# Week 6

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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*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)

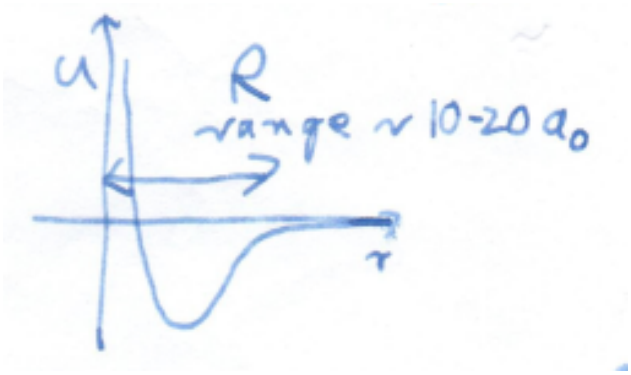
$$\hat{H} = \sum_{k=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_{\mathbf{x}_k}^2 + V(\mathbf{x}_k) \right) + \frac{1}{2} \sum_{k,l=1}^{N} U(\mathbf{x}_k - \mathbf{x}_l) \tag{3.18}$$

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.

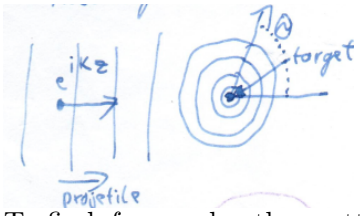
**Important fact I:** Densities in dilute gas BEC are such that the mean distance $d$ between atoms $d \gg R$, since $d \sim 0.1\mu$m. $\implies$ When interactions take place, they are mostly binary scattering of two atoms, so let us look at that.

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 $\theta$ 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.

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

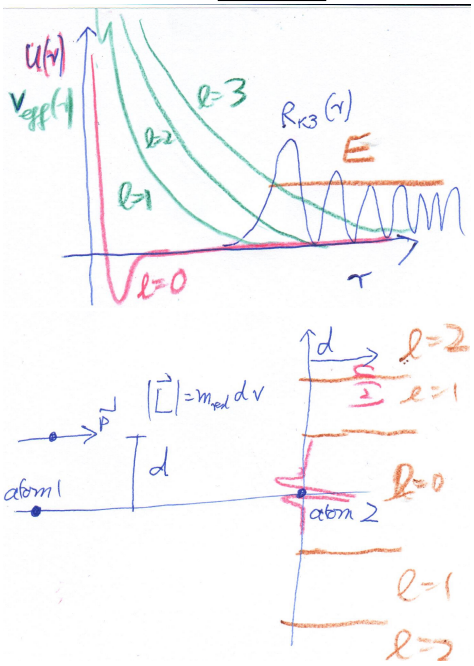
**Partial wave expansion (PWE):** (*Also reminder only.* ) A useful tool for the solution of Eq. (3.21) in scattering theory is the PWE. Here we expand both, $f$ and the incoming wave in terms of Legendre polynomials in $\theta$.

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

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:

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

**s-wave scattering:** As in usual solutions of the TISE, the wavefunction $R(r)$ will not significantly extend into regions where $0 < E < V_{\text{eff}}(r)$ (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 $V_{\text{eff}}(r)$ 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 $\theta$, 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

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

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

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

So now $f$ no longer depends on scattering energy/momentum through $k$ nor on angle $\theta$. 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, $\phi$ 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 $\psi$.
- 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 $\phi$ and $\phi^*$ 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 [3] 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

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

- 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.

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

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

- 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 math example)

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

### 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

**Time-independent GPE**

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

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

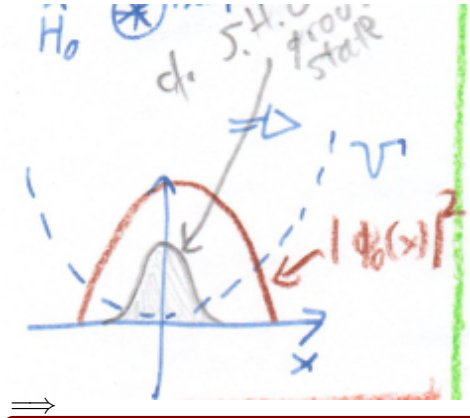
**Ground State Solutions:**

**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 $U_0 n > \underbrace{\frac{\hbar\omega}{2}}_{\text{Approximate K.E. in GS oscillator}}$ the kinetic energy can be neglected relative to the interaction energy.

