Lecture-1: Weakly Interacting Bose Gas
Gross-Pitaevskii Formalism

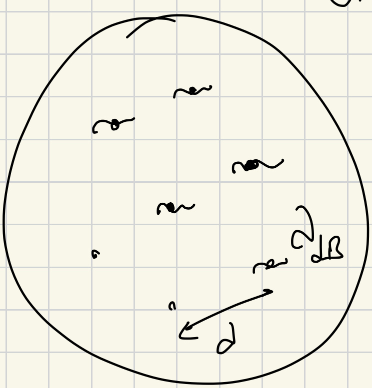
Q1) Consider a many-body system of non-interacting particles at temperature T. In the 'classical' regime of the many-body statistics, the system/particles are distributed among the possible states by respecting Boltzmann distribution $\propto e^{-E/k_B T}$.

When do the quantum nature of the particles start to reveal themselves and how is the classical distribution is modified? How does the particle being Boson or Fermion change the distribution? How does the concept of 'chemical potential' rise in this context?

1) As we derive the partition function for a system of N indistinguishable particles $Z = \frac{Z_1^N}{N!}$, we implicitly assume that the particles rarely tend to occupy the same eigenstate of the single particle Hamiltonian. The system is supposed to be in the 'classical statistical regime' in which the temperature is sufficiently high such that the available thermal energy easily raises the particles to the excited levels.

As we lower the temperature, this picture needs to be revised:

(No interactions)



$d \gg \lambda_{dB}$

Classical stat. mech.

$d \sim \lambda_{dB}$

de Broglie wavelength on the same order of magnitude with the inter-particle distance

$$\lambda_{dB} = \frac{h}{P} \quad , \qquad KE = \frac{P^2}{2m} = \frac{3k_BT}{2}$$

$$\Rightarrow \quad \left(\frac{h}{\lambda_{dB}}\right)^2 \cdot \frac{1}{2m} \simeq \frac{3k_BT}{2}$$

$$\Rightarrow \quad \sqrt{\frac{h^2}{3k_BTm}} \sim \lambda_{dB} \qquad \left.\begin{array}{l}\text{Low } T \\ \text{Low mass}\end{array}\right\} \underline{\underline{\lambda_{dB}\uparrow}}$$

When the system becomes 'degenerate' in the sense that the particles start to occupy the same eigenstate, the particles being Boson or Fermion revise the statistics dramatically:

* Bosons can occupy the same eigenstate, whereas Fermions cannot.

This fact is also clear from their distribution functions:

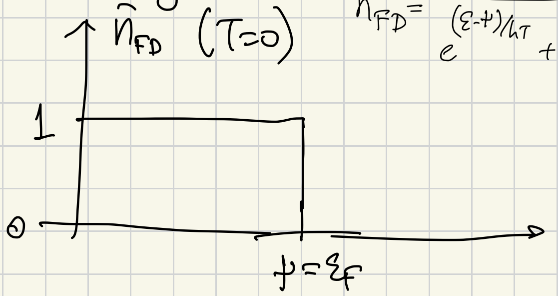
$$\bar{n}_{BE}(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} - 1}, \quad \bar{n}_{FD}(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} + 1}$$

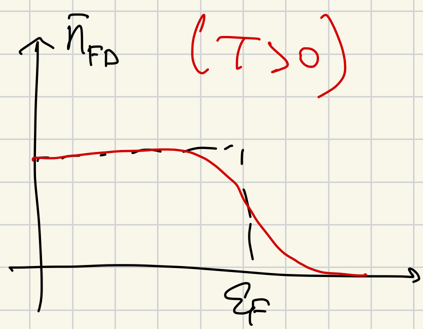
where ε is the energy of the state and μ is the chemical potential of the system:

$$dE = TdS - PdV + \mu dN \Rightarrow \mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$$

For a degenerate gas, $\mu \simeq E(N+1) - E(N)$ as the addition of a single particle leads negligible change in both entropy S and volume V. Therefore the chemical potential can be regarded as the energy needed to add a single particle to the system:

$$\bar{n}_{FD} = \frac{1}{e^{(\varepsilon-\mu)/kT} + 1}$$



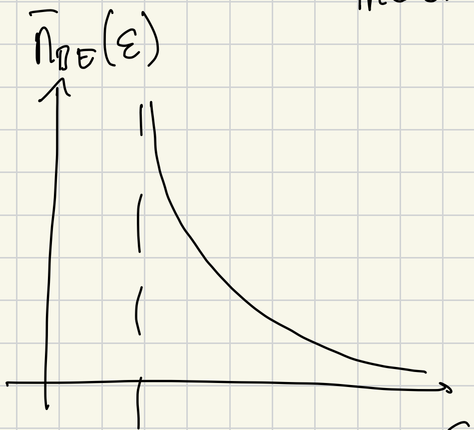


$$\bar{n}_{BE}^{(s)} = \frac{1}{e^{(\varepsilon_s-\mu)/k_BT} - 1}$$

As $\varepsilon \to \mu$, $\bar{n}_{BE}$ diverges!

As $T \to 0$, the occupation increases its density near ε.

