combine states (2.50) for multiple single-particles states (modes) into

Many-mode coherent state (Bosons):

$$\hat{a}_k|\boldsymbol{\alpha}\rangle = \alpha_k|\boldsymbol{\alpha}\rangle, \quad \boldsymbol{\alpha} = \{\alpha_1 ... \alpha_N\}, \quad \alpha_k \in \mathbb{C} \tag{2.51}$$

which exhibit one coherent amplitude α_k for each single-particle basis state k

- The slightly messy formal decomposition of (2.51) into Fock-states is

$$|\boldsymbol{\alpha}\rangle = e^{-\sum_k \frac{|\alpha_k|^2}{2}} \sum_{n_1 n_2 ... n_N} \frac{\alpha_1^{n_1}\alpha_2^{n_2}...\alpha_N^{n_N}}{\sqrt{n_1!}\sqrt{n_2!}...\sqrt{n_N!}}|n_1 n_2 ... n_N\rangle. \tag{2.52}$$

2.4.4 Fermionic coherent states (not used here)

If we assume a definition like (2.51) for fermionic operators we run into trouble:

$$\{\hat{a}_k, \hat{a}_l\}|\boldsymbol{\alpha}\rangle = (\alpha_k\alpha_l + \alpha_l\alpha_k)|\boldsymbol{\alpha}\rangle \stackrel{!}{=} 0 \qquad (\text{since}\{\hat{a}_k, \hat{a}_l\} = 0)$$

For two non-zero complex numbers $\alpha_k\alpha_l + \alpha_l\alpha_k = 2\alpha_k\alpha_l \neq 0$ of course.

Solution: We use

Grassmann-numbers Defined as an anti-commuting set of complex numbers

- Based on this we can also use the coherent state concept for fermions. Mainly useful for fermionic path integrals
- Not further used in this lecture

Week 5

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3 Bose-Einstein Condensates

3.1 Quantum statistical physics

For large systems, we cannot know all microscopic detail $\implies$ describe with density-matrix (see 1.3.2).

All essential postulates take a very similar form to classical statistical physics.

Quantum statistical ensembles:

Microcanonical ensemble (fixed N,V,E)

$$\hat{\rho} = \frac{1}{\Gamma(E)} \sum_{\substack{k \\ E_k \approx E}} |\,\psi_k\,\rangle\langle\,\psi_k\,| \tag{3.1}$$

- the sum runs over all many-body states k with energy in energy range $E \leq E_k \leq E + \Delta E$, for a small ΔE. See Eq. (1.23) for the definition of $|\,\psi_k\,\rangle$, E_k, i.e., they are generic many-body states.

Canonical ensemble (fixed N,V,T)

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}, \tag{3.2}$$

where $\beta = (k_B T)^{-1}$ and Z is the partition function, $Z = \mathrm{Tr}[e^{-\beta \hat{H}}]$.

- Z normalizes $\hat{\rho}$ to fulfill $\mathrm{Tr}[\hat{\rho}] = 1$.
- The exponential of an operator is defined via the power series of exp.

- In eigenbasis of $\hat{H}$, $\langle\,\psi_k\,|$, we can write

$$\hat{\rho} = \frac{1}{Z}\sum_k e^{-\beta E_k}|\,\psi_k\,\rangle\langle\,\psi_k\,|. \tag{3.3}$$

- (3.3) is however more general. We may not know the eigenbasis, since finding it is hard for interacting many-body systems.

Grand-canonical ensemble (fixed μ,V,T)

$$\hat{\rho} = \frac{1}{Z_G}e^{-\beta(\hat{H}-\mu\hat{N})}, \tag{3.4}$$

where μ is the chemical potential (operationally defined later), $\hat{N}$ the total number operator for the system and $Z_G = Tr[e^{-\beta(\hat{H}-\mu\hat{N})}]$ the grand-canonical partition function.

- In eigenbasis of $\hat{H}$ and $\hat{N}$, $\langle\,\psi_k\,|$, we can write:

$$\hat{\rho} = \frac{1}{Z_G}\sum_k e^{-\beta(E_k-\mu N_k)}|\,\psi_k\,\rangle\langle\,\psi_k\,|, \tag{3.5}$$

where N_k is the number of particles in the state $|\,\psi_k\,\rangle$.

We focus on the latter example, and explore the
Consequences for Indistinguishable particles:

Consider single particle basis $H_0|\,\varphi_m\,\rangle = \varepsilon_m|\,\varphi_m\,\rangle$ and non-interacting many-body Hamiltonian

$$\hat{H} = \sum_m \varepsilon_m \hat{a}_m^\dagger \hat{a}_m. \tag{3.6}$$

- Convince yourself that Fock states $|\,\mathbf{N}\,\rangle = |\,N_1N_2N_3\cdots\rangle$ in (2.2) are eigenstates of $\hat{H}|\,\mathbf{N}\,\rangle = E_{\mathbf{N}}|\,\mathbf{N}\,\rangle$ with $E_{\mathbf{N}} = \sum_m N_m\varepsilon_m$.
- From (3.5)

$$\hat{\rho} = \sum_{\mathbf{N}} P_{\mathbf{N}}|\,\mathbf{N}\,\rangle\langle\,\mathbf{N}\,|$$

with (define $N_{\mathbf{N}} = \sum_m N_m$)

$$P_{\mathbf{N}} = \frac{e^{-\beta(E_{\mathbf{N}}-\mu N_{\mathbf{N}})}}{\sum_{\mathbf{N}} e^{-\beta(E_{\mathbf{N}}-\mu N_{\mathbf{N}})}} = \frac{\exp\left[-\beta\left(\sum_m N_m\varepsilon_m\right)+\beta\mu\left(\sum_m N_m\right)\right]}{\sum_{N_1,N_2,N_3,\ldots}\exp\left[-\beta\left(\sum_m N_m\varepsilon_m\right)+\beta\mu\left(\sum_m N_m\right)\right]} \tag{3.7}$$

$$= \frac{\prod_m \exp[\beta N_m(\mu-\varepsilon_m)]}{\prod_l\left[\sum_{N_l}\exp[\beta N_l(\mu-\varepsilon_l)]\right]} = \prod_m P_m(N_m) \tag{3.8}$$

with

$$P_m(N_m) = \frac{\exp[\beta N_m(\mu - \varepsilon_m)]}{\sum_{N_l} \exp[\beta N_l(\mu - \varepsilon_l)]}, \tag{3.9}$$

the probability to have N_m particles in mode number m. To see the latter statement more rigorously, define this probability as $P_m(N_m) = \bar{\sum}_{\mathbf{N}'} P_{\mathbf{N}'}$ with $\bar{\sum}$ running *only* over all $\bar{\mathbf{N}}'$ that fulfill $N'_m = N_m$. Starting from (3.7) you then reach (3.9) (excercise).

Now: What is the mean number of particles in state $|\,\psi_b\,\rangle$, with energy ε_b?

$$\begin{aligned} \bar{m}_b = \langle \hat{N}_b \rangle &= \mathrm{Tr}[\hat{\rho}\hat{N}_b] = \sum_{\mathbf{N}} P_{\mathbf{N}} \mathrm{Tr}\,(N_b|\,\mathbf{N}\,\rangle\langle\,\mathbf{N}\,|) \\ &\quad \downarrow \\ &\quad = \hat{a}_b^\dagger \hat{a}_b \\ &= \sum_{\mathbf{N}} P_{\mathbf{N}} N_b \overset{\text{as } \circledast}{=} \sum_{N_b} P_b(N_b) N_b \end{aligned} \tag{3.10}$$

So far, our discussion was valid for both, Bosons and Fermions. Now we have to specifiy.

Fermions: Allowed values of $N_b = 0, 1$

$$\Longrightarrow \bar{m}_b = 0 + P_b(1) \times 1 = \frac{\exp(\beta(\mu - \varepsilon_b))}{1 + \exp(\beta(\mu - \varepsilon_b))} \Longrightarrow$$

Fermi-Dirac distribution Mean number of indistinguishable Fermions in a given state b with energy ε_b:

$$\bar{m}_b = \frac{1}{\exp(\beta(\varepsilon_b - \mu)) + 1}. \tag{3.11}$$

Bosons: All values of $N_b = 0, 1, 2, ..., \infty$ are allowed

- Define $a = \exp[\beta(\mu - \varepsilon_b)]$ and note that we can then write

$$\bar{m}_b = \sum_{N_b} P_b(N_b) N_b = \frac{a \frac{d}{da} \left(\sum_{N_b} a^{N_b} \right)}{\sum_{N_b} a^{N_b}}$$

- Use geometric series $\sum_n a^n = 1/(1-a)$ to reach[3]

Bose-Einstein distribution Mean number of indistinguishable Bosons in a given state b with energy ε_b:

$$\bar{m}_b = \frac{1}{\exp(\beta(\varepsilon_b - \mu)) - 1}. \tag{3.12}$$

[3] Using this expression requires $a < 1$, which is the case since $\mu < 0$, as we shall see shortly.

- The classical limit $\bar{m}_b \ll 1$ is reached when the occupation of each state is very small. $\implies \exp \gg 1$

$$\implies \bar{m}_b = \exp(-\beta(\varepsilon_b - \mu)),$$

so we recover the Boltzmann-distribution from classical physics.

- For given system (i.e. fixed ε_k and temperature), the chemical potential controls the mean total particle number via $N = \sum_k \bar{m}_k$.

3.2 Bose-Einstein condensation

Consider non-interacting Bosonic atoms in a harmonic trap, with

$$\varepsilon_{\mathbf{n}} = \hbar\omega(n_x + n_y + n_z + \frac{3}{2}).$$

⚠ In section 3.2, n_x, n_y, n_z label oscillator states not occupation numbers. For those we use capital N as before

The mean total atom number now is

$$N = \sum_{n_x n_y n_z} \bar{m}_{n_x n_y n_z} \overset{(3.12)}{=} \sum_{n_x n_y n_z} \frac{1}{\exp[\beta(\hbar\omega(n_x + n_y + n_z + \frac{3}{2}) - \mu)] - 1}$$

- Define $\tilde{\mu} = \mu - \frac{3}{2}\hbar\omega$. We need $\tilde{\mu} < 0$ for reasonable results, which means positive mean occupation, $\bar{m}_{\mathbf{n}>}0$.

- We see that, for a given state $\mathbf{n} = (n_x, n_y, n_z)$, if we lower the temperature (T↓) then all mean occupations go down ($\bar{m}_{\mathbf{n}} \downarrow$). On the other hand, for a given state $\mathbf{n}$ and T, if we increase the adjusted chemical potential ($\tilde{\mu} \uparrow$) then all mean occupations go up ($\bar{m}_{\mathbf{n}} \uparrow$).

- Thus, if we would want to keep the total particle numbers N fixed as we lower the temperature T, we need to simultaneously increase μ.

- But in that we are limited by the requirement $\tilde{\mu} < 0$, so the question is what happens when we reach $\tilde{\mu} = 0$? In that case we see for the groundstate occupation: $\underset{\substack{\downarrow \\ \text{Ground-state occupation}}}{\bar{m}_{000}} = \frac{1}{e^{\beta.0}-1} \to \infty$, which is a problem, while for all other states the formula (3.12) could still be OK.

- The solution is to separately write the occupation of the ground-state as in:

$$N = N_0 + \sum_{\mathbf{n} \neq (000)} \bar{m}_{\mathbf{n}} \tag{3.13}$$

Let us find the lowest temperature T_c where $N_0 \approx 0$ is still possible. In other words, what is the lowest temperature for which we are still able to distribute "enough" atoms among all the excited

states, using the B.E. distribution function (3.12). This will correspond to $\tilde{\mu} = 0$. Hence:

$$N = \sum_{\mathbf{n}\neq(000)} \frac{1}{\exp[\beta_c(\hbar\omega(n_x+n_y+n_z)) - \underbrace{\tilde{\mu}}_{=0}] - 1} \qquad \beta_c = \frac{1}{k_B T_c}$$

$$\approx \int dn_x dn_y dn_z \frac{1}{\exp[\beta_c(\hbar\omega(n_x+n_y+n_z))] - 1} \qquad \text{Let } n'_{x/y/z} = \hbar\omega n_{x/y/z}$$

$$\approx \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \int_0^\infty dn'_x dn'_y dn'_z \frac{1}{e^{n'_x+n'_y+n'_z} - 1} = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \int d^3\mathbf{n} e^{-p(n'_x+n'_y+n'_z)} \qquad \underbrace{\left[\because \sum_{p=1}^\infty e^{-p\alpha} = \frac{1}{e^\alpha - 1}\right]}_{\text{geometric series}}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \underbrace{\left(\int_0^\infty dn'_x e^{-pn'_x}\right)}_{=1/p} \left(\int_0^\infty dn'_y e^{-pn'_y}\right)\left(\int_0^\infty dn'_z e^{-pn'_z}\right)$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \frac{1}{p^3} = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \zeta(3)$$

where $\zeta(s) = \sum_{p=1}^\infty \frac{1}{p^s}$ is the Riemann-Zeta function. Below T_C, we have to allow $N_0 > 0$ in (3.13) in order to allocate all our N atoms into a quantum state. We thus derived the

Critical temperature for Bose-Einstein condensation in a 3D isotropic harmonic trap

$$k_B T_c = \hbar\omega N^{1/3} \zeta(3)^{-1/3} = 0.94 N^{1/3} \hbar\omega \tag{3.14}$$

- depends on the dimension and trap details.
- numerical estimate: $N = 10000, \omega = (2\pi)100\text{Hz} \implies T_c = 97$ nK (nano-Kelvin)

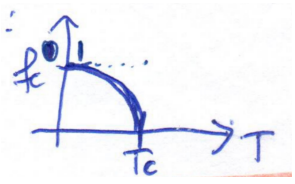
Now let $T < T_c$. From (3.13) $\implies$

$$N = N_0(T) + \sum_{\mathbf{n}\neq(000)} \underbrace{\bar{m}_{\mathbf{n}}}_{\text{as before}} = N_0(T) + \int dn_x dn_y dn_z \frac{1}{\exp[\underbrace{\beta}_{\beta = 1/k_B T \text{ (not } T_c \text{ now)}}(\hbar\omega(n_x+n_y+n_z))] - 1}$$

$$= N_0(T) + \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) = N_0(T) + \left(\frac{k_B T}{k_B T_c}\right)^3 N \implies$$

Fraction of Bose condensed atoms:

$$f_c = \frac{N_0(T)}{N} = \left[1 - \left(\frac{T}{T_c}\right)^3\right] \tag{3.15}$$

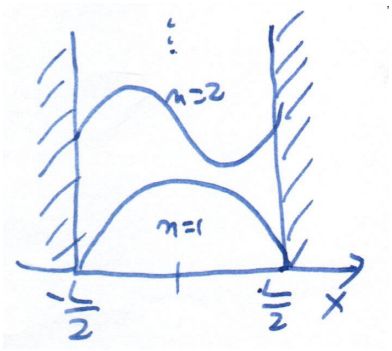


- Bose Einstein condensation has the properties of a second order phase transition.
- Unlike most of those, it does not require interactions (except indirectly, for thermalization).
- At $T = 0$, the system is in the state of $N_0 = N$, with

$$\hat{\rho} = |\, N000...\,\rangle\langle\, N000...\,| \longleftrightarrow |\, \psi_0\,\rangle = |\, \underset{\substack{\downarrow \\ \text{Fock-state with all N atoms in the ground state}}}{N}000...\,\rangle \tag{3.16}$$

3.2.1 De-Broglie Wave overlap

To work out one more aspect of condensation, let us redo the derivation in 3.2 for Bosons in a 3D infinite square (cubic) well (of volume $L^3 = V$).



$$E_{\mathbf{n}} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \qquad\qquad \mathbf{k} = \frac{\mathbf{n}\pi}{L}$$

Using a similar calculations as in 3.2 (bit harder due to $E \sim n^2$) one can show:

$$T_c \approx \frac{\hbar^2}{2m\pi k_b}\left(\frac{N}{2.6V}\right)^{2/3}.$$ Let us define the

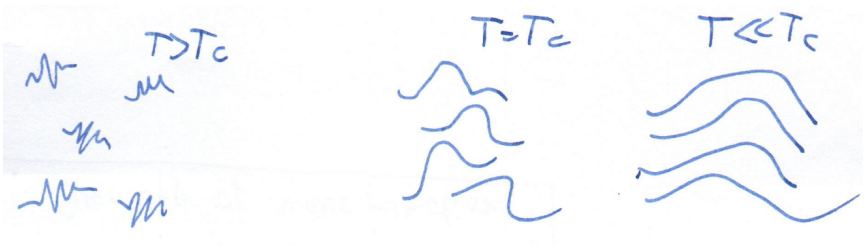
Thermal de-Broglie Wavelength

$$\lambda_T = \frac{\hbar}{\sqrt{mk_BT}}. \tag{3.17}$$

as the wavelength of a particle with kinetic energy $E_{\text{kin}} \approx k_BT$. Mean nearest neighbour distance of randomly distributed atoms at density $\rho = N/V$ is $\bar{d} = \frac{1}{3}\left(\frac{3}{4\pi\rho}\right)^{1/3}\Gamma(1/3) \approx 0.5\rho^{-1/3}$. Thus

$$\lambda_{T_c} = \hbar\sqrt{\frac{1}{mk_B}\left(\frac{2\pi mk_B}{\hbar^2}\left(\frac{2.6V}{N}\right)^{2/3}\right)} = \frac{\sqrt{2\pi(2.6)^{2/3}}}{\rho^{1/3}} \approx 3\rho^{-1/3}$$

Thus around T_c, the atomic de-Broglie waves begin to overlap:



Week 6

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

3.3 Gross-Pitaevskii Equation

- Previously, we considered Bose gases with non-interacting atoms.
- However BEC occurs also if (weak) interactions are present.
- These can be treated very simply for dilute-gas BEC.

3.3.1 Contact Interactions

Consider N interacting Bosons with Hamiltonian (2.16)

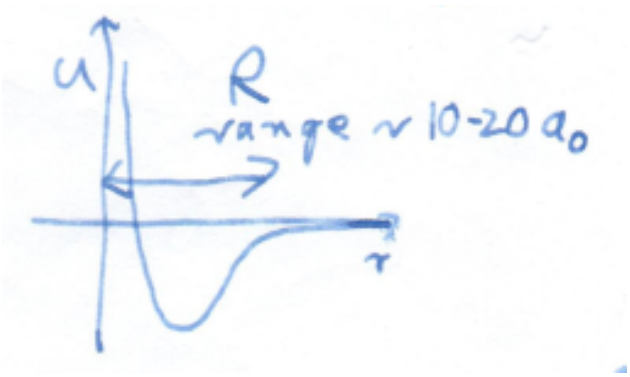
$$\hat{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}_k} + V(\mathbf{x}_k) \right) + \frac{1}{2}\sum_{k,l=1}^{N} U(\mathbf{x}_k - \mathbf{x}_l) \tag{3.18}$$

with $V(\mathbf{x}_k) = \frac{1}{2}m\omega^2\mathbf{x}_k^2$ (*harmonically trapped, e.g. magnetic or optical trap, see PHY402 lecture notes*).

Realistically, atoms interact with a finite range potential

$$U(\mathbf{x}_k - \mathbf{x}_l) = \frac{A}{r^{12}} - \frac{B}{r^6} \qquad r = |\mathbf{x}_k - \mathbf{x}_l|, \tag{3.19}$$

that has an attractive van-der-Waals components ($\sim -r^{-6}$), due to interactions of dipole fluctuations and a repulsive component ($\sim +r^{-12}$) due to electron overlapp. This is called Lennard-Jones Potential.



left: Sketch of Lennard-Jones Potential. Note the range is of the order $10a_0$ ∼nm.

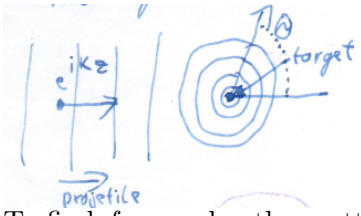
Important fact I: Densities in dilute gas BEC are such that the mean distance d between atoms $d \gg R$, since $d \sim 0.1\mu$m. $\implies$ When interactions take place, they are mostly binary scattering of two atoms, so let us look at that.

We need to consider atomic collisions in quantum scattering theory.

Quantum scattering theory: (*This box is a reminder only. Please read up quantum scattering theory basics in a text book, if required.*) An atom scatters of an target (assumed immobile) at $\mathbf{r} = 0$ with interaction potential $U(r)$. We can write

$$\varphi_k(\mathbf{r}) = e^{ik_i x} + f_k(\theta)\frac{e^{ikr}}{r} \tag{3.20}$$

for the scattering wave function of the particle. This includes that the incoming particle has a known initial momentum $\mathbf{p}_i = \hbar k_i \mathbf{e}_x$ along the x direction, while after the scattering it may go in any direction (with final momentum $\mathbf{p}_f$, with a scattering angle θ while $|\mathbf{p}_i| = |\mathbf{p}_f|$. The amplitude for a certain scattering angle is encoded in $f_k(\theta)$.



left: Schematic of the setup in quantum scattering theory. The x direction goes to the right.

To find f, we solve the scattering TISE, inserting (3.20). $m_r = m/2$ is the reduced mass.

$$(\boldsymbol{\nabla}^2 + k^2)\varphi_k(\mathbf{r}) = \frac{2m_r}{\hbar^2}U(r)\varphi_k(\mathbf{r}). \tag{3.21}$$

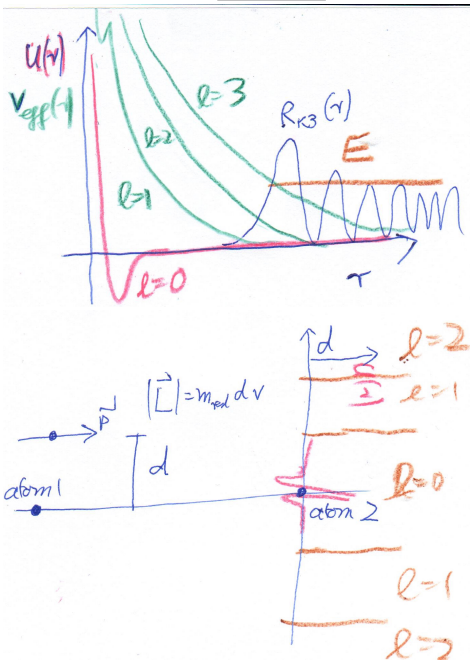
Partial wave expansion (PWE): (*Also reminder only.*) A useful tool for the solution of Eq. (3.21) in scattering theory is the PWE. Here we expand both, f and the incoming wave in terms of Legendre polynomials in θ.

$$\varphi_k(\mathbf{r}) = \sum_{l=0}^{\infty} A_l P_l(\cos\theta) R_{kl}(r). \tag{3.22}$$

The interpretation of l is that it quantifies the angular momentum wrt. the scattering centre, which depends on the impact parameter, and is conserved in a central potential $V(r)$.
Due to that conservation we can solve (3.21) separately in each angular momentum channel. There the corresponding radial wave function $R_{kl}(r)$ satisfies:

$$R''_{kl}(r) + \frac{2}{r}R'_{kl}(r) + \left[k^2 \underbrace{- \frac{l(l+1)}{r^2} - \frac{2m_r}{\hbar^2}U(r)}_{\equiv -\frac{2m_r}{\hbar^2}U_{\text{eff}}(r)}\right] R_{kl}(r) = 0. \tag{3.23}$$

s-wave scattering: As in usual solutions of the TISE, the wavefunction $R(r)$ will not significantly extend into regions where $0 < E < U_{\text{eff}}(r)$ (see below). Thus if the range of the interaction potential $U(r)$ is sufficiently short, higher angular momentum channels will not be affected by it. This means that scattering at very low temperatures can be fully described by $l = 0$, which is called s-wave scattering. Since for $l = 0$, $P_l(\theta) = 1$, in this case the scattering is isotropic.



left: Interaction potential $U(r)$ (magenta), and complete effective potential $U_{\text{eff}}(r)$ for higher l (green). An exemplary incoming partial wave in channel 3 with energy $E = \hbar^2 k^2/(2m_r) > 0$ is also shown.

left: Alternatively think that angular momentum quantisation is dividing the continuous axis of different impact parameters d into regions with discrete angular momentum. If the potential is short ranged, collisions with impact parameter yielding $l > 0$ will not involve it. The lower the velocity, the larger the "l=0" region. **Hence...**

Important fact II: At low temperatures (low scattering velocities) only $l = 0$ (s-wave) will contribute. Since the s-wave component of the PWE $P_0(\cos\theta) = 1$ does not depend on θ, scattering is isotropic (all outgoing directions are equally likely)

s-wave scattering length: To first order perturbation theory (Born approximation), one can show that the scattering amplitude in Eq. (3.20) is given by

$$f_k(\theta) = -\frac{2m_r}{4\pi\hbar^2}\int d^3\mathbf{r}' e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}'}U(\mathbf{r}'), \tag{3.24}$$

that is, $f_k(\theta)$ is related to a Fourier transform of $V(\mathbf{r})$. For very low temperatures, and hence small momenta of the scattering particles, their de-Broglie wavelengths are much longer than the range of the interaction potential. Then $e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}'} \approx 1$ in Eq. (3.25) and we have

$$f = -\frac{2m_r}{4\pi\hbar^2}\int d^3\mathbf{r}' U(r') \equiv a_s \tag{3.25}$$

So now f no longer depends on scattering energy/momentum through k nor on angle θ. The quantity a_s is called s-wave scatteing length.

Important fact III: At very low temperatures for dilute gases, a single number, the s-wave scatteing length contains all the information about the scattering.

Together, the three "important facts" above allow the use of the

Contact interaction potential. (chosen to give same s-wave scattering as (3.19))

$$U(\mathbf{x}_k - \mathbf{x}_l) \implies U_0 \delta(\mathbf{x}_k - \mathbf{x}_l) \tag{3.26}$$

with $U_0 = \frac{4\pi\hbar^2 a_s}{m}$

- a_s is the s-wave scattering length, that quantifies the amplitude of the scattering process (or total cross-section).
- sign of a_s tells if interactions are repulsive ($a_s > 0$) or attractive ($a_s < 0$).
- Exercise: Show that (3.26) indeed gives the same scattering amplitudes as (3.19) when inserted into (3.25).

3.3.2 Condensate Wave function

Let us assume something like Eq. (3.16) [$|\,\psi_0\,\rangle = |\,N000...\,\rangle$] holds even in the interacting case. Thus again all Bosons shall be in the same state $\implies$

Ansatz for many-body wave-function (N Bosons, 1D)

$$\psi(\mathbf{x}, t) = \prod_{l=1}^{N} \phi(x_l, t) \tag{3.27}$$

$$\text{with} \quad \int_{-\infty}^{\infty} |\phi(x,t)|^2 dx = 1 \tag{3.28}$$

Unlike in the non-interacting case, ϕ may not be the trap ground-state, and we now want to find which state it is.

Determine $\phi(\mathbf{x}, t)$ from $\hat{H}$ in Eq. (2.16) with potential (3.26) using the time-dependent variational principle: $\delta S = 0$, with

Action S:

$$S = \int dt d^N x \underbrace{\frac{i\hbar}{2}[\psi^*(\mathbf{x},t)\frac{\partial}{\partial t}\psi(\mathbf{x},t) - \psi(\mathbf{x},t)\frac{\partial}{\partial t}\psi^*(\mathbf{x},t)] - \psi^*(\mathbf{x},t)\hat{H}\psi(\mathbf{x},t)]}_{\text{Lagrangian density}} \tag{3.29}$$

- To test this we could show that it gives the correct many-Body SE upon variation of ψ.
- Variational principle allows us to "enforce" the guess (3.27) and then ask "what equation does $\phi(\mathbf{x},t)$ have to follow if this is true?"

