TA 13. Wave solutions in Hartree-Fock and vortex solutions in Gross-Pitaevskii

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1 Introduction

In this tutorial we will look at some simple solutions of the Hartree-Fock Equation (HFE) and of the Gross-Pitaevskii Equation (GPE).

The HFE is a mean field equation for a many fermion system; the physical application we will discuss is the gas of electrons in an homogeneous positive ions background, which is a good approximation of a metal at low temperatures. We will see that for such system, plane waves satisfy the HFE.

The GPE is instead a mean field equation for many bosons system in their ground state. Differently from fermions, in fact, bosons can occupy the same quantum state. Such a system is called condensate. Superfluids, i.e. fluids which show no viscosity, are an example of application of the GPE. We will discuss a particular solution of the GPE, which is the vortex.

2 Wave solutions in HFE

The HFE for N particles $\psi_i(\vec{r}, s)$, where i labels the particle, reads

$$\left(\underbrace{\frac{-\hbar^2\nabla^2}{2m}}_{(1)} + U(\vec{r}) + \underbrace{\int \mathrm{d}^3 r'\, V(|\vec{r}-\vec{r'}|)\rho(\vec{r'})}_{(2)}\right)\psi_i(\vec{r}, s) - \underbrace{\sum_{s'}\int \mathrm{d}^3 r'\, V(|\vec{r}-\vec{r'}|)\rho(\vec{r}, s, \vec{r'}, s')\psi_i(\vec{r'}, s)}_{(3)} = \epsilon_i \psi_i(\vec{r}, s) \ , \tag{2.1}$$

where U is the one-body (external) potential, V is the 2-body potential and

$$\rho(\vec{r'}) = \sum_j n_j \sum_s \left|\psi_j(\vec{r'}, s)\right|^2 \ , \ \rho(\vec{r}, s, \vec{r'}, s') = \sum_j n_j \psi_j(\vec{r}, s)\psi_j^*(\vec{r'}, s') \ ; \tag{2.2}$$

we will assume $\psi_i(\vec{r}, s) =: \psi_i(\vec{r})\chi_s$, i.e. that we can decompose the spin part χ_s.

If the potential $U(\vec{r}) = U_0$, i.e. it is just a constant, then we can prove that plain waves

$$\psi_i(\vec{r}) = \frac{1}{\sqrt{\Omega}} \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} \ , \tag{2.3}$$

where Ω is a volume factor[1], is solution of the HFE. We look at the pieces of the HFE one at a time.

$$(1)\ \left(\frac{-\hbar\nabla^2}{2m}+U_0\right)\psi_i(\vec{r},s)=\left(\frac{\hbar k^2}{2m}+U_0\right)\psi_i(\vec{r},s)\ ; \tag{2.4}$$

$$\begin{aligned}(2)\ \frac{1}{\Omega}\int \mathrm{d}^3r' V(|\vec{r}-\vec{r'}|)\sum_j n_j \mathrm{e}^{\mathrm{i}\vec{k}_j\cdot\vec{r}}\mathrm{e}^{-\mathrm{i}\vec{k}_j\cdot\vec{r}}\sum_s \chi_s^{(j)}{\chi^{(j)}}^\dagger_s &= \frac{1}{\Omega}\int \mathrm{d}^3r'\, V(|\vec{r}-\vec{r'}|)\sum_{js} n_{js} \\ &= \frac{N}{\Omega}\int \mathrm{d}^3r'\, V(|\vec{r}-\vec{r'}|) = N\tilde{V}(0)\ ;\end{aligned} \tag{2.5}$$

$$\begin{aligned}(3)\ &\int \mathrm{d}^3r'\, V(|\vec{r}-\vec{r'}|)\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r'}}\frac{\chi_s}{\Omega^{3/2}}\sum_j n_j \mathrm{e}^{\mathrm{i}\vec{k}_j\cdot(\vec{r}-\vec{r'})}\sum_{s'}\chi_s^{(j)}{\chi^{(j)}}^\dagger_{s'} = \frac{\chi_s}{(2\pi)^3}\int \mathrm{d}^3q\,\mathrm{d}^3r'\,\frac{\tilde{V}(\vec{q})}{\sqrt{\Omega}}\mathrm{e}^{\mathrm{i}\vec{q}\cdot(\vec{r}-\vec{r'})} \\ &\times\sum_{js} n_{js}\mathrm{e}^{\mathrm{i}\vec{r'}\cdot(\vec{k}-\vec{k}_j)}\mathrm{e}^{\mathrm{i}\vec{r}\cdot\vec{k}_j} = \frac{\chi_s}{\sqrt{\Omega}}\int \mathrm{d}^3q\sum_{js} n_{js}\delta(\vec{k}-\vec{k}_j-\vec{q})\tilde{V}(\vec{q})\mathrm{e}^{\mathrm{i}\vec{r}\cdot(\vec{k}_j+\vec{q})} = \psi_i(\vec{r},s)\sum_{js} n_{js}\tilde{V}(\vec{k}-\vec{k}_j)\ ;\end{aligned} \tag{2.6}$$