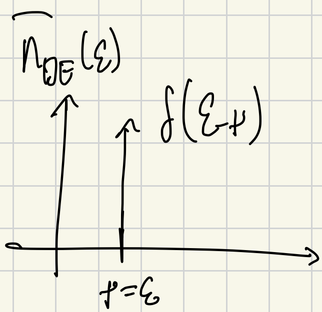
$T \simeq 0$:



$\mu = \varepsilon_0$: Grand state energy of the single particle states

$\mu \leq \varepsilon_0$ for an ideal BEC

$T = 0$:

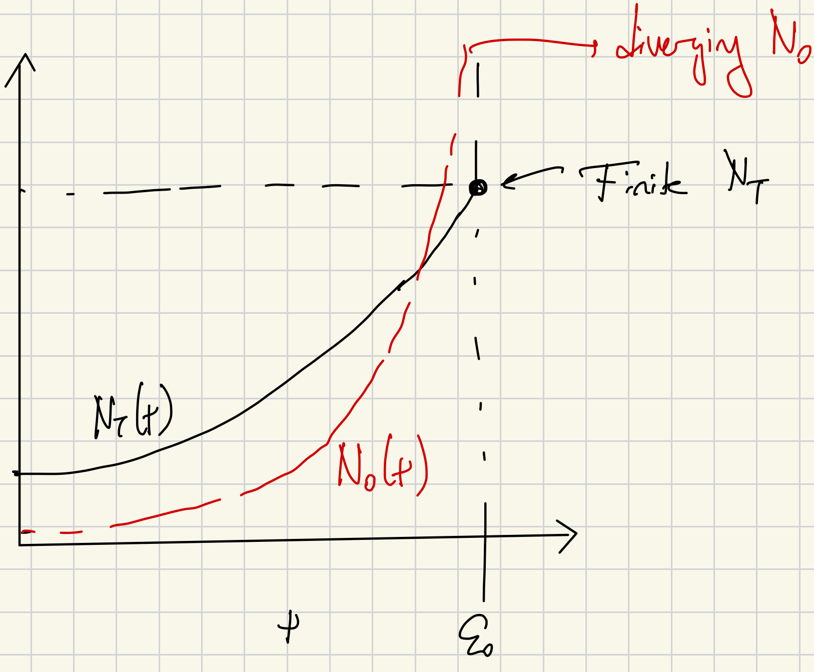


All particles in the same grand state with energy ε_0.

As $\mu \to \varepsilon_0$, the # of particles in the ground state, N_0, diverges while the thermal cloud:

$$N_T = \sum_{\nu \neq 0} \frac{1}{e^{(\varepsilon_\nu - \varepsilon_0)/kT} - 1}$$ is still finite,

where the total # of particles $N = N_0 + N_T$.

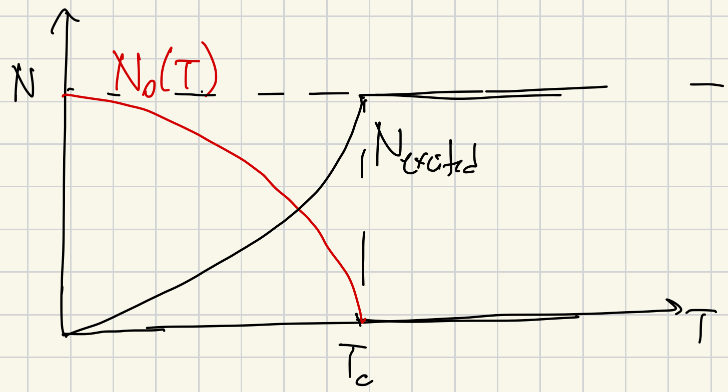


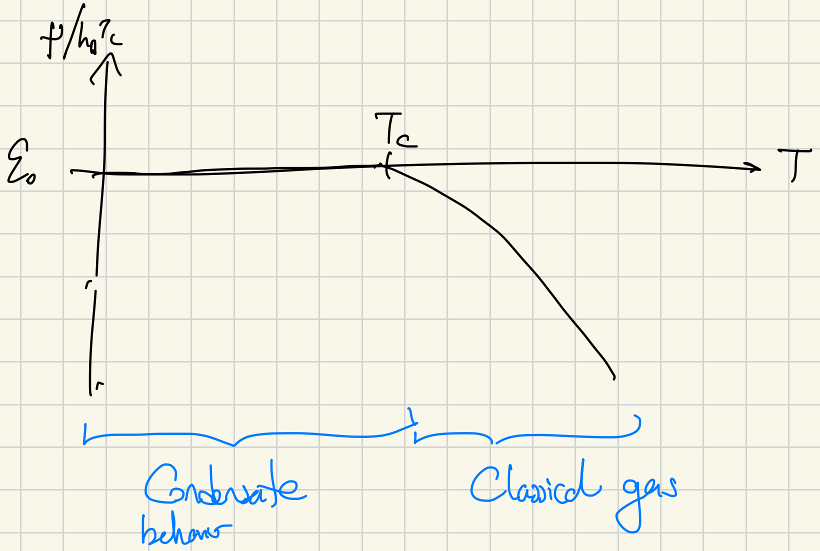
So if $N = N_T + N_0 > N_T(\mu = \varepsilon_0, T)$, the condensation starts!

The condensation criteria:

$$\boxed{N_T(T_c, \mu = \varepsilon_0) = N}$$

Below T_c, the chemical potential is the ground state energy since the added particle directly occupies the ground state.





2) Consider an ideal BEC inside a harmonic oscillator. Find the critical temperature T_c and the condensate fraction N_0/N for $T \leq T_c$.

2) Isotropic harmonic potential:

$$V_{ext}(\vec{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2)$$

The single particle Hamiltonian:

$$\hat{H}_1 = -\frac{\hbar^2}{2m^2}\nabla^2 + V_{ext}(\vec{r})$$

The eigenenergies are:

$$\varepsilon_{n_x, n_y, n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$$

where $n_{x,y,z} = 0, 1, 2, \ldots$

The grand state wavefunction

$$\psi_0(\vec{r}) = \left(\frac{m\omega}{\hbar\pi}\right)^{3/4} e^{-\frac{m\omega}{2\hbar} r^2}, \quad r^2 \equiv x^2 + y^2 + z^2$$

Since the particles inside the condensate occupy the same eigenstate at $T=0$, it is meaningful to introduce the concept of macroscopic wavefunction:

$$\Psi_0(\vec{r}) = \sqrt{N}\, \psi_0(\vec{r})$$

where N is the # of particles. This new wavefunction normalizes the state up to the integral $\int |\Psi_0|^2 d^3r = N$ instead $\int |\psi_0|^2 d^3r = 1$.

$$\int n(\vec{r})\, d^3\vec{r} = N \Rightarrow n(\vec{r}) = |\Psi_0(\vec{r})|^2$$

is the condensate density.

