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Introduction to quantum liquids
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TD4: Applications of the Gross-Pitaevskii equation

In this TD we will concentrate on the study of the Gross-Pitaevskii equation (GPE)

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm ext}(\boldsymbol{r}) + g|\Psi_0(\boldsymbol{r})|^2\right)\Psi_0(\boldsymbol{r}) = \mu\Psi_0(\boldsymbol{r}) \qquad (1)$$

for the study of inhomogeneous condensates.

1) Thomas-Fermi approximation

1.1) Be R the characteristic length scale for the variations of the macroscopic wavefunction

$$\frac{R^2\ \nabla^2\Psi_0}{\Psi_0} \sim 1 \quad . \qquad (2)$$

Show that, if $R \gg \xi$ (where $\xi = \hbar/\sqrt{2gmn}$ is the healing length), the kinetic part of the GPE can be neglected with respect to the non-linear term.
Conclude that, under the above assumption (the so-called Thomas-Fermi approximation), the condensate density satisfies the simple equation

$$|\Psi_0(\boldsymbol{r})|^2 = n(\boldsymbol{r}) = \frac{\mu - V_{\rm ext}(\boldsymbol{r})}{g} \qquad (3)$$

1.2) Consider the case of a confining harmonic potential, $V_{\rm ext} = (1/2)m\omega^2 r^2$. Draw the radial density profile $n(r)$, and calculate the radius of the condensate (Thomas-Fermi radius). If N is the total number of particles, show that the related chemical potential is

$$\mu(N) = \left(\frac{15}{8}\frac{gN}{\pi}\right)^{2/5}\left(\frac{m\omega^2}{2}\right)^{3/5} \qquad (4)$$

Calculate the compressibility, $\kappa = \partial N/\partial\mu$, and comment on its dependence on g.

2) Condensate at a hard-wall potential

Consider the hard-wall potential in one dimension

$$V_{\rm ext}(x) = \begin{cases} 0 & x \geq 0 \\ \infty & x < 0\ . \end{cases} \qquad (5)$$

What are the boundary conditions for the GPE at $x = 0$ and $x = \infty$?
Writing

$$\Psi_0 = \sqrt{n}\ f\left(\frac{x}{\sqrt{2}\ \xi}\right) \qquad (6)$$

where $n = |\Psi_0(x\to\infty)|^2$, show that the GPE takes the form

$$\frac{d^2 f(y)}{dy^2} = -2(f - f^3) \qquad (7)$$

where $y = x/(\sqrt{2}\,\xi)$. Show that $f(y) = \tanh(y)$ is a solution to the above equation. Draw the full solution to the GPE equation: do you understand now why they call ξ the "healing" length?

3) Vortex solution

We look now for a solution to the GPE with finite vorticity. Taking a system with cylindrical symmetry, consider a macroscopic wavefunction of the form

$$\Psi_0(r,\phi,z) = |\Psi_0(r)|\; e^{ip\phi} \qquad p \in \mathbb{Z} \quad . \tag{8}$$

3.1) What is the angular momentum of this wavefunction? Calculate the related velocity field

$$\boldsymbol{v}_s(\boldsymbol{r}) = \frac{\hbar}{m}\boldsymbol{\nabla} S(\boldsymbol{r}) \tag{9}$$

where S is the phase of the wavefunction.
Calculate the vorticity of the velocity field, and show that the vorticity is quantized. By using Stokes' theorem, show that

$$\boldsymbol{\nabla} \times \boldsymbol{v}_s(\boldsymbol{r}) = \frac{h}{m}\, p\, \delta^{(2)}(r)\, \boldsymbol{e}_z \quad . \tag{10}$$

3.2) Show that the GPE equation takes the form

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right)|\Psi_0| + \frac{\hbar^2}{2m}\frac{p^2}{r^2}|\Psi_0| + g|\Psi_0|^3 - \mu|\Psi_0|^2 = 0 \tag{11}$$

Writing $|\Psi_0| = \sqrt{n} f(y)$ with $|\Psi_0(r \to \infty)| = \sqrt{n}$ and $y = r/\xi$, rewrite the GPE in the form

$$\left(\frac{d^2}{dy^2} + \frac{1}{y}\frac{d}{dy}\right) f + \left(1 - \frac{p}{y^2}\right) f - f^3 = 0 \tag{12}$$

3.3) For $y \to 0$, we look for a solution in the form $f \sim y^{\alpha}$. Show that this works if $\alpha = |p|$. In the opposite limit, $y \to \infty$, show that the GPE equation reduces to the same form as that of the hard-wall potential.
Interpolating between the two limits, sketch the form of the radial wavefunction $|\Psi_0(r)|$. What is the characteristic size of the vortex core?