where we defined

$$\tilde{V}(\vec{q})=\frac{1}{\Omega}\int \mathrm{d}^3r\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}}V(\vec{r}) \implies V(\vec{r})=\frac{\Omega}{(2\pi)^3}\int \mathrm{d}^3q\,\tilde{V}(\vec{q})\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}}\ . \tag{2.7}$$

This will result in the following energies in the HFE

$$\epsilon_{\vec{k}}=\frac{\hbar k^2}{2m}+U_0+N\tilde{V}(0)-\sum_{js} n_{js}\tilde{V}(\vec{k}-\vec{k}_j)\ ; \tag{2.8}$$

this ends the proof that plane waves solve HFE.

3 The homogeneous electron gas

We want to apply what we saw before to an homogeneous electron gas in an uniform background of positive charges (so that the overall system is neutral); in this case, the external potential $U(\vec{r})$ is the one coming from the Coulomb interaction with positive charges. We can write

$$U(\vec{r})=-\int \mathrm{d}^3r'\,\rho_{\mathrm{ion}}(\vec{r'})V(\vec{r}-\vec{r'})\sim-\frac{N}{\Omega}\int \mathrm{d}^3r'\,V(\vec{r'})=-N\tilde{V}(0)\ , \tag{3.1}$$

where we used $\rho_{\mathrm{ion}}\sim N/\Omega$, since we assumed an homogeneous background (and charge neutrality, hence the number of positive ions matches the number of electrons). Notice that this term exactly cancels the $N\tilde{V}(0)$ term in Eq. (2.8).

In order to compute the last term in Eq. (2.8), we need $\tilde{V}(\vec{q})$ for the Coulomb potential

$$V(\vec{r})=\frac{e^2}{r}\mathrm{e}^{-\epsilon r}\ , \tag{3.2}$$

where we added a regulator ϵ to make the following integrals doable (we will set the regulator to zero at the end of the calculation). Hence (using spherical coordinates),

$$\tilde{V}(\vec{q})=\frac{e^2}{\Omega}2\pi\int_0^\infty \mathrm{d}r\,\mathrm{e}^{-\epsilon r}\int_{-1}^1 \mathrm{d}\cos\theta\, r\mathrm{e}^{-\mathrm{i}qr\cos\theta}=\frac{4\pi e^2}{\Omega q}\int_0^\infty \mathrm{d}r\,\mathrm{e}^{-\epsilon r}\sin qr=\frac{4\pi e^2}{\Omega}\frac{1}{q^2+\epsilon^2}\ , \tag{3.3}$$

where the integral on the last step is the same we solved in the Weisskopf-Wigner method tutorial. Sending the regulator to zero, we obtain the Coulomb field in Fourier space (which you will encounter other times)

$$\tilde{V}(\vec{q})=\frac{4\pi e^2}{\Omega}\frac{1}{q^2}\ . \tag{3.4}$$

[1] Dimensional analysis demands $|\psi|^2$ to have dimensions of an inverse volume, since its integral over space should give a probability.

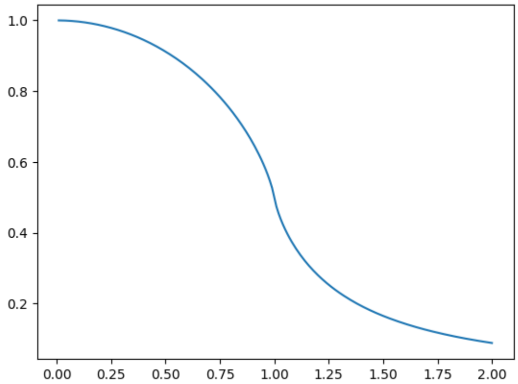

Figure 1: The function F.