The condensation will occur if $N \geq N_c = N_T(T_c, \mu = \varepsilon_0)$

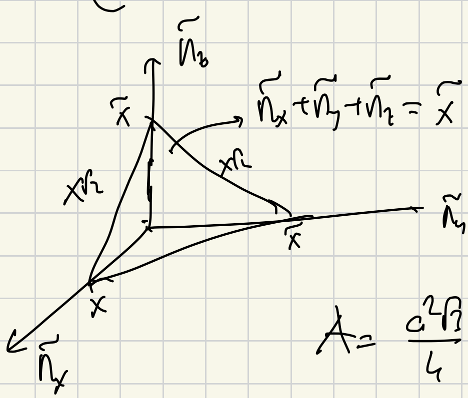
where $\varepsilon_0 = \frac{3}{2}\hbar\omega$.

$$N_T = \sum_{n_x, n_y, n_z} \frac{1}{\exp\left[\beta\left(n_x+n_y+n_z+\frac{3}{2}-\frac{3}{2}\right)\hbar\omega\right]-1}$$

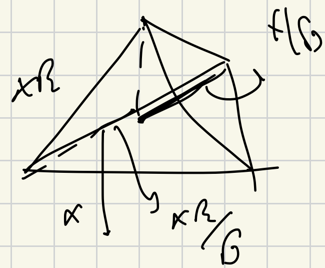
$$\simeq \int dn_x\, dn_y\, dn_z \cdot \frac{1}{e^{\beta(n_x+n_y+n_z)\hbar\omega}-1}$$

Define $\tilde{n}_i \equiv \beta\hbar\omega n_i$, $d\tilde{n}_i = \beta\hbar\omega\, dn_i$

$$\Rightarrow N_T = \frac{1}{(\beta\hbar\omega)^3} \int d\tilde{n}_x\, d\tilde{n}_y\, d\tilde{n}_z \frac{1}{e^{(\tilde{n}_x+\tilde{n}_y+\tilde{n}_z)}-1} \Rightarrow$$



$$A = \frac{a^2\sqrt{3}}{4} = \frac{\tilde{x}^2\sqrt{3}}{2}$$



$$N_T = \frac{1}{(\beta\hbar\omega)^3}\int_0^\infty d\tilde{x}\,\frac{1}{\sqrt{3}}\cdot\frac{\tilde{x}^2\sqrt{3}/2}{e^{\tilde{x}}-1}$$

$$= \frac{1}{(\beta\hbar\omega)^3}\,\frac{1}{2}\underbrace{\int_0^\infty d\tilde{x}\,\frac{\tilde{x}^2}{e^{\tilde{x}}-1}}_{\underbrace{\zeta(3)}_{\text{Zeta-function}}\cdot\underbrace{\Gamma(3)}_{\text{Gamma function}}} = \frac{\zeta(3)}{(\beta\hbar\omega)^3}$$

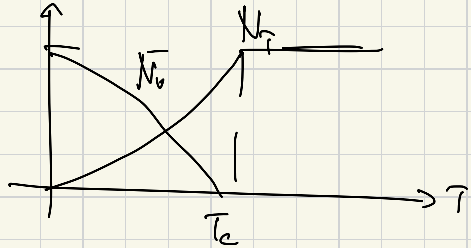
$$N_T = \frac{\zeta(3)}{(\hbar\omega)^3}(k_B T)^3 \Rightarrow \quad N_T = N = \frac{\zeta(3)}{(\hbar\omega)^3}(k_B\cdot T_c)^3$$

$$\Rightarrow \boxed{k_B T_c \cong 0.94\,\hbar\omega\, N^{1/3}}$$ Critical temperature

Fraction of the condensed particles for $T<T_c$:

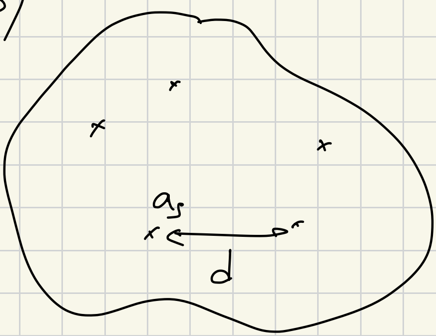
$$\frac{N_0}{N} = 1 - \frac{N_T}{N} = 1 - \frac{\zeta(3)(k_BT)^3}{(\hbar\omega)^3}\cdot\frac{(\hbar\omega)^3}{\zeta(3)(k_BT_c)^3} \Rightarrow$$

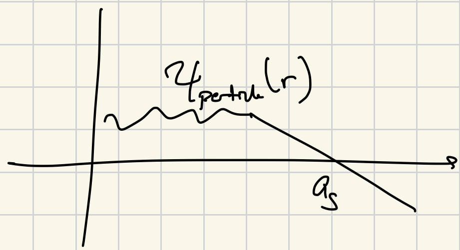
$$\boxed{\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3}$$



3) Until now, we only considered the non-interacting particles. How can we study the interacting Bose gas? Can we derive an equation for the macroscopic wavefunction of the Bose condensate?