Note:

$$\frac{\partial}{\partial t}\psi(\mathbf{x},t) \overset{(3.27)}{=} [\sum_{k=1}^{N}\frac{\partial}{\partial t}\phi(x_k,t)] \prod_{\substack{l=1\\l\neq k}}^{N}\phi(x_l,t) \tag{3.30}$$

Let us insert (3.27) into (3.29) and simplify

$$\begin{aligned} S \overset{(3.30)}{=} \int dt d^N\mathbf{x} \quad & [\frac{i\hbar}{2}[\prod_{l'=1}^{N}\phi^*(x_{l'},t)\sum_{k=1}^{N}\prod_{\substack{l=1\\l\neq k}}^{N}\phi(x_l,t)\frac{\partial}{\partial t}\phi(x_k,t) - \prod_{l'=1}^{N}\phi(x_{l'},t')\sum_{k=1}^{N}\prod_{\substack{l=1\\l\neq k}}^{N}\phi^*(x_l,t)\frac{\partial}{\partial t}\phi^*(x_k,t)] \\ & - \prod_{l'=1}^{N}\phi^*(x_{l'},t')[\sum_{k=1}^{N}\hat{H}_0(x_k) + \frac{1}{2}\sum_{\substack{k,m=1\\k\neq m}}^{N}U_0\delta(x_k-x_m)]\prod_{l=1}^{N}\phi(x_l,t)] \end{aligned} \tag{3.31}$$

We have to integrate $\int d^N x = \int dx_1 \int dx_2 .... \int dx_i ..... \int dx_N$. All integrals with $x_i \neq (x_k \text{ or } x_m)$ give $\int |\phi(x_i,t)|^2 dx_i = 1 \implies$

$$\begin{aligned} S = & \sum_{k=1}^{N}\int dt \int dx_k \quad [\frac{i\hbar}{2}[\phi^*(x_k,t)\frac{\partial}{\partial t}\phi(x_k,t) - \phi(x_k,t)\frac{\partial}{\partial t}\phi^*(x_k,t)] \\ & - \phi^*(x_k,t)\hat{H}_0(x_k)\phi(x_k,t) + \underbrace{\frac{U_0}{2}\sum_{\substack{m=1\\k\neq m}}^{N}\int dx_m \quad \phi^*(x_k,t)\phi^*(x_m,t)\delta(x_k-x_m)\phi(x_k,t)\phi(x_m,t)}_{=\frac{U_0(N-1)}{2}\phi^*(x_k,t)^2\phi(x_k,t)^2}] \end{aligned} \tag{3.32}$$

Note all pieces of the sum $\sum_{k=1}^{N}$ are the same:

$$\begin{aligned} S = & N\int dt \int dx \quad [\frac{i\hbar}{2}[\phi^*(x,t)\frac{\partial}{\partial t}\phi(x,t) - \phi(x,t)\frac{\partial}{\partial t}\phi^*(x,t)] \\ & - \phi^*(x,t)\hat{H}_0\phi(x,t) + \frac{U_0(N-1)}{2}\phi^*(x,t)^2\phi(x,t)^2] \end{aligned} \tag{3.33}$$

Variation of S:

$$\delta S = S[\phi+\delta\phi,\phi^*] + S[\phi,\phi^*+\delta\phi^*] - 2S[\phi,\phi^*] \tag{3.34}$$

(We treat ϕ and ϕ^* as independent). Demand

$$\begin{aligned} 0 \quad = \quad \delta S \quad = \quad N \int dt \int dx \quad & \frac{i\hbar}{2}[\delta\phi^* \frac{\partial}{\partial t}\phi + \phi^* \frac{\partial}{\partial t}\delta\phi - \delta\phi \frac{\partial}{\partial t}\phi^* - \phi \frac{\partial}{\partial t}\delta\phi^* \\ & - \delta\phi^*[H_0\phi + U_0(N-1)\phi^*\phi^2] - [\phi^* H_0 \delta\phi + U_0(N-1)\phi^{*2}\phi\delta\phi]] \end{aligned} \tag{3.35}$$

Now this should be zero for **all** small functions $\delta\phi(x,t) \implies$
coefficient of $\delta\phi(x,t)$ and $\delta\phi^*(x,t)$ must vanish inside the integral $\forall x, t$. From coefficient of $\delta\phi^*(x,t)$ we finally obtain the

time-dependent Gross-Pitaevskii Equation (GPE)

$$i\hbar\frac{\partial}{\partial t}\phi(x,t) = \Big(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)}_{=\hat{H}_0(x)} + U_0(N-1)|\phi(x,t)|^2\Big)\phi(x,t). \tag{3.36}$$

- $\phi(x,t)$ is the condensate wave function. Here $(\int_{-\infty}^{\infty}|\phi(x,t)|^2 dx = 1)$
- $U_0 = \frac{4\pi\hbar^2 a_s}{m}$ from (3.26).
- This is similar to single-particle Schrödinger equation but with a term that is non-linear in the wave function. This completely changes the mathematics and solutions to do with this equation.
- $(N-1)|\phi(x,t)|^2 = \rho =$ atom density. This makes sense, since the non-linear term describes interactions, and the interaction energy for one atom should be dependent on the density of other atoms.

3.3.3 Mean Field Theory

We can derive (3.36) differently (and much easier), starting from quantum field theory. Consider $\hat{H}$ in (2.27) with $U(\mathbf{x}-\mathbf{y})$ from (3.26), thus

$$\hat{H} = \int dx \left[\hat{\psi}^\dagger(x) H_0 \hat{\Psi}(x) + \frac{U_0}{2}\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x)\right] \tag{3.37}$$

Consider the field operator in Heisenberg picture $\hat{\Psi}(x,t)$, which must fulfill the

Heisenberg equation for the field operator

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(x,t) = [\hat{\Psi}(x,t), \hat{H}] = \hat{H}_0\hat{\Psi}(x,t) + U_0\hat{\Psi}^\dagger(x,t)\hat{\Psi}(x,t).\hat{\Psi}(x,t) \tag{3.38}$$

We ought to specify an (initial) quantum state, but let's not, rather we make the :

Mean-Field Ansatz

$$\langle\hat{\Psi}(x,t)\rangle = \tilde{\phi}(x,t) \tag{3.39}$$

- $\tilde{\phi}$ is again the condensate wave-function [4] or order parameter of the BEC.

Taking the expectation value of (3.38) we reach

$$i\hbar\frac{\partial}{\partial t}\tilde{\phi}(x,t) = \hat{H}_0\tilde{\phi}(x,t) + U_0 \underbrace{\langle\hat{\Psi}^\dagger(x,t)\hat{\Psi}(x,t)\hat{\Psi}(x,t)\rangle}_{\text{factorisation: } \langle\hat{\Psi}^\dagger(x,t)\rangle\langle\hat{\Psi}(x,t)\rangle\langle\hat{\Psi}(x,t)\rangle} \tag{3.40}$$

We now assume the factorization as shown and reach:

Gross-Pitaevskii Equation (again)

$$i\hbar\dot{\tilde{\phi}}(x,t) = \hat{H}_0(x)\tilde{\phi}(x,t) + U_0|\tilde{\phi}(x,t)|^2\tilde{\phi}(x,t) \tag{3.41}$$

- Same as (3.36) for $N \approx N-1$.
- A possible quantum-state that justifies (3.3.3) is the many-body coherent state (2.51). We assume the S.H.O single-particle basis and $|\,\psi\,\rangle = |\,\alpha_0,\alpha_1,.....\,\rangle$ (see (2.51)) Thus

$$\begin{aligned}\underset{\text{state}}{\langle\psi} \;\Big|\; \underset{\text{field op.}}{\hat{\Psi}} \;\Big|\; \underset{\text{state}}{\psi\rangle} &= \langle\alpha_0,\alpha_1,.....|\sum_{k=1}^{\infty}\varphi_k(x)\hat{a}_k|\alpha_0,\alpha_1,.....\rangle \\ &= \langle\alpha_0,\alpha_1,.....|\sum_{k=1}^{\infty}\varphi_k(x)\alpha_k|\alpha_0,\alpha_1,.....\rangle \\ &= \sum_{k=1}^{\infty}\varphi_k(x)\alpha_k \equiv \tilde{\phi}(x,t=0) \in \mathbb{C}\end{aligned} \tag{3.42}$$

- Due to the use of coherent states, we have an uncertainty in the particle number here ($\approx$ N in the mean).
- $\langle\frac{\partial}{\partial t}\hat{\Psi}\rangle = \frac{\partial}{\partial t}\langle\hat{\Psi}\rangle$ since in Heisenberg picture state is time-independent.

[4] Here $\int_{-\infty}^{\infty}|\tilde{\phi}(x,t)|^2dx = N$, in contrast to the normalisation used for (3.36). We try to distinguish the two conventions with the ˜ symbol.

•

$$\langle \hat{H}_0(x)\hat{\Psi}\rangle = \underset{\substack{\downarrow \\ \text{many body fock state}}}{\langle\psi|}\hat{H}_0(x)\sum_n \varphi_n(x)\hat{a}_n|\psi\rangle = \hat{H}_0(x)\sum_n \varphi_n(x)\langle\psi|\hat{a}_n|\psi\rangle$$
$$= \hat{H}_0(x)\underbrace{\langle\psi|\sum_n \varphi_n(x)\hat{a}_n|\psi\rangle}_{=\langle\hat{\Psi}\rangle} = \hat{H}_0(x)\tilde{\phi}(x) \tag{3.43}$$

- For coherent state $|\,\psi\,\rangle = |\,\alpha_0, \alpha_1, \cdots\rangle$ we have $\langle\alpha_0, \alpha_1, \cdots|\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}|\alpha_0, \alpha_1, \cdots\rangle = \langle\hat{\Psi}^\dagger\rangle\langle\hat{\Psi}\rangle\langle\hat{\Psi}\rangle$ (exercise), thus the coherent state would also justify the factorization used in (3.40).

Counter-example where factorization does not work: (just <u>math</u> example)

$$|\,\psi\,\rangle = \frac{1}{\sqrt{2}}(|\,300...\,\rangle + |\,200...\,\rangle) \implies \langle\psi|\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x)|\psi\rangle \underset{\substack{\downarrow \\ \text{all other terms of } \sum_{k=1}^{\infty}\varphi_k(x)a_k^\dagger \text{ vanish}}}{=} \frac{1}{2}\langle\psi||\varphi_0(x)|^2\varphi_0(x)\hat{a}_0^\dagger\hat{a}_0\hat{a}_0|\psi\rangle$$
$$= \frac{1}{2}|\varphi_0(x)|^2\varphi_0(x)(\langle 300| + \langle 200|)(2\sqrt{3}|200\rangle + \sqrt{2}|100\rangle) = \sqrt{3}|\varphi_0(x)|^2\varphi_0(x) \text{ But:}$$
$$\langle\psi\rangle = \frac{\varphi_0(x)}{2}(\langle 300|+\langle 200|)(\sqrt{3}|200\rangle+\sqrt{2}|100\rangle) = \frac{\sqrt{3}}{2}\varphi_0(x) \implies \langle\hat{\Psi}^\dagger\rangle\langle\hat{\Psi}\rangle\langle\hat{\Psi}\rangle = \frac{3\sqrt{3}}{8}|\varphi_0(x)|^2\varphi_0(x)$$

3.3.4 Condensate Ground State

Stationary states of (3.3.3) evolve as

$$\tilde{\phi}(x,t) = \exp\left[\frac{-i\mu t}{\hbar}\right]\tilde{\phi}_0(x). \tag{3.44}$$

Inserting this into (3.3.3) gives a

<u>Time-independent GPE</u>

$$\mu\phi_0(x) = \left[\hat{H}_0(x) + U_0|\phi_0(x)|^2\right]\phi_0(x) \tag{3.45}$$

- We renamed $\tilde{\phi}_0 \longrightarrow \phi_0$ but still $\int_{-\infty}^{\infty}|\phi_0(x)|^2dx = N$.
- μ is the chemical potential if ϕ_0 is the ground state.
- Same as for the TISE, also Eq. (3.45) has multiple (excited state) solutions.

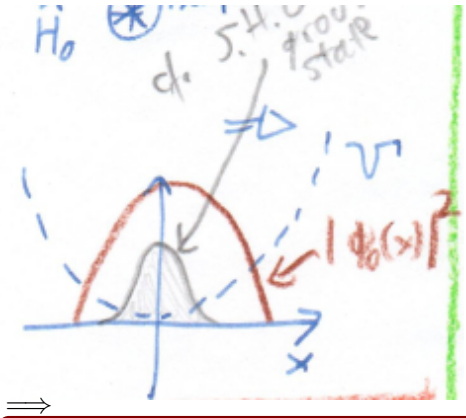
Ground State Solutions:

Example (i):

Very strong repulsive interactions $U_0 \gg \underbrace{\hbar\omega}_{trap} > 0$. In that case, neglect $-\frac{\hbar^2}{2m}\nabla^2$ in $\hat{H}_0$.

$$\mu\phi_0(x) = V(x)\phi_0(x) + U_0|\phi_0(x)|^2\phi_0(x)$$

$$|\phi_0(x)|^2 = \begin{cases} \frac{\mu - V}{U_0} & \text{if} > 0 \\ 0 & \text{else} \end{cases}$$



left: In a harmonic trap (blue dashed), non-interacting atoms condense into the SHO ground state (grey shape). Due to interactions, atoms instead settle into the Thomas-Fermi shape (brown line).

$\Longrightarrow$

Wave-function in Thomas-Fermi Approximation

$$\phi_0(x) = \begin{cases} \sqrt{\frac{\mu - V}{U_0}} & \text{if}(\mu - V) > 0 \\ 0 & \text{else} \end{cases} \tag{3.46}$$

• Why do we neglect $\frac{-\hbar^2}{2m}\nabla^2$ and not the trap? We see that both, the repulsive interaction $U_0|\phi_0(x)|^2$ for $U_0 > 0$ and the kinetic energy cause a spread of the wave-function. In contrast, the trap V causes localization. The final shape is determined by a balance of spread versus localization. For $U_0 n > \frac{\hbar\omega}{2}$ the kinetic energy can be neglected relative to the interaction energy.

↓

Approximate K.E. in GS oscillator

Example (ii): Very weak interactions $|U_0| \ll \hbar\omega$.

For $U_0 = 0$, we know harmonic oscillator ground state φ_0 solves (**??**). So,

Ansatz :

$$\phi_0(x) = N\exp\left[-\frac{x^2}{2\sigma(U_0)^2}\right] \tag{3.47}$$

Determine $\sigma(U_0)$ from variational principle $\delta E = 0$ using

$E = \int dx \quad \phi_0^*(x)[\hat{H}_0 + U_0(|\phi_0(x)|)^2]\phi_0(x)$ (Pethick-Smith (Exercise))

Example (iii): Any other interaction strength: We can use the imaginary time method, where we solve (3.3.3) for t $\longrightarrow -i\tau$

Imaginary Time GPE

$$-\hbar\frac{\partial}{\partial\tau}\tilde{\phi}(x,\tau) = \left[\hat{H}_0(x) + U_0|\tilde{\phi}(x,\tau)|^2\right]\tilde{\phi}(x,\tau) \tag{3.48}$$

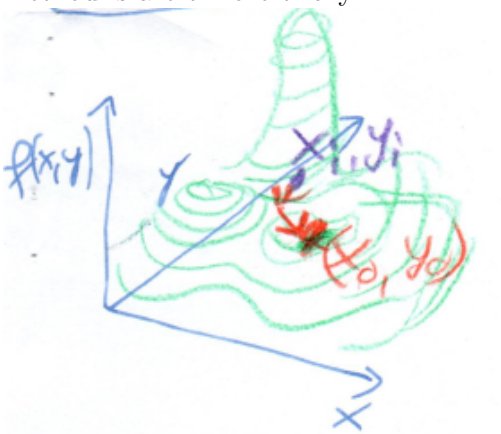
subject to constraint $\int_{-\infty}^{\infty}|\tilde{\phi}(x,\tau)|^2dx \stackrel{!}{=} N$

This typically rapidly converges to the lowest energy solutions $\phi_0(x)$ of (**??**), (almost) regardless of initial state.

heuristic motivation:

Take the (linear) Schrödinger equation ($U_0 = 0$). Then $\psi(x,t) = \sum_n c_n(0)e^{\frac{-iE_nt}{\hbar}}\phi_n(x)$ Replace $t \longrightarrow -i\tau \implies \psi(x,\tau) = \sum_n c_n(0)e^{\frac{-E_n\tau}{\hbar}}\phi_n(x)$ $\psi(x,\tau) \longrightarrow 0$ for $\tau \longrightarrow \infty$ since all components exponentially decay. But among all of them, the groundstate component ($n = 0$) decays the slowest. $\implies$ If we enforce $\int_{-\infty}^{\infty}|\psi|^2dx = 1$, the ground-state eventually becomes the only one to survive, so the scheme converges to the groundstate.

BONUS TEXT: In the presence of interactions $U_0 > 0$, the justification for the imaginary time method is a bit more tricky:



left: Let $f(x,y)$ be a 2D function. To find the minimum value and its location $f_0(x_0,y_0)$, go opposite to the gradient (along red arrow in figure) from some initial test-point (x_i,y_i). TThis is called the steepest descent method in optimization.

Now consider the GP energy functional

$$E = \int d^3x \quad \phi^*(x)\left[\hat{H}_0(x) + \frac{U_0}{2}|\phi_0(x)|^2\right]\phi_0(x$$

as ∞-dimensional function, using the identification $f \longrightarrow E$, $(x,y) \longrightarrow \phi(x)$.

The analog of $\frac{\partial f}{\partial x}$ is $\frac{\delta E}{\delta\phi(x)}$ (functional derivative). Let us consider ϕ, ϕ^* as independent.

$$\frac{\delta E}{\delta\phi^*(x)} = \left[H_0(x) + \frac{U_0}{2}|\phi_0(x)|^2\right]\phi_0(x)$$

Thus going for a short step $\frac{\delta\tau}{\hbar}$ into direction of negative gradient.

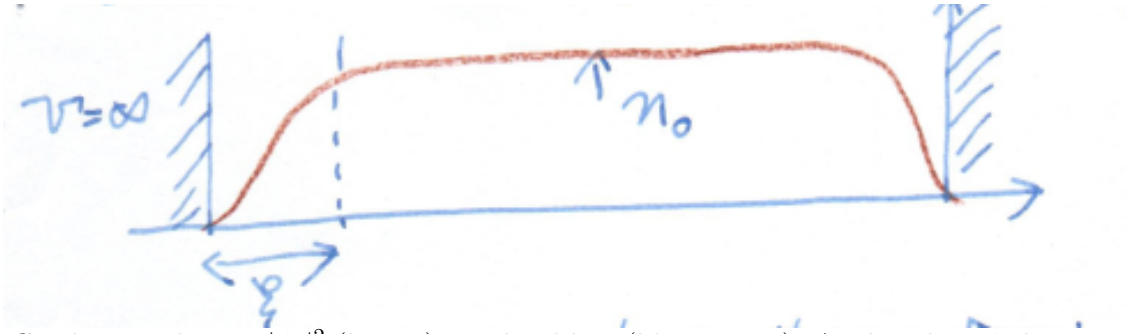
$$\phi(x,\tau+\delta\tau) - \phi(x,\tau) = -[H_0 + U_0|\phi_0(x)|^2]\phi_0(x)$$

$$\phi(x,\tau+\delta\tau)-\phi(x,\tau)=-[H_0+U_0|\phi_0(x,\tau)|^2]\phi_0(x,\tau)$$

$\Longrightarrow$ which is a discrete time-derivative version of Eq. (3.48).

3.3.5 Condensate Healing Length

Consider a condensate in a hard box, for large U_0.



top: Condensate density $|\phi_0|^2$ (brown) in a hard box (blue stripes). At the edges ϕ_0 has to vanish due to boundary conditions.

- Far away from the edges, the Thomas-Fermi approximation (3.46) gives us a density

$$n_0=\frac{\mu}{U_0} \tag{3.49}$$

- Near the edge however, we can not neglect kinetic term. Rewrite (3.45) as

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_0(x)+U_0[(\phi_0(x))^2-n_0]\phi_0(x)=0$$

  Define $\phi_0(x)=\sqrt{n_0}f(\frac{x}{\zeta})$ $\Longrightarrow$

$$\frac{-\hbar^2}{2mU_0n_0\zeta^2}f''(\frac{x}{\zeta})+[f^2-1]f=0 \tag{3.50}$$

  This equation becomes scale-free if we set

Healing Length

$$\zeta=\frac{\hbar}{\sqrt{2mU_0n_0}} \tag{3.51}$$

- This is the shortest scale on which the BEC can respond to perturbations in the bulk.

3.3.6 Hydrodynamic equations and vortices

Let us rewrite the condensate wave function as

$$\phi(x,t) = \underbrace{\sqrt{\rho(x,t)}}_{amplitude} e^{\underbrace{i\varphi(x,t)}_{phase}} \qquad \phi \in \mathbb{C}, \quad \rho, \varphi \in \mathbb{R}. \tag{3.52}$$

The ρ, φ have the interpretation of

Hydrodynamic variables

$$\underline{\text{atomic density}} \quad \rho = |\phi|^2 \tag{3.53}$$

$$\text{and } \underline{\text{flow velocity}} \quad \mathbf{v} = \frac{\hbar}{m}\boldsymbol{\nabla}\varphi$$

To see that this makes sense we insert (3.52) into (3.3.3) split into real- and imaginary parts and thus derive the

Hydrodynamic equations for a BEC

$$\text{Continuity equation} \quad \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \cdot \mathbf{v}) \tag{3.54}$$

$$\text{“Bernoulli's eqn”} \quad m\frac{d\mathbf{v}}{dt} = -\boldsymbol{\nabla}[P_q + \frac{1}{2}m\mathbf{v}^2 + U\rho + V(x)] \tag{3.55}$$

$$\text{with } \underline{\text{quantum pressure term}} \quad P_q = -\frac{\hbar^2\boldsymbol{\nabla}^2\sqrt{\rho}}{2m\sqrt{\rho}} \tag{3.56}$$

- Whenever P_q is small, we can think of the BEC as a “fluid”.
- quantum nature still has interesting consequence such as

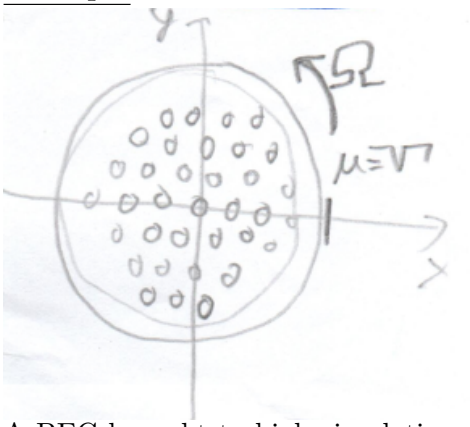
Quantisation of circulation

$$\underbrace{\oint_C}_{\underline{\text{circulation}}} \mathbf{v} \cdot d\mathbf{x} = (2\pi n)\frac{\hbar}{m} = n(\underbrace{\frac{h}{m}}_{\text{circulation quantum}}) \tag{3.57}$$

Here $n \in \mathbb{N}_0$ is called the Winding number.

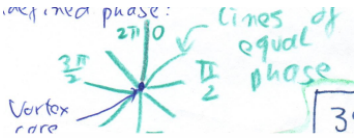
- Proof : show that $\int_L \mathbf{v} \cdot d\mathbf{x} = \frac{\hbar}{m}[\varphi(\mathbf{b}) - \varphi(\mathbf{a})]$ for a non-closed loop between two points $\mathbf{a}$ and $\mathbf{b}$. Then (3.57) follows because the phase at $\mathbf{x}$ has to be unique $\Longrightarrow$

Example: **Abrikosov-lattice of Vortices** :



left: Abrikosov-lattice of vortices (circles). Ω indicates and externally enforced rotation of the BEC cloud.

A BEC brought to high circulation state $n \ggg 1$ forms an Abrikosov-lattice of n vortices, each vortex-core has zero density $\rho = 0$ due to the undefined phase at that point:



left: vortex core

3.3.7 Condensate excitations

What happens to a stationary state (3.44) if it is slightly perturbed? Let us look for periodic (eigenmode) solutions with Ansatz :

Perturbed BEC

$$\phi(x,t) = e^{-\frac{i\mu t}{\hbar}}[\phi_0(x) + u(x)e^{-i\omega t} - v^*(x)e^{i\omega t}] \tag{3.58}$$

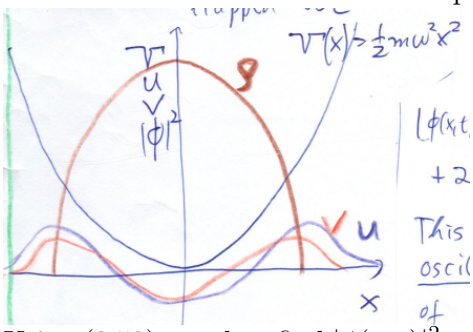
- Be careful: In this section v has nothing to do with velocity.
- We need to include $e^{i\omega t}$ AND $e^{-i\omega t}$ because (3.3.3) couples ϕ with ϕ^*.
- Insert (3.58) into (3.3.3), use (3.45) then seperately consider coefficients of $e^{i\omega t}$ and $e^{-i\omega t}$ to get the

Bogoliubov equations for elementary excitations of BEC

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(x) + 2U_0|\phi_0(x)|^2 - \mu - \hbar\omega\right] u(x) - U_0\phi_0(x)^2 v(x) = 0,$$
$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(x) + 2u_0|\phi_0(x)|^2 - \mu + \hbar\omega\right] v(x) - U_0\phi_0^*(x)^2 u(x) = 0. \tag{3.59}$$

Here ω is the mode frequency.

Example: Breathing mode of harmonically trapped BEC. Assume a BEC in a harmonic trap has the Thomas-Fermi shape for $\rho(x) = |\phi_0(x)|^2$ in (3.46) (brown). Solving (3.59), you would then find one mode with shapes u (blue), v (red) $\in \mathbb{R}$ as shown below.



left: Breathing mode of a trapped BEC

Using (3.58), we then find $|\phi(x,t)|^2 \approx |\phi_0(x)|^2 + 2\phi_0(u-v)\cos(\omega t) + \mathcal{O}(u^2, v^2)$ This represents breathing oscillations that arise from a competition of trapping and repulsive interactions. It turns out we find a breathing frequency (for large U_0) of $\omega = \sqrt{5}\omega_{\text{trap}}$.

Week 7

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

3.4 Quasiparticles/quantized excitations

In section 3.3 we had assumed the gas is fully condensed and thus effectively replaced $\underbrace{\hat{\psi}(\mathbf{x})}_{\text{operator}} \rightarrow \underbrace{\phi(\mathbf{x})}_{\text{complex function}}$, completely.

Let us now retain some possibly non-condensed atoms, by writing the

Field operator with fluctuations (c.f. Eq. (3.58))

$$\hat{\psi}(\mathbf{x}) = \phi_0(\mathbf{x}) + \underbrace{\sum_n u_n(\mathbf{x})\hat{\alpha}_n - v_n^*(\mathbf{x})\hat{\alpha}_n^\dagger}_{\hat{\chi}(\mathbf{x})} \tag{3.60}$$

In this expression:

$\hat{\psi}$	Bose atomic field operator
$\langle\hat{\psi}\rangle = \phi_0$	(still) condenstate mean field
$u_n(\mathbf{x}), v_n(\mathbf{x})$	Bogoliubov mode function
$\hat{\alpha}_n, \hat{\alpha}_n^\dagger$	Bogoliubov creation and destruction operators (Bosonic)
$\hat{\chi}(\mathbf{x})$	fluctuation operator, assumed small ($\mathcal{O}(\hat{\chi}^3) = 0$)

We now insert (3.60) into Hamiltonian (3.37) and choose u_n, v_n such that the Hamiltonian is diagonalized.