With a large amount of electrons, we can write the following sum as an integral ($(2\pi)^3 \sum_{\vec{k}} /\Omega \sim \int \mathrm{d}^3k$),

$$\begin{aligned}&\sum_{js} n_{js}\tilde{V}(\vec{k}-\vec{k}_j) \sim \frac{\Omega}{(2\pi)^3}\int \mathrm{d}^3k'\,\tilde{V}(\vec{k}-\vec{k'}) = \frac{e^2}{\pi}\int \mathrm{d}k'\,k'^2 \int_{-1}^{1} \frac{\mathrm{d}\cos\theta}{k^2+k'^2-2kk'\cos\theta} \\ &= -\frac{e^2}{\pi k}\int_0^\infty \mathrm{d}k'\,k'\ln\frac{k-k'}{k+k'} = -\frac{e^2 k}{\pi}\int_0^\infty \mathrm{d}x\,x\ln\frac{1-x}{1+x}\ ,\end{aligned} \tag{3.5}$$

where on the last step we changed variable $x = k'/k$. Using

$$\int \mathrm{d}x\,x\ln(1+bx) = \frac{b^2x^2-1}{2b^2}\ln(1+bx)+\frac{x}{2b}-\frac{x^2}{4} \implies \int_0^A \mathrm{d}x\,x\ln\frac{1-x}{1+x} = \frac{A^2-1}{2}\ln\frac{1-A}{1+A}-A\ , \tag{3.6}$$

we see that the integral diverges; if we limit the integration over momenta to k_F (the Fermi momentum, which is the maximum momentum of a system of fermions at zero temperature), we have

$$\epsilon_{\vec{k}} = \frac{\hbar^2k^2}{2m} - \frac{2e^2k_\mathrm{F}}{\pi}F\left(\frac{k}{k_\mathrm{F}}\right)\ ,\quad F(x) = \frac{1}{2}+\frac{1-x^2}{4x}\ln\frac{1+x}{|1-x|}\ . \tag{3.7}$$

We see that the energy dispersion is changed; this can be seen as an effect of the exchange potential, or equivalently as an effect of the Fermi-Dirac statistic for fermions, here represented by the function F. Notice that it is a negative contribution; this negative exchange energy can explain the cohesion of electrons in metal.

4 Vortex solution in GPE

The GPE is basically HFE but for boson condensates (i.e. bosons which are all in the ground state), in particular there is no exchange term (no Pauli exclusion principle). The GPE reads

$$\left(\frac{-\hbar^2\nabla^2}{2m} + U(\vec{r}) + N\int \mathrm{d}^3r'\,V(|\vec{r}-\vec{r'}|)\left|\phi_0(\vec{r'})\right|^2\right)\phi_0(\vec{r}) = \epsilon_0\phi_0(\vec{r})\ . \tag{4.1}$$

We will use the short-range interaction approximation, i.e. we assume $V(|\vec{r}-\vec{r'}|) \simeq V_0\delta(|\vec{r}-\vec{r'}|)$. Moreover, we will set $U(\vec{r}) = 0$; the GPE then reads

$$\left(\frac{-\hbar^2\nabla^2}{2m} + NV_0|\phi_0(\vec{r})|^2\right)\phi_0(\vec{r}) = \epsilon_0\phi_0(\vec{r})\ . \tag{4.2}$$

It is a non linear Schrödinger equation, where the non-linear term $NV_0|\phi_0(\vec{r})|^2$ describes the mean field potential from other bosons.

We are after a particular solution of the GPE, the vortex solution. To find it, consider

$$\phi_0(\vec{r}) = \frac{f(\vec{r})}{\sqrt{N}}\mathrm{e}^{\mathrm{i}\chi(\vec{r})}\ , \tag{4.3}$$

where f is real. We can define the particle density ρ and current $\vec{j}$ as always

$$\rho = N|\phi_0|^2 = f^2(\vec{r}) \ , \ \vec{j} = -\frac{\mathrm{i}\hbar N}{2m}\phi_0^* \boldsymbol{\nabla}\phi_0 + \text{h.c.} = -\frac{\mathrm{i}\hbar}{2m} 2\mathrm{i} f^2 \boldsymbol{\nabla}\chi = \rho\vec{v} \ , \ \vec{v} := \frac{\hbar}{m}\boldsymbol{\nabla}\chi \ , \tag{4.4}$$

where on the last step we defined the velocity of the field (this kind of decomposition is called Madelung transformation). Before inserting this form of ϕ_0 into the GPE, let's first discuss some properties of this decomposition.