3)





If $d \gg a_s$, the system can be regarded as weakly interacting: $n \simeq \frac{1}{d^3} \Rightarrow \frac{a_s}{d} \ll 1$

$$a_s n^{1/3} \ll 1$$

$\Rightarrow$ $\boxed{n a_s^3 \ll 1}$ Condition for the weakly interacting regime

For a weakly interacting system, one can model the interaction between two particles as 'contact potential' or 'Fermi pseudo-potential':

$$V_{int}(\vec{r}_2, \vec{r}_2) = g\, \delta(\vec{r}_1 - \vec{r}_2)$$

coupling constant

$$g = \frac{4\pi a_s \hbar^2}{m}$$ (First order Born approximation)

The Hamiltonian of the weakly interacting Bose gas with N particles under an external potential $V_{ext}(\vec{r})$

$$\hat{H} = \text{Kinetic} + \text{External potential} + \text{Interaction potential}$$

$$= \sum_{i=1}^{N} \frac{\hat{P}_i^2}{2m} + \sum_{i=1}^{N} V_{ext}(\vec{r}_i)$$

$$+ \sum_{i=1}^{N} \sum_{j \neq i} V_{int}(\vec{r}_i, \vec{r}_j)$$

$\Rightarrow$ The interaction Hamiltonian can be written for the contact potential as:

$$\hat{V}_{int} = \sum_{i=1}^{N} \sum_{j>i} V_{int}(\vec{r}_i, \vec{r}_j)$$

$$= g \sum_{i=1}^{N} \sum_{j>i} \delta(\vec{r}_i - \vec{r}_j)$$

$$\Rightarrow \boxed{\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \hat{V}_{ext}(\vec{r}_i) + g \sum_{i=1}^{N} \sum_{j>i} \hat{\delta}(\vec{r}_i - \vec{r}_j)}$$

Gross-Pitaevskii approach: Product-state ansatz

Assume all the particles occupy the same quantum state $\phi(\vec{r})$:

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) = \prod_{i=1}^{N} \phi(\vec{r}_i)$$

$\phi(\vec{r})$ is not necessarily the eigenstate of the non-interacting

Single particle Hamiltonian:

$$\hat{h}_i = \frac{\vec{p}_i^{\,2}}{2m} + V_{ext}(\vec{r}_i)$$

since the system is now changed by the two-particle interaction,

So one of the limits to check to see if the product state ansatz yields a macroscopic wavefunction correctly: $g \to 0$.
The solution in this limit should converge to the solution of the Schrödinger eqn. with the Hamiltonian $\hat{h}_i$.
In order to find the state $\Psi(\vec{r})$ using the variational approach, we follow the steps:

(1) Find $\langle \Psi(\vec{r}_1, \ldots \vec{r}_N) | \hat{H} | \Psi(\vec{r}_1, \ldots \vec{r}_N) \rangle = E$

(2) Minimize the energy E with the constraint that the total # of particles N is conserved:

Consider the function $E[\Psi] - \mu N[\Psi]$ and

$$\delta \left[E[\Psi] - \mu N[\Psi] \right] = 0 \Rightarrow$$

$$\boxed{\frac{\delta\left[E-\mu N\right]}{\delta\psi^*}=0}$$ (Functional variation w.r.t. ψ^*)

(1) $\langle \Psi(\vec{r}_1,\ldots\vec{r}_N) \,|\, \hat{H} \,|\, \Psi(\vec{r}_1,\ldots\vec{r}_N)\rangle = ?$

where $\Psi(\vec{r}_1,\ldots\vec{r}_N) = \prod_i \phi(\vec{r}_i)$ and

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{P}_i^2}{2m} + \hat{V}_{ext}(\vec{r}_i) + g\sum_{i=1}^{N}\sum_{j\neq i} \hat{\delta}(\vec{r}_i-\vec{r}_j)$$

* Extenal potential $\langle \Psi | V_{ext} | \Psi\rangle$

$$= \int d^3r_1\, d^3r_2 \ldots d^3\vec{r}_N \left(\prod_{i=1}^{N} \phi^*(\vec{r}_i)\right) \sum_{i=1}^{N} V_{ext}(\vec{r}_i) \left(\prod_{i=1}^{N} \phi(\vec{r}_i)\right)$$

$$= \int d^3r_1\, \phi^*(r_1)\, V_{ext}(r_1)\, \phi(r_1) \cdot \underbrace{\int d^3r_2 \ldots d^3r_N \prod_{i=2}^{N} |\phi(r_i)|^2}_{=1} + (2,2) + \ldots$$

$$= N \cdot \int d^3\vec{r}\; \phi^*(r)\, V_{ext}(r)\, \phi(r)$$

$$= \int d^3\vec{r}\; \psi^*(\vec{r})\, V_{ext}(\vec{r})\, \psi(\vec{r}) \;,\; \text{where } \psi(\vec{r}) = \sqrt{N}\,\phi(\vec{r})$$