Diagonalized: in terms of Fock states for Bogoliubov operators means it takes the form

$$\hat{H} \approx \sum_n \varepsilon_n \hat{\alpha}_n^\dagger \hat{\alpha}_n$$

This is achieved when u_n and v_n fulfill the

Bogoliubov-de-Gennes (BdG) equations

$$\begin{aligned}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{x}) + 2U_0|\phi_0(\mathbf{x})|^2 - \mu - \hbar\omega_n\right] u_n(\mathbf{x}) - U_0\phi_0(\mathbf{x})^2 v_n(\mathbf{x}) = 0 \\ \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{x}) + 2U_0|\phi_0(\mathbf{x})|^2 - \mu + \hbar\omega_n\right] v_n(\mathbf{x}) - U_0\phi_0^*(\mathbf{x})^2 u_n(\mathbf{x}) = 0\end{aligned} \tag{3.61}$$

and

Orthonormality conditions

$$\begin{aligned}&\int d^3x \phi_0^*(\mathbf{x}) u_n(\mathbf{x}) = \int d^3x \phi_0^*(\mathbf{x}) v_n^*(\mathbf{x}) = 0 \quad \text{(modes are orthogonal to condensate)} \\ &\int d^3x \left[u_n(\mathbf{x}) u_m^*(\mathbf{x}) - v_n(\mathbf{x}) v_m^*(\mathbf{x})\right] = \delta_{mn} \\ &\int d^3x \left[u_n(\mathbf{x}) v_m(\mathbf{x}) - v_n(\mathbf{x}) u_m(\mathbf{x})\right] = 0\end{aligned} \tag{3.62}$$

Using (3.61) the Hamiltonian takes the form of a

Quasi-particle Hamiltonian

$$\hat{H} = E[\phi] + \sum_n (\mu + \hbar\omega_n)\hat{\alpha}_n^\dagger \hat{\alpha}_n \tag{3.63}$$

where we used the

$$E[\phi] = \int d^3x \ \phi^*(\mathbf{x}) \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla} + V(\mathbf{x}) + U_0|\phi(\mathbf{x})|^2 \phi(\mathbf{x})\right] \tag{3.64}$$

Gross-Pitaevskii energy functional

- Eq. (3.63) takes the form of a Hamiltonian for non-interacting entities created by $\hat{\alpha}_n^\dagger$.
- For that reason $\hat{\alpha}_n, \hat{\alpha}_n^\dagger$ are called quasi-particle operators.
- Eq. (3.61) takes the same form as Eq. (3.59), which we got starting with a seemingly quite different question. We will comment on this later.
- Eq. (3.62) ensure that the quasi-particles are Bosons:

$$\begin{aligned}\left[\hat{\alpha}_n, \hat{\alpha}_m^\dagger\right] &= \int d^3\mathbf{x} \int d^3\mathbf{y} \left(u_n^*(\mathbf{x}) u_m(\mathbf{y}) \left[\hat{\Psi}(\mathbf{x}), \hat{\Psi}^\dagger(\mathbf{y})\right] + v_n^*(\mathbf{x}) v_m(\mathbf{y}) \left[\hat{\Psi}^\dagger(\mathbf{x}), \hat{\Psi}(\mathbf{y})\right] \right) \\ &= \int d^3\mathbf{x} \left(u_n^*(\mathbf{x}) u_m(\mathbf{x}) - v_n^*(\mathbf{x}) v_m(\mathbf{x}) \right) \overset{Eq.\ (3.62)}{=} \delta_{nm}.\end{aligned} \tag{3.65}$$

- Using (3.62), we can "invert" (3.60) [exercise] to find

$$\begin{aligned}\hat{\alpha}_n &= \int dx \left[u_m^*(\mathbf{x})\hat{\psi}(\mathbf{x}) + v_m^*(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\right] \\ \hat{\alpha}_n^\dagger &= \int dx \left[u_m(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}) + v_m(\mathbf{x})\hat{\psi}(\mathbf{x})\right]\end{aligned} \tag{3.66}$$

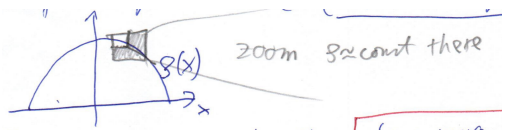
  Hence we also call

$$\begin{aligned}u_m(\mathbf{x}) &- \text{particle amplitude} \\ v_m(\mathbf{x}) &- \text{hole amplitude}\end{aligned}$$

  $\implies$ A BdG excitation is a superposition of added & subtracted particles.

3.4.1 Phonons

Let us proceed to solve the BdG equations (3.61) for the simple case of a homogenous, constant condensate $\implies \phi_0(\mathbf{x}) = \underbrace{\sqrt{\rho}}_{\text{(indep of x)}}$; $\rho =$ atom density.



left: This can be realistic when concentrating on a small piece of a large BEC cloud. This would be called the local density approximation (LDA).

For this case, we make the

Plane-wave Ansatz

$$u_q(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\bar{u}_q e^{iqx} \qquad v_q(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\bar{v}_q e^{iqx} \tag{3.67}$$

- $\mathcal{V}$ is the quantisation volume
- q - wave number
- $\bar{u}_q$, $\bar{v}_q$ - are amplitudes, these are just complex numbers

Insert (3.67) into (3.61) and use $-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 u_q(\mathbf{x}) = \underbrace{\frac{\hbar^2 q^2}{2m}}_{\equiv E_q} u_q(\mathbf{x})$ etc., we can find the matrix equation

$$\underbrace{\begin{pmatrix} E_q + 2U_0\rho - \mu - \hbar\omega_q & -U_0\rho \\ -U_0\rho & E_q + 2U_0\rho - \mu + \hbar\omega_q \end{pmatrix}}_{\equiv M} \begin{pmatrix} \bar{u}_q \\ \bar{v}_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.68}$$

For this to have any non-trivial solution, we need $\det(M) = 0$, hence

$$\det(M) = -(\hbar\omega_q)^2 + (E_q + 2U_0\rho - \mu)^2 - U_0^2\rho^2 = 0. \tag{3.69}$$

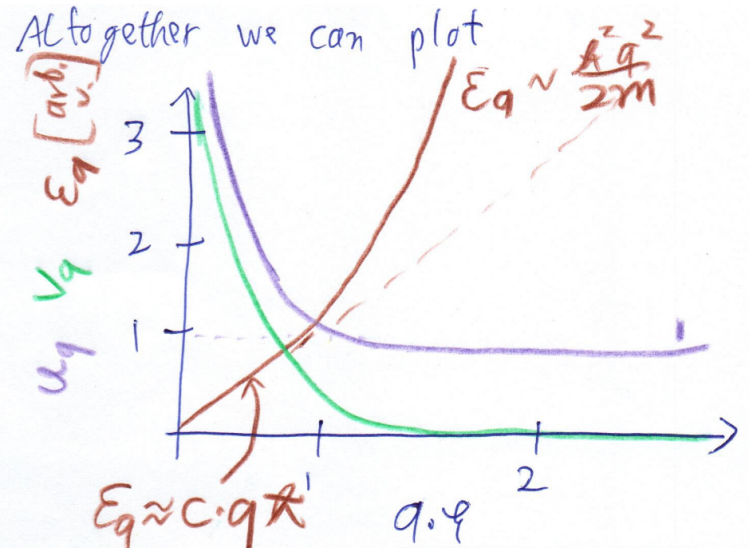
For a homogeneous condensate we know that $\mu = U_0\rho$, which follows from Eq. (3.45). Using that, we find for the excitations of the condensate the

Bogoliubov dispersion relation

$$\varepsilon_q \equiv \hbar\omega_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + 2U_0\rho\right)} \tag{3.70}$$

Using (3.62), (3.68) and (3.70) we can show, after defining the abbreviation $\zeta_q \equiv E_q + U_0\rho$, that

$$\bar{u}_q^2 = \frac{1}{2}\left(\frac{\zeta_q}{\varepsilon_q} + 1\right), \quad \bar{v}_q^2 = \frac{1}{2}\left(\frac{\zeta_q}{\varepsilon_q} - 1\right). \tag{3.71}$$



left: Combined plot of Bogoliubov energy ε_q (3.70) (brown), particle amplitude $\bar{u}_q$ (violet) and hole amplitude $\bar{v}_q$ (green) (3.71).

In the figure we have used the definition of the

Speed of sound

$$c = \sqrt{\frac{U_0\rho}{m}} \tag{3.72}$$

Comments about Bogoliubov excitations:

- for $q \ll \xi$, we have $\varepsilon_q \approx cq\hbar$ and $|\bar{u}_q|^2 + |v_q|^2 \gg 1$. $\varepsilon_q \approx cq\hbar$ is a linear dispersion relation as for sound-waves. $|\bar{u}_q|^2 + |v_q|^2 \approx N_{\text{atoms}}$, the number of atoms involved in an exciation (see yellow box * below). So long wavelength excitations with $q \ll \xi$ are collective excitations/ sound-waves.
- for $q \gg \xi$, we can approximate $\varepsilon_q \sim \frac{\hbar^2 q^2}{2m}$, which is the energy of a free particle. Also $|\bar{u}_q|^2 + |v_q|^2 \to 1$. This is a single-atom excitation ($\sim$ 1 atom got kicked so hard, it no longer feels the others).

Number of excited atoms*: Let us consider the number of excited atoms

$$N_{\text{exc}} = \int \langle \hat{\chi}^\dagger \hat{\chi} \rangle dx \quad \text{(see(3.60))}$$

Let $|\,\psi\,\rangle = |\,N_1 N_2 ...\,\rangle$ be the Fock state for occupation of Bogoliubov excitations. $\Longrightarrow$

$$N_{\text{exc}} = \int_V dx \sum_{qq'} \left(u_q^*(\mathbf{x}) u_{q'}(\mathbf{x}) \underbrace{\hat{\alpha}_q^\dagger \hat{\alpha}_{q'}}_{\sim \delta_{qq'} \text{ in state} |\,\psi\,\rangle} + v_q(\mathbf{x}) v_{q'}^*(\mathbf{x}) \underbrace{\hat{\alpha}_q \hat{\alpha}_{q'}^\dagger}_{= \hat{\alpha}_{q'}^\dagger \hat{\alpha}_q + \delta_{qq'}} \right)$$

$$= \sum_q \left(|u_q|^2 + |v_q|^2 \right) N_q + \sum_q |v_q|^2. \tag{3.73}$$

Since N_q here is the number of excitations, this motivates the allocation of $|\bar{u}_q|^2 + |\bar{v}_q|^2$ as "number of atoms within a single excitation".

3.4.2 Time-dependence

The overall time-dependence of the field operator in Eq. (3.60) is

Time-dependence of BdG modes

$$\hat{\psi}(x,t) = e^{-i\frac{\mu}{\hbar}t} \left[\phi_0(\mathbf{x}) + \sum_n u_n(\mathbf{x}) \hat{\alpha}_n e^{-i\omega_n t} - v_n^*(\mathbf{x}) \hat{\alpha}_n^\dagger e^{i\omega_n t} \right] \tag{3.74}$$

- c.f. Eq. (3.58)
- to see this insert (3.60) into $\underset{\text{Heisenberg}}{Eq.\ (3.38)}$ using $\underset{\text{GPE}}{Eq.\ (3.3.3)}$ and $\underset{\text{BdG}}{Eq.\ (3.61)}$

3.4.3 Coherent vs incoherent excitation

We have now addressed two seemingly different questions:

(A) In section 3.3.7: If we slightly perturb the GPE solution $\phi(x,t) = \phi_0(\mathbf{x}) + \delta\phi(x,t)$, how does the perturbation $\delta\phi$ evolve in time?

(B) In section 3.4: In a QFT problem, which fluctuation modes outside the BEC diagonalize the Hamiltonian?

Seemingly different questions give the same BdG equations for condensate excitations, compare (3.59) and (3.61).

The reason is that (A) is included in (B). Consider a single Bogoliubov mode only (say $n = 1$). Assume its quantum state is $|\,\psi\,\rangle = |\,\beta\,\rangle$ where $\beta \in \mathbb{C}$.
$\downarrow$
coherent state

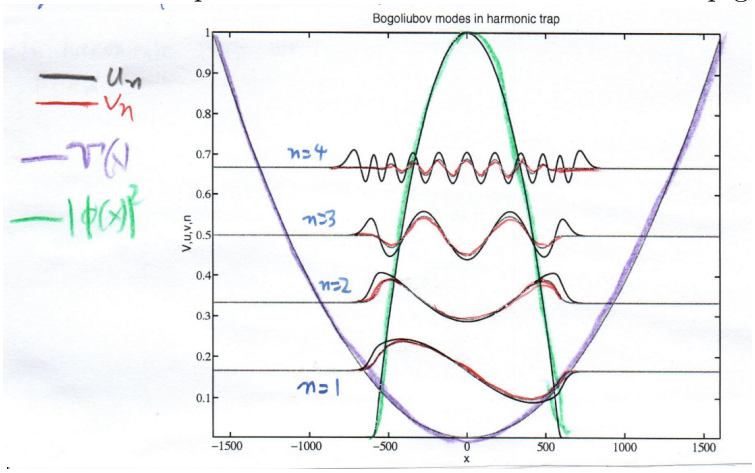
Then

$$\langle\hat{\psi}(x,t)\rangle = e^{-i\frac{\mu}{\hbar}t}\left[\phi_0(\mathbf{x}) + u_1(\mathbf{x})\beta e^{-i\omega_1 t} - v_1^*(\mathbf{x})\beta^* e^{i\omega_1 t}\right]$$
$\downarrow$
Eq. (3.74)

which is a BEC mean field perturbation as in (3.59) (So here the population in mode number one has phase-coherence with the BEC). Had we used $\hat{\rho} = \sum_n p_n |\,n\,\rangle\langle\,n\,|$ for mode one, we keep $\langle\hat{\psi}\rangle = e^{-i\frac{\mu}{\hbar}t}\phi_0(\mathbf{x})$ with no perturbation of the mean field itself, so in that setting the p_n correspond to incoherent thermal population.

3.4.4 The thermal cloud

In general (3.61) has to be solved numerically, but see Pethick & Smith for some analytical approximation techniques. The numerical solution in a 1D trap gives the following:



left: BdG modes in 1D trap (violet) are shown as black lines (u_n) and red lines (v_n). We also show the Thomas-Fermi shape of the condensate (green).

As $n \to \infty$, the modes approach the following

$$u_n \to \varphi_n \quad \text{(S.H.O states, see 1.9)}$$
$$v_n \to 0$$

As for the homogeneous case, we see that high energy BdG modes essentially become like single-particle excitations.

The modes now allow us to describe the "thermal cloud": BEC experiments never reach $T = 0$, hence we write

Thermal cloud state

$$\hat{\rho} = \sum_{\mathbf{N}} P_{\mathbf{N}} |\,\mathbf{N}\,\rangle\langle\,\mathbf{N}\,| \qquad P_{\mathbf{N}} - \text{see Eq. (3.5)} \tag{3.75}$$

for the state of thermal uncondensed atoms.

- We assume there is a (much larger) BEC component co-existing (not described by Eq. (3.75), but Eq. (3.60), in $\hat{\psi} = \phi + \hat{X}$).

  Let us now try to determine the total atom density

$$n(\mathbf{x}) = \langle\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\rangle = |\phi_0(\mathbf{x})|^2 + \underbrace{0}_{\mathrm{Tr}[\hat{\rho}\hat{\alpha}]} + \sum_{nn'} \mathrm{Tr}\left[\hat{\rho}(u_n^*(\mathbf{x})\hat{\alpha}_n^\dagger - v_n(\mathbf{x})\hat{\alpha}_n)(u_{n'}(\mathbf{x})\hat{\alpha}_{n'} - v_{n'}^*(\mathbf{x})\hat{\alpha}_{n'}^\dagger)\right] \tag{3.76}$$

$$= |\phi_0(\mathbf{x})|^2 + \sum_n \mathrm{Tr}\left[\hat{\rho}\left\{\left(|u_n(\mathbf{x})|^2 + |v_n(\mathbf{x})|^2\right)\hat{\alpha}_n^\dagger\hat{\alpha}_n + |v_n(\mathbf{x})|^2\right\}\right], \tag{3.77}$$

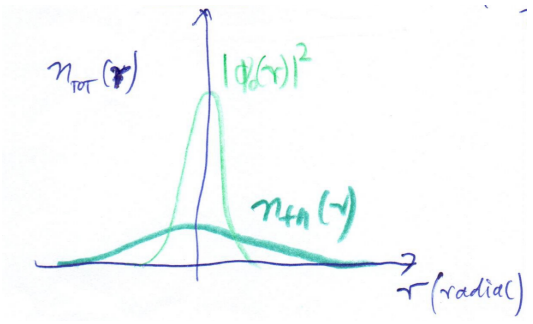
  where, to reach the second line, we have used that the expectation value of terms like $\alpha_n\alpha_{n'}^\dagger$ in the Fock states appearing in (3.75) is zero, unless $n = n'$. We thus have a total

Atom density

$$n_{\mathrm{tot}}(\mathbf{x}) = \underbrace{|\phi_0(\mathbf{x})|^2}_{\mathrm{BEC}} + \sum_n \left\{ \underbrace{\left(|u_n(\mathbf{x})|^2 + |v_n(\mathbf{x})|^2\right)}_{\text{thermal cloud}} \underset{\text{see Eq. (3.12) } (b \leftrightarrow n)}{\bar{m}_n} + \underbrace{|v_n(\mathbf{x})|^2}_{\text{quantum fluctuations}} \right\} \tag{3.78}$$

Example: Approximate $v \approx 0$, $u_n \to \varphi_n \implies$, then do some technical calculation to reach the thermal cloud shape (spatial density of thermal atoms) $n_{th}(\mathbf{x})$ for N_{th} thermal atoms:

$$n_{th}(\mathbf{x}) = \frac{N_{th}}{\pi^{3/2}R_xR_yR_z} e^{-\frac{x^2}{2R_x^2}} e^{-\frac{y^2}{2R_y^2}} e^{-\frac{z^2}{2R_z^2}}. \tag{3.79}$$



left: Thus the thermal cloud shape is Gaussian, with widths $R_i = \sqrt{\frac{2k_BT}{m\omega_i}}$, which depend on the temperature. Together with the condensate, we thus have a bi-modal density distribution, which can often be used to measure temperature T.

3.4.5 Superfluidity

We can give a phenomenological definition. A substance is a superfluid if it shows the following properties:

(i) flow without friction through small capillaries

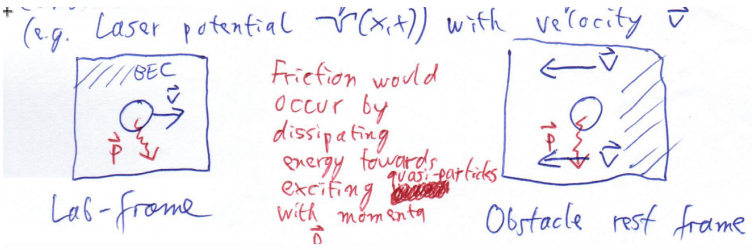
(ii) perfect heat conductivity (via convection)

(iii) rotation only via quantized vortices (see section 3.3.6)

Found e.g. in dilute gas BEC & cold liquid helium. How does it arise?

Critical velocity:

Consider a BEC through which we drag an obstacle (e.g. Laser potential $V(\mathbf{x},t)$) with velocity $\mathbf{v}$.



left: Sketch of moving obstacle in BEC medium in the lab-frame versus obstacle rest frame.

Consider energy of gas in the two frames

	Lab-frame	Rest frame
Ground-state (BEC only)	E' (some internal energy)	$E' + \frac{1}{2} N m v^2$ (N: N_{atoms}; m: mass of one atom)
Excited state (BEC plus one excitation $\mathbf{p}$)	$E' + \varepsilon_p$ (ε_p: see Eq. (3.70))	$E' + \varepsilon_p - \mathbf{p}\cdot\mathbf{v} + \frac{1}{2}Nmv^2$ ($\mathbf{p}\cdot\mathbf{v}$: Doppler shift)
	V(x,t), Hamiltonian time-dependent energy NOT CONSERVED	V(x), energy conserved, can only create excitation if ΔE=0

Energy needed to create excitation:

$$\Delta E = \varepsilon_p - \mathbf{p}\cdot\mathbf{v} \tag{3.80}$$

Smallest gap at $\mathbf{p} \parallel \mathbf{v} \implies$ critical velocity for $\Delta E = 0 \implies 0 = \varepsilon_p - |\mathbf{p}||\mathbf{v}| \implies \mathrm{v}_{\text{crit}} = \min_{\mathbf{p}} \left[\frac{\varepsilon_p}{|\mathbf{p}|}\right]$.
If it moves slower than v_{crit}, the obstacle cannot create any excitation. From Eq. (3.70) we then find

Critical velocity: below $\mathrm{v}_{\mathrm{crit}}$, there is superfluidity

$$\mathrm{v}_{\mathrm{crit}} = \underset{\mathbf{p}}{\mathrm{Min}} \left[\frac{\sqrt{\frac{p^2}{2m}\left(\frac{p^2}{2m} + 2U_o\rho\right)}}{p} \right] = \sqrt{\frac{\rho U_o}{m}} = c \quad \text{speed of sound} \tag{3.81}$$

$(\mathbf{p} \leftrightarrow \hbar\mathbf{q})$

- In a usual fluid, there are single particle excitations $\varepsilon_p \sim \frac{p^2}{2m}$ for arbitrarily small $\mathbf{p}$ (unlike here) $\implies$ No superfluidity.
- Thus superfluidity relies on interactions.

3.4.6 Condensate stability

Lets return to Eq. (3.58) for perturbations of the mean field, the same conclusions can be found from Eq. (3.60).

$$\phi(x,t) = e^{-i\frac{\mu}{\hbar}t}\left[\phi_0(\mathbf{x}) + u(\mathbf{x})e^{-i\omega t} - v^*(\mathbf{x})e^{i\omega t}\right]$$

- Solutions to the BdG equations (3.61) do not have to have real frequencies $\omega \in \mathbb{R}$, the frequency can in general be complex $\omega \in \mathbb{C}$.

  Example: Homogeneous condensate with attractive interactions $U_0 < 0$

  $$\hbar\omega_q = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\frac{\hbar^2 q^2}{2m} + U_0\rho\right)} \qquad \mathrm{Im}(\hbar\omega_q) \neq 0 \text{ for } q < \frac{\sqrt{4|U_0|\rho m}}{\hbar}$$

- They also do not guarantee that $\mathrm{Re}[\omega] > 0$, which would make sure that the excitation has in fact a higher energy than the BEC. For the following, let us write $\omega = \underset{\mathrm{Re}}{\omega'} + i\underset{\mathrm{Im}}{\omega''}$ for the real and imaginary parts of ω.

We can classify results into three cases:

$\omega' > 0, \omega'' = 0$: Usual stable case, oscillatory modes

$\omega'' \neq 0$: The condensate is dynamically (modulationally) unstable. Small perturbations in Eq. (3.58) will grow exponentially with growth rate $\sim (\omega'')$

Examples:

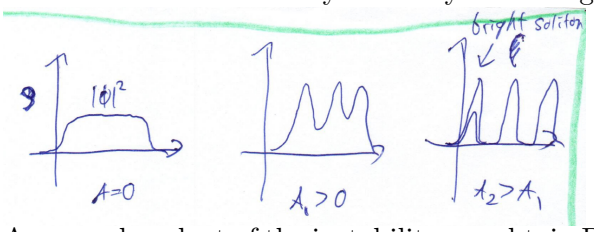
homogeneous $U_0 \longrightarrow$	bright solitons
rotated BEC $\longrightarrow$	vortices
BEC $U_0 > 0$ $\overset{\text{optical-lattice}}{\longrightarrow}$ (Band-gap)	gap-solitons

Usually the end-product of this instability is a new (stable) non-linear solution of TIGPE.

$\omega' < 0$: The condensate is energetically unstable

– All is fine in Eq. (3.58), which assumes unitary evolution, but $\phi_0(\mathbf{x})$ is NOT a local minimum of $E[\phi]$ Eq. (3.64). Hence any dissipation will destroy $\phi_0(\mathbf{x})$.

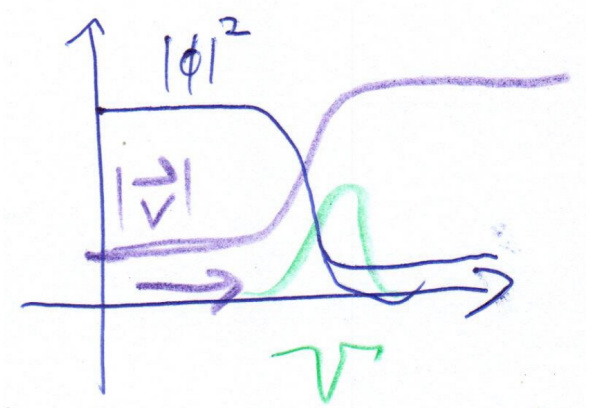
Examples: (i) Collapse of a homogenous BEC collapse with attractive interactions $U_0 < 0$. Here the initial state is dynamically and energetically unstable.



left: Density of initially almost homogenous BEC during dynamical instability. Unstable modes grow into bumps in time, the end-result is a train of bright solitons plus excess heating.

As an endproduct of the instability, we obtain Bright solitons: Non-linear solutions of TIGPE for $U_0 < 0$. Using $\phi_0 \sim \text{sech}(\mathbf{x})$ [soliton] in Eq. (3.61) instead of the initial homogenous state, all BdG modes are stable in the final state.

(ii) A partially supersonic ($v_{\text{flow}} > c$) flow of a BEC with repulsive interactions $U_0 > 0$. This can be dynamically stable but is energetically unstable.



left: Sketch of condensate which makes a subsonic-supersonic transition when flowing over an external potential hump $V(x)$ (green). Density (blue), velocity $|\mathbf{v}|$ (violet) can be inferred from Eq. (3.54) and Eq. (3.55).

Again, we can use a Doppler shift argument as in section 3.4.5 $\hbar\omega' = \hbar\omega - vk \implies v_{crit}$ previous section = some phonons become energetically unstable.

We would reach similar conclusions looking at quantized, incoherent excitations.

How do they all (mean-field BEC, thermal & quantum excitations) play together in a time-dependent manner? $\longrightarrow$ Next chapter.

Week 8

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

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3.5 Quantum Field theory of Bose-Einstein Condensates

- – In section 3.4 we dealt with non-interacting quasi particles.
  – There also was no conversion from condensed to uncondensed component (heating).
- This section discusses one QFT method that can address both, and mentions few others.