The velocity field, as defined previously, is irrotational, hence one would expect that, for a closed path C,

$$\int_C \vec{v}\cdot \mathrm{d}l = \int_S \boldsymbol{\nabla}\times\vec{v}\cdot \mathrm{d}\vec{S} = 0 \ , \tag{4.5}$$

hence the line integral of $\vec{v}$ on a closed path is zero, unless we are not allowed to apply Stokes theorem. This, again (Berry phase tutorial), happens the moment we do not have a simply connected space. For example, consider

$$\chi = s\phi \ , \tag{4.6}$$

where we used cylindrical coordinates (r, ϕ, z); then, the mapping from cylindrical coordinates to physical coordinates is singular at $r = 0$ (every ϕ, for $r = 0$, represent the same point). For a closed path around the axis $r = 0$, Stokes theorem cannot be applied for such a configuration, but to ensure the single valuedness of ϕ_0, we should impose

$$\delta\chi = \int_C \boldsymbol{\nabla}\chi\cdot \mathrm{d}\vec{l} = 2\pi s \ , \tag{4.7}$$

where $s \in \mathbb{Z}$. Recalling that in cylindrical coordinates,

$$\boldsymbol{\nabla} = \hat{e}_r\frac{\partial}{\partial r} + \frac{\hat{e}_\phi}{r}\frac{\partial}{\partial\phi} + \hat{e}_z\frac{\partial}{\partial z} \ , \ \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2} \ , \tag{4.8}$$

we can write

$$\boldsymbol{\nabla}\chi = \frac{s}{r}\hat{e}_\phi \implies \int_C \boldsymbol{\nabla}\chi\cdot \mathrm{d}\vec{l} = 2\pi s \implies \int_C \vec{v}\cdot \mathrm{d}l = \frac{2\pi\hbar}{m}s \ , \tag{4.9}$$

hence the line integral around $r = 0$, i.e. the vortex axis, is quantized. This is an example of a vortex. Notice that, for ϕ_0 to be continuous, it must be that $f(r\to 0)\to 0$ (otherwise, coming to $r = 0$ from different ϕ angles would give a different ϕ_0; this can be viewed as the fact that, at the center of a vortex, you do not feel his presence). Moreover, at large distances from the vortex, you are expected to recover the homogeneous solution (i.e. constant density) you encountered in the lecture notes,

$$\phi_0^{\text{constant}} = \sqrt{\frac{\epsilon_0}{NV_0}} \implies f(r\to\infty)\to\sqrt{\frac{\epsilon_0}{V_0}} \ . \tag{4.10}$$

A suggestive way to see how the vortex solution arises, is to start from the constant solution and see what happens when a phase is attached to it (the addition of a phase gives another acceptable solution). The moment χ gives rise to the ("topological") singularity, the constant solution is "changed" to this vortex solution.

Let's try to insert ϕ_0 in the GPE, with the simplifying assumption $f(\vec{r}) = f(r)$ (i.e. we do not care about the z axis). Then, the GPE can be written as

$$-\frac{\hbar^2}{2m}\left(f'' + \frac{f'}{r} - \frac{s^2}{r^2}f\right) + V_0 f^3 = \epsilon_0 f \ . \tag{4.11}$$

Looking at its asymptotics, assuming $f\sim r^k$ for $r\to 0$ for some $k > 0$, keeping only the smallest power of r, we have

$$k(k-1) + k - s^2 = 0 \implies k = |s| \ . \tag{4.12}$$

At large distances, we look for $f(r)\sim A + B/r^\alpha$ (where we expect to obtain $A = \sqrt{\epsilon_0/V_0}$), we have

$$A(\epsilon_0 - V_0A^2) + \frac{\hbar^2}{2m}\frac{As^2}{r^2} - 3V_0A^2\frac{B}{r^\alpha} + \mathcal{O}(r^{-\alpha-1}) = 0 \implies A = \sqrt{\frac{\epsilon_0}{V_0}} \ , \ \alpha = 2 \ , \ B = \frac{\hbar^2 s^2}{6m\sqrt{\epsilon_0 V_0}} =: \xi^2 s^2\sqrt{\frac{\epsilon_0}{V_0}} \ ; \tag{4.13}$$

this means that the vortex solution has the behaviors

$$f(r\to 0)\to r^{|s|} \ , \ f(r\to\infty)\to\sqrt{\frac{\epsilon_0}{V_0}}\left(1 - \frac{\xi^2 s^2}{r^2}\right) \ . \tag{4.14}$$

