Superfluids of vanishing roton gap

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Abstract –Dense Bose superfluids, as HeII, differ from dilute ones by the existence of a roton minimum in their excitation spectrum. When the roton energy gap is small, the shape of this roton minimum controls the superfluid behaviour close to any singularity, such as vortex cores, or close to solid boundaries. The obtained density oscillations close to the singularity are shown to be fully described by a linear perturbation theory, that relates their frequency and exponential damping to the shape of the roton minimum. This allows for general conclusions, for superfluids in porous media, or in transcient high pressure state.

Introduction. – HeII is the low temperature, low pressure superfluid phase of ^{4}He. The roton minimum, in its excitation spectrum, has been inferred by Landau [1] from the viscosity measurements of Andronikashvili [2]. It has been shown, by Feynman [3] to be due to the dense packing of ^{4}He atoms. Solidification, which occurs above 2.5MPa for low temperature ^{4}He, can be seen as a condensation of rotons, due to their interactions.

The low value of the excitation energy at the roton minimum also suggests that the superfluid has a strong susceptibility for spatial perturbations of wave number k_o, the position of the roton minimum. Localized perturbations will then produce oscillations in the superfluid density in their neighborhood [4–6]. Determining the parameters which control the extension and amplitude of these oscillations, and discussing their implications are the goals of this paper.

The existence of density oscillations can be of tremendous importance in the study of quantum turbulence in which a central role is played by vortex reconnections [7,8] and thus it is useful to quantify how these oscillations depend on the shape of the roton minimum. In particular, this study is necessary to the design of numerical investigations of vortex reconnections, as it was done formerly without taking into account the roton gap [9].

This paper is organized as follows. First and foremost, the universal influence of the roton minimum is shown on a simple example, the Pomeau-Rica version [5] of the Gross-Pitaevskii equation [10]. The density oscillations around a vortex core are then compared, in this model, to the linear response to a localized perturbation. The last section is devoted to the same problem with a more realistic model [6], able to reproduce the dispersion relation of superfluid Helium close to the melting curve. We finally conclude on the implications for real systems.

Linear treatment of the non-local Gross-Pitaevskii equation. – The Pomeau-Rica [5] version of the Gross-Pitaevskii [10] equation reads:

$$i\hbar\partial_t\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) - \mu\psi(\vec{r},t) + U_o\psi(\vec{r},t)\int d^3\vec{r}'\,\theta(|\vec{r}-\vec{r}'|/a)|\psi(\vec{r}',t)|^2 \quad (1)$$

where $U_o\theta(|\vec{r}-\vec{r}'|/a)$ represents the interaction potential between two atoms located at $\vec{r}$ and $\vec{r}'$, a is the range of the potential. The interaction $\theta(\vec{x})$ is 1 if $|\vec{x}| < 1$, 0 for $|\vec{x}| > 1$ and μ is the chemical potential, fixing the equilibrium density $n = |\psi(\vec{r},t)|^2$.

Using the transformation $\vec{r} \to a\vec{r}$, $\psi \to \sqrt{n}\psi$, $t \to (2ma^2/\hbar)t$, Eq. 1 can be written in the following non-dimensional form:

$$i\partial_t\psi(\vec{r},t) = -\Delta\psi(\vec{r},t) - 4\pi\Lambda\psi(\vec{r},t)/3 + \Lambda\psi(\vec{r},t)\int d^3\vec{r}'\,\theta(|\vec{r}-\vec{r}'|)|\psi(\vec{r}',t)|^2 \quad (2)$$

where

$$\Lambda = \frac{2ma^2U_ona^3}{\hbar^2} \quad (3)$$

remains the only parameter. Any static perturbation will appear as an additional term $V(\vec{r}) = \psi(\vec{r})\mathcal{V}(\vec{r})$ in the right hand side of equation (2). Far from the perturbation, the solution of Eq. 2 can be written to linear order as $\psi = 1 + \delta\psi$, with $\delta\psi$ and its complex conjugate $\delta\psi^*$ verifying the linear system

$$i\partial_t\delta\psi(\vec{r},t) + \Delta\delta\psi(\vec{r},t) \\ -\Lambda\int d^3\vec{r}'\,\theta(|\vec{r}-\vec{r}'|)(\delta\psi(\vec{r}',t) + \delta\psi^*(\vec{r}',t)^*) = V(\vec{r}) \quad (4)$$

$$-i\partial_t\delta\psi^*(\vec{r},t) + \Delta\delta\psi^*(\vec{r},t) \\ -\Lambda\int d^3\vec{r}'\,\theta(|\vec{r}-\vec{r}'|)(\delta\psi(\vec{r}',t) + \delta\psi^*(\vec{r}',t)) = V(\vec{r}) \quad (5)$$