3.5.1 Hartree-Fock Bogoliubov Method

We start again with the Heisenberg equation for the field operator (3.38).

$$i\hbar\dot{\hat{\psi}} = \hat{H}_0\hat{\psi} + U_0\hat{\psi}^\dagger\hat{\psi}\hat{\psi} \tag{3.82}$$

and take the expectation value, using $\hat{\psi}(\mathbf{x},t) = \phi(\mathbf{x},t) + \hat{\chi}(\mathbf{x},t)$, Eq. (3.60), assuming $\langle\hat{\chi}\rangle = 0$

$$\begin{aligned}\dot{\phi}(\mathbf{x},t) &= \hat{H}_0\phi(\mathbf{x},t) + U_0\langle(\phi^\star + \hat{\chi}^\dagger)(\phi+\hat{\chi})(\phi+\hat{\chi})\rangle \\ &= \hat{H}_0\phi(\mathbf{x},t) + U_0[|\phi(\mathbf{x},t)|^2\phi(\mathbf{x},t) + 2\langle\hat{\chi}^\dagger\hat{\chi}\rangle\phi(\mathbf{x},t) + \langle\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle + \langle\hat{\chi}\hat{\chi}\rangle\phi^*(\mathbf{x},t) + \langle\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle]\end{aligned} \tag{3.83}$$

We in general do not know $\langle\hat{\chi}^\dagger\hat{\chi}\rangle$. Let us define

Normal correlation function:

$$G_N(\mathbf{x},\mathbf{x}') = \langle\hat{\chi}^\dagger(\mathbf{x}')\hat{\chi}(\mathbf{x})\rangle \tag{3.84}$$

Anomalous correlation function:

$$G_A(\mathbf{x},\mathbf{x}') = \langle\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x})\rangle \tag{3.85}$$

- Now we see that we can express pieces of Eq. (3.83) using $G_N(\mathbf{x},\mathbf{x})$ and $G_A(\mathbf{x},\mathbf{x})$.
- For $\langle\hat{\chi}^\dagger\hat{\chi}^\dagger\hat{\chi}\rangle$ we use

Wick's Theorem For a Gaussian quantum state we have

$$\langle \hat{O}_1\hat{O}_2\hat{O}_3\rangle = \langle \hat{O}_1\hat{O}_2\rangle\langle \hat{O}_3\rangle + \langle \hat{O}_1\rangle\langle \hat{O}_2\hat{O}_3\rangle + \langle \hat{O}_1\hat{O}_3\rangle\langle \hat{O}_2\rangle - 2\langle \hat{O}_1\rangle\langle \hat{O}_2\rangle\langle \hat{O}_3\rangle \tag{3.86}$$
$$\langle \hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4\rangle = \underbrace{\hat{O}_1\hat{O}_2}\underbrace{\hat{O}_3\hat{O}_4} + \underbrace{\hat{O}_1\hat{O}_3}\underbrace{\hat{O}_2\hat{O}_4} + \underbrace{\hat{O}_1\hat{O}_4}\underbrace{\hat{O}_2\hat{O}_3} + \langle \hat{O}_1\rangle\langle \hat{O}_2\rangle\langle \hat{O}_3\rangle\langle \hat{O}_4\rangle$$

Here $\underbrace{\hat{O}_A\hat{O}_B} = \langle \hat{O}_A\hat{O}_B\rangle - \langle \hat{O}_A\rangle\langle \hat{O}_B\rangle$ is called a contraction.

• If the operators $\hat{O}_k$ are Fermionic, there are some additional minus signs. For each term on the rhs. of (3.86), first reorder the $\hat{O}_k$ by swapping neighbors such that those to be contracted are adjacent. For each swap, multiply a factor (-1).

BONUS MATERIAL, Gaussian quantum state:
Single mode example: $\rho = \mathcal{N}\exp(-\bar{n}\hat{a}^\dagger\hat{a} - \frac{1}{2}\bar{m}(\hat{a}^\dagger)^2 - \frac{1}{2}\bar{m}^*\hat{a}^2)$
e.g. a Coherent State or a thermal State: $\bar{m} = \bar{m}^* = 0, \bar{n} = -\beta(\epsilon - \mu)$ [See Eq. (3.4)]

Many mode generalisation:

$$\hat{\rho} = \mathcal{N}\exp(\sum_{i,j=1}^{2M} K_{ij}\hat{C}_i^\dagger\hat{C}_j) \quad \hat{C} = \begin{bmatrix} \hat{a_1} \\ . \\ . \\ . \\ \hat{a_M} \\ \hat{a}_1^\dagger \\ . \\ . \\ . \\ \hat{a}_M^\dagger \end{bmatrix} \tag{3.87}$$

- See e.g. Gardiner/ Zoller "Quantum Noise" 3rd ed. page 119

- See Blaizot and Ripka "Quantum theory of finite systems"(P. 93, Eq (4.47))
- Many variants of Wick's theorem exist all over QFT. They all express the final result of bringing operator products involving $\hat{a}, \hat{a}^\dagger$ into some default order.
- Using Wick's theorem in the form above, we see $\langle \hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle = 0$ since $\langle \hat{\chi}\rangle = 0$

We arrive at a

Modified GPE

$$i\hbar\frac{\partial\phi(\mathbf{x},t)}{\partial t} = \bar{H}_0\phi(\mathbf{x},t) + U_0|\phi(\mathbf{x},t)|^2\phi(\mathbf{x},t) + 2U_0\overbrace{G_N(\mathbf{x},\mathbf{x},t)}^{\equiv\bar{G}_N(\mathbf{x})}\phi(\mathbf{x},t) + U_0\overbrace{G_A(\mathbf{x},\mathbf{x},t)}^{\equiv\bar{G}_A(\mathbf{x})}\phi^*(\mathbf{x},t) \tag{3.88}$$

- We can see that $G_N(\mathbf{x},\mathbf{x}) = n_{\text{unc}}(\mathbf{x})$ is the density of uncondensed (thermal) atoms, by comparison with the discussion in section 3.4.4.
- The interpretation of the term $\sim G_N$, would thus be an interaction between condensed and un-condensed atoms.
- To make use of Eq. (3.88), we need to know $G_N(\mathbf{x},\mathbf{x},t)$ and $G_A(\mathbf{x},\mathbf{x},t)$

We can get those from the Heisenberg equation for $\hat{\chi}^\dagger(\mathbf{x}')\hat{\chi}(\mathbf{x})$ and $\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x})$:

Hartree-Fock Bogulibov equations

$$\begin{aligned}
i\hbar\frac{\partial G_A(\mathbf{x},\mathbf{x}')}{\partial t} &= \langle[\hat{\chi}(\mathbf{x}')\hat{\chi}(\mathbf{x}),\hat{H}]\rangle \qquad (3.89)\\
&= [H_0(\mathbf{x}) + H_0(\mathbf{x}')]G_A(\mathbf{x},\mathbf{x}') + 2U_0\Big[|\phi(\mathbf{x})|^2 + |\phi(\mathbf{x}')|^2 + \bar{G}_N(\mathbf{x})\\
&\quad + \bar{G}_N(\mathbf{x}')\Big]G_A(\mathbf{x},\mathbf{x}') + U_0\Big[\phi(\mathbf{x})^2G_N^*(\mathbf{x},\mathbf{x}') + \phi(\mathbf{x}')^2G_N(\mathbf{x},\mathbf{x}')\\
&\quad + \bar{G}_A(\mathbf{x})G_N^*(\mathbf{x},\mathbf{x}') + \bar{G}_A(\mathbf{x}')G_N(\mathbf{x},\mathbf{x}')\Big] + U_0\Big[\phi(\mathbf{x})^2 + G_A(\mathbf{x},\mathbf{x})\Big]\delta^3(\mathbf{x}-\mathbf{x}')\\
i\hbar\frac{\partial G_N(\mathbf{x},\mathbf{x}')}{\partial t} &= [\hat{H}_0(\mathbf{x}) - \hat{H}_0(\mathbf{x}')]G_N(\mathbf{x},\mathbf{x}') + 2U_0\Big[\phi(\mathbf{x})|^2 - |\phi(\mathbf{x}')|^2 + \bar{G}_N(\mathbf{x})\\
&\quad + \bar{G}_N(\mathbf{x}')\Big]G_N(\mathbf{x},\mathbf{x}') + U_0\Big[\bar{G}_A(\mathbf{x})G_A^*(\mathbf{x},\mathbf{x}') - \bar{G}_A(\mathbf{x}')G_A(\mathbf{x},\mathbf{x}')\Big]\\
&\quad + U_0\Big[\phi(\mathbf{x})^2G_A^*(\mathbf{x},\mathbf{x}') - \phi^*(\mathbf{x}')G_A(\mathbf{x},\mathbf{x}')\Big] \qquad (3.90)
\end{aligned}$$

- These form a coupled system of equations together with (3.88).
- We have again used Wick's theorem on terms like $\langle\hat{\chi}^\dagger\hat{\chi}^\dagger\hat{\chi}\hat{\chi}\rangle$
- The general idea where
  1. equation for $\langle\hat{\psi}\rangle$ couples to
  2. $\langle\hat{\psi^\dagger\psi}\rangle$ couples to
  3. $\langle\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\rangle$

  is called cumulant expansion. It has to be truncated at some order, here this is done by using Wick's theorem.

We can define:

- Condensate density $|\phi(\mathbf{x})|^2$, and condensate number $N_{\text{cond}} = \int |\phi|^2 dx$
- Thermal density $\bar{G}_N(\mathbf{x})$ and thermal number $N_{\text{unc}} = \int \bar{G}_N(\mathbf{x}) dx$

- In the HFB equations (3.88) and (3.89), terms have the following interpretation (please see color file or printout)
  - $\cdots$ interactions between condensed and uncondensed atoms
  - $\cdots$interactions of uncondensed atoms among each other
  - $\cdots$ conversion of condensed and uncondensed atoms (heating)

Example, Relation to Bogulibov equations (3.61): Let us consider $|\,\psi\,\rangle = 0$, the Bogulibov vacuum with zero quasiparticles in any mode, as our initial-state (eternal state in thre Heisenberg picture). Then we can see that

$$G_N(\mathbf{x}, \mathbf{x}') = \sum_n v_n(\mathbf{x}') v_n^*(\mathbf{x}), \tag{3.91}$$

$$G_A(\mathbf{x}, \mathbf{x}') = -\sum_n u_n(\mathbf{x}') v_n^*(\mathbf{x}). \tag{3.92}$$

For these G_A, G_N, a lengthy calculation gives from HFB equations Eq. (3.89):

$$i\hbar \dot{G}_N(\mathbf{x}, \mathbf{x}') = 0 \tag{3.93}$$

$$i\hbar \dot{G}_A(\mathbf{x}, \mathbf{x}') = -2\mu G_A(\mathbf{x}, \mathbf{x}') \to G_A(\mathbf{x}, \mathbf{x}', t) = e^{\frac{i2\mu t}{\hbar}} G_A(\mathbf{x}, \mathbf{x}', 0) \tag{3.94}$$

To reach this we ignore G relative to ϕ^2 (=fluctuations are small) and assume $\phi(t) = \phi_0(t = 0)$
•Thus the Bogulibov vacuum is a steady state of the HFB-equations.

3.5.2 Depletion and Renormalisation

Let us further look at the density of uncondensed atoms $n_{\text{unc}}(\mathbf{x}) = G_N(x, x)$ in the Bogoliubov vacuum $|\,\psi\,\rangle = |\,0\,\rangle$. Let us calculate $n_{\text{unc}}(\mathbf{x})$ for a homogenous BEC, with constant density ρ, as used in section 3.4.1:

$$n_{\text{unc}} = \sum_n |v_n(\mathbf{x})|^2 \to \frac{1}{\mathcal{V}} \sum_q v_q^2 \xrightarrow[3D]{} \frac{1}{\mathcal{V}} \int_{q=0}^{\infty} dq\, q^2 (4\pi) \underbrace{D}_{=\frac{2\pi}{L}^3}^{\text{(Density of states)}} v_q^2 \tag{3.95}$$

[We have converted sum $\to$ integral, using the density of states D for quantised particles in 3D box ($K_i = \frac{n\pi}{L}$) [But only one k_i per cell not two ($\pm|k_i|$)]]

$$= \frac{1}{2\pi^2} \int_0^{\infty} dq\, q^2 v_q^2 \overset{Eq.\ (3.71)}{=} \frac{8(mU_0\rho)^{\frac{3}{2}}}{3\hbar^3\pi^2}$$

Using also $U_0 = \frac{4\pi\hbar^2 a_s}{m}$, we find the

Condensate Depletion:

$$\frac{n_{\text{unc}}}{\rho} = \frac{8}{3\sqrt{\pi}}(\rho a_s^3)^{\frac{1}{2}} \tag{3.96}$$

- Depletion implies that, even though we are in the BdG vacuum with zero phonon excitations, interactions cause some atoms to remain outside of the condensate.
- Typical numbers: $a_s = 5.5nm$ for Rubidium, $\rho = 10^{19}/m^3 \implies \frac{n_{\text{unc}}}{\rho} = 0.2\%$ uncondensed density.

Let us also calculate

$$\bar{G}_A(\mathbf{x}) = G_A(x,x) = \sum_n u_n(\mathbf{x})v_m^*(\mathbf{x}) \overset{\text{trying as above}}{=} \infty \quad \text{We have a divergent integral}$$

$$\overset{\text{cut-off integral at } K}{=} -\frac{4}{\pi^2}\int_0^K dq\, q^2 u_q v_q^* \overset{\text{large } K}{=} -\frac{4mU_0\rho K}{\pi^2\hbar^2} \equiv -\kappa U_0 \rho \tag{3.97}$$

This divergence has the same cause as in the other local quantum-field theories (e.g. particle physics): The implicit mathematical (but not physical) assumption that the theory is valid up to arbitrarily high energy scales. Solution: Renormalisation = we absorb "infinities" (in our case K) into parameters into the Hamiltonian (rather than having them in observables) and define the

Renormalised interaction U

$$U_0 = \frac{U}{1-\kappa U} \quad \text{where } \kappa = \frac{4mK}{\pi^2\hbar^2} \tag{3.98}$$

- κ "infinite", U_0 "infinite" (parameter in $\hat{H}$), U "finite" (observable quantity)
- "Infinite" means ∞ in the limit $K \to \infty$
- To see that Eq. (3.98) makes sense, we can calculate e.g. the Born scattering amplitude from $\hat{H}$

Example, Renormalised mean-field interaction in modified GPE Eq. (3.88):

$$i\hbar\dot{\phi} = \hat{H}_0\phi + U_0|\phi|^2\phi + \overbrace{2U_0 G_N\phi}^{\text{lets ignore } \bar{G}_N\text{, assuming small}} + U_0\bar{G}_A\phi_0^* \tag{3.99}$$

We now use Eq. (3.97) with the replacement $U_0 \to U$

$$\bar{G}_A = -\kappa U\rho \tag{3.100}$$

in (3.99) to replace $U_0 \to U$. Then

$$i\hbar\dot{\phi} = \hat{H}_0\phi + \underbrace{(U_0(1-\kappa U))}_{=U \text{ from Eq. (3.98) , which is finite}}|\phi|^2\phi + 2U\bar{G}_N\phi \tag{3.101}$$

(Steps in brown a is allowed because perturbations $\hat{\chi}$ (hence $G_N, G_A, \bar{G}_N, \bar{G}_A$) are "small")
• For numerical implementation : K frequently small enough that renormalisation can be ignored.

Appraisal of HFB:

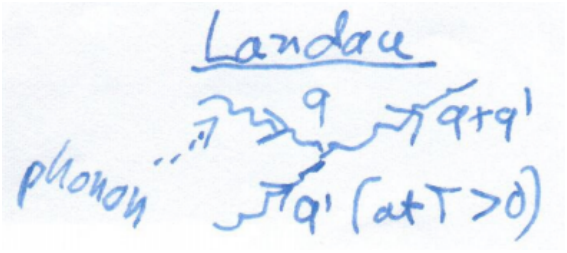
PROS:

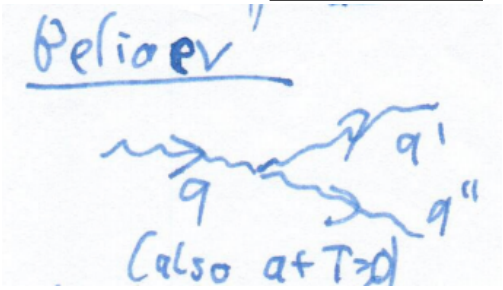
- Seemingly straightforward implementation
- Easy implementation conceptually
- Includes repulsion between BEC and thermal cloud

CONS:

- Subtleties with renormalisation
- Excitations in this formalism have an energy gap, which means that $E_q \to$ nonzero for q$\to$ 0. However they should be gapless, according to a Hugenholtz-Pines theorem (related to the Goldstone theorem).
- Computationally hard in general 3D (in which case correlation functions G_A, G_N are 6D.
- No $\hat{\chi}^\dagger\hat{\chi}\hat{\chi}$ terms

  due to assumption of Gaussian state/ use of Wick theorem. $\implies$ Absence of phonon damping:





$\Rightarrow$ This led to the design of various "fixes" of HFB and alternatives. Some of those are listed below.

3.5.3 Other Bose-gas quantum field methods

HFB is straightforward to derive but has some issues listed on the previous page. Let us thus list some alternative methods to study quantum-field corrections beyond the GPE, or fully quantum models.

I: Truncated Wigner approximation:

- We write $W(\alpha, \alpha^*) = F[\hat{\Lambda}(\alpha, \alpha^*), \hat{\rho}(t)]$, where F denotes some functional, Λ is an operator basis and $\hat{\rho}$ the time evolving density matrix. In essence this is using the Wigner function (2.49) in a many-body setting.
- We next convert the time evolution equation for the density matrix into one for the Wigner function: $\dot{\hat{\rho}}$=... $\rightarrow \dot{W} = ...$
- The result can be mapped to a set of stochastic differential equations $i\hbar\dot{\alpha}(\mathbf{x}) = ...$
- These take the same form as the GPE + random noise on the initial state.
- We can obtain all quantum observables, which are correlation functions such has $\langle\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x})\rangle$ from corresponding classical correlation functions over the noisy wave function, e.g. $\langle\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x})\rangle = \overline{\alpha^*(\mathbf{x}')\alpha(\mathbf{x})} - \frac{1}{2}$"$\delta(x - x')$".

II: t-DMRG:

This is short for **t**ime-dependent **d**ensity **m**atrix **r**enormalisation **g**roup. We discretise the full quantum many body problem (3.38) for example in the position basis: $\hat{\Psi}(\mathbf{x}) \rightarrow \hat{\Psi}(x_k)$, and then use an approximate method invented in the quantum information and condensed matter communities. It works well in 1D and if there is "not too much entanglement" in the system.

III: MCTDH(B):

Multi-**c**onfigurational **t**ime-**d**ependent **H**artree for **B**osons. Starts with a more complicated Ansatz than Eq. (3.27) into the many-body SE, that allows multiple strongly occupied states.

IV: Few exact solutions:

In some cases there are a few exact solutions of interesting many-body problems. One example is the exactly one dimensional system with Hamiltonian

$$\bar{H} = -\sum_{n=1}^{N} \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_n^2} + \sum_{n,m=1}^{N} \frac{U_0}{2}\delta(x_n - x_m) \tag{3.102}$$

This is the first quantised Hamiltonian that we get for a bunch of Bosons in 1D, with no external potential $V(x) = 0$ and contact interactions U just as discussed in section 3.3.1. For the case

$U_0 < 0$ (attractive interactions), this is called Lieb-Liniger Hamiltonian, and has quantum soliton solutions:

$$\psi(x_1, ..., x_N) \sim e^{iKX_{CM}} \exp\left[-\frac{m|U_0|}{2\hbar} \sum_{i<j} |x_i - x_j|\right] \tag{3.103}$$

[Compare assignment 1, Q1(ii) and last page of week 7]

Week 9

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

4 Degenerate Fermi Gases

4.1 Ideal Fermi Gases

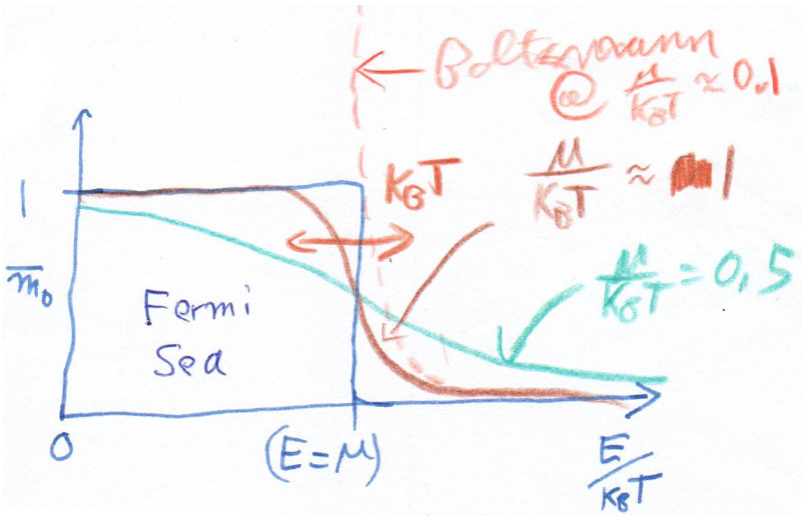
In section 3.2 we explored what happens to N non-interacting Bosons as the temperature is decreased $T \downarrow 0$. Now we follow the same question for Fermions, thus using the Fermi-Dirac distribution [Eq. (3.11)]:

$$\bar{m}_b = \frac{1}{\exp[\beta(\varepsilon_b - \mu)] + 1}$$

- First difference: $\bar{m}_b > 0 \ \forall \varepsilon_b, \mu \rightarrow$ no constraint on μ in contrast to Bose case.
- We can also much more easily take the limit

$$\lim_{T\to 0} \bar{m}_b = \begin{cases} +1 & \varepsilon_b < \mu \\ 0 & \varepsilon_b > \mu \end{cases}$$

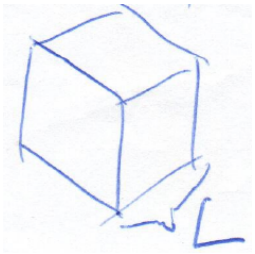
- Let us plot Eq. (3.11) for various parameters



We see that for $T = 0$, all states with energy below μ are occupied, and above are not. This sharp transitions "softens" up, as we increase the temperature.

- We again find, that the Fermi-Dirac distribution approaches the classical Boltzmann distribution, once states are weakly occupied ($m_n \ll 1 \to \exp[\cdots] \gg 1$) and energies much higher than μ.

It is clear in the plot above, that $E = \mu$ seems to be a special energy. To figure out what it means, lets look at non-interacting Fermions in a 3D box potential of cube-side-length L with spin s ($|\vec{s}| = \frac{1}{2}$).



left: Particle in a cubic box: We recall that wave-numbers in trigonometric eigenfunctions $\sin(k_l x)$ are quantized in each spatial dimension with condition

$$k_l = \frac{n_l \pi}{L}$$

$$l \in \{x, y, z\}$$

$$n_l = 1, 2, ...\infty$$

Let us first consider the $T = 0$ case. As before in our discussion of Bosons, μ sets the total (mean) number of particles according to

$$N = \sum_{\text{all states } b} \bar{m}_b \tag{4.1}$$

$$\Rightarrow N \overset{\text{here}}{=} \sum_{n_x, n_y, n_z, s} \bar{m}_{n_x, n_y, n_z, s} \tag{4.2}$$

At zero temperature, we have simply

$$\bar{m}_{n_x, n_y, n_z, s} = \begin{cases} 1 & E_{\mathbf{n}} < \mu \\ 0 & E_{\mathbf{n}} \geq \mu \end{cases}$$

where $E_{\mathbf{n}} = \frac{\mathbf{n}^2 \pi^2 \hbar^2}{2mL^2}$ is the particle in the box energy. Since the latter is always positive, we see the first important difference to the Bose case, that we require $\mu > 0$ in order to have any particles. Then

$$\Rightarrow N = \sum_{n_x, n_y, n_z, s} \bar{m}_{n_x, n_y, n_z, s} \approx \frac{2}{8} \int d^3\mathbf{n}\ \bar{m}_{\mathbf{n}} \tag{4.3}$$

$$= \frac{4\pi}{4} \int_0^{n_{\max}} dn\ n^2 \text{ (use 3D spherical coordinates)} \tag{4.4}$$

$$= \frac{1}{3} \pi n_{\max}^3 \tag{4.5}$$

where $n_{\max} = \sqrt{\frac{2mL^2\mu}{\pi^2\hbar^2}}$. At the first $\approx$ we approximate the sum by an integration. We get a factor of 2 from summation over the two spin-states $m_s = +1/2, -1/2$, and we get a factor of $1/8$ since the original sum runs only over positive n_x, n_y, n_z, while the integration runs over all 8 sign quadrants. In the second line, we built in that $\bar{m}$ will be zero for $|\mathbf{n}| > n_{\max}$

Altogether we obtained N as a function of μ and can then solve for μ to find the

Fermi-energy (for non-interacting $s = \frac{1}{2}$ Fermions in a box)

$$\mu_0 = E_F = (3\pi^2)^{2/3} \frac{\hbar^2}{2m} \left(\frac{N}{V}\right)^{2/3}, \; V = L^3 \tag{4.6}$$

- Thus at $T = 0$ (or for $k_B T \ll E_F$), the Fermions occupy all energy states up to (approx up to) E_F. See blue line (brown line) in the earlier figure. This configuration, where μ is somewhat more important for the distribution than T, is called degenerate Fermi gas (DFG).
- In phase space, the surface where particles have exactly the Fermi energy E_F, is called Fermi surface.
- The transition to a DFG is less sharp than for a BEC, roughly we can say that the degeneracy temperature to DFG is

$$k_B T \approx E_F \tag{4.7}$$

- Had we used only a single spin-state, the pre-factor would be $(3\pi^2)^{2/3} \to (6\pi^2)^{2/3}$, we shall require this later. We also define the

Fermi-momentum or Fermi-wavenumber via

$$\frac{\hbar^2 k_F^2}{2m} = \frac{p_F^2}{2m} = E_F, \text{ i.e. momentum at Fermi surface} \tag{4.8}$$

$$k_F = [(3\pi^2)\rho]^{1/3}, \; \rho = \frac{N}{V} \text{ (density)} \tag{4.9}$$

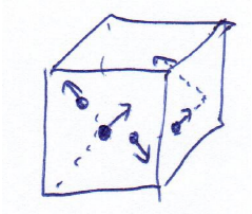
Examples:
Electrons in a conductor: Iron (Fe) has a mass density of $\rho \sim 7.8$ g/cm^3, which gives roughly an atom number density of $\rho_{\text{Fe}} \approx 8.3 \times 10^{28}/\text{m}^3$. There are two conduction electrons per atom, hence $\rho_{\text{e}^-} = 16.6 \times 10^{28}/\text{m}^3$. Using Eq. (4.7) and Eq. (4.6) we can find that $T_F \approx 1.3 \times 10^5$K and $E_F \approx$ 2-10 eV. $\Rightarrow$ Conduction electrons are DFG at all reasonable temperatures (where the metal still exists).

Cold Fermionic atoms: E.g. ^{6}Li. In atom traps (as discussed for BEC) the density is very low $\rho \approx 10^{17}/\text{m}^3$. Using the equations above, we find $T_F \approx 80$ nK, so this is again the same range of temperatures as for BEC. We shall later re-calculate E_F in a harmonic trap, see Eq. (4.17), which would be more appropriate for this case.

- We see that how cold is cold enough for degeneracy of Fermions strongly depends on the system.