* Kinetic energy $\langle \Psi | \sum_{i=1}^{N} \frac{p_i^2}{2m} | \Psi \rangle$:

$$= \int d^3\bar{r}_1 \dots d^3\bar{r}_N \left(\prod_{i=1}^{N} \phi^*(\bar{r}_i) \right) \left(\sum_{i=1}^{N} \frac{p_i^2}{2m} \right) \left(\prod_{i=1}^{N} \phi(\bar{r}_i) \right)$$

where $\hat{p}_i = i\hbar \nabla_i$ $\qquad \hat{p}_i^\dagger = -i\hbar \overleftarrow{\nabla}_i$

$$= \int d^3 r_1 \, \phi^*(\bar{r}_1) (+i\hbar \overleftarrow{\nabla}_1) \frac{(-i\hbar \overrightarrow{\nabla}_1)}{2m} \phi(\bar{r}_1) \underbrace{\int d^3 r_2 \dots d^3 r_N \prod_{i=2}^{N} \phi^*(\bar{r}_i) \prod_{i=2}^{N} \phi(\bar{r}_i)}_{=1}$$

$$+ \int d^3 r_2 \, \phi^*(\bar{r}_2) (+i\hbar \overleftarrow{\nabla}_2) \frac{(-i\hbar \overrightarrow{\nabla}_2)}{2m} \phi(\bar{r}_2) \underbrace{\int d^3\bar{r}_1 d^3\bar{r}_3 \dots d^3\bar{r}_N \prod_{i\neq 2}^{N} \phi^*(\bar{r}_i) \prod_{i\neq 2}^{N} \phi(\bar{r}_i)}_{=1}$$

$\vdots$

$$= N \int d^3 r \, \phi^*(\bar{r}) (+i\hbar \overleftarrow{\nabla}) \frac{(-i\hbar \overrightarrow{\nabla})}{2m} \phi(\bar{r})$$

$$= \int d^3 r \, \psi^*(\bar{r}) (i\hbar \overleftarrow{\nabla}) \frac{(-i\hbar \overrightarrow{\nabla})}{2m} \psi(\bar{r}) = \int d^3 r \, \frac{\hbar^2 |\nabla \psi|^2}{2m}$$

✱ Interaction energy $\langle \Psi | \hat{V}_{int} | \Psi \rangle$:

$$= \int d^3\bar{r}_1 \dots d^3\bar{r}_N \left[\prod_{i=1}^{N} \phi^*(\bar{r}_i)\right] \left[g \cdot \sum_{i=1}^{N} \sum_{\substack{j\neq i \\ j>i}} \delta(\bar{r}_i - \bar{r}_j)\right] \left[\prod_{i=1}^{N} \phi(\bar{r}_i)\right]$$

$$= \int d^3\bar{r}_1 \, d^3\bar{r}_2 \; \phi^*(\bar{r}_1)\, \phi^*(\bar{r}_2) \cdot g \cdot \delta(\bar{r}_1 - \bar{r}_2)\, \phi(\bar{r}_1)\, \phi(\bar{r}_2)$$

$$\underbrace{\left(\int d^3\bar{r}_3 \dots d^3\bar{r}_N \prod_{i=3}^{N} \phi^*(\bar{r}_i) \cdot \prod_{i=3}^{N} \phi(\bar{r}_i) \right)}_{=1}$$

$$+ (1,3) + (1,4) \dots + (2,3) + (2,4) \dots + \dots + (N-1, N)$$

$$= \int d^3\bar{r}_1 \; \phi^*(\bar{r}_1)\, \phi^*(\bar{r}_1)\, g \, \phi(\bar{r}_1)\, \phi(\bar{r}_1) + (1,3) + (1,4) \dots$$

$$= g \int d^3\bar{r}_1 \; |\phi(\bar{r})|^2 \cdot |\phi(\bar{r})|^2 + (1,3) + (1,4) + \dots + (2,3) + \dots$$

$$= g \int d^3\bar{r}_1 \; |\phi(\bar{r})|^4 + \dots$$

How many terms? $(N-1) + (N-2) + \dots + 1 = \dfrac{N(N-1)}{2}$

$$\simeq \frac{N^2}{2} \text{ if } N \gg 1.$$

$$\Rightarrow \quad \langle \Psi | V_{int} | \Psi \rangle \simeq \frac{g N^2}{2} \int d^3\bar{r}_i \, |\phi(\bar{r})|^4$$

$$\simeq \frac{g}{2} \int d^3\bar{r}_i \, |\psi(\bar{r})|^4 = \frac{g}{2} \cdot \int d^3\bar{r}_i \, [n(\bar{r})]^2$$

Therefore, the total energy functional becomes:

$$E = \int d^3\bar{r} \left\{ \frac{\hbar^2}{2m} |\nabla \psi(\bar{r})|^2 + V_{ext}(\bar{r}) \cdot |\psi(\bar{r})|^2 + \frac{g}{2} |\psi(\bar{r})|^4 \right\}$$

where $N = \int d^3\bar{r} \, |\psi(\bar{r})|^2$. and $\psi(\bar{r}) = \sqrt{N} \, \phi(\bar{r})$

$$\Rightarrow \quad E - \mu N = \int d^3\bar{r}_i \left\{ \frac{\hbar^2}{2m} |\nabla \psi(\bar{r})|^2 + V_{ext}(\bar{r}) |\psi(\bar{r})|^2 + \frac{g}{2} |\psi(\bar{r})|^4 - \mu |\psi(\bar{r})|^2 \right\}$$

Remember that $|\psi(\bar{r})|^2 = \psi^* \psi$ $\quad |\nabla \psi|^2 = (\nabla \psi^*)(\nabla \psi)$

$|\psi(\bar{r})|^4 = \psi^* \psi^* \psi \psi$

(2) Functional variational $\dfrac{\delta[E-\mu N]}{\delta\psi^*}=0$:

$$\frac{\delta}{\delta\psi^*}\int d^3\bar{r}_i\left[\frac{\hbar^2}{2m}[\nabla\psi]^2+V_{ext}|\psi|^2+\frac{g}{2}|\psi|^4-\mu|\psi|^2\right]=0$$

Consider $\dfrac{\delta}{\delta\psi^*}\left[\int d^3\bar{r}_i\left(V_{ext}(\bar{r})-\mu\right)|\psi|^2\right]$

$$=\int d^3\bar{r}_i\left(V_{ext}-\mu\right)\cdot\frac{\delta|\psi|^2}{\delta\psi^*}$$

$$\frac{\delta|\psi|^2}{\delta\psi^*}=\frac{\delta(\psi^*\psi)}{\delta\psi^*}=\psi$$

