2.2 Gross-Pitaevskii equation: a variational derivation

To derive Gross-Pitaevskii equation, we start from the general hamiltonian:

$$\mathcal{H} = \underbrace{\sum_{i=1}^{N} \frac{p_i^2}{2m}}_{\text{kinetic}} + \underbrace{\sum_{i=1}^{N} V(r_i)}_{\text{trap}} + \underbrace{\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} U(|r_i - r_j|)}_{\text{interactions}} \tag{I.16}$$

and compute the energy with the following variational wave-function: it considers that all atoms are in the lowest energy level, the wave-function of which is denoted by $\phi_0(r)$:

$$|\psi(r_1, r_2, \ldots, r_N)\rangle = |\phi_0(r_1)\rangle \otimes |\phi_0(r_2)\rangle \otimes \cdots \otimes |\phi_0(r_N)\rangle \tag{I.17}$$

Interactions actually induce correlations and at $T = 0$ the condensed fraction is not 1 because interactions can couple the ground-state to excited state but this approximation is fairly good for dilute gas. At non-zero temperature, we should rather describe the system using a density-matrix formalism. The derivation of GP equation relies on the variational method. The energy functional $E[\psi] = \langle\psi|\mathcal{H}|\psi\rangle/\langle\psi|\psi\rangle$ has a minimum E_0 for the true ground-state wave-function $|\psi_0\rangle$. When making a small variation $\psi \to \psi + \delta\psi$, the normalization of $|\psi\rangle$ may change. In order to work in the subspace of normalized wave-functions, we introduce a Lagrange multiplier μ, which will appear to be equal to the chemical potential at the end of the calculation. We thus rather minimize the functional $F[\psi] = \langle\psi|\mathcal{H}|\psi\rangle - \mu\langle\psi|\psi\rangle$. Let us compute the different terms using (I.17). We choose $\phi_0(r) \equiv \phi(r)$ to be normalized ($\int dr|\phi|^2 = 1$) and assumes that it vanishes at the boundary of the integration volume. The kinetic term reads ($p = -i\hbar\nabla$):

$$\begin{aligned}
\langle\psi|\sum_{i=1}^{N} \frac{p_i^2}{2m}|\psi\rangle &= \sum_{i=1}^{N} \frac{\hbar^2}{2m}\int dr_i \nabla\phi^*(r_i)\nabla\phi(r_i) \\
&= +N\frac{\hbar^2}{2m}\int dr|\nabla\phi(r)|^2 = -N\frac{\hbar^2}{2m}\int dr\phi^*(r)\Delta\phi(r)
\end{aligned} \tag{I.18}$$

potential term:

$$\langle\psi|\sum_{i=1}^{N} V(r_i)|\psi\rangle = N\int dr\phi^*(r)V(r)\phi(r) \tag{I.19}$$

interaction term:

$$\begin{aligned}
\langle\psi|\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} U(|r_i - r_j|)|\psi\rangle &= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\int dr_i \int dr_j \phi^*(r_i)\phi^*(r_j)U(|r_i - r_j|)\phi(r_j)\phi(r_i) \\
&= \frac{N(N-1)}{2}\int dr \int dr'\phi^*(r)\phi^*(r')U(|r - r'|)\phi(r')\phi(r)
\end{aligned} \tag{I.20}$$

Lagrange multiplier term (written in a way to get the variations easily):

$$\mu\langle\psi|\psi\rangle = \mu\left(\int dr\phi^*(r)\phi(r)\right)^N \tag{I.21}$$

Now, we make a small variation of our unknown wave-function $\phi(r) \to \phi(r) + \delta\phi(r)$. ϕ is a complex function, instead of varying the real and imaginary parts, we take ϕ and ϕ^* as independent variables. The functional derivatives $\delta\{\ldots\}/\delta\phi^*$ are easily computed for terms (I.18), (I.19). For the interactions term, there is two contributions from each ϕ^* but the r variable can be permuted which removes the factor 2:

$$N(N-1)\int dr\delta\phi^*(r)\left(\int dr'|\phi(r')|^2 U(|r-r'|)\right)\phi(r) \tag{I.22}$$

For the chemical potential, we have:

$$\frac{\delta\langle\psi|\psi\rangle}{\delta\phi^*} = N\left(\int dr\phi^*(r)\phi(r)\right)^{N-1}\int dr\delta\phi^*(r)\phi(r) = N\int dr\delta\phi^*(r)\phi(r) \tag{I.23}$$