4.2 Degeneracy Pressure

One consequence of populating all states up to energies E_F is that these particles may move "fast" and hence contribute to significant pressure.



left: pressure = elastic collisions off wall

Basic thermodynamic P, V, E relation

$$P \cdot V = \frac{2}{3} N \langle \varepsilon_{\text{kin}} \rangle, \;\; P \to \text{Pressure}$$

For the DFG of particles in box

$$\begin{aligned} \langle \varepsilon_{\text{kin}} \rangle &= \frac{2}{8} \frac{\int d^3\mathbf{n}\; E(\mathbf{n})}{N}, \qquad \left(E(\mathbf{n}) = \frac{\mathbf{n}^2 \pi^2 \hbar^2}{2mL^2} \right) \\ &= \frac{4\pi}{4} \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) \frac{\int_0^{n_{\max}} dn\; n^4}{N} \\ &\underset{\text{(exercise)}}{=} \frac{3}{5} E_F \end{aligned}$$

We arrive at the

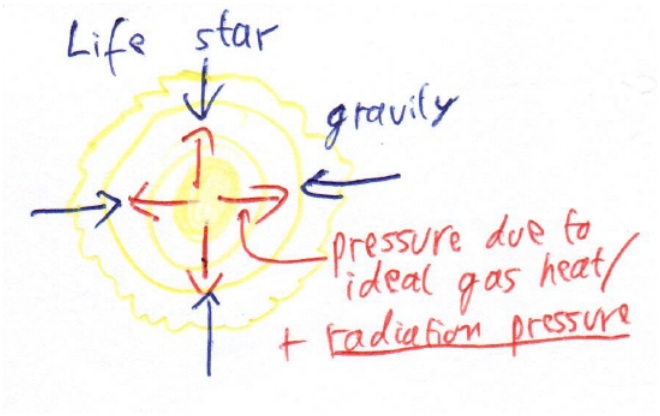
Fermi-pressure , also called degeneracy pressure:

$$P_F = \frac{2}{5} \underbrace{\left(\frac{N}{V} \right)}_{\rho} E_F \sim \rho^{5/3} \tag{4.10}$$

- This is valid for $T \lesssim T_F$ and unlike the classical case, there is non-zero pressure all the way to $T = 0$.
- You can think of this as Fermions resisting being sqeezed into "same state". (But note, there are no interactions.)

4.3 Applications in Astrophysics

4.4 White dwarf stars



- In our sun, inward gravity is balanced by outward pressure and radiation pressure due to fusion reaction H+H $\rightarrow$ He sustaining temperature T.
- When fuel runs out, heavy stars shrink and get hotter, then do fusion of He $\rightarrow$ C,...,Fe.
- The latter won't work for solar-mass star, because they are too light, so we can ask what happens when they run out of H, thus only contain He, and can no longer provide fusion? $\Rightarrow$ In some cases we get a white-dwarf where gravity is balanced by Fermi-pressure (4.10).

Stellar DFG: Assume a compressed star with mass $M = 10^{30}$ kg, central density $\rho_{\text{center}} = 10^{10}$ kg/m^3, temperature $T = 10^7$ K. [c.f Sun $M_\odot = 2\times10^{30}$ kg, $\rho_{\text{center}} = 1.6\times10^5$ kg/m^3, $T = 1.57\times10^7$ K]. We assume the old star contains now only ionized Helium.

$$\begin{aligned}\Rightarrow M &\approx N_{\text{elec}}m_{\text{e}} + N_{\text{nucleons}}m_{\text{p}} \\ &= N_{\text{elec}}(m_{\text{e}} + 2m_{\text{p}}) \\ &\approx 2N_{\text{elec}}m_{\text{p}}\end{aligned}$$

Estimate number density of electrons roughly (turns out, pressure by He nuclei is negligible),

$$\rho_{\text{e}} = \frac{N}{V} = \frac{M/2m_{\text{p}}}{M/\rho_{\text{center}}} = \frac{\rho_{\text{center}}}{2m_{\text{p}}} \approx 3\times10^{-9}\text{electrons/fm}^3$$

Fermi temperature $T_F \overset{Eq.\ (4.7)}{=} 8.8\times10^9$ K
$\Rightarrow$ Despite being very hot, electrons at these high densities form DFG!

Stable equilibrium radius R of star (simplify star as a uniform sphere):

$$0 = dE = \frac{\partial}{\partial R}\underbrace{\left(-\frac{3}{5}\frac{M^2}{R}G\right)}_{E_{\text{grav}}}dR \qquad \underbrace{-P_F(R)(4\pi R^2 dR)}_{\text{using } dE=-PdV \text{ from thermodynamics}} \tag{4.11}$$

We can solve this for the

White-dwarf radius:

$$R_* = \mathcal{N} \frac{\hbar^2}{G m_e m_{He}^{5/3} M^{1/3}} \tag{4.12}$$

- Here $\mathcal{N} = 3(6\pi^2)^{1/3} \approx 11.69$ is a numerical pre-factor. Proof: Assigment 5. Test: Sirius B, $M = 1.05 M_\odot$, $R = 5100$ km (Formula (4.12) gives 7030 km)

4.4.1 Relativistic DFG

For very dense (massive) white dwarfs, e^- near the Fermi surface become so fast that they have to be treated relativistically. We have to recalculate section 4.1 and section 4.2 using

$$E_{kin} = mc^2 \left(\sqrt{1 + \left(\frac{p}{mc} \right)^2} - 1 \right). \tag{4.13}$$

After a technical calculation, we find the relativistic Fermi-pressure

$$P_F \sim \text{const.} \cdot \rho^{4/3} \tag{4.14}$$

If we redo 4.11 with this, we find there is no stable R_* for a stellar mass above the

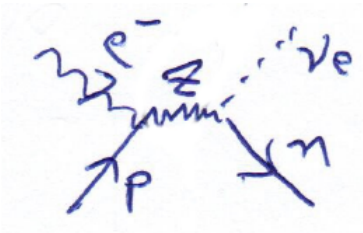
Chandrasekhar-limit:

$$M \approx 1.44 M_\odot \tag{4.15}$$

where $M_\odot$ is the solar mass. This is the maximal mass for white dwarf stars.

4.4.2 Neutron stars

- For heavier stars, e^- degeneracy pressure cannot halt gravitational collapse once fusion runs out.
- Once matter reaches density of $\rho \sim 10^{17}$ kg/m^3 (density of nuclei), electrons and protons form neutrons via inverse beta decay



- At equal density, P_F from neutrons is $\frac{m_e}{m_p}$ times that of electrons, and thus intrinsically much smaller, see Eq. (4.6)-(4.10). However, at some point the density becomes so high that also the degeneracy pressure P_F of neutrons becomes relevant, and may halt collapse.

Neutron star:
The result, when all matter is converted to neutrons and neutron degeneracy pressure has halted gravitational collapse. Their typical mass range is

$$1.4M_\odot < M < 3M_\odot,$$

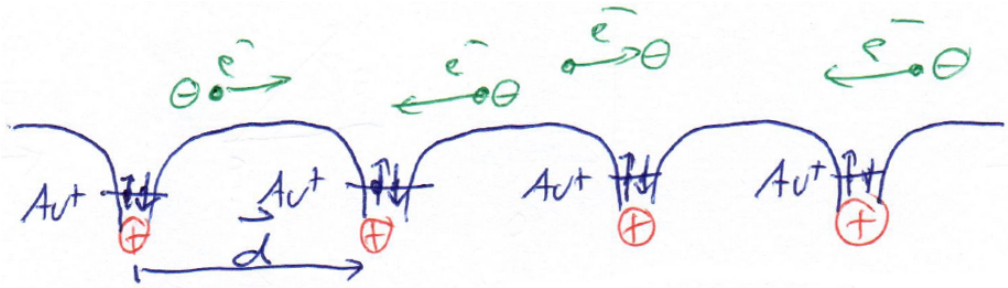
with a radius of

$$R \sim 20\text{km}.$$

- If neutron Fermi-pressure is overcome as before in section 4.4.1 (by neutrons becoming relativistic) $\rightarrow$ total gravitational collapse, black-hole.

4.5 Electron gas in metals

- Alkali metals or Copper, Silver, Gold: 1 valence e^- per atom. Picture:



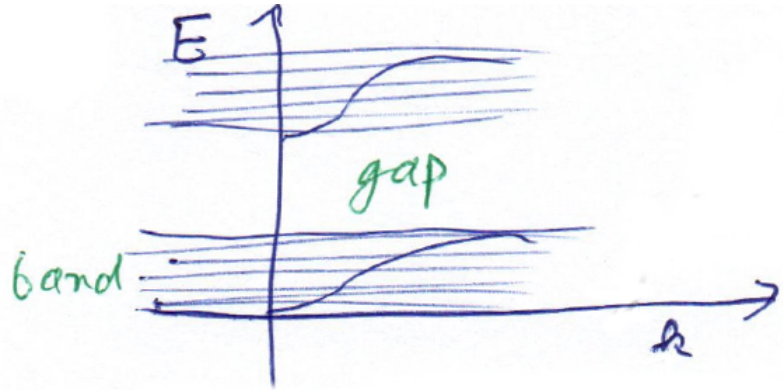
- Ions bound by "immersion" in electron gas (metallic binding)
- Electron-electron Coulomb interactions are screened due to background ion sea and hence weak
- Electron-ion interactions: electrons aren't really "free", but see periodic potential $V(\mathbf{x}) = V(\mathbf{x}+\mathbf{d})$

Bloch theorem: Eigenstates for electrons in the periodic ion potential are of the form

$$\phi_{\mathbf{k},j}(\mathbf{x}) = u_j(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}} \tag{4.16}$$

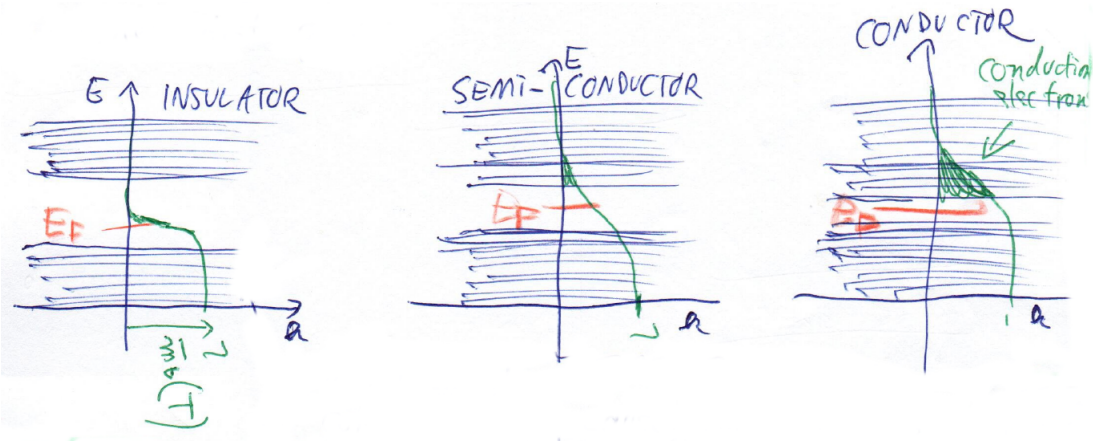
where $u_j(\mathbf{x}) = u_j(\mathbf{x}+\mathbf{d})$, i.e the function u possesses the same periodicity properties as the ionic potential $V(\mathbf{x})$

Gives rise to band-structure[5] (note, energies for negative k are the same $E(-k) = E(k)$):



Example, solid material properties:

- From numbers in example on pg. 73, valence electrons form a degenerate Fermi-gas. 3 pictures distinguish:



In the sketches above, blue lines are the bands. We then draw the Fermi distribution function Eq. (3.11) as green line, with energy axis vertical, and population axis horizontal (so transposed compared to the figures at the beginning of "week 9").

4.6 Ultra-cold atomic Fermi-gas

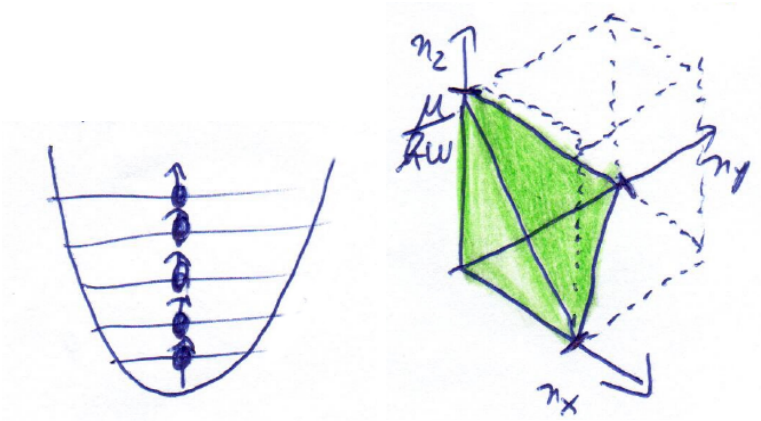
- As in section 3.2, we now focus on a dilute gas of ultra-cold atoms in a harmonic trap, but here now fermionic atoms.
- Recall that compound objects of an even number of constituent Fermions are Bosons, while those of an odd number of constituent Fermions are Fermions. Since all items making up

[5] Top band $E(k)$ curve should be flipped.

andatom are Fermions (electrons and nucleons, or more fundamentally, electrons and quarks), we need $N_{\text{elec}} + N_{\text{protons}} + N_{\text{neutrons}}$ to be odd for a fermionic atom. Since $N_{\text{elec}} = N_{\text{protons}}$ for neutral atoms, the sum of the two is always even. Thus fermionic atoms are all those with an odd number of neutrons.

- We assume spin-polarization for now, (e.g all $\uparrow$).
- We neglect interactions (but show shortly this is even realistic when all $|\uparrow\rangle$).

  Expected picture:



- At $t = 0$, $\bar{m}_b = 1$ up to $\mu = E_F$.
- Harmonic trap $E_{n_x,n_y,n_z} = \hbar\omega(n_x + n_y + n_z)$

$$\Rightarrow N(\mu) = \sum_{n_x,n_y,n_z} 1 \text{ (with } (n_x + n_y + n_z) < \frac{\mu}{\hbar\omega}) = \text{ Volume of the green object above}$$
$$= (\mu/\hbar\omega)^3/6$$

With same reasoning as before, we obtain the

Fermi energy in trap

$$E_F = \hbar\omega(6N)^{1/3} \tag{4.17}$$

- Using numbers as for the degeneracy temperature of Bose-atoms earlier [after Eq. (3.14)], we obtain $T_F \approx 187$ nK ($N = 10000$, $\omega = (2\pi)100$ Hz)
- Seems slightly "easier" to reach than BEC, but making a degenerate Fermi gas of cold atoms turned out harder.
  Reasons:

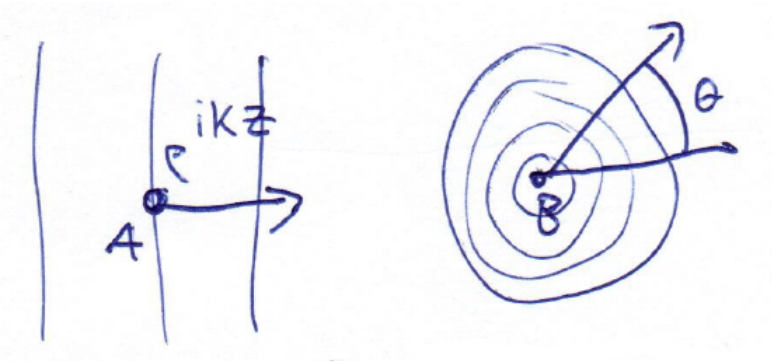
  (i) Evaporative cooling (see PHY402 p.89) relies on interactions for remnant atoms to rethermalize.

(ii) Fermi-blocking (section 2.2.4): atom has to scatter exactly into the right "empty" state. We see in the next section that spin-polarized ultracold Fermions barely interact.

- Solution: e.g sympathetic cooling: mix Bosons and Fermions, cool Bosons, Fermions can interact with Bosons, thus cool down together.

4.7 Ultra-cold Fermion interactions

Let us revisit quantum scattering theory as in section 3.3.1.



The wavefuntion corresponding to this cartoon is

$$\psi_0(\mathbf{r}) = \exp(ikz) + \frac{f(\theta)}{r}\exp(ikr)$$

where $\mathbf{r} = \mathbf{r}_B - \mathbf{r}_A$ is the relative coordinate between the two collision partners, and $r, \theta, (\varphi)$ the corresponding 3D spherical coordinates.

For Fermions, to fulfill the anti-symmetrisation requirement, we need $\psi(\mathbf{r}) \stackrel{!}{=} -\psi(-\mathbf{r})$.
We could try the usual trick:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{2}}\big(\psi_0(\mathbf{r}) - \psi_0(-\mathbf{r})\big). \tag{4.18}$$

Note

$$\psi_0(-\mathbf{r}) = \exp(-ikz) + \frac{f(\theta+\pi)}{r}\exp(ikr).$$

But for S-wave scattering (see pg. 42), $f(\theta) =$ const. (indep. of θ), so construction doesn't work, because the scattering part of the wavefunction vanishes in (4.18). We would need $f(\theta) = -f(\theta+\pi)$, which would be true only for P-wave scattering ($l = 1$ relative angular momentum).
But our arguments to neglect P-wave scattering in the ultra-cold regime in section 3.3.1. hold also for Fermions.

No s-wave scattering or identical Fermions ⇒ Ultra-cold, spin-polarized Fermions are to a very good approximation effectively non-interacting.

- It implies that results such as Eq. (4.17) are actually useful.
- Importantly, the basic interatomic interaction potential as sketched in section 3.3.1 [Eq. (3.19)] would not be much different between Bosonic or Fermionic isotopes of the same atom. The statement above only arises effectively in ultra-cold scattering, since the Fermion symmetry of the many-body wave-function makes it less likely at cold temperatures for the two Fermions to be ever close to each other.
- The situation changes if we have 2 spin-states $\uparrow, \downarrow$, which can take care of symmetrization in (4.18) $\Rightarrow$ then S-wave interactions are possible.

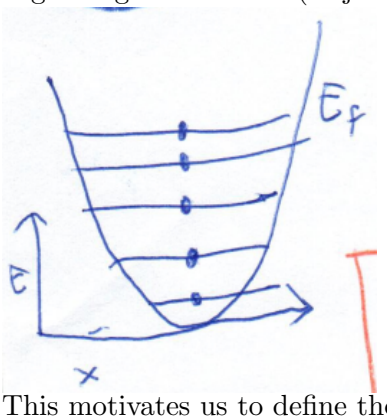
Week 10

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

4.8 Trapped Atomic Fermi Gases

Now we explore the ultra-cold atomic Fermi gas further, within a harmonic trap, but initially neglecting interactions (as justified in section 4.7). We then find



left: Non-interacting ground state: All single particle states $|\,\varphi_n\,\rangle$ up to $E = E_F$ are filled with exactly one atom (or $(2S+1)$ atoms if we consider them to have spin S).

This motivates us to define the

Fermi-Sea State:

$$|\,FS\,\rangle_N = \prod_{n=0}^{N-1} \hat{a}_n^\dagger |\,0\,\rangle \tag{4.19}$$

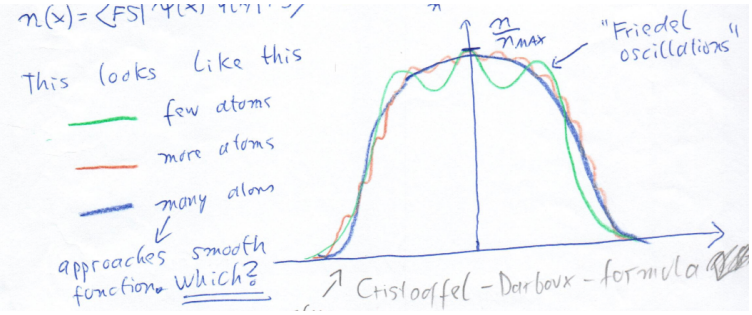
N = Atom-number and $E_n < E_F(N)$

Using the Fermi-field operator

$$\hat{\Psi}(x) = \sum_n \varphi_n(x)\hat{a}_n, \tag{4.20}$$

we obtain a total density

$$n(x) = \langle FS|\hat{\psi}^\dagger(x)\hat{\psi}(x)|FS\rangle \underset{\text{exercise}}{=} \sum_n |\varphi(x)|^2. \tag{4.21}$$



left: Results of (4.21) are plotted on the left for different numbers of atoms. The oscillations visible for smaller N are called Friedel Oscillations.

4.8.1 Thomas-Fermi-approximation

To find the density shape shown as the blue line (for many atoms) in the figures above, we can again use the Thomas-Fermi approximation, see section 3.3.4, however in a slightly different formulation.

Let us assume a large gas, so that we can use the local density approximation. This means we use the results derived in section 4.1, which were assuming a homogeneous system, by instead inserting a slowly varying density $N/V \to n(r)$.

From Eq. (4.6) and Eq. (4.8) we can then find relations between a local Fermi wavenumber/momentum and density and local Fermi-energy, as:

$$\underset{\text{(ignoring spin)}}{n(r) = \frac{k_F^3(r)}{6\pi^2}}, \qquad \varepsilon_F(r) = \frac{\hbar^2 k_F(r)^2}{2m}. \tag{4.22}$$

The equillibrium density is such that adding one more atom has the same energy everywhere, thus:

$$\underset{\substack{\text{added on}\\ \text{Fermi surface}}}{\frac{\hbar^2 k_F^2(r)}{2m}} + \underset{\text{trap}}{V(r)} = \mu \tag{4.23}$$

Solving for $n(r)$ gives us the

Thomas-Fermi profile for Fermi gas

$$n(r) = \frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}[\mu - V(r)]\right)^{\frac{3}{2}} \quad \text{if} \quad \mu > V(r) \quad \text{else} \quad n(r) = 0 \tag{4.24}$$

- This gives the blue line in the previous figure.
- Note for BEC we have $[\mu - V(r)]^1$.

We can extend this local semiclassical/like WKB approach to include the momentum distribution and finite temperature effects with the resultant

Semiclassical distribution function for a Fermi gas:

$$f(\mathbf{r},\mathbf{p}) = \frac{1}{\exp[\beta(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \mu)] + 1} \tag{4.25}$$

- From this we can obtain the total atom number

$$N = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{r}d^3\mathbf{p} f(\mathbf{r},\mathbf{p}) \tag{4.26}$$

or density/momentum density

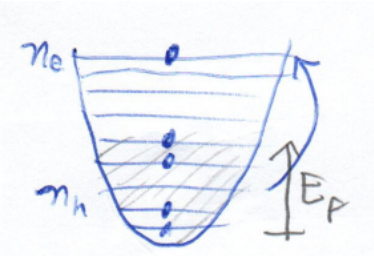
$$n(\mathbf{r}) = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{p} f(\mathbf{r},\mathbf{p}) \tag{4.27}$$

$$\tilde{n}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{r} f(\mathbf{r},\mathbf{p}) \tag{4.28}$$

- The same view-point adopted here can give the Thomas-Fermi profile for bosons, derived with different methods for Eq. (3.46). In a (locally) homogeneous BEC there is no kinetic energy, but instead interaction energy $U_0 n(r)$, unlike the Fermionic case. Replacing in Eq. (4.23) the Fermi-(kinetic) energy $\frac{\hbar^2 k_F^2(r)}{2m}$ by $U_0 n(r)$, we then find Eq. (3.46).

4.8.2 Excitations of the ideal gas

The simplest excited state of $|FS\rangle$ is obtained, when we move any atom with $E < E_F$ to $E > E_F$.



left: Excitation of a degenerate Fermi gas, an atom has jumped from state n_h (h for hole) to n_e (e for excited).

In this we are actually doing two things: creating a hole at n_h (oscillator quantum number) and excited atom at n_e.

We can consider these both separately as excited states of a system with $N-1$ atoms (for the hole) or $N+1$ atoms (for the excited atom). Energy of hole: $E[\hat{a}_{n_h}|FS\rangle_N] - E[|FS\rangle_{N-1}] = E_F - E_{n_h} = E_F - \hbar\omega(n_h + \frac{1}{2})$

Similarly for excitation $E[\hat{a}^\dagger_{n_e}|FS\rangle_N] - E[|FS\rangle_{N+1}] = E_{n_e} - E_F$

If we denote by n_F the oscillator state quantum number up to which all states are filled in the Fermi sea, we have

Energy of particle or hole excitation

$$E_n = \hbar\omega|n - n_F| \tag{4.29}$$

(homogeneous system would have $\varepsilon_k = \frac{\hbar^2|k^2 - k_F^2|}{2m}$)

4.9 (Weak) Repulsive interactions in spin mixtures

- So far, we only considered non-interacting Fermi gases, which as per the discussion in section 4.7, is actually realistic for a cold single species gas.
- For two species (e.g. $\frac{N}{2}$ atoms in one spin state $|\uparrow\rangle$ and $\frac{N}{2}$ atoms in another $|\downarrow\rangle$) interactions become relevant since $|\uparrow\rangle$ atoms do have s-wave interactions with $|\downarrow\rangle$ atoms.
- Thus also evaporative cooling works again.
- Let us assume interactions are fully repulsive everywhere, that is $U(r) > 0 \quad \forall r$.

4.9.1 Landau Fermi Liquid

Let us consider "slow" turning on of interactions, so we start with perturbation theory. We use the

Hamiltonian for spin-mixture of a Fermi-gas

$$\hat{H} = \int d^3\mathbf{x}\Big\{ \sum_{s=\uparrow,\downarrow} \hat{\psi}_s^\dagger(\mathbf{x}) H_0 \hat{\psi}_s(\mathbf{x}) + U_0 \hat{\psi}_\uparrow^\dagger(\mathbf{x})\hat{\psi}_\downarrow^\dagger(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x})\Big\}. \tag{4.30}$$

- The field operator now has a spin index

$$\hat{\psi}_s(\mathbf{x}) = \sum_n \hat{a}_{s,n}\, \varphi_n(\mathbf{x})\chi_s$$

(χ_s = spinor i.e. $s = \uparrow \longrightarrow \begin{pmatrix}1\\0\end{pmatrix}$ and $s = \downarrow \longrightarrow \begin{pmatrix}0\\1\end{pmatrix}$)

($\hat{a}_{s,n}|\,0\,\rangle = |\,n, s\,\rangle$, $\quad n \to$ trap single particle state, $\qquad s = |\uparrow\rangle, |\downarrow\rangle$)

- We have,

$$\{\hat{\psi}_s(\mathbf{x}), \hat{\psi}_{s'}^\dagger(\mathbf{x}')\} = \delta_{ss'}\delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{4.31}$$

- The Hamiltonian already includes the fact that only atoms in two different spin-states can interact, see section 4.7.

For simplicity, we only consider a homogeneous system, with the following expansion for the

Fermion field operator:

$$\hat{\psi}_s(\mathbf{x}) = \sum_{\mathbf{k}} \frac{\hat{a}_{s,\mathbf{k}}}{\sqrt{2\pi}^3} \underbrace{\varphi_{\mathbf{k}}(\mathbf{x})}_{planewaves} \chi_s, \quad \varphi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\mathbf{x}}, \tag{4.32}$$

where $\mathcal{V}$ is a box-normalisation factor.