Similarly, $\dfrac{\delta|\psi|^4}{\delta\psi^*}=\dfrac{\delta[\psi^2\psi^{*2}]}{\delta\psi^*}=2.\psi^2\psi^*$

$$=2|\psi|^2\psi$$

$$\frac{\delta}{\delta\psi^*}|\nabla\psi|^2=\frac{\delta}{\delta\psi^*}(\nabla\psi^*)(\nabla\psi)=-\frac{\delta}{\delta\psi^*}\left(\psi^*\nabla\nabla\psi\right)$$

integration by parts!

$$=-\nabla^2\psi$$

Therefore,

$$\int d^3\bar{r}_i \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(\bar{r}) + V_{ext}(\bar{r})\,\psi(\bar{r}) + g|\psi(\bar{r})|^2 \psi(\bar{r}) - \mu \psi(\bar{r}) \right] = 0$$

$\Rightarrow$ The Gross–Pitaevskii equation (time-independent form):

$$\boxed{-\frac{\hbar^2}{2m} \nabla^2 \psi(\bar{r}) + V_{ext}(\bar{r})\,\psi(\bar{r}) + g|\psi(\bar{r})|^2 \psi(\bar{r}) = \mu \psi(\bar{r})}$$

Schrödinger eqn: (time-independent form)

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\bar{r}) + V(\bar{r})\,\psi(\bar{r}) = E\,\psi(\bar{r})$$

(1) $g \to 0$ and $\mu \to E$.

The chemical potential μ is the eigenstate energy E of the state $\psi(\bar{r})$ when $g \to 0$, expectedly!

(2) The equation is nonlinear due to the $|\psi|^2\psi$ term!

(3) $\mu = g|\psi|^2$ for a homogeneous condensate without external potential.

$\mu = gn_0$: The energy needed to add an extra particle: $\mu = E(N+1) - E(N) \simeq gn_0$.

(4) Time-dependent form can be obtained by minimizing the action $S = \int d^3r \int dt \cdot \left[\mathrm{Re}(i\psi^* \partial_t \psi) - \mathcal{E}(\psi,\psi^*) + \mu|\psi|^2\right]$ instead of $E - \mu N$:

$$i\hbar \frac{\partial \Psi(\hat{r})}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\hat{r}) + g|\Psi(\hat{r})|^2 - \mu\right]\Psi(\hat{r})$$

instead of free energy $F = E - \mu N$

(5) $$i\hbar \frac{\partial \Psi(\vec{r})}{\partial t} = \Big[\underbrace{-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r})}_{\text{Single particle Hamiltonian}} + \underbrace{g|\Psi(\vec{r})|^2}_{\text{Interaction among the particles}} \Big] \Psi(\vec{r})$$

The condensate particles feel the interaction as if it is inside a mean-field of $g|\Psi(\vec{r})|^2$!

* It is a self-consistent mean-field theory in the sense that the solution $\Psi(\vec{r})$ depends on the mean-field interaction created by $|\Psi(\vec{r})|^2$!

* Single particle operator energy $\propto N$
* Two-body interaction energy $\propto N^2$

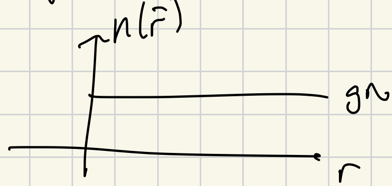
4) What are the length/energy scales of the GP equation? What is the Thomas-Fermi limit? What is the healing length of the condensate?

4) $$-\frac{\hbar^2}{2m}\nabla^2\psi + V_{ext}(\vec{r})\psi + g|\psi|^2\psi = \mu\psi$$

$$E = \int d^3\vec{r}\left\{ \underbrace{\frac{\hbar^2}{2m}|\nabla\psi|^2}_{\substack{\text{Kinetic}\\ \text{energy}\\ \text{density}}} + \underbrace{V_{ext}(\vec{r})|\psi|^2}_{\substack{\text{External}\\ \text{potential energy}\\ \text{density}}} + \underbrace{g|\psi|^4}_{\substack{\text{Interaction}\\ \text{energy}\\ \text{density}}} \right\}$$

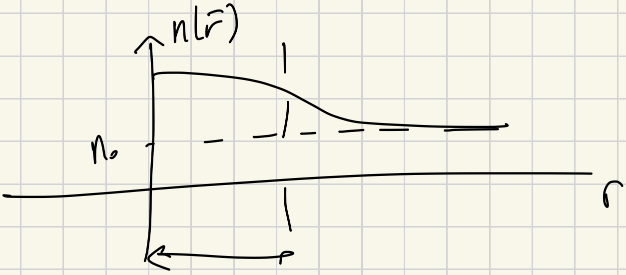
Consider the uniform condensate : $V_{ext}(\vec{r}) = 0$

$\nabla\psi = 0$



$$\Rightarrow \quad \mu = g|\psi|^2 = gn$$

Now look for solutions that include a perturbation / kick in the condensate:



healing length ξ: The length of the condensate to 'heal' itself into the uniform condensate density in the absence of external potential.

$$\frac{\hbar^2}{2m}\nabla^2\psi \simeq g|\psi|^2 \Rightarrow \quad \frac{\hbar^2}{2m\xi^2} \simeq g n_0$$

$\Rightarrow$ Healing length: $\xi^2 \simeq \dfrac{\hbar^2}{2mgn_0}$

$$\xi^{-1} = \sqrt{\frac{2mgn_0}{\hbar^2}} = \sqrt{\frac{2\cancel{m}\,\frac{4\pi a_s \cancel{\hbar^2}}{\cancel{m}} n_0}{\cancel{\hbar^2}}} \Rightarrow$$

$$\boxed{\xi = \sqrt{\frac{1}{8\pi a_s n_0}}}$$

* Healing length must exceed interparticle spacing in GP formalism.