Collecting terms, we find for the variation:

$$\frac{\delta F[\phi,\phi^*]}{\delta\phi^*} = N\left\{-\frac{\hbar^2}{2m}\Delta\phi(r) + V(r)\phi(r) + (N-1)\left(\int dr'|\phi(r')|^2 U(|r-r'|)\right)\phi(r) - \mu\phi(r)\right\} = 0 \tag{I.24}$$

Thus, what is inside the brackets must vanish and the resulting equation is the Gross-Pitaevskii one. It is usually more tractable for a point-contact interaction $U(r-r') = U_0\delta(r-r')$, with U_0 positive or negative (see models for interactions between atoms), and using $N-1 \simeq N$, it has the nice form:

$$-\frac{\hbar^2}{2m}\Delta\phi(r) + V(r)\phi(r) + NU_0|\phi(r)|^2\phi(r) = \mu\phi(r) \tag{I.25}$$

It resembles a time-independent Schrödinger equation $\hat{\mathcal{H}}\phi = E\phi$ except that it has a non-linear "self-trapping" term $NU_0|\phi(r)|^2$ coming from the mean-field approximation and the right hand side is the chemical potential rather than the energy per particle E/N. People often remove the N factor by changing the normalization of $\phi(r)$ using $\Psi(r) = \sqrt{N}\phi(r)$. We can also check that $\mu = \delta E/\delta N$. Indeed, we have

$$\frac{\delta E}{\delta N} = \frac{\partial E}{\partial N} + \frac{\delta E}{\delta\phi}\frac{\partial\phi}{\partial N} \tag{I.26}$$

but $\frac{\delta E}{\delta\phi} = 0$ because ϕ is the variational solution. All terms in the energy are linear in N but the interaction one which is proportional to $N(N-1)/2$ and gives after derivation $N - 1/2$

$$\frac{\partial E}{\partial N} = (\text{non-interacting terms}) + (N-1/2)\times(\text{interaction term})\ . \tag{I.27}$$

On the other side, multiplying (I.25) by $\phi^*(r)$ and integrating over r gives

$$\mu = (\text{non-interacting terms}) + (N-1)\times(\text{interaction term})\ . \tag{I.28}$$

and since $N - 1 \simeq N - 1/2$, we may identify μ to $\delta E/\delta N$.

2.3 Variational solution of Gross-Pitaevskii equation

$$\phi(r) = \frac{1}{\pi^{3/4}(\eta\sigma)^{3/2}} e^{-(x^2+y^2+z^2)/2\eta^2\sigma^2} \tag{I.29}$$

$$\int_{-\infty}^{+\infty} dx\; e^{-x^2} = \sqrt{\pi} \tag{I.30}$$

$$\int_{-\infty}^{+\infty} dxdydz\; \phi(r)^4 = \frac{1}{(2\pi)^{3/2}(\eta\sigma)^3} \tag{I.31}$$

$$\int_{-\infty}^{+\infty} dxdydz\; x^2\phi(x,y,z)^2 = \frac{(\eta\sigma)^2}{2} \tag{I.32}$$

$$\int_{-\infty}^{+\infty} dxdydz\; \left|\frac{\partial\phi}{\partial x}\right|^2 = \frac{1}{2(\eta\sigma)^2} \tag{I.33}$$

2.4 Stability of the BEC for repulsive and attractive interactions

$$E^{\text{tot}} = \frac{3}{4}N\hbar\omega_0\left[\frac{1}{\eta^2} + \eta^2 + \frac{\chi}{\eta^3}\right] \quad \text{with} \quad \chi = \frac{2}{3}\sqrt{\frac{2}{\pi}}\left(\frac{aN}{\sigma}\right) \tag{I.34}$$