Using

$$(2\pi)^3 \delta^3(\mathbf{x}) = \int d^3\mathbf{x}\, e^{i\mathbf{k}\mathbf{x}}$$

we obtain,

Momentum-space Hamiltonian for the spin-mixture

$$\hat{H} = \underbrace{\sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}^\dagger_{\uparrow k} \hat{a}_{\uparrow k} + \hat{a}^\dagger_{\downarrow k} \hat{a}_{\downarrow k})}_{\hat{H}_0} + \underbrace{\frac{U_0}{\mathcal{V}} \sum_{\substack{k_1,k_2,k_3,k_4: \\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} \hat{a}^\dagger_{\uparrow k_3} \hat{a}^\dagger_{\downarrow k_4} \hat{a}_{\downarrow k_2} \hat{a}_{\uparrow k_1}}_{\hat{V}} \tag{4.33}$$

From this Hamiltonian, let us first find the energy of the unperturbed/ non-interacting Fermi-sea itself. The expectation value is

$$\begin{aligned} E^{(0)} =& \langle FS| \sum_k \frac{\hbar^2 k^2}{2m} (\hat{a}^\dagger_{\uparrow k} \hat{a}_{\uparrow k} + \hat{a}^\dagger_{\downarrow k} \hat{a}_{\downarrow k}) |FS\rangle \qquad (\hat{H}_0 \quad \text{only!}) \\ =& (4\pi) \int_0^{k_F,\uparrow} dk k^2 \underbrace{D}_{\substack{\downarrow \\ \text{density} \\ \text{of states}}} \frac{\hbar^2 k^2}{2m} + (4\pi) \int_0^{k_F,\downarrow} dk k^2 D \frac{\hbar^2 k^2}{2m} \\ \underset{\substack{Eq.\ (4.6), Eq.\ (4.8) \\ D=\mathcal{V}/(2\pi)^3}}{=}& \frac{3}{5} (E_{F\uparrow} N_\uparrow + E_{F\downarrow} N_\downarrow) \end{aligned}$$

In the second equality, we used the fact that number operators give 0 for wave-numbers above the Fermi-level and 1 below. Then we also already did the angular integration in spherical 3D coordinates for $\mathbf{k}$. Since energies are apparently separately found for each spin species, we have also derived the

Total energy of an ideal Fermi gas

$$E_{Tot} = \frac{3}{5} E_F N \tag{4.34}$$

Now let us find the change of the energy due to some small interactions U_0 using Rayleigh-

Schödinger perturbation theory. The first order energy correction, as usual, is:

$$E^{(1)} = \langle FS|\hat{V}|FS\rangle \underset{\substack{k_1=k_3,\\ k_2=k_4}}{=} \frac{U_0}{V}\sum_{k_1,k_2}\langle \hat{a}^\dagger_{\uparrow k_1}\hat{a}_{\uparrow k_1}\rangle\langle \hat{a}^\dagger_{\downarrow k_2}\hat{a}_{\downarrow k_2}\rangle = \frac{U_0}{V}N_\uparrow N_\downarrow \tag{4.35}$$

Below the first equality, we indicate that for a non-vanishing matrix elements, indices in $\hat{V}$ have to be equal as shown. We show (4.35) here mainly as example for perturbation theory in a many-body context.

Let us also look in the first order correction to the quantum state $|\,FS\,\rangle$:

The formula you know from basic quantum mechanics perturbation theory is:

$$\underbrace{|n^{(1)}\rangle}_{\text{perturbed state}} = \sum_{k\neq n}\frac{\langle\, k^{(0)}\,|\hat{V}\quad \overbrace{|\,n^{(0)}\,\rangle}^{\text{unpert. state}}}{E_n^{(0)}-E_k^{(0)}}\underbrace{|k^{(0)}\rangle}_{\text{basis}} \tag{4.36}$$

In our many-body context this translates to

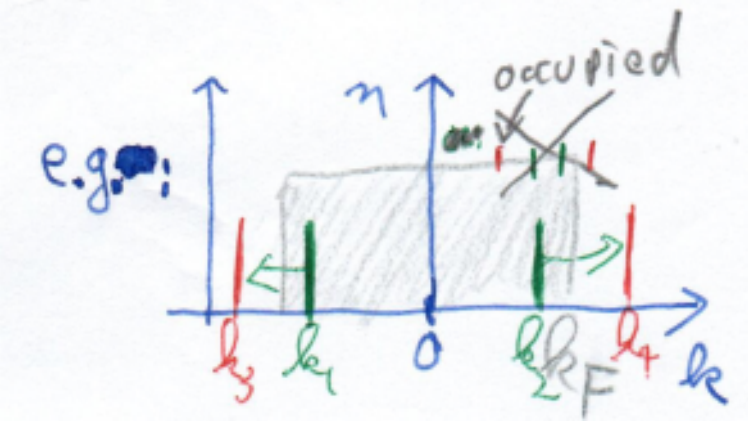
$$|\,FS^{(1)}\,\rangle = \sum_{\mathbf{N}}{}' \frac{\langle\,\mathbf{N}\,|\hat{V}|\,FS^{(0)}\,\rangle}{E^{(0)}-E_{\mathbf{N}}}|\,\mathbf{N}\,\rangle \tag{4.37}$$

- The prime $'$ on the sum shall denote that the sum does not include the state $|\,FS\,\rangle$ itself.
- We use Fock-states $|\,\mathbf{N}\,\rangle$, see Eq. (2.2), for Fermions, taking into account occupations of different spin states also.
- We find
$$E_{\mathbf{N}} = \sum_k \frac{\hbar^2k^2}{2m}(N_{k\uparrow}+N_{k\downarrow})$$
- For $\hat{V}$, see Eq. (4.33).

Let's evaluate the required Matrix elements:

$$\langle\,\mathbf{N}\,|\hat{V}|\,FS^{(0)}\,\rangle = \frac{U_0}{V}\sum_{\substack{k_1,k_2,k_3,k_4:\\ \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}} \underbrace{\langle\,\mathbf{N}\,|\hat{a}^\dagger_{\uparrow k_3}\hat{a}^\dagger_{\downarrow k_4}\ \underbrace{\hat{a}_{\downarrow k_2}\hat{a}_{\uparrow k_1}|\,FS^{(0)}\,\rangle}_{\substack{\text{we need}\\ |k_1|,|k_2|<k_F}}}_{\substack{\text{we need}\quad k_1=k_3,k_2=k_4\\ \text{Or,}\quad |k_3|,|k_4|>k_F}} \tag{4.38}$$

Below the braces we indicate conditions for operators acting on states to gives something non-zero. One choice, $k_1 = k_3$, $k_2 = k_4$ is boring, because we end up coupling $|\,FS\,\rangle$ with itself. However for the second choice $|k_3|, |k_4| > k_F$ we mix $|\,FS\,\rangle$ with the "double particle-hole excitation" state sketched below:



left: Double particle-hole excitation: A state with the filled Fermi sea, but then two atoms at momenta k_1 and k_2 were removed, and lifted above the Fermi surface to k_3 and k_4.

Let us give this is definition:

Particle-hole state

$$| \underbrace{(k_3 \uparrow)^e}_{\substack{\text{excitation with} \\ \text{wave-vector } \mathbf{k}_3}} \quad (k_4 \downarrow)^e \quad (k_2 \downarrow)^h \quad \underbrace{(k_1 \uparrow)^h}_{\substack{\text{hole with} \\ \text{wave-vector } \mathbf{k}_1}} \quad \rangle \tag{4.39}$$

eg: spin↑ spin↓

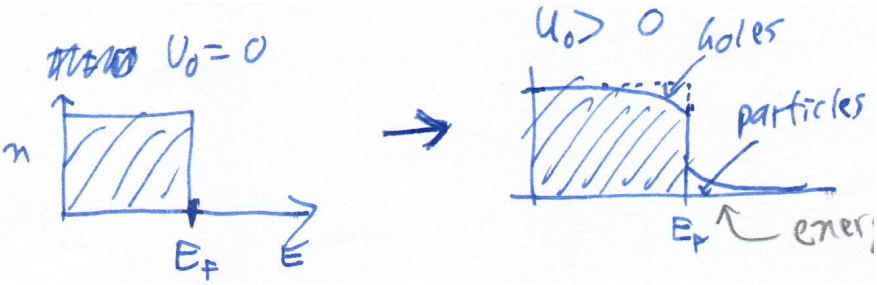
The perturbed Fermi-sea from Eq. (4.37) thus is

$$|\, FS^{(1)} \,\rangle = |\, FS^{(0)} \,\rangle + \frac{U_0}{V} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} \frac{|\, (k_3 \uparrow)^e (k_4 \downarrow)^e (k_2 \downarrow)^h (k_1 \uparrow)^h \,\rangle}{E^{(0)} - [\sum_{l=1,\cdots,4} \frac{\hbar^2 |k_l^2 - k_F^2|}{2m} + E^{(0)}]} \tag{4.40}$$

It is said that the interactions dress the FS with particle+hole pairs: A

Fermi-liquid is a Fermi sea, which interactions dress with particle+hole pairs as in Eq. (4.40).

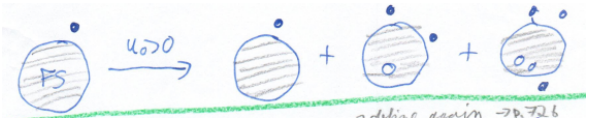
This leads to a softening/smearing out of the Fermi edge even at $T = 0$:



left: Fermion energy distribution without interactions (left), and with weak repulsive interactions (right), forming a Fermi-liquid. Particle and hole excitation becomes increasingly unlikely away from the Fermi surface, due to the energy denominator in (4.40).

Similarly to the ground-state, in the Fermi-liquid, also excited-states get dressed with other excited many-body states.

Fermi liquid theory can be understood as free fermions $|\, k, \underset{spin}{\sigma} \,\rangle$ evolving into fermionic quasi-particles with the same momentum and spin, due to interaction/dressing. These have a slightly modified effective mass m^*.

Quasi-particle cartoon: 

- Most properties of Fermi-liquid system are (surprisingly) similar to the non-interacting cases.
- Applied to electrons in a metal, this describes most non-superconducting metals.
- Cold-atom experiments:
  See Nascimbine et al. Nature 463 1057 (2010).
  Horikoshi et al. Science 327 442 (2010).

Week 11

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

4.10 Attractive interactions, pairing

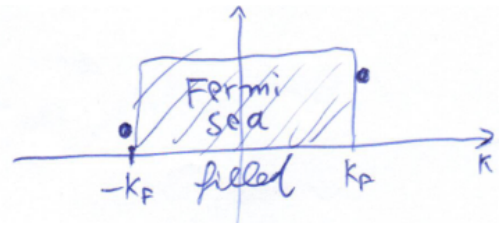
Lots of credit: Gora Shlyapnikov "Ultracold quantum gases, Degenerate Fermi gases". Part-II (internet).

- On first sight our previous discussion should be equally valid for weak attractive interactions ($U_0 < 0$ in Eq. (4.33)).
- However, another phenomenon precludes this, by making a filled Fermi-sea up to E_F, a bad starting point: Superfluid pairing.

4.10.1 Two-body Cooper-pairing

- The same pairing phenomenon gives rise to superconductivity in condensed matter systems (example D in section 2.3.1, free electron gas), we will discuss the condensed matter case here, not the cold-atom case, for a reason given at end of this section.

Assume a degenerate Fermi system at $T = 0 \implies$ all momentum states filled up to k_F. We assume for simplicity that these particles don't interact, but importantly Pauli-block all states up to $|k| = k_F$. (see section 2.2.2):



Now we add two interacting particles on top of this Fermi-sea, with Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\nabla^2_{\mathbf{x}_1} + \nabla^2_{\mathbf{x}_2}\right) + V(\underbrace{\mathbf{x}_1 - \mathbf{x}_2}_{\equiv \mathbf{r}}). \tag{4.41}$$

We make the Ansatz

$$\psi_0(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2\pi}^3}\int d^3\mathbf{k}\frac{g_\mathbf{k}}{\sqrt{\mathcal{V}}}\underbrace{\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2))}_{\text{symmetric}}\frac{1}{\sqrt{2}}\big[\underbrace{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}_{\text{anti-symmetric}}\big] \tag{4.42}$$

for the complete wavefunction including relative motion and spin, but ignoring the irrelevant center-of-mass co-ordinate. Note that the Ansatz has the correct symmetry for Fermions.

Insertion into relative-motion Schrödinger equation following from (4.41):

$$\int d^3\mathbf{k}\ \underbrace{\frac{\hbar^2\mathbf{k}^2}{m}}_{\equiv 2\epsilon_\mathbf{k}} g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2))+V(\mathbf{x}_1-\mathbf{x}_2)\int d^3\mathbf{k}\ \ g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)) = E\int d^3\mathbf{k}\ \ g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)). \tag{4.43}$$

($\hat{H}$ is spin independent)

- Write $\cos(\mathbf{kr}) = \frac{1}{2}(e^{i\mathbf{kr}}+e^{-i\mathbf{kr}})$, then apply on both sides $\frac{1}{\sqrt{2\pi}^3}\int d^3\mathbf{r}\,e^{-i\mathbf{k}'\mathbf{r}}$... and use that $\int d^3\mathbf{r}\,e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}} = (2\pi)^3\delta(\mathbf{k}'-\mathbf{k})$:

$$2\epsilon_{\mathbf{k}'}\underbrace{\frac{(g_{\mathbf{k}'}+g_{-\mathbf{k}'})}{2}}_{\substack{=g_{\mathbf{k}'}\text{ assume}\\ \text{symmetric}}} - Eg_{\mathbf{k}'} = -\frac{1}{(2\pi)^3}\int d^3\mathbf{k}\int d^3\mathbf{r}\,e^{-i\mathbf{k}'\mathbf{r}}V(\mathbf{r})\frac{g_\mathbf{k}}{2}(e^{i\mathbf{kr}}+e^{-i\mathbf{kr}}). \tag{4.44}$$

We define:

$$V_{\mathbf{k}'\mathbf{k}} = \frac{1}{(2\pi)^3}\int d^3\mathbf{r}\,e^{-i\mathbf{k}'\mathbf{r}}V(\mathbf{r})\,e^{i\mathbf{kr}}$$

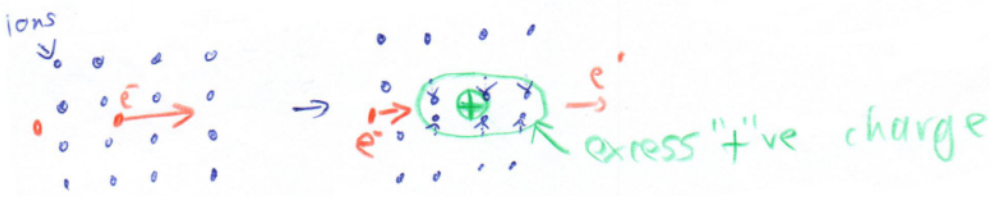
and then can write (4.44) as

$$\implies g_{\mathbf{k}'}(2\epsilon_{\mathbf{k}'}-E) = -\frac{1}{2}\int d^3\mathbf{k}\ \ (V_{\mathbf{k}'\mathbf{k}}g_\mathbf{k} + V_{\mathbf{k}'(-\mathbf{k})}\,g_\mathbf{k}). \tag{4.45}$$

Before proceeding, let us now ask how or why our two Fermions on top of the Fermi sea would interact, for the specific case of electron in a solid crystal.

Electrons in crystal:

- Surprisingly these effectively experience a weakly attractive interaction due to phonon-exchange.



- Negative charge of electron causes distortion of positively charged ion lattice with a lot of delay, due to inertia of the ions. The resulting local excess charge after the ions have finally moved, can attract another electron, see sketch.
- This effect can even be dominant over the direct $e^- - e^-$ Coulomb repulsion for large distances between the electrons, since the direct Coulomb interaction is heavily screened by the crystal ions.
- A QM treatment of the phonon mediated interactions in the figure, gives an energy cutoff for these interactions at the Debye frequency $\hbar\omega_D$, or equivalently a momentum cutoff $\equiv \Delta k$.

We thus take an attractive interaction for $V_{\mathbf{k}'\mathbf{k}}$ and assume it to be constant below the cutoff for simplicity:

$$V_{\mathbf{k}'\mathbf{k}} = \begin{cases} -|V| & ; k_F < |\mathbf{k}|, |\mathbf{k}'| < k_F + \Delta k \leftarrow \text{Debye cutoff} \\ 0 & ; \text{otherwise} \end{cases} \tag{4.46}$$

Hence $V_{\mathbf{k}'\mathbf{k}} = V_{\mathbf{k}'(-\mathbf{k})}$. Setting $V_{\mathbf{k}'\mathbf{k}} = 0$ for $|\mathbf{k}|, |\mathbf{k}'| < k_F$ incorporates the fact that due to the filled Fermi sea in the background, electrons cannot get scattered to these momenta through any interaction [6].

Our Schrödinger equation (Eq. (4.45)) can then be written as

$$g_{\mathbf{k}'} = \frac{+|V|}{(2\epsilon_{\mathbf{k}'} - E)} \int d^3\mathbf{k}\Big|_{\mathbf{k}:k_F<|\mathbf{k}|<k_F+\Delta k} g_{\mathbf{k}} \tag{4.47}$$

Next we perform the integral $\int d^3\mathbf{k}$ on both sides and cancel terms $\int d^3\mathbf{k} g_{\mathbf{k}}$, to reach

$$\frac{1}{|V|} = \int d^3\mathbf{k}\Big|_{\mathbf{k}:k_F<|\mathbf{k}|<k_F+\Delta k} \frac{1}{(2\epsilon_{\mathbf{k}} - E)}.$$

We convert the integral to spherical polar coordinates and reach

$$\frac{1}{|V|} = (4\pi) \int_{k_F}^{k_F+\Delta k} dk \frac{k^2}{(2\epsilon_k - E)}. \tag{4.48}$$

[6] Note, that we can interpret $\mathbf{k}$ as indicating both$^{(*)}$, the relative momentum of the pair $\mathbf{p}_{rel} = \hbar\mathbf{k}$, or the momentum of one of the members of the pair, e.g. $\mathbf{p}_1 = \hbar\mathbf{k}$ (the other member has momentum $\mathbf{p}_2 = -\mathbf{p}_1$ in that case. The constraints written above on possible values of $\mathbf{k}$ arise from the latter view.

$^{(*)}$ *[This slightly confusing fact is due to the need to have CM momentum $\mathbf{k}_{CM} \approx 0$ and the relative momentum being defined as $\mathbf{p}_{rel} = (\mathbf{p}_1 - \mathbf{p}_2)/2$. See some texts on QM of the two-body problem. One way to justify this, is that we want $[\hat{\mathbf{r}}, \hat{\mathbf{p}}_{rel}] = i\hbar$, where $\hat{\mathbf{r}} = \hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2$]*

Change integration variable to energy $dk = m/\hbar^2 k\, d\epsilon$

$$\frac{1}{|V|} = \left(\frac{4\pi m}{\hbar^2}\right) \int_{\epsilon_F}^{\epsilon_F + \hbar\omega_D} d\epsilon \frac{\overbrace{k}^{\approx k_F \text{ due to } \hbar\omega_D \ll \epsilon_F}}{(2\epsilon - E)}. \tag{4.49}$$

We finally arrive at

$$\frac{1}{|V|} = \mathcal{N} \int_{\epsilon_F}^{\epsilon_F + \hbar\omega_D} \frac{d\epsilon}{(2\epsilon - E)} = \frac{\mathcal{N}}{2} \log\left(\frac{2E_F - E + 2\hbar\omega_D}{2E_F - E}\right), \tag{4.50}$$

where we have used the shortcut notation $\mathcal{N} = 4\pi m k_F/\hbar^2$. For $\mathcal{N}|V| \ll 1$ (weak coupling approximation), we can solve this for E and then obtain the

Cooper pair energy:

$$E_{\text{pair}} = E = 2E_F - 2\hbar\omega_D \exp\left[-\frac{2}{\mathcal{N}|V|}\right]. \tag{4.51}$$

(size $\gg$ inter-particle distance in medium)

Comments:

- $E < 2E_F$ for arbitrarily weak interactions. This signals an instability of the Fermi-sea towards bound states (Cooper pairs) (relative to E_F). (Unlike the repulsion case, non-interacting scenario is not a good starting point here.)
- A cooper pair is a bound state of Fermions above the Fermi sea, bound together by very weak attractive, phonon-mediated interactions.
- In the discussion in this section, we only concluded that the Cooper pair is a bound-state since the pairing gives a negative energy shift to the energy of two unpaired Fermions on the Fermi surface. This view is further corroborated when evaluating the coefficients $g_{\mathbf{k}}$ to first write the wave function of a Cooper pair first in Fourier space, and then in position space. One finds a wavefunction for relative motion $\psi_0(\mathbf{x}, \mathbf{y}) \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, with symmetric $\psi_0(\mathbf{x}, \mathbf{y})$, that goes to zero for large $|\mathbf{x} - \mathbf{y}|$, hence is a bound state. See [A. Kadin, Journal of Superconductivity and Novel Magnetism, "*Spatial Structure of the Cooper Pair*" (2007)] for a discussion of the spatial Cooper pair wave function.
- For repulsive interactions $E > 2E_F$ (no problem).
- Without blocked Fermi-sea (let $\int_0^{\hbar\omega_D} d\epsilon$ in Eq. (4.50)), we get $E > 0$ (no bound states).
- The size (orbital radius)(of a Cooper pair is typically much larger than the inter-particle distance in medium.
- Without Debye cutoff: Eq. (4.50) is UV divergent $\rightarrow$ need regularisation/renormalisation, see section 3.5.2.

The last point is the reason why we did the calculation for a solid-state setup rather cold atom Fermion gases: In the Fermi-gas there is no natural cutoff, so the calculation would need renormalisation, which we want to avoid here. But Cooper-pairs form in cold atomic Fermi gases for the same reason as in an electron gas. One finds a

Cooper pair energy in an atomic Fermi gas that is a spin-mixture of $\uparrow$ and $\downarrow$:

$$E_{\text{pair}} = E = 2E_F - 2E_F \exp\left[-\frac{\pi}{2k_F|a_s|}\right]. \tag{4.52}$$

This sets the right order of magnitude.

- Roughly, to reach this keep variable k in Eq. (4.49), change cutoff from $\hbar\omega_D$ to $\to E_F$ and use $|V| = 4\pi\hbar^2|a_s|/m$.

4.10.2 Many Cooper pairs

- In the previous section we saw that an attractively interacting degenerate Fermi-gas is unstable to pair formation, but we dealt with a single pair. What happens for many?
- Tight pairs (molecules) would be Bosons, they could condense. What does that cause? But these pairs are not that tightly bound....
- Also: Now we also want to include all versus all interactions, not just among a single pair as in section 4.10.

As we did in section 3.3.2 for a BEC, we want to build the statements above into a useful mathematical Ansatz for the many-body wave function. Unlike there, we would want to now describe the condensation of pairs.

In first quantization, we could write

$$\psi(\mathbf{x}) = \hat{\mathcal{P}}_F \left[\psi_0(x_1, x_2)\,\psi_0(x_3, x_4)...\psi_0(x_{N-1}, x_N)\right], \tag{4.53}$$

where ψ_0 is the pairing wave function we had found in section 4.10.1. Here, $\hat{\mathcal{P}}_F$ is the anti-symmetrisation operator introduced in Eq. (2.1).

We could write Eq. (4.53) more elegantly as

$$\hat{c}^{\dagger N}\,|\,0\,\rangle$$

for N Cooper pairs, with

$$\hat{c}^\dagger = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x}, \mathbf{y}) \hat{\Psi}^\dagger_\uparrow(\mathbf{x}) \hat{\Psi}^\dagger_\downarrow(\mathbf{y}), \tag{4.54}$$

the Cooper-pair creation operator.[7]

Using the operator (4.54), we could write a Cooper pair condensate as a

Coherent state of pairs

$$|\psi_{\rm BCS}\rangle = \mathcal{N} e^{\gamma \hat{c}^\dagger} |\,0\,\rangle \tag{4.55}$$

where, $\mathcal{N}$ is normalisation factor, and γ the complex number characterising the coherent state (c.f. α in (2.42)).

- If $\hat{c}^\dagger$ was a bosonic operator, this would be analogous to our earlier treatments of BEC. But in general, we can neither clearly associate commutation, nor anti-commutation relations with $\hat{c}^\dagger$.
- We need some more powerful theory....

4.10.3 BCS-Theory

Let us consider the BCS Many-body theory of Fermion pairing due to Bardeen-Cooper-Schrieffer, which also explains superconductivity. Instead of attempting to deal with Cooper pairs, this starts out with the following trick Where for a BEC, we had assumed a non-zero mean-field, now we can assume a

non-zero pairing-field: (also "**Order parameter**")

$$0 \neq \Delta(\mathbf{x}) = U_0 \langle \hat{\Psi}_\uparrow(\mathbf{x}) \hat{\Psi}_\downarrow(\mathbf{x}) \rangle \tag{4.56}$$

- It shall turn out only after we did the ensuing calculation, that this assumption is in fact related to Cooper pairing.
- Clearly (4.56) involves an assumption on the many-body quantum state. All states that we find in the following, have to be checked for consistency with (4.56) in the end.
- For the moment just take (4.56) as a mathematical assumption, and let's see where it leads us....

[7] To see that this name makes sense, write $\hat{c}^\dagger|\,0\,\rangle$ and apply the field operators to the vacuum to reach a Fermionic Fock state $|\,\mathbf{y}\downarrow, \mathbf{z}\uparrow\rangle$ expressed using the position basis. Then write the position-space representation: $\langle\,\mathbf{x}'\mathbf{y}'\,|\hat{c}^\dagger|\,0\,\rangle$. Using $\langle\,\mathbf{x}\,|\,\mathbf{x}'\,\rangle = \delta(\mathbf{x}-\mathbf{x}')$, you should find the result discussed at the end of section 4.10.1.

From these initial considerations, we will now approximately diagonalize the interacting Hamiltonian (4.30) with $U_0 < 0$, assuming equal numbers of $\uparrow, \downarrow$ Fermions in a homogeneous system.

We "simplify" the interaction term as

$$U_0 \hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) \approx \frac{1}{2}\Big\{\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\rangle\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \langle\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x}) + \langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\psi^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x}) \tag{4.57}$$

$$+ \langle\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle\psi^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) - \Big(\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle\psi^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \langle\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\psi^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\Big)\Big\}. \tag{4.58}$$

***Comments*:**

- This is motivated again by Wick's theorem (3.86), use Fermionic signs as discussed earlier.
- Wick's theorem gets some minus signs when Fermions are involved.
- The red factor of 1/2 is required to make the assumption consistent with Wick's theorem. I am confused as it is not there in some of the literature.

We further define:

Hartree fields	$\mathcal{U}_\uparrow(\mathbf{x}) = U_0\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle$ (same for $\downarrow$)	(4.59)
Fock fields	$\mathcal{F}_\uparrow(\mathbf{x}) = U_0\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$ (same for $\uparrow\leftrightarrow\downarrow$)	(4.60)

- In the paired state (Eq. (4.55)), $\mathcal{F}_{\uparrow,\downarrow} = 0$ (Proof $\rightarrow$ Assignment 6).
- In a homogeneous system, $\Delta(\mathbf{x}) = \Delta$ ($\Delta \in \mathbb{R}$), $\mathcal{U}_\uparrow(\mathbf{x}) = \mathcal{U}_\downarrow(\mathbf{x}) = U$ can be constant. Note: $U \neq U_0$, but includes it.