Now assume that the condensate wavefunction is sufficiently smooth such that the kinetic energy term is negligible with respect to the external potential and interaction energies:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V_{ext}(\bar{r})\psi + g|\psi|^2\psi = \mu\psi$$

$$V_{ext}(\bar{r})\psi(\bar{r}) + |\psi(\bar{r})|^2\psi(\bar{r}) = \mu\psi(\bar{r})$$

$$\Rightarrow \boxed{V_{ext}(\bar{r}) + |\psi(\bar{r})|^2 = \mu}$$

This is the TF limit. This limit can generally be realized for sufficiently high # of particles N, since

$$E_{int} \propto N^2$$
$$E_{kin} \propto N.$$

In the TF limit,

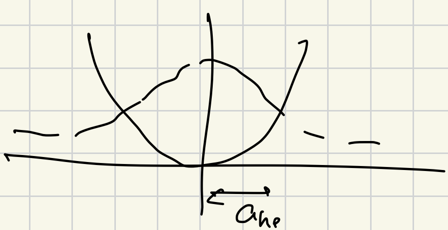
$$V_{ext}(\bar{r}) + g n(\bar{r}) = \mu \Rightarrow n(\bar{r}) = \frac{\mu - V_{ext}(\bar{r})}{g}$$

The chemical potential μ can be calculated by the constraint $\int n(\bar{r})\, d^3\bar{r} = N$

$$\boxed{\int \frac{\mu - V_{ext}(\bar{r})}{g}\, d^3\bar{r} = N.}$$

Another important length scale is the harmonic oscillator length scale:

$$\frac{\hbar^2}{2m a_{ho}^2} = \frac{1}{2} m\omega^2 a_{ho}^2 \Rightarrow \boxed{a_{ho} = \sqrt{\frac{\hbar}{m\omega}}}$$

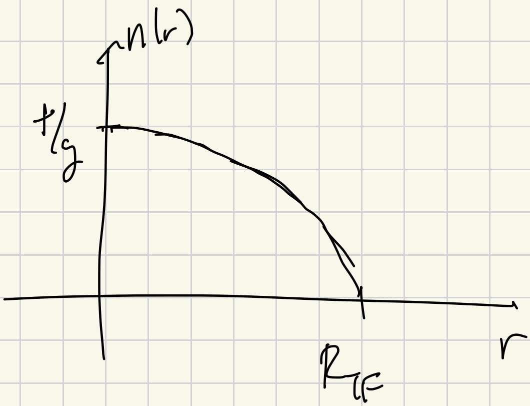


5) Find the Thomas-Fermi solution of the Bose condensate in an isotropic Bose condensate.

5)

$$n(\bar{r}) = \frac{\mu - V_{ext}(\bar{r})}{g} = |\psi(\bar{r})|^2$$

$$V_{ext}(\bar{r}) = \frac{1}{2} m\omega^2 r^2 \Rightarrow n(r) = \frac{\mu - \frac{1}{2} m\omega^2 r^2}{g}$$



$$\frac{1}{2} m\omega^2 R_{TF}^2 = \mu$$

$$R_{TF} = \sqrt{\frac{2\mu}{m\omega^2}}$$

In the TF limit, there exist a finite radius at and above which $n(\bar{r}) = 0$!

$$\int n(r)\,d^3\vec{r} = N = \int \left(\frac{\mu - \frac{1}{2} m\omega^2 r^2}{g} \right) d^3\vec{r}$$

$$= 4\pi \cdot \int_0^{R_{TF}} dr \cdot r^2 \left[\frac{\mu}{g} - \frac{m\omega^2}{2g} r^2 \right]$$

$$= 4\pi \cdot \left[\frac{\mu}{g} \cdot \frac{R_{TF}^3}{3} - \frac{m\omega^2}{2g} \cdot \frac{R_{TF}^5}{5} \right] = N$$

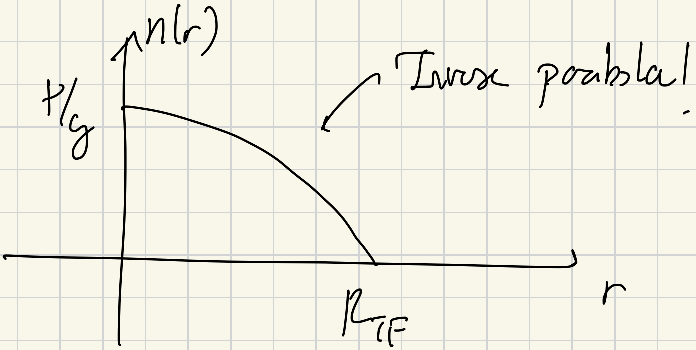
$$\frac{4\pi\mu}{g} \left[\frac{R_{TF}^3}{3} - \frac{m\omega^2}{2\mu} \cdot \frac{R_{TF}^5}{5} \right] = N$$