2.5 The Thomas-Fermi regime

useful relations:

$$\text{trap length scale: } \sigma = \sqrt{\frac{\hbar}{m\omega_0}} \tag{I.35}$$

$$\text{scattering length: } a\,, \quad U_0 = \frac{4\pi\hbar^2}{m}a = 4\pi\,\hbar\omega_0\, a\sigma^2 \tag{I.36}$$

$$\text{healing length: } \xi_0 = \frac{1}{\sqrt{8\pi n_0 a}} \tag{I.37}$$

$$\text{Radius in Thomas-Fermi regime: } R \simeq \sigma\left(\frac{aN}{\sigma}\right)^{1/5} \tag{I.38}$$

$$\text{Inter-particle distance: } d \simeq R\,N^{-1/3} \tag{I.39}$$

2.6 The healing length

3 Time-dependent Gross-Pitaevskii equation

3.1 Let us try from the Schrödinger equation

The Schrödinger equation for N-particles reads:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{r_i}\psi + \sum_{i=1}^{N}V(r_i,t)\psi + \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}U(r_i-r_j)\psi \tag{I.40}$$

with $\psi(r_1,\ldots,r_N,t)$ the many-body wave-function. Note that the external potential V can depend on time (the interaction term could also depend on time). To derive time-dependent Gross-Pitaevskii equation, we now take the same ansatz as for the time-independent one except that now we have the time depedence:

$$|\psi(r_1,r_2,\ldots,r_N,t)\rangle = |\phi(r_1,t)\rangle|\phi(r_2,t)\rangle\cdots|\phi(r_N,t)\rangle \tag{I.41}$$

Up to $i\hbar$, the left-hand term reads

$$\frac{\partial\psi}{\partial t} = \sum_{i=1}^{N}\phi(r_1,t)\cdots\frac{\partial\phi(r_i,t)}{\partial t}\cdots\phi(r_N,t) \tag{I.42}$$

We want an equation on $\phi(r,t)$ only. To get it, we integrate over all other particles but the first one. To do so, we multiply left and right terms by $\int\prod_{j=1}^{N}dr_j\phi^*(r_j,t)$ and use the normalization constraint $\int dr_j|\phi(r_j,t)|^2=1$. The right hand side and non-interacting part of the right-hand side is simply reduced to

$$N\int dr\phi(r,t)^*\left\{i\hbar\frac{\partial\phi(r,t)}{\partial t} - \frac{\hbar^2}{2m}\Delta\phi(r,t) - V(r,t)\phi(r,t)\right\} \tag{I.43}$$

The interactions contribution reads:

$$\sum_{i=1}^{N}\int\prod_{j=1}^{N}dr_j\phi^*(r_j)\sum_{k\neq i}^{N}\left(\prod_{l\neq i,k}\phi(r_l)\right)U(r_i-r_k)\phi(r_i)\phi(r_k)$$

The contribution on the i^{th} particle is:

$$\begin{aligned}\int\prod_{j=1}^{N}dr_j\phi^*(r_j)\sum_{k\neq i}^{N}\left(\prod_{l\neq i,k}\phi(r_i)\right)U(r_i-r_k)\phi(r_i)\phi(r_k) &= \int dr_i\phi(r_i)^*\sum_{k\neq i}\int dr_k|\phi(r_k)|^2U(r_i-r_k)\phi(r_i)\\ &= \int dr_i\phi(r_i)^*(N-1)U_0|\phi(r_i)|^2\phi(r_i)\end{aligned}$$

where we took a delta interaction $U(r_i-r_k)=U_0\delta(r_i-r_k)$ in the last equality. Collecting terms, we find:

$$N\int dr\phi(r,t)^*\left\{i\hbar\frac{\partial\phi(r,t)}{\partial t} - \frac{\hbar^2}{2m}\Delta\phi(r,t) - V(r,t)\phi(r,t) - \frac{1}{2}(N-1)U_0|\phi(r,t)|^2\phi(r,t)\right\} = 0 \tag{I.44}$$

But what can we infer from that? It is however tempting to say that the term within brackets is zero. But this is not true because the interaction term would have a 1/2 factor which does not correspond to the correct equation. The derivation can be done more properly using variational principle.

3.2 Variational derivation of time-dependent Gross-Pitaevskii equation

The derivation of the time-dependent GP equation relies on the minimization of the action. This is the least action principle. For a single particule, we may write the action $\mathcal{S}$:

$$\mathcal{S}[\psi] = \int_{t_1}^{t_2} dt \int dr\ \mathcal{L}(\psi, \psi^*, \dot{\psi}, \dot{\psi^*}, \nabla\psi, \nabla\psi^*) \tag{I.45}$$

with $\dot{\psi} = \partial\psi/\partial t$. Assuming that ψ vanishes at the boundaries of the integration volume and that the variations satisfy $\delta\psi(t_1, r) = \delta\psi(t_2, r)$ for all points r, it is easy to derive the Lagrange equations for the Lagrangian:

$$-\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{\psi^*}} + \frac{\partial \mathcal{L}}{\partial \psi^*} - \nabla \cdot \left(\frac{\partial \mathcal{L}}{\partial \nabla \psi^*}\right) = 0 \tag{I.46}$$

the last term is a scalar product $\sum_{j=x,y,z} \partial_j \left(\frac{\partial \mathcal{L}}{\partial(\partial_j \psi^*)}\right)$. The Lagrange formalism should give back the correct equation of motion which is nothing but the Schrödinger equation. For that, we must choose the good $\mathcal{L}$. For a single particle in a trap:

$$\mathcal{L} = i\frac{\hbar}{2}\left[\psi^*\dot{\psi} - \dot{\psi^*}\psi\right] - \frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi - \psi^* V(r,t)\psi \tag{I.47}$$

You can check that applying (I.46) gives the Schrödinger equation. In the case of many particles, the action and Lagrangian can easily be generalized to N-particles making the Lagrangian depends on all $\nabla_{r_i}\psi$ where r_i is the position of the i^{th} particle and the integration inside the action running over all particle positions $\int dr_1 \cdots dr_N$. The Lagrange equation is

$$-\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{\psi^*}} + \frac{\partial \mathcal{L}}{\partial \psi^*} - \sum_{i=1}^{N} \nabla_{r_i} \cdot \left(\frac{\partial \mathcal{L}}{\partial \nabla_{r_i} \psi^*}\right) = 0 \tag{I.48}$$

with $\psi(r_1, \ldots, r_N, t)$ the many-body wave-function. The good choice for our many-body Lagrangian is now

$$\mathcal{L} = i\frac{\hbar}{2}\left[\psi^*\dot{\psi} - \dot{\psi^*}\psi\right] - \frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_{r_i}\psi^*\nabla_{r_i}\psi - \sum_{i=1}^{N}\psi^* V(r_i,t)\psi - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\psi^* U(r_i - r_j)\psi \tag{I.49}$$

Applying the Lagrange equations (I.48) to (I.49) gives the Schrödinger equation that we expect:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{r_i}\psi + \sum_{i=1}^{N}V(r_i,t)\psi + \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}U(r_i - r_j)\psi \tag{I.50}$$

Note that the external potential V can depend on time (the interaction term could also depend on time).

To derive time-dependent Gross-Pitaevskii equation, we now take the same ansatz as for the time-independent one, namely

$$|\psi(r_1, r_2, \ldots, r_N, t)\rangle = |\phi(r_1, t)\rangle|\phi(r_2, t)\rangle \cdots |\phi(r_N, t)\rangle \tag{I.51}$$

so that

$$\dot{\psi}(r_1, r_2, \ldots, r_N, t) = \sum_{i=1}^{N} \phi(r_1, t) \cdots \frac{\partial \phi(r_i, t)}{\partial t} \cdots \phi(r_N, t) \tag{I.52}$$

We the help of the previous calculations done for the try with the Schrödinger equation, we find for the total action:

$$\begin{aligned} \mathcal{S}[\phi] = N \int_{t_1}^{t_2} dt \int dr \, \Big\{ i\frac{\hbar}{2}\left[\phi^* \frac{\partial \phi}{\partial t} - \frac{\partial \phi^*}{\partial t}\phi\right] - \frac{\hbar^2}{2m}\nabla\phi(r,t)^*\nabla\phi(r,t) \\ -V(r,t)|\phi(r,t)|^2 - \frac{1}{2}(N-1)U_0|\phi(r,t)|^4 \Big\} \end{aligned} \tag{I.53}$$

The action of the N-particles many-body system has reduced to N-times the action of a one-particle system. This is mean-field theory. This action is called the ϕ^4 model and appears quite often in physical models. Using the Lagrange equations on (I.53), one finds:

$$i\hbar\frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\phi(r,t) + V(r,t)\phi(r,t) + (N-1)U_0|\phi(r,t)|^2\phi(r,t) \tag{I.54}$$

Note that the factor $1/2$ in the interaction term drops because of the $(\phi^*)^2$ dependence of the $|\phi|^4$ term. It is important to understand that this is an equation of motion for the system so it resembles more a Schrödinger equation than the time-independent GP equation. In particular, one can calculate the spectrum of excitations $E(k) = \hbar\omega(k)$ with this equation.

3.3 Linearization and Bogoliubov spectrum

3.4 Solitons