From (4.58) we now have:

$$U_0 \hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) \approx \Delta^*\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \Delta\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x}) + U\big(\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\big).$$

Finally, we re-assemble the Hamiltonian (4.30) and augment it to a grand-canonical one $\hat{K} = \hat{H} - \mu\hat{N}$:

$$\hat{K} = \sum_{s=\uparrow,\downarrow} \int d^3\mathbf{x}\, \hat{\Psi}_s^\dagger(\mathbf{x}) \Big[-\frac{\hbar^2\nabla^2}{2m} + U - \mu \Big] \hat{\Psi}_s(\mathbf{x}) + \int d^3\mathbf{x} \Big[\Delta^* \hat{\Psi}_\downarrow(\mathbf{x}) \hat{\Psi}_\uparrow(\mathbf{x}) + \Delta\, \hat{\Psi}_\uparrow^\dagger(\mathbf{x}) \hat{\Psi}_\downarrow^\dagger(\mathbf{x}) \Big].$$

In the homogeneous case, it is again simpler to work in the momentum basis. As we did for (4.33), we reach the

BCS/pairing Hamiltonian:

$$\hat{K} = \hat{H}_{\rm BCS} = \sum_{\mathbf{k},s=\uparrow,\downarrow} \xi_\mathbf{k} \hat{a}_{\sigma\mathbf{k}}^\dagger \hat{a}_{\sigma\mathbf{k}} + \Delta \sum_\mathbf{k} \left(\hat{a}_{\downarrow\mathbf{k}} \hat{a}_{\uparrow(-\mathbf{k})} + \hat{a}_{\uparrow(-\mathbf{k})}^\dagger \hat{a}_{\downarrow\mathbf{k}}^\dagger \right) \tag{4.61}$$

where,

$$\xi_\mathbf{k} = \frac{\hbar^2 k^2}{2m} + U - \mu.$$

- In section 3.4, we had kept only Bose-gas excitations up to order $\hat{\chi}^2$, and then diagonalized the Hamiltonian using the Bogoliubov transformation (e.g. Eq. (3.66)).
- This trick works generically for Hamiltonians up to quadratic in $\hat{a}$, $\hat{a}^\dagger$, thus also here, for Eq. (4.61) . Here we define the

Bogoliubov-transformation (BCS-system)

$$\begin{aligned} \hat{\alpha}_{\uparrow\mathbf{k}} &= u_\mathbf{k} \hat{a}_{\uparrow\mathbf{k}} - v_\mathbf{k} \hat{a}_{\downarrow(-\mathbf{k})}^\dagger \\ \hat{\alpha}_{\downarrow\mathbf{k}} &= u_\mathbf{k} \hat{a}_{\downarrow\mathbf{k}} + v_\mathbf{k} \hat{a}_{\uparrow(-\mathbf{k})}^\dagger \end{aligned} \tag{4.62}$$

Comparison to BEC: In Chapter-3, we were more ambitious and did the Bogoliubov transformation directly for an inhomogeneous system. For the homogeneous case, Eq. (3.66) gives:

$$\hat{\alpha}_\mathbf{k} = u_\mathbf{k} \hat{a}_\mathbf{k} + v_\mathbf{k} \hat{a}_\mathbf{k}^\dagger, \tag{4.63}$$

which is quite similar to (4.62). To reach this, use $\hat{\Psi}(\mathbf{x}) = \int d^3\mathbf{k} \frac{\hat{a}_\mathbf{k}}{\sqrt{2\pi}^3} \varphi_\mathbf{k}(\mathbf{x})$ and the definition of a δ function.

The quasi-particle operators (Eq. (4.62)) should satisfy Fermi commutation relations:

$$\left\{ \hat{\alpha}_{s\mathbf{k}}, \hat{\alpha}_{s'\mathbf{k}'}^\dagger \right\} \overset{\text{exercise}}{=\!=} (u_\mathbf{k}^2 + v_\mathbf{k}^2) \delta_{\mathbf{k}\mathbf{k}'} \delta_{ss'}.$$

We thus have to require the normalisation $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$.

Using the latter, we can derive the

inverse Bogoliubov transformation (Proof → exercise, signs might be wrong)

$$\begin{aligned}\hat{a}_{\uparrow\mathbf{k}} &= u_{\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}\\ \hat{a}_{\downarrow\mathbf{k}} &= u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}.\end{aligned} \tag{4.64}$$

Inserting Eq. (4.62) into Eq. (4.61) gives

$$\begin{aligned}\hat{K} = \sum_{\mathbf{k}}\Big\{&\Big[\Big(\xi_{\mathbf{k}}u_{\mathbf{k}} + \Delta v_{\mathbf{k}}\Big)u_{\mathbf{k}} - \Big(\xi_{\mathbf{k}}v_{\mathbf{k}} - \Delta u_{\mathbf{k}}\Big)v_{\mathbf{k}}\Big]\Big(\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} + \hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\Big)\\ &+ \Big[\Big(\Delta v_{\mathbf{k}} + \xi_{\mathbf{k}}u_{\mathbf{k}}\Big)v_{\mathbf{k}} - \Big(\Delta u_{\mathbf{k}} - \xi_{\mathbf{k}}v_{\mathbf{k}}\Big)u_{\mathbf{k}}\Big]\Big(\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} + \hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}}\Big)\\ &+ 2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}\Big\} \qquad \text{(steps see p.786)}\end{aligned}$$

Detailed steps: Note: ($u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$ from parity invariance).

$$\begin{aligned}\hat{K} = \sum_{\mathbf{k}}\xi_{\mathbf{k}}\Big[&\Big(\overbrace{u_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}_{\downarrow(-\mathbf{k})}}^{\hat{a}^\dagger_{\uparrow\mathbf{k}}}\Big)\Big(\overbrace{u_{\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}}^{\hat{a}_{\uparrow\mathbf{k}}}\Big) + \Big(\overbrace{u_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}}^{\hat{a}^\dagger_{\downarrow\mathbf{k}}}\Big)\Big(\overbrace{u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}}^{\hat{a}_{\downarrow\mathbf{k}}}\Big)\Big]\\ + \Delta\Big[&\Big(\underbrace{u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}}_{\hat{a}_{\downarrow\mathbf{k}}}\Big)\Big(\underbrace{u_{-\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} - v_{-\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}}_{\hat{a}_{\uparrow(-\mathbf{k})}}\Big) + \Big(\underbrace{u_{-\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} - v_{-\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}}_{\hat{a}^\dagger_{\uparrow(-\mathbf{k})}}\Big)\Big(\underbrace{u_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}}_{\hat{a}^\dagger_{\downarrow\mathbf{k}}}\Big)\Big]\\ = \sum_{\mathbf{k}}\xi_{\mathbf{k}}\Big[&u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}_{\uparrow\mathbf{k}} + v_{\mathbf{k}}^2\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}\\ &+ u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}^2\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\Big]\\ + \Delta\Big[&u_{\mathbf{k}}^2\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}} - v_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}}\\ &+ u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\uparrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} - v_{\mathbf{k}}^2\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\Big]\end{aligned}$$

$$\Big(\text{Use } \sum_{\mathbf{k}}\xi_{\mathbf{k}}\hat{\alpha}^\dagger_{(-\mathbf{k})}\hat{\alpha}_{(-\mathbf{k})} = \sum_{\mathbf{k}}\xi_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}, \text{ since } \xi_{\mathbf{k}} = \xi_{-\mathbf{k}}\Big)$$

$$\begin{aligned}= \sum_{\mathbf{k}}\Big[&\xi_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) + 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}\Big]\big(\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} + \hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\big) + \underbrace{2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}}_{\text{from commutators}}\\ + \Big[&2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} - (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2)\Delta\Big]\big(\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + \hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}}\big)\end{aligned}$$

By demanding the

Bololiubov de Gennes equations (BCS, Fermions)

$$\begin{aligned} \xi_{\mathbf{k}} u_{\mathbf{k}} + \Delta v_{\mathbf{k}} &= \epsilon_{\mathbf{k}} u_{\mathbf{k}} \\ -\xi_{\mathbf{k}} v_{\mathbf{k}} + \Delta u_{\mathbf{k}} &= \epsilon_{\mathbf{k}} v_{\mathbf{k}}. \end{aligned} \tag{4.65}$$

We diagonalize the Hamiltonian into

$$\hat{K} = E_0 + \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k},s} \hat{\alpha}_{\mathbf{k},s} \tag{4.66}$$

where, $E_0 = \sum_{\mathbf{k}} 2(\xi_{\mathbf{k}} v_{\mathbf{k}}^2 - \Delta u_{\mathbf{k}} v_{\mathbf{k}})$.

- This again has the form of non-interacting quasi-particles.

To find out more about the excitations of the system, we have to solve Eq. (4.65). In matrix form

$$\begin{pmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \epsilon_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}. \tag{4.67}$$

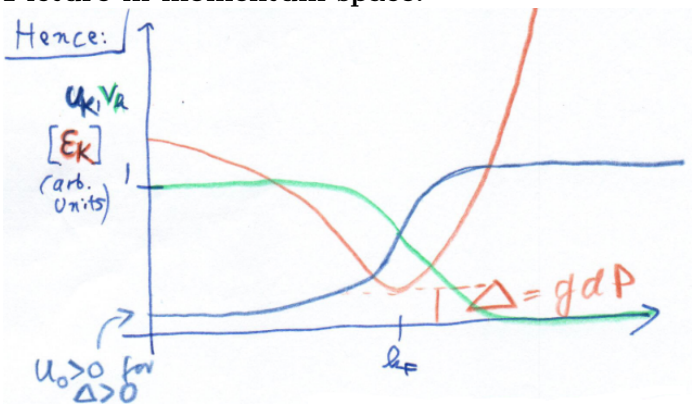
Using also $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$, we proceed as for (3.68). The solutions are:

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right), v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right), \epsilon_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} \tag{4.68}$$

for particle amplitude $u_{\mathbf{k}}$, hole amplitude $v_{\mathbf{k}}$ and dispersion relation, quasiparticle-energy $\epsilon_{\mathbf{k}}$.

- Recall $\xi_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m + U - \mu = \hbar^2\mathbf{k}^2/2m - \tilde{\mu}$ (see Eq. (4.61)), using $\tilde{\mu} = \mu - U$.
- $\tilde{\mu}$ is the Fermi-energy at $T = 0$.

Picture in momentum space:



- k_f comes in via $\mu = E_F$.
- Behavior of u, v logical from particle/hole excitation interpretation (look at $\alpha^\dagger$). Above the Fermi energy, there are no holes to make.
- Crucial feature of dispersion relation is the energy gap $\epsilon_{\min} = \Delta$. Thus, if $\Delta > 0$, ϵ_k is never zero.

Discussion of diagonalized Hamiltonian (4.66):

Ground state:

Already from (Eq. (4.66)), we can understand the system better:

- As was the case for Bose-gas, the ground state of the system is one with no quasi-particles (c.f. Eq. (3.63)). We call this state the quasi-particle vacuum $|\psi_0\rangle$, and define it via

$$\hat{\alpha}_{s\mathbf{k}}|\psi_0\rangle = 0. \tag{4.69}$$

  (compare $\hat{\alpha}_{s\mathbf{k}}|\,0\,\rangle = 0$ for the bare vacuum)

- We can easily write one such state explicitly, namely

$$|\psi_0\rangle = \prod_{\mathbf{k}'s'} \hat{\alpha}_{\mathbf{k}'s'}|\,0\,\rangle \tag{4.70}$$

Reason: This works since $\hat{\alpha}_{s\mathbf{k}}^2 = 0$ (from $\{\hat{\alpha}_{s\mathbf{k}}, \hat{\alpha}_{s\mathbf{k}}\} = 0$).

We can then use Eq. (4.62) to explicitly obtain the

BCS state:

$$|\psi_{\text{BCS}}\rangle = |\psi_0\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}\uparrow} \hat{a}^\dagger_{(-\mathbf{k})\downarrow}\right)|\,0\,\rangle. \tag{4.71}$$

- To see this, start by first evaluating $\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}_{\uparrow(\mathbf{k})}|\,0\,\rangle = \cdots = v_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}\uparrow}\hat{a}^\dagger_{(-\mathbf{k})\downarrow})|\,0\,\rangle$. Then do the same for all other $\mathbf{k}'$. Finally a factor $\prod_{\mathbf{k}} v_{\mathbf{k}}$ is taken care of by normalising the state.
- Each possible pair can be either occupied (v) or unoccupied (u).

Ground state energy:

We can now verify that the pairing assumption $\Delta \neq 0$ has lowered the energy compared to the unpaired Fermi-sea.

$$\langle\psi_{\text{BCS}}|\hat{K}|\psi_{\text{BCS}}\rangle - \langle FS|\hat{K}|FS\rangle = \sum_{\mathbf{k}} \big(\underbrace{2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}}_{E_0,\text{ see (4.66)}}\big) - \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} \underbrace{2}_{\substack{\text{spin}\\ \uparrow\downarrow}} \underbrace{\xi_{\mathbf{k}}}_{\substack{\text{energy relative}\\ \text{to Fermi-sea}}}$$

$$= \frac{\hbar^2k^2}{2m} - \tilde{\mu} = \frac{\hbar^2}{2m}(k^2 - k_F^2)$$

$$= \sum_{\mathbf{k}} \big\{2v_{\mathbf{k}} \underbrace{(\xi_{\mathbf{k}}v_{\mathbf{k}} - \Delta u_{\mathbf{k}})}_{\substack{=-\epsilon_{\mathbf{k}}v_{\mathbf{k}}\\ Eq.\ (4.65)}}\big\} - \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} 2\xi_{\mathbf{k}} \overset{*}{=} \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} \big\{-2\epsilon_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\xi_{\mathbf{k}}\big\}$$

$$\overset{\text{Eq. (4.68)}}{=\!=} \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} \left(-\epsilon_{\mathbf{k}}\left(1 - \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right) - 2\xi_{\mathbf{k}}\right) = \underbrace{\sum_{\mathbf{k}} \big(\underbrace{-\xi_{\mathbf{k}}}_{>0} - \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}\big)}_{<0}$$

(*): The reason we can restrict the first sum also to $|\mathbf{k}| < k_F$ is that $v_{\mathbf{k}}^2 \to 0$ for $|k| > k_F$, see figure on page 98

- Overall we lower the total energy of the system only for a non-zero gap Δ.

We can now finally actually see that the BCS state we got is the pair-coherent state we guessed in Eq. (4.55). By going to Fourier-space, we can rewrite the pair operator

$$\hat{c}^\dagger = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y})\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{y}) \qquad \text{(see Eq. (4.54))}$$

as

$$\hat{c}^\dagger = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}. \tag{4.72}$$

(see details A below). Then, using Campbell Baker Hausdorff formula (see assignment 2) and $[\hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{(-\mathbf{k})}, \hat{a}^\dagger_{\mathbf{k}'}\hat{a}^\dagger_{(-\mathbf{k}')}] = 0$ (see details A&B below)

$$\mathcal{N}e^{\gamma\hat{c}^\dagger} = \mathcal{N}e^{\sum_{\mathbf{k}}\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}} \overset{(*)}{=\!=} \mathcal{N}\prod_{\mathbf{k}} e^{\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}}$$
$$\overset{\text{Fermions}}{=\!=} \mathcal{N}\prod_{\mathbf{k}}\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right).$$

With moving $\mathcal{N}$ into the product (detail C below), we reach the the form

BCS state as coherent pair state

$$|\psi_{\text{BCS}}\rangle = e^{\gamma\hat{c}^\dagger}|\,0\,\rangle = \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)|\,0\,\rangle \tag{4.73}$$

Proof details
A:

$$\hat{c}^\dagger = \int d^3\mathbf{x}\int d^3\mathbf{y}\,\varphi_0(\mathbf{x},\mathbf{y})\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{y})$$
$$\left(\text{Use } \hat{\Psi}_\uparrow(\mathbf{x}) = \sum_{\mathbf{k}}\frac{1}{\sqrt[3]{2\pi}}\hat{a}_{\uparrow\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{\mathcal{V}}}\right)$$
$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{(2\pi)^3}\int d^3\mathbf{x}\int d^3\mathbf{y}\varphi_0(\mathbf{x}-\mathbf{y})e^{-i\mathbf{k}\cdot\mathbf{x}}e^{-i\mathbf{k}'\cdot\mathbf{y}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$

change to relative and C.M. co-ordinates $\mathbf{r} = \mathbf{x}-\mathbf{y},\ \mathbf{R} = (\mathbf{x}+\mathbf{y})/2$

$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{(2\pi)^3}\int d^3\mathbf{r}\int d^3\mathbf{R}\varphi_0(\mathbf{r})e^{-i\mathbf{k}\cdot(\mathbf{R}-\frac{\mathbf{r}}{2})}e^{-i\mathbf{k}'\cdot(\mathbf{R}+\frac{\mathbf{r}}{2})}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$
$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\underbrace{\left(\frac{\int d^3\mathbf{r}}{\sqrt[3]{2\pi}}\varphi_0(\mathbf{r})e^{-i(\frac{\mathbf{k}'-\mathbf{k}}{2})\cdot\mathbf{r}}\right)}_{F.T.\ \tilde{\varphi}_0\left(\frac{\mathbf{k}'-\mathbf{k}}{2}\right)}\underbrace{\left(\frac{\int d^3\mathbf{R}}{\sqrt[3]{2\pi}}e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{R}}\right)}_{=\sqrt[3]{2\pi}\delta(\mathbf{k}+\mathbf{k}')}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$
$$= \sum_{\mathbf{k}}\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})} \ \text{ with } \varphi_{\mathbf{k}} = \frac{\sqrt[3]{2\pi}\tilde{\varphi_0}(-\mathbf{k})}{\mathcal{V}}.$$

B:

$$\left[\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}}, \hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\right] = \hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'} - \hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}} \overset{\text{use anti-commutators}}{=\!=} 0$$

C: Determine $\mathcal{N}$ for which $|\,\psi_{pair}\,\rangle \equiv \mathcal{N}\prod_{\mathbf{k}}\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)$ is normalized $\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle = 1$. Let us rewrite $|\,0\,\rangle = |\,0_{\mathbf{k}\uparrow}, 0_{\mathbf{k}\downarrow}, 0_{-\mathbf{k}\uparrow}, 0_{-\mathbf{k}\downarrow}\,\rangle \otimes |\,0_{\text{other }\mathbf{k}}\,\rangle$, where we have singled out the Fock space occupations for the forward and backward direction of a specific $\mathbf{k}$, with all possible spins. Since $\hat{a}_{\pm\mathbf{k}'}$ for any other $\mathbf{k}' \neq \mathbf{k}$ do not affect this sub-space, we can calculate normalisation separately

in each of these segments. Then

$$\begin{aligned}\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle &= \mathcal{N}^2\prod_{\mathbf{k},\mathbf{k}'}\langle\,0\,|\left(1+\gamma^*\varphi^*_{\mathbf{k}}\hat{a}_{\downarrow(-\mathbf{k})}\hat{a}_{\uparrow\mathbf{k}}\right)\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)|\,0\,\rangle \\ &= \mathcal{N}^2\prod_{\mathbf{k},\mathbf{k}'(halfspace)}\langle\,0\,|\left(1+\gamma^*\varphi^*_{\mathbf{k}}\hat{a}_{\downarrow(-\mathbf{k})}\hat{a}_{\uparrow\mathbf{k}}\right)\left(1+\gamma^*\varphi^*_{-\mathbf{k}}\hat{a}_{\downarrow(\mathbf{k})}\hat{a}_{\uparrow(-\mathbf{k})}\right) \\ &\times\left(1+\gamma\varphi'_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow(-\mathbf{k}')}\right)\left(1+\gamma\varphi_{-\mathbf{k}'}\hat{a}^\dagger_{\uparrow(-\mathbf{k}')}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\right)|\,0\,\rangle \qquad (4.74)\end{aligned}$$

In the second equality we have split the products over $\mathbf{k}$ such that the symbol only contains half of space (say with positive k_x) and the pieces in the other half are made explicit by writing a part with $\mathbf{k}\to(-\mathbf{k})$. We can now collect the combination in which operators may act so that rhs and lhs are not orthogonal in the end. You shall find

$$\begin{aligned}\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle &= \mathcal{N}^2\prod_{\mathbf{k},\mathbf{k}'(halfspace)}\left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right)\left(1+|\gamma|^2|\varphi'_{\mathbf{k}}|^2\right) = \mathcal{N}^2\left(\prod_{\mathbf{k}(halfspace)}\left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right)\right)^2 \\ &\overset{\varphi_{\mathbf{k}}=\varphi_{-\mathbf{k}}}{=} \mathcal{N}^2\prod_{\mathbf{k}}\left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right) \qquad (4.75)\end{aligned}$$

We now see that a way to normalize the state is the choice $\mathcal{N}=\prod_{\mathbf{k}}\frac{1}{\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}}$. Inserting this into $|\,\psi_{pair}\,\rangle$ and distributing each factor for $\mathbf{k}$ from $\mathcal{N}$ onto the main expression gives the form (4.73) if we call $u_{\mathbf{k}}=1/\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}$ and $v_{\mathbf{k}}=\gamma\varphi_{\mathbf{k}}/\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}$.

4.10.4 Self consistency of BCS-Theory

Before we move to the consequences of the gap, let us calculate it. (Recall, we just assumed $\langle\hat{\Psi}\hat{\Psi}\rangle=\Delta$ at the onset of section 4.10.3.)

Recall that the BCS calculation started with an input non-vanishing pairing field $\Delta=U_0\langle\hat{\Psi}_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$. Now we have actually found the quantum ground state with which to evaluate the right hand side, namely (4.71). That state depends on u, v and these in turn depend on Δ through (4.65). We now have to check that the theory is self consistent, which means we can correctly get Δ out, when we evaluate $U_0\langle\hat{\Psi}_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$.

Starting state (**): We assume $\langle\ \rangle$ pertains to a Fock-state (or thermal mixture of those) with $N_{\mathbf{k}}$ Bogoliubov excitations in mode k. For all $N_{\mathbf{k}}=0$, this includes the BCS ground state (4.71).

Let us evaluate the pairing field. Since we are in a homogenous system $\Delta(\mathbf{x})$ does not depend on $\mathbf{x}$ and is equal to its mean value over space $\Delta=\int d^3\mathbf{x}\,\Delta(\mathbf{x})/\mathcal{V}$, where $\mathcal{V}$ is some quantisation volume.

Then

$$\Delta = U_0 \int d^3\mathbf{x} \langle \hat{\Psi}_\uparrow(\mathbf{x}) \hat{\Psi}_\downarrow(\mathbf{x}) \rangle / \mathcal{V} = \frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle \hat{a}_{\uparrow\mathbf{k}} \hat{a}_{\downarrow\mathbf{k}'} \underbrace{\int d^3\mathbf{x} \frac{\exp\left[i(\mathbf{k}+\mathbf{k}')\mathbf{x}\right]}{\mathcal{V}}}_{=\delta_{\mathbf{k},\mathbf{k}'}} \rangle$$

$$= \frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \langle \hat{a}_{\uparrow\mathbf{k}} \hat{a}_{\downarrow(-\mathbf{k})} \rangle$$

$$\overset{\text{Eq. (4.64)}}{=\!=} \frac{U_0}{\mathcal{V}} \int d^3\mathbf{k} \big\langle \big(u_{\mathbf{k}} \hat{\alpha}_{\downarrow(-\mathbf{k})} + v_{\mathbf{k}} \hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\big)\big(u_{\mathbf{k}} \hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}} \hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}\big) \big\rangle$$

$$\overset{(**)}{=\!=} -\frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} (1 - 2N_{\mathbf{k}})$$

where,

$$N_{\mathbf{k}} = \frac{1}{\exp(\epsilon_{\mathbf{k}}/k_B T) + 1}.$$

We have $u_{\mathbf{k}} v_{\mathbf{k}} = \Delta / 2\epsilon_{\mathbf{k}}$ from Eq. (4.68), hence

$$\Delta = -\frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \frac{\Delta}{2\epsilon_{\mathbf{k}}} \left(1 - 2\frac{1}{\exp(\epsilon_{\mathbf{k}}/k_B T) + 1}\right). \tag{4.76}$$

We divide both sides by Δ, use $U_0 = -|U_0|$ and reform exp into tanh and turn the sum into an integration to reach

the **gap-equation** (consistency condition)

$$|U_0| \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\tanh(\epsilon_{\mathbf{k}}/2k_B T)}{2\epsilon_{\mathbf{k}}} = 1. \tag{4.77}$$

- Here we really needed $U_0 < 0$, else this would <u>not</u> have a solution. That means that for repulsive interactions, our assumption of pairing $\Delta \neq 0$ could never be consistent.

At zero temperature:

$$|U_0| \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\sqrt{\Delta_0^2 + \xi_{\mathbf{k}}^2}} = 1. \tag{4.78}$$

The main contribution to the integral is from $|\mathbf{k}| \approx k_F$ (there the denominator is smallest, *see picture of Δ earlier*). Near k_F, we Taylor expand $\xi_{\mathbf{k}}$ to first order:

$$\xi_{\mathbf{k}} \approx \underbrace{\frac{\hbar^2 k_F^2}{2m}}_{E_F} + \underbrace{\frac{\hbar^2}{m} k_F}_{\hbar v_F} (k - k_F) + \mathcal{O}(k - k_F)^2 + U - \underbrace{\mu}_{=E_F}. \tag{4.79}$$

Also assuming small U, we then reach

$$|\xi_{\mathbf{k}}| \approx \hbar v_F (|\mathbf{k}| - k_F) \ll E_F. \tag{4.80}$$

and can find

$$\Longrightarrow |U_0|(4\pi)\int_0^{\overbrace{\kappa}^{\text{cutoff}}} dk \frac{k^2}{2\sqrt{\Delta_0^2+(\hbar v_F)^2(k-k_F)^2}} \overset{\text{nasty integration}}{=\!=} \lambda \ln\left(\frac{\epsilon_{cut}}{\Delta_0}\right) \overset{!}{=\!=} 1$$

where, after inserting $U_0 = 4\pi\hbar^2 a_s/m$,

$$\lambda = \frac{2k_F|a_s|}{\pi}. \tag{4.81}$$

We choose an energy-cutoff $\epsilon_{\text{cut}} = E_F = \hbar^2\kappa/2m$, then find

zero-temperature gap:

$$\Delta_0 = E_F \exp\left(-\frac{\pi}{2k_F|a_s|}\right) \ll E_F. \tag{4.82}$$

- Comparison with Eq. (4.52) now gives a neat interpretation: Since $\Delta_0 = 1/2|E_{\text{pair}} - 2E_F|$, i.e., half the binding energy of a Cooper pair: Excitations become gapped, since in order to make one, I would have to break a pair.
- Since we have found that $\Delta \neq 0$ in the end, we have in retrospect justified our initial assumption in (4.56). Thus the equation turned out self-consistent (iff, Δ is chosen as (4.82)).

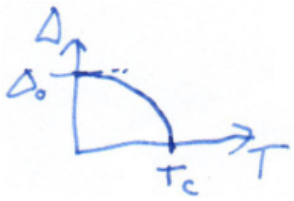
We could also evaluate Δ from Eq. (4.77) for $T > 0$ and would find

finite-temperature gap

$$\Delta = 3.06 T_c\left(1 - \frac{T}{T_c}\right)^{1/2} \tag{4.83}$$

and **critical temperature**

$$T_c \approx 0.57\,\Delta_0 \ll T_F. \tag{4.84}$$



4.10.5 Fermionic superfluidity and superconductivity

Now we come to the main consequence of the paired ground-state and gapped excitation spectrum:

Return to our discussion in section 3.4.5 of conditions "when an obstacle with velocity $\mathbf{v}$ can create excitations within the quantum gas". Nothing there was specific to Bosons, so also for Fermions no excitations are possible below an obstacle velocity of

$$v_{\text{crit}} = \min_{\mathbf{k}} \left(\frac{\epsilon_{\mathbf{k}}}{\hbar \mathbf{k}} \right). \tag{4.85}$$

Wee see from Eq. (4.68) (and the plot underneath it), that

Fermion critical velocity for superconductivity

$$v_{\text{crit}} = \frac{\Delta}{\hbar k_F}. \tag{4.86}$$

Superfluidity arises here because we cannot create excitations of our Cooper-pair condensate.

Because the condensate again has a coherent order parameter $\Delta(\mathbf{r}) = \langle \hat{\Psi}_\uparrow(\mathbf{r}) \hat{\Psi}_\downarrow(\mathbf{r}) \rangle \in \mathbb{C}$, we again have the consequence of quantized-circulation $\implies$ vortices just as in a BEC.

This is used as an experimental signature of Fermionic superfluidity.

4.11 Outlook

- We looked only at $N_\uparrow = N_\downarrow =$ spin-balanced Fermi gases. New physics for spin-imbalanced $N_\uparrow \neq N_\downarrow$, or impurities $N_\uparrow = 1$, $N_\downarrow = N - 1 \to$ Polarons.
- Fermionic superfluidity and superconductivity are probably one of the most involved and surprising quantum-many-body effects.

  The effect is not there at all in a two-body picture.