5 Vortex-antivortex

We will see that the vortex solution has a logarithmically divergent part. The energy associated to a vortex reads

$$E = N \int \mathrm{d}^3 r\, \phi_0^* \left(\frac{-\hbar^2 \nabla^2}{2m} + \frac{1}{2} N V_0 |\phi_0|^2 \right) \phi_0 \ , \tag{5.1}$$

where you should notice the 1/2 factor in front of the potential energy part (remember that it is a many-body term; this 1/2 factor is the analogous to what happens when one wants to compute the gravitational energy of a many-body system). We can split the previous as

$$\begin{aligned} E &= N \int \mathrm{d}^3 r\, \phi_0^* \frac{1}{2} \left(\frac{-\hbar^2 \nabla^2}{2m} + \frac{1}{2} N V_0 |\phi_0|^2 \right) \phi_0 - \frac{N\hbar^2}{4m} \int \mathrm{d}^3 r\, \phi_0^* \nabla^2 \phi_0 \\ &= \frac{N\epsilon_0}{2} - \frac{2\pi L_z \hbar^2}{4m} \int_0^\infty \mathrm{d}r\, r f \left(f'' + \frac{f'}{r} - \frac{s^2}{r^2} f \right) = \text{const.} + \frac{\pi L_z \hbar^2}{2m} \int_0^\infty \mathrm{d}r\, r \left((f')^2 + \frac{s^2}{r^2} f^2 \right) \ , \end{aligned} \tag{5.2}$$

where we integrated by parts in the last step (and integrated $\int_0^\infty f f' \,\mathrm{d}r = \left. f^2 \right|_0^\infty /2 = \text{finite}$). We see that

$$r(f')^2 \sim \frac{1}{r^5} \implies \text{converges} \ , \ \frac{s^2}{r} f^2 \sim \frac{A^2}{r} \implies \text{log divergent} \ ; \tag{5.3}$$

hence we obtain a formally divergent contribution to the energy.

It is interesting to notice that this divergence disappears if one consider a vortex-antivortex pair, i.e. two vortices with opposite value of s; more specifically, $s_\mathrm{V} := s$ and $s_\mathrm{A} = -s$ with $s > 0$, for the vortex and antivortex respectively (in the following, $_\mathrm{V}$ and $_\mathrm{A}$ subscript refers to vortex and antivortex quantities respectively). The solution will look like

$$\sqrt{N} \phi_0 \sim \ f(|\vec{r} - \vec{r}_\mathrm{V}|) \mathrm{e}^{\mathrm{i}\phi_\mathrm{V}} + f(|\vec{r} - \vec{r}_\mathrm{A}|) \mathrm{e}^{\mathrm{i}\phi_\mathrm{A}} ; \tag{5.4}$$

we are just interested in the log divergent part. Since we have two vortices, we cannot use cylindrical coordinates to describe both (or better, it is not convenient); with this in mind, we can schematically write

$$f^2 \frac{s^2}{r^2} \to f^2 |\vec{v}|^2 \ , \ \vec{v} = \frac{\hbar s}{m r^2} (-y, x) \ ; \tag{5.5}$$

for the two vortices system, we can write ($\Delta x_\mathrm{V} := x - x_\mathrm{V}$ and so on)

$$\vec{v} = \frac{\hbar s_\mathrm{V}}{m} \left(\frac{(-\Delta y_\mathrm{V}, \Delta x_\mathrm{V})}{|\Delta \vec{r}_\mathrm{V}|^2} - \frac{(-\Delta y_\mathrm{A}, \Delta x_\mathrm{A})}{|\Delta \vec{r}_\mathrm{A}|^2} \right) \ ; \tag{5.6}$$

far from the vortices centers, $r \gg r_\mathrm{V}, r_\mathrm{A}$, the behavior of $\vec{v} \sim 1/r^2$. This means that the term containing $f^2 |\vec{v}|^2$ will now converge, and the vortex-antivortex configuration is favoured energetically. Taking superfluids as an example, vortex-antivortex pairs are expected to be formed upon stirring.