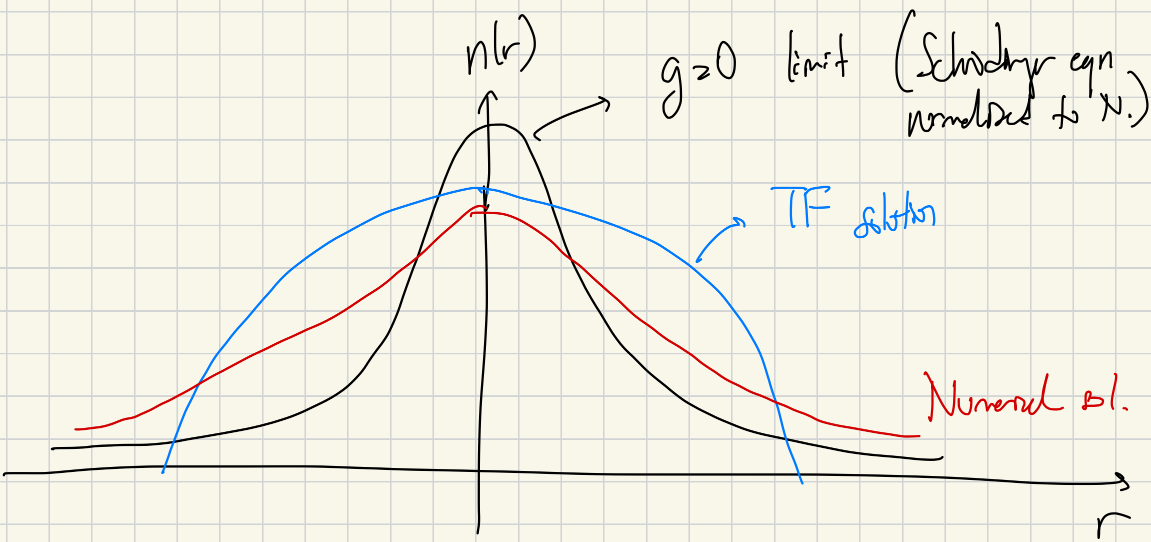
where $R_{TF} = \sqrt{\frac{2\mu}{m\omega^2}}$, $\frac{(R_{TF})^2}{2\mu/m\omega^2} = 1$

$$\frac{2R_{TF}^3}{15} \cdot \frac{4\pi\mu}{g} = N \Rightarrow \frac{2}{15} \cdot \frac{2\sqrt{2}}{(m\omega^2)^{3/2}} \cdot \frac{4\pi\mu^{5/2}}{g} = N$$

$$\Rightarrow \mu^{5/2} = \frac{15\, gN \cdot m^{3/2}\omega^3}{16\pi\sqrt{2}} \Rightarrow \boxed{\mu = \left(\frac{15\, gN\, m^{3/2}\omega^3}{16\pi\sqrt{2}} \right)^{2/5}}$$

$$\mu \propto (gN)^{2/5} \qquad n(r) = \frac{\mu - \frac{1}{2} m\omega^2 r^2}{g}$$





6) How to solve the GP equation numerically?

Imaginary time evolution to solve the ground state of the interacting Bose condensate.

Consider a general form of a time-development equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$$

The aim is to find the ground state wavefunction Ψ_{GS}.

Any wavefunction Ψ can be expanded in terms of the eigenstates including:

$$\Psi = \sum_n c_n \cdot \Psi_n \, , \qquad n \equiv GS, 1, 2, \ldots$$

$$\Psi(t) = c_0(t)\Psi_{GS} + c_1(t)\Psi_1 + c_2(t)\Psi_2 + \ldots$$

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

$$i\hbar \frac{\partial}{\partial t}\left[c_0(t)\psi_{GS} + c_1(t)\psi_1 + \dots\right] = \hat{H}\left[c_0(t)\psi_{GS} + c_1(t)\psi_1 + \dots\right]$$

$$i\hbar \left\{ \psi_{GS}\, c_0' + \psi_1\, c_1' + \dots \right\} = c_0 \cdot E_{GS}\,\psi_{GS} + c_1 \cdot E_1 \psi_1 + \dots$$

$$\int d^3r\ \psi_i^* \left\{ \dots \right\} \Rightarrow i\hbar\, c_i' = c_i E_i$$

$$\Rightarrow c_i = e^{-E_i t/\hbar}$$

$$\Rightarrow \psi(t) = \sum_{i=GS} e^{-iE_i t/\hbar}\, \psi_i$$

Now consider the following hypothetical evolution:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \xrightarrow[\substack{t \to \tau = it \\ t = \tau_i}]{} -\hbar \frac{\partial \psi}{\partial \tau} = \hat{H}\psi \Rightarrow$$

$$-\hbar \frac{\partial \psi}{\partial \tau} = \hat{H}\psi \Rightarrow \psi(\tau) = \sum_{i=GS} e^{-E_i \tau/\hbar} \psi_i$$

$$\psi(\tau) = e^{-E_{GS}\tau/\hbar} \psi_{GS} + e^{-E_1 \tau/\hbar} \psi_1 + \ldots$$

For a sufficiently long evolution in imaginary time, the only term that survives is the ground state: ψ_{GS}, since $E_{GS} < E_{i>1}$

$$\boxed{\psi(\tau \to \infty) \propto \psi_{GS}}$$

Imaginary time algorithm:

1. Assign an initial wavefunction ψ_{init}
2. $\psi_i = \psi_{init} - \frac{\hat{H}\psi_{init}}{\hbar} \cdot \Delta\tau$, where $H[\psi] = H[\psi_{init}]$
3. Renormalize $\int |\psi_i|^2 d\vec{r} = N$.
4. Calculate μ: $\hat{H}\psi = \mu\psi$
5. Check $\hat{H}\psi - \mu\psi$ to converge.
6. Repeat (2-6).

7) Compare the solutions of the non-interacting limit of GP equation (Schrödinger eq.), analytical solution of TF limit and the numerical solution of the GP equation.

Discuss in which limits the numerical solution approaches the Schrödinger eqn and TF solution.