Week 12

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

5 Quantum Simulations

We have seen that solving quantum many-body problems almost always requires smart approximations ($\langle\hat{\psi}\rangle \approx \phi$, $\langle\hat{\psi}\hat{\psi}\rangle \approx \Delta$) or validity of perturbation theory. In principle, we could use a brute force approach

$$|\,\psi(t)\,\rangle = \sum_{N_1\ldots N_n} c_{N_1\ldots N_n}(t)\underbrace{|\,N_1\ldots N_n\,\rangle}_{Eq.\ (2.2)} \tag{5.1}$$

and solve the

Many-body SE in the Fock-state representation

$$i\hbar\dot{c}_{N_1\ldots N_n}(t) = \sum_{N_1'\ldots N_n'} \langle\, N_1\ldots N_n\,|\hat{H}|\,N_1'\ldots N_n'\,\rangle c_{N_1'\ldots N_n'} \tag{5.2}$$

• Exercise: derive this from $i\hbar|\,\dot{\psi}(t)\,\rangle = \hat{H}|\,\psi\,\rangle$.

However, even if we allow <u>at most N</u> particles in M modes (single particle basis states), we have

Dimension of Fock space d: Fock-space dimension for max N bosons in M modes

$$d = (N+1)^M \tag{5.3}$$

• e.g 9 particles, 10 modes $\Rightarrow d = 10^{10}$. Assuming a complex number is 16 Bytes, this corresponds to 150 GB of storage. A many-body state thus very quickly cannot fit into a computer. $\Rightarrow$

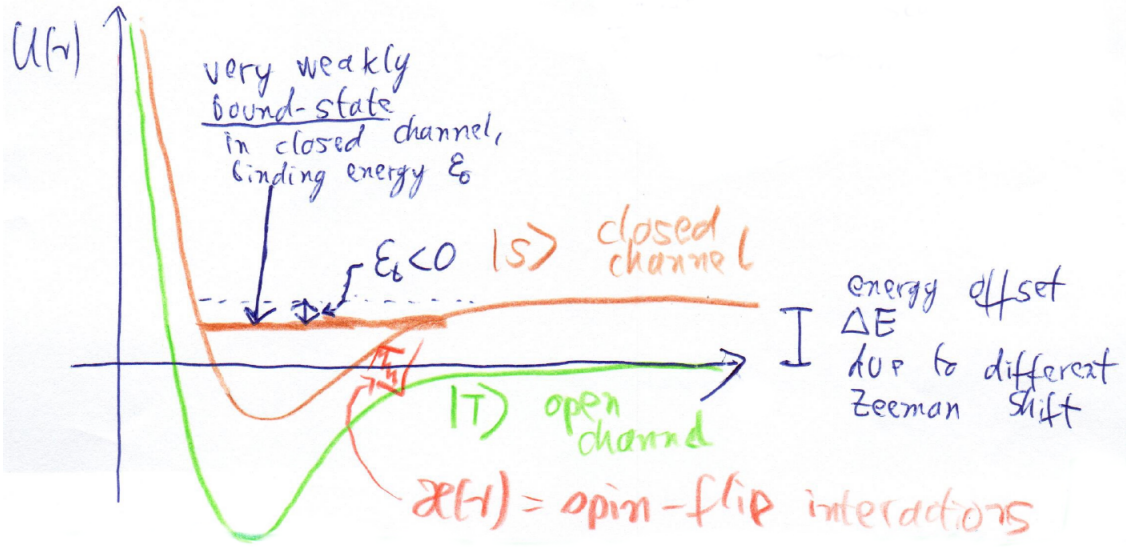
Quantum simulation concept: (Richard Feynman)
Find an experimentally accessible system, with the same Hamiltonian (mathematically) but on which we can do easier measurements and where parameters in the Hamiltonian are experimentally controllable.

- Disambiguation: the term "quantum simulation" can also refer to numerical simulation of any quantum problem.
- We now will sketch two examples using cold degenerate gases.
- Before that, let us revisit atomic interactions.

5.1 Fano-Feshbach Resonances

- So far, we have ignored electron spin dependence of atomic interactions (we had only looked at symmetry (boson/fermion)).
- In reality, interactions depend slightly on **electron**-spin.
- Careful: In chapter 4, when discussing atomic spin, we referred to two selected Hyperfine-states e.g
$$|\uparrow\rangle = \left|F = \frac{1}{2}, m_F = +\frac{1}{2}\right\rangle \quad \text{and,} \quad |\downarrow\rangle = \left|F = \frac{1}{2}, m_F = -\frac{1}{2}\right\rangle$$
The states entering scattering properties are (pair) electron spin singlet $|\,S\,\rangle = |\,s = 0, m_s = 0\,\rangle$ and triplet $|\,T\,\rangle = |\,s = 1, m_s = +1, 0, -1\,\rangle$.
- Due to unspecified nuclear spin, both $|\uparrow\uparrow\rangle, |\downarrow\uparrow\rangle$ may contain both $|\,S\,\rangle, |\,T\,\rangle$.
- Energy of $|\,S\,\rangle, |\,T\,\rangle$ depends differently on magnetic field through Zeeman-shift (see PHY402, pg. 25).

Multi-channel scattering: (channel "=" certain choice of initial/final state quantum numbers) We can have the following picture: To find scattering length a_s ($|\uparrow\downarrow\rangle$):



- Consider two incoming scattering partners in $|\uparrow\downarrow\rangle$ with energy $E \gtrsim 0$ (ultra-cold regime)
- Calculate 2nd order perturbation theory (in $\kappa(r)$, spin-flip Hamiltonian) energy correction to scattering state

$$E_n^{(2)} = \sum_{k \neq n} \frac{\left|\langle k^{(0)}|\hat{V}|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \tag{5.4}$$

(see QM lecture).

- Schematically here

$$\begin{aligned} &|\, n^{(0)}\,\rangle \sim |\uparrow\downarrow\rangle \otimes |\, E \approx 0,\ \text{scattering state}\,\rangle, && E_n^{(0)} \approx 0 \\ &|\, k^{(0)}\,\rangle \sim |\uparrow\uparrow\rangle \otimes |\, \text{bound state}\,\rangle, && E_k^{(0)} \approx \Delta E \\ &\left|\langle\, k^{(0)}\,|\hat{V}|\, n^{(0)}\,\rangle\right|^2 \sim |\kappa|^2, && \frac{1}{E_n^{(0)} - E_k^{(0)}} \sim -\frac{1}{\Delta E} \end{aligned}$$

Three cases: If

$\Delta E \to 0$ (Resonance), $E_n^{(2)} \to \infty$

$\Delta E < 0$, $E_n^{(2)} > 0 \Rightarrow$ (more) repulsive interactions

$\Delta E > 0$, $E_n^{(2)} < 0 \Rightarrow$ (more) attractive interaction

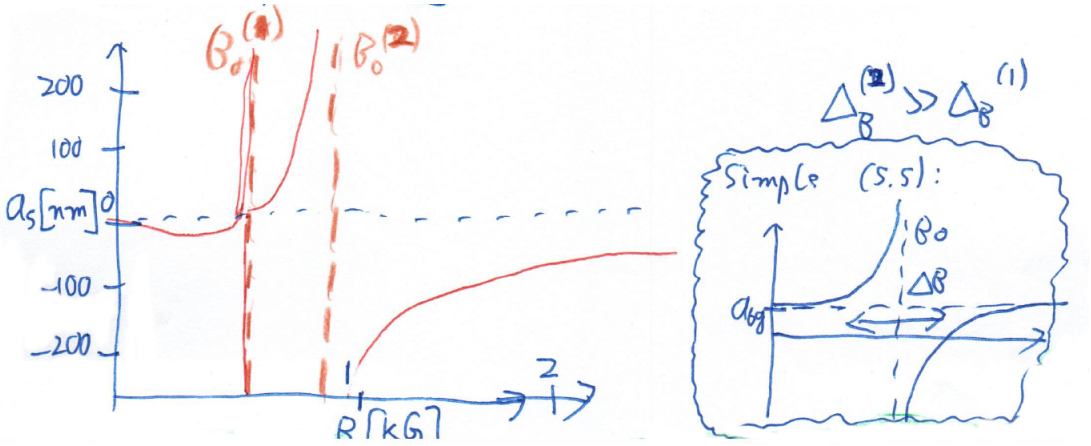
- Since ΔE depends on magnetic field B, it is now plausible that:

Scattering length near Feshbach resonance

$$a_s(B) = a_{\text{bg}}\Big(1 - \frac{\Delta B}{B - B_0}\Big) \tag{5.5}$$

a_{bg} = background scattering length,
B_0 = position of resonance,
ΔB = width of resonance.

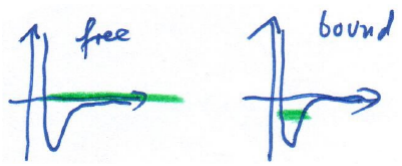
Example: Scattering length with 2 Feshbach resonances [^{6}Li: $B_0^{(1)} = 543$ G, $B_0^{(2)} = 834$ G]



- Feshbach resonances effectively make the interaction strength an experimentally controllable parameter.
- We can reach $a_s = 0$, $a_s > 0$, $a_s < 0$ and (almost) $a_s = \infty$.

5.2 BEC-BCS Crossover

- Using Feshbach resonances, we can now realize DFG with interactions ranging from repulsive to attractive (see week 10 vs week 11).
- Let us reconsider the repulsive $a_s > 0$ side: Do we get a Fermi-liquid as ground state as in section 4.9.1?
- Answer: when considering the scenario with a Feshbach resonance, that would be only a meta-stable (excited) state/phase, since the scattering state with $E \approx 0$ for which we found $a_s > 0$ in section 5.1 has higher energy than a bound state in the closed channel.



- Bound-states and Cooper pairs are related (the latter *are* a type of weak bound state). It turns out, with rigorous renormalization we can actually apply BCS theory all the way from $U_0 = -\infty$ to $U_0 = \infty$.

5.2.1 From Cooper-pairs to Molecules

Let us again look at the pair creation operator

$$\hat{C}^\dagger = \sum_{\mathbf{k}} \varphi_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}\uparrow} \hat{a}^\dagger_{(-\mathbf{k})\downarrow} \tag{5.6}$$

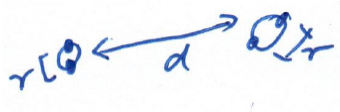
Commutator:

$$\left[\hat{C}, \hat{C}^\dagger\right] = \sum_{\mathbf{k},\mathbf{k}'} \varphi^*_{\mathbf{k}} \varphi_{\mathbf{k}'} \left[\hat{a}_{(-\mathbf{k})\downarrow} \hat{a}_{\mathbf{k}\uparrow}, \hat{a}^\dagger_{\mathbf{k}'\uparrow} \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\right] \overset{\text{(yellow box below)}}{=} \sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 (1 - \hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow}) \tag{5.7}$$

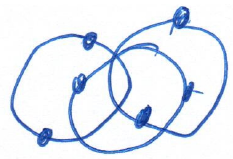
We can show (see steps on page 95) that $\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 = 1$ due to normalization of our starting pair state $\varphi_0(\mathbf{x} - \mathbf{y})$.

Thus when acting on states with few fermions "per momentum mode", we have $\left[\hat{C}, \hat{C}^\dagger\right] = 1$, and our pair behaves like a boson. (You can show $\left[\hat{C}, \hat{C}\right] = \left[\hat{C}^\dagger, \hat{C}^\dagger\right] = 0$ also).

For this we require a broad Fourier transform $\tilde{\varphi}_0(k) \to$ tightly bound pairs in position space. This corresponds to molecules with spacing $d \gg$ orbital radius r,



In other limit, where $r \gg d$, we will have high occupations of all momentum modes ($\hat{n} \sim 1$), and we talk of Cooper-pairs (that are not quite bosons, but have some "bosonic-character").



Through this change of the interpretation/details of the many-body paired state, we are able to smoothly interpolate between a BEC of bosonic molecules (made of two fermionic atoms) at $a_s > 0$ and a BCS-superfluid due to Cooper-pairing at $a_s < 0$.

More on composite-Bosons: [*Disclaimer: The following is mainly custom improvised for this course, and BONUS material. Please alert me to mistakes, or to any reference where this is discussed satisfactorily*]. It is a central theme in this course, that atoms can be Bosons or Fermions, depending on the number of fundamental Fermions (electrons, protons, neutrons) that they are made of. One way to see that this makes sense is through the rules for angular momentum addition (QM or AMol lecture), which tell you that adding an even number of half-integer spins (Fermions) gives integer spins (Bosons), but odd numbers remain half-integer (Fermions).
Here we explore how to see this in an alternative way, using commutation relations. Consider the expression (5.6) for the creation operator of a bound-state (see proof/sketch after (4.73)). We assume $\{\hat{a}^\dagger_{\mathbf{k}s}, \hat{a}^\dagger_{\mathbf{k}'s'}\} = \delta_{ss'}\delta_{\mathbf{k}\mathbf{k}'}$, so the constituents of the bound-state are Fermions.
Now let's find the commutator $\left[\hat{C}, \hat{C}^\dagger\right]$ (see above for first step). Then

$$\begin{aligned}
&\left[\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}_{\mathbf{k}\uparrow}, \hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\right] = \hat{a}_{(-\mathbf{k})\downarrow}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}^\dagger_{(-\mathbf{k}')\downarrow} - \hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}_{\mathbf{k}\uparrow} \\
&= \hat{a}_{(-\mathbf{k})\downarrow}\hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow} - \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}_{\mathbf{k}\uparrow} \\
&= \hat{a}_{(-\mathbf{k})\downarrow}\hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow} + \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow} - \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow} - \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}_{\mathbf{k}\uparrow} \\
&= \left\{\hat{a}_{(-\mathbf{k})\downarrow}, \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\right\}\hat{a}_{\mathbf{k}\uparrow}\hat{a}^\dagger_{\mathbf{k}'\uparrow} - \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\left\{\hat{a}^\dagger_{\mathbf{k}'\uparrow}, \hat{a}_{\mathbf{k}\uparrow}\right\} = -\delta_{\mathbf{k}\mathbf{k}'}\left(\hat{a}^\dagger_{\mathbf{k}'\uparrow}\hat{a}_{\mathbf{k}\uparrow} + \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\hat{a}_{(-\mathbf{k})\downarrow}\right)
\end{aligned} \tag{5.8}$$

In the second equality we have anti-commuted one operator past the other spin species, and im the third equality inserted zero in form of the red terms. The purpose was to reach the anti-commutators in the last line. Inserting Eq. (5.8) into (5.7), assuming $\varphi_{\mathbf{k}} = \varphi_{-\mathbf{k}}$, $\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 = 1$ and one more anti-commutation give the result in the main text.
Clearly whenever we can neglect the $\hat{n}_{\mathbf{k}}$ terms, the commutator behaves as for Bosons. When is this justified? For this lets look at the expectation value of the commutator in the state $\hat{c}^\dagger|\,0\,\rangle$, i.e. one that contains precisely one of the bound-states in question. We can show (exercise)

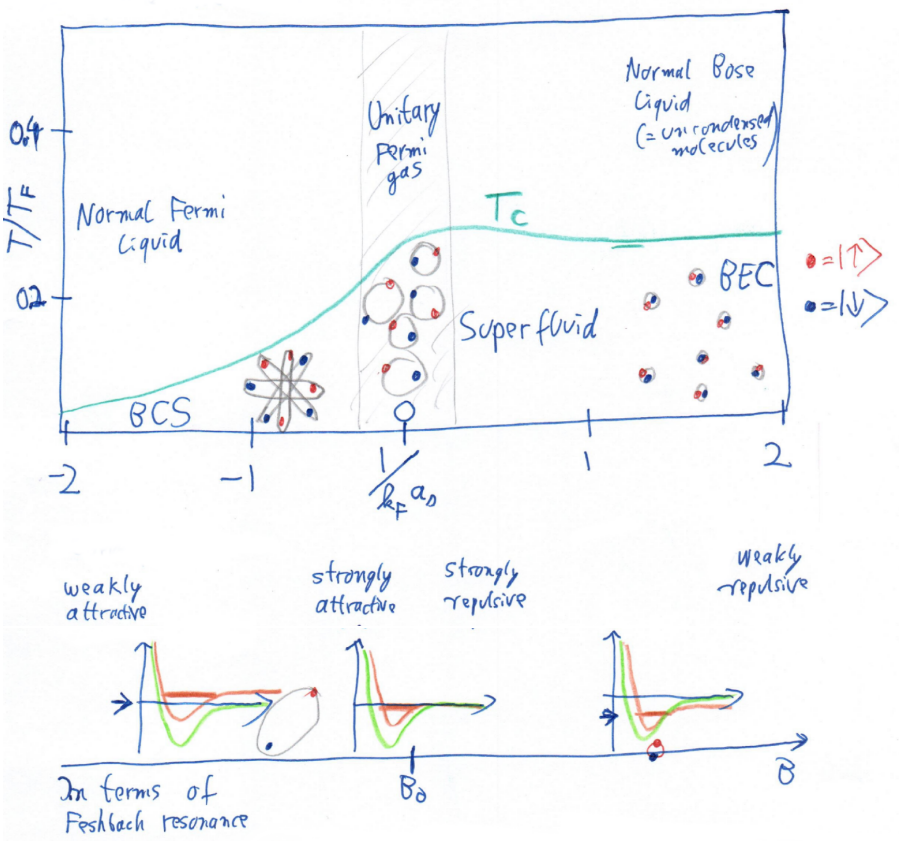
$$\langle\left[\hat{C}, \hat{C}^\dagger\right]\rangle = 1 - 2\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^4. \tag{5.9}$$

An expression such as $\mathcal{P} = \sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^4$ for $\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 = 1$ is called participation ratio, it measures "how many of the total number of available states are involved". If only one, e.g. $\varphi_{\mathbf{k}} = \delta_{\mathbf{k},\mathbf{k}_0}$, then $\mathcal{P} = 1$. If many, you shall find $\mathcal{P} \to 0$.

Composite Bosons continued: Now let us quantify the statement, that we observe our composite Boson on large scales, where internal details don't matter. Assuming everything is in a cubic box of side-length L, we then say our bound-state wavefunction is a delta-function in real space. That means it becomes constant in momentum space, with <u>all</u> $\varphi_{\mathbf{k}}$ equal and non-zero. Thus $\mathcal{P} = 0$ and the composite behaves like a Boson. In contrast, an example in which our relative wavefunction fills a significant fraction of our box, is if it was made of a superposition of just a few box-eigenstates. In that cases only a few $\varphi_{\mathbf{k}}$ are non-zero, and there is no well defined bosonic character.

5.2.2 Crossover phase diagram

Altogether we have the following phase diagram:



- CORRECTION: The magnetic field increases to the left, please flip axis.
- Very close to resonance, interactions are very large, such that $r_{\text{range}} \ll k_F^{-1} \ll a_s$. This is called unitary case (for non-obvious reasons), here the only scale is k_F (physics universal).

on the left: BCS

$$\mu = E_F > 0$$

$$\Delta \approx E_F e^{-\frac{\pi}{2k_F|a_s|}}$$

on the right: BEC

$$\mu = -\frac{1}{2}\underbrace{\left(\frac{\hbar^2}{ma_s}\right)}_{\varepsilon_b} + U_m\rho_m < 0$$

$$U_m = \frac{\pi\hbar^2 a_s}{m_{\text{at}}}$$

5.3 Quantum-simulation aspects of BEC-BCS crossover

High T_C superconductivity
While not being directly related, these share several features with the crossover region:

- Pair size $\sim$ average distance (see p. 89)
- Normal state (above T_C) not ordinary Fermi-liquid

Neutron stars/ Quark matter
Particularly in the unitary limit, there is only one scale in the interacting fermion problem (details don't matter). It should thus also apply to other DFG systems than ultra-cold gases, such as neutron stars (see section 4.4.2). This is particularly useful, since calculations in this strongly interacting regime are very challenging.

Week 13

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
Instructor: Sebastian Wüster, IISER Bhopal, 2019

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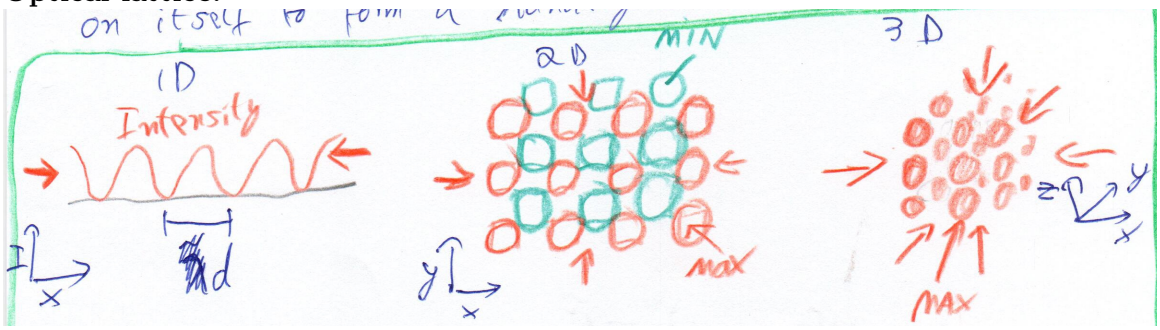
5.4 Lattice Models

We have mentioned few times, the similarities between an electron gas in a crystal lattice and a cold atomic gas in an optical lattice. Now few more details on the latter:

5.4.1 Optical lattices

Consider a coherent laser beam which is back-reflected on itself to form a standing wave in

Optical lattice:



- We obtain an intensity pattern for the light that can be written as,

$$I(x) = I_0 \cos^2(k_L x) \tag{5.10}$$

where $d = \frac{\lambda_L}{2}$ is the distance between adjacent sites, λ_L is laser wavelength and $k_L = \frac{2\pi}{\lambda_L}$.

We can calculate the energy shift of an atom due to exposure to the rapidly varying E-field of the laser (AC Stark shift). This shifts turns I(x) into a spatial potential

$$V(x) = -\frac{1}{2}\alpha(\omega) \underbrace{\langle \epsilon(t)^2 \rangle_t}_{\substack{\text{time avg of} \\ \text{light intensity}}} \tag{5.11}$$

where α is the atomic polarizability and ω is the laser frequency.

We find $\alpha(\omega) < 0$, just above an atomic resonance (blue detuned) $\implies V > 0$.

$\cdots\ \cdots\ \alpha(\omega) > 0$, just below $\cdots\ \cdots\ \cdots\ \cdots\ \cdots$ (red detuned) $\implies V < 0$.

(See PHY 402, Assignment 4, also c.f. section 5.1 and Mid-sem exam). We thus have an

Optical lattice potential

$$V(x) = V_0 \cos^2(k_L x), \tag{5.12}$$

where V_0 can be positive or negative dependent on light detuning.

5.4.2 Bose-Hubbard Model

You had shown in the mid-term exam how starting from Eq. (3.37) [$\hat{H}$ for Bose gas in form with $\hat{\Psi}$], we can derive

Bose-Hubbard Hamiltonian

$$\hat{K} = \hat{H} - \mu\hat{N} = \sum_m \left[J(\hat{a}^\dagger_{m+1}\hat{a}_m + \hat{a}^\dagger_{m-1}\hat{a}_m) + \frac{U}{2}\hat{n}_m(\hat{n}_m - 1) - \tilde{\mu}\hat{n}_m \right] \tag{5.13}$$

- $\hat{a}^\dagger_m$ creates an atom "on site m". 

- J allows tunneling/hopping from site to site.
- U are repulsive on-site interactions $\hat{n}_m = \hat{a}^\dagger_m \hat{a}_m$
- $\tilde{\mu} = \mu - E$ ($E \to$ on site energy) is the chemical potential.

Let us try to find ground-states of $\hat{K}$ in two simple cases

[A] $J = 0$, no tunelling:

No tunneling, $[\hat{K}, \hat{n}_m] = 0 \implies$ We can write eigenstates as Fock-states $|\,\mathbf{N}\,\rangle$. Since all sites are equivalent, we pick $|\,\mathbf{N}_0\,\rangle = |\,M, M, \cdots, M\,\rangle$, i.e. a state with exactly M bosons per site. Its energy is

$$\langle\,\mathbf{N}_0\,|\mathbf{K}|\,\mathbf{N}_0\,\rangle = N_{\text{sites}}[\frac{U}{2}M(M-1) - \tilde{\mu}M]. \tag{5.14}$$

This is minimized by $M = \frac{\tilde{\mu}}{U} + \frac{1}{2}$. Since M has to be an integer, for parameters $\tilde{\mu}$, U in the range $M - 1 < \frac{\tilde{\mu}}{U} < M$ we have exactly M bosons per site. This is called the

Mott-insulating state

$$|\,\psi_{\text{Mott}}\,\rangle = \sum_m \frac{(\hat{a}_m^\dagger)^M}{\sqrt{M!}}|\,0\,\rangle, \tag{5.15}$$

- The sum here runs over the lattice sites.
- Mott-insulator in condensed matter: A material that should conduct from band-theory (i.e. based on single particle physics), but does not due to $e^- - e^-$ interactions (i.e. due to many-body physics).

[B] $\underline{U = 0}$ **no interactions, let** $J < 0$**:** This becomes a single particle problem

Find eigen-states of the single-particle Hamiltonian, it turns out the lowest state is

$$|\,\varphi_0\,\rangle = \frac{1}{\sqrt{N_{\text{states}}}} \sum_m \hat{a}_m^\dagger |\,0\,\rangle \tag{5.16}$$

(particle fully de-localized on lattice)

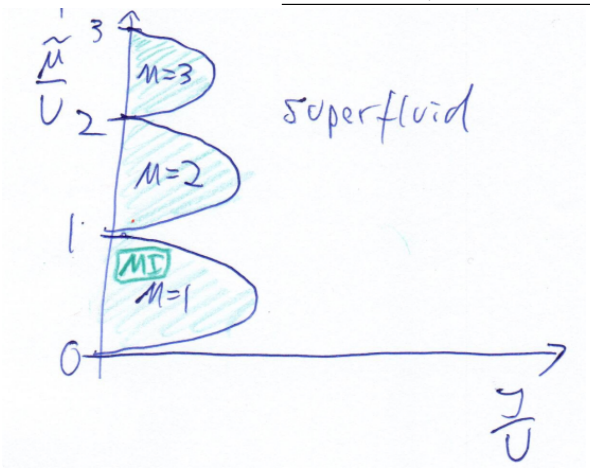
- We know at $T = 0$ we will have a BEC condensed in $|\,\varphi_0\,\rangle$ and can use mean-field theory.

Super-fluid state

$$|\,\psi_{\text{BEC}}\,\rangle = \mathcal{N}\left(\sum_m \hat{a}_m^\dagger\right)^M |\,0\,\rangle \qquad \mathcal{N} \text{ is a Normalization factor,} \tag{5.17}$$

[C] For both, non-vanishing interactions and hopping, $U \neq 0, J = 0$**, we require a more complicated analysis. The result of that would be:**

Phase-diagram for superfluid/Mott-insulator Quantum phase transition:



left:

- Mott insulating phase is shown in green.
- Transitions between green and white are called quantum phase transition, because they can happen due to change of parameters in the Hamiltonian, but at zero temperature $T = 0$.

From Eq. (5.15) and Eq. (5.17) we can calculate the inter-site coherence

$$g_{m,m+1} = \langle \hat{a}_m^\dagger \hat{a}_{m+1} \rangle \tag{5.18}$$

We find $g = 0$ for the Mott insulator (5.15) and $g \neq 0$ for the superfluid (5.17) (Exercise).

This means atoms from different sites interfere in a superfluid state after time-of-flight expansion, but not in the Mott-insulator $\implies$ clear experimental signature, see Greiner *et. al*, Nature **415** 39 (2002).

The End

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