3.4) To conclude, we calculate the energy of the solution to the GPE containing one quantized vortex. Knowing that the energy functional is given by

$$E = \int d^3r \left(\frac{\hbar^2}{2m}|\boldsymbol{\nabla}\Psi_0|^2 + \frac{g}{2}|\Psi_0|^4\right) \tag{13}$$

we consider a cylindrical sample, with radius R and height L. Show that the energy difference between the macroscopic wavefunction containing a vortex and the uniform wavefunction (without vortices) can be written as

$$E_v = \frac{L\pi\hbar^2 n}{m}\int_0^{R/\xi} dy\; y\left[\left(\frac{df}{dy}\right)^2 + \frac{p^2}{y^2}f^2 + \frac{1}{2}(f^4 - 1)\right] \tag{14}$$

To estimate this integral, we drastically approximate $f(y)$ with the function $f(y) = y$ for $y < 1$ and $f(y) = 1$ for $y \geq 1$. Show that this leads to the estimate

$$E_v \approx \frac{L\pi\hbar^2 n}{m} p^2 \ln\left(\frac{bR}{\xi}\right) \tag{15}$$

where $b = 2.3$ (The exact result gives the same form for the energy, but a different coefficient $b = 1.46$, so the above estimate is not that bad after all).
Explain the fact that the energy of the vortex diverges with the system size $L, R \to \infty$, although the vortex excitation only leads to a localized depletion in the density profile around the vortex core.

3.5) Imagine that the cylindrical bucket containing the condensate is put into rotation at an angular velocity Ω. In the rotating reference frame the Hamiltonian takes the form

$$\mathcal{H} = \mathcal{H}_0 - \Omega L_z \tag{16}$$

where $\mathcal{H}_0$ and L_z are the Hamiltonian and the angular momentum in the laboratory frame. Show that for $\Omega > \Omega_c$ (to be determined) the vortex configuration becomes stable, so that vortices start to appear in the system.

4) Vortex-vortex interactions

Imagining to rotate the bucket even faster, we want to investigate whether the vortex we have created acquires a higher vorticity, or whether we add instead more vortices with unit vorticity to the system. To this end we need to calculate the interaction energy between two vortices with cores at a distance $d \gg \xi$.
In presence of two vortices the velocity field takes the form

$$\boldsymbol{v}_s = \frac{\hbar}{m}\frac{p_1}{r}\,\boldsymbol{e}_\phi^{(0)} + \frac{\hbar}{m}\frac{p_2}{r-d}\,\boldsymbol{e}_\phi^{(d)} = \boldsymbol{v}_0 + \boldsymbol{v}_d \tag{17}$$

where the $\boldsymbol{e}_\phi^{(0)}$ and $\boldsymbol{e}_\phi^{(d)}$ vectors are referred to cylindrical reference frames with origins at $r = 0$ and $r = d$ respectively.
Similarly to what seen at 3.4) (but even more drastically) we neglect the spatial variation of the density of the condensate, and we take

$$\Psi(\boldsymbol{r}) \approx \sqrt{n}\, e^{iS(\boldsymbol{r})} \tag{18}$$

where $n = \text{const.}$, and $\boldsymbol{v}_s = (\hbar/m)\boldsymbol{\nabla} S$.

4.1) Show that the energy of interaction between the two vortices can be written as

$$E_{\text{int}} = mn \int d^3r\, \boldsymbol{v}_0 \cdot \boldsymbol{v}_d \quad . \tag{19}$$

4.2) If $r \gg d$ we have that $\boldsymbol{e}_\phi^{(0)} \approx \boldsymbol{e}_\phi^{(d)}$. Considering that $R \gg d$, the points with $r \gg d$ will dominate the above integral, so that we can take this approximation all over the volume of the system. In this case, show that

$$E_{\text{int}} \approx \frac{2L\hbar^2\pi n}{m} p_1 p_2 \ln\left(\frac{R}{d}\right) \quad . \tag{20}$$

Comment on the nature of the interaction.

4.3) Now we are ready to respond to the initial question: what happens when rotating the condensate faster and faster? Compare the energy of a vortex with vorticity $p = 2$, $E_v(p = 2)$, with the energy of two vortices $2E_v(p = 1) + E_{\text{int}}$. Which solution is energetically favored?

4.4) Let us look now at the experiment, shown in Fig. **??**. Can you interpret what you see in light of the previous results? Can you understand the structure of the vortex arrays appearing in the system?

Mathematical appendix

Gradient in cylindrical coordinates

$$\boldsymbol{\nabla} = \boldsymbol{e}_r \, \frac{\partial}{\partial r} \; + \; \boldsymbol{e}_\phi \, \frac{1}{r} \frac{\partial}{\partial \phi} \; + \; \boldsymbol{e}_z \, \frac{\partial}{\partial z} \tag{21}$$

Laplacian in cylindrical coordinates

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \tag{22}$$

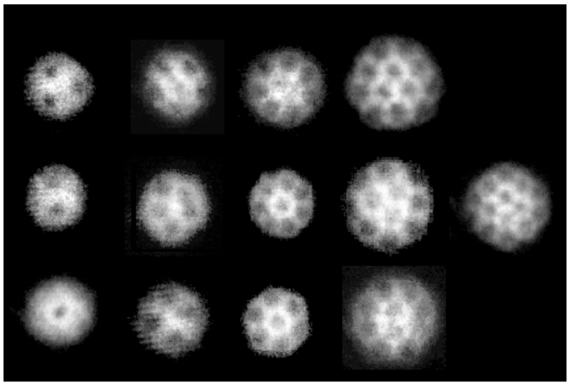

Figure 1: Vortex arrays appearing in a condensate under rotation at increasing angular velocity. From F. Chevy's PhD thesis, ENS-Paris (2001).