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

For $U_0 = 0$, we know harmonic oscillator ground state $\varphi_0$ 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 $\infty$-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 $\phi, \phi^*$ 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.

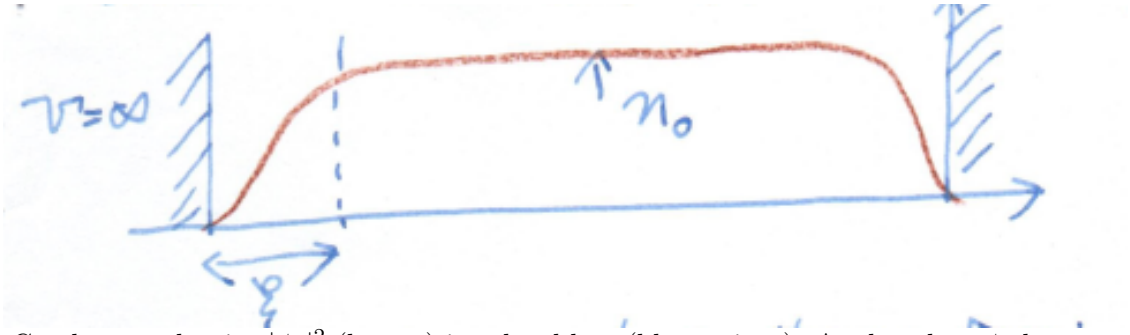
$$\phi(x,\tau+\delta\tau) - \phi(x,\tau) = -[H_0 + U_0|\phi_0(x)|^2]\phi_0(x)$$

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

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

$$\frac{-\hbar^2}{2mU_0 n_0 \zeta^2} f''(\frac{x}{\zeta}) + [f^2 - 1]f = 0 \tag{3.50}$$

This equation becomes scale-free if we set

**Healing Length**

$$\zeta = \frac{\hbar}{\sqrt{2mU_0 n_0}} \tag{3.51}$$

- 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 $\rho$, $\varphi$ 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

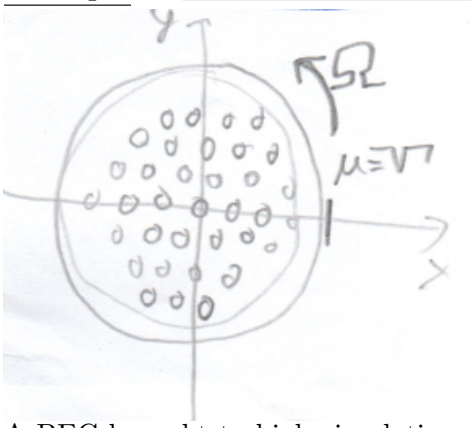
  **Quantisation of circulation**

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

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

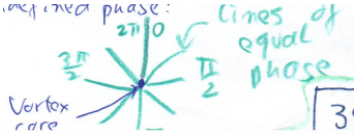
- Proof : show that $\int_L \mathbf{v} \cdot d\mathbf{x} = \frac{\hbar}{m}[\varphi(\mathbf{b}) - \varphi(\mathbf{a})]$ for a non-closed loop between two points $\mathbf{a}$ and $\mathbf{b}$. Then (3.57) follows because the phase at $\mathbf{x}$ has to be unique $\Longrightarrow$

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




**left:** Abrikosov-lattice of vortices (circles). $\Omega$ 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**

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

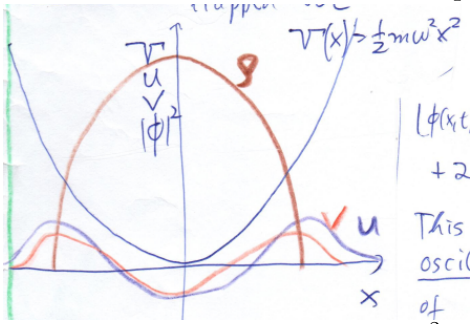
- Be careful: In this section $v$ has nothing to do with velocity.
- We need to include $e^{i\omega t}$ AND $e^{-i\omega t}$ because (3.3.3) couples $\phi$ with $\phi^*$.
- Insert (3.58) into (3.3.3), use (3.45) then seperately consider coefficients of $e^{i\omega t}$ and $e^{-i\omega t}$ to get the

**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 $\omega$ 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 $\omega = \sqrt{5}\omega_{\text{trap}}$.