By Fourier transforming, we get:

$$(\omega - k^2 - \Lambda\tilde{\theta}(k))\tilde{\delta\psi}(\vec{k},\omega) - \Lambda\tilde{\theta}(k)\tilde{\delta\psi}^*(\vec{k},\omega) = \tilde{V}(\vec{k}) \\ (\omega + k^2 + \Lambda\tilde{\theta}(k))\tilde{\delta\psi}^*(\vec{k},\omega) + \Lambda\tilde{\theta}(k)\tilde{\delta\psi}(\vec{k},\omega) = -\tilde{V}(\vec{k}) \quad (6)$$

where $\tilde{\theta}(k)$ is the Fourier transform of the normalized interaction potential θ:

$$\tilde{\theta}(k) = \frac{4\pi}{k^3}(\sin(k) - k\cos(k)) \quad (7)$$

Eliminating $\tilde{\delta\psi}^*$ from the former system (Eq. 6) gives:

$$(\omega^2 - \omega(k)^2)\tilde{\delta\psi}(\vec{k},\omega) = (\omega + k^2)\tilde{V}(\vec{k}) \quad (8)$$

where $\omega(k)$ is the dispersion relation of the linear excitations, namely

$$\omega(k)^2 = k^2(k^2 + 2\Lambda\tilde{\theta}(k)) \ . \quad (9)$$

The frequency $\omega = \omega(k)$ allows a non zero $\tilde{\delta\psi}(\vec{k},\omega)$ without any perturbation ($\tilde{V}(\vec{k}) = 0$). The static ($\omega = 0$) solution of equation (8) is:

$$\tilde{\delta\psi}(\vec{k}) = -\frac{k^2\tilde{V}(\vec{k})}{\omega(k)^2} \ . \quad (10)$$

Finally, the form of the pertubation $\delta\psi(\vec{r})$ in the physical space is given by the inverse Fourier transform

$$\delta\psi(\vec{r}) = \frac{1}{(2\pi)^3}\int \tilde{\delta\psi}(\vec{k})e^{i\vec{k}.\vec{r}}d\vec{k} \ . \quad (11)$$

In the case of interest for us, $\omega(k)^2/k^2$ has a deep minimum (the roton minimum) at $k = k_o$ that will clearly dominate the right hand side (RHS) of Eq. 10. Let us write in its neighbourhood $\omega(k)^2/k^2 = \Omega^2 + c^2(k - k_o)^2$, where $\hbar\Omega$ is the energy roton gap and $m_* = \hbar\Omega/c^2$ the "roton mass".

Rectilinear vortex. – To model the pertubation induced by a vortex line, let us consider a localized perturbation that depends only on the distance r from the z-axis[1] (cylindrical symmetry). In this case, the Fourier transform of V can be written as $\tilde{V}(\vec{k}) = \tilde{v}(k_\perp)\delta(k_z)$, where δ is the Dirac function. Because the roton minimum is assumed deep, i.e. Ω^2 is assumed small, the RHS of Eq. 10 has a sharp maximum at $k = k_o$. Thus, the very precise shape of the perturbation is not important as long as it is localized, i.e. the Fourier transform $\tilde{v}(k_\perp)$ is smooth. In this spirit, we can Taylor expand the perturbation as $\tilde{v}(k_\perp) \approx \tilde{v}(k_o) + \tilde{v}'(k_o)(k_\perp - k_o)\delta(k_z)$. Using Eq. 10, we can approximate $\tilde{\delta\psi}(\vec{k})$ as:

$$\tilde{\delta\psi}(\vec{k}) \approx -\frac{\tilde{v}(k_o) + \tilde{v}'(k_o)(k_\perp - k_o)}{\Omega^2 + c^2(k - k_o)^2}\delta(k_z) \ . \quad (12)$$

Clearly, this approximation goes beyond the particular case of the Pomeau-Rica model (Eq. 2). The first order correction to the order parameter ψ, due to a localized perturbation, will obey an equation like (8), with a smooth function on the RHS, for any superfluid Bose system at low temperature. In the following, we shall use the approximation (12) for $\tilde{\delta\psi}(\vec{k})$.

Then, using the approximative form of $\tilde{\delta\psi}(\vec{k})$ (Eq. 12) and Eq. 11 , we get $\delta\psi(\vec{r}) = \delta\psi(r)$ with

$$\delta\psi(r) \propto \int_0^\infty \frac{\tilde{v}(k_o) + \tilde{v}'(k_o)(k_\perp - k_o)}{\Omega^2 + c^2(k_\perp - k_o)^2}J_0(k_\perp r)k_\perp dk_\perp \ , \quad (13)$$

where $J_0(x) = \int_0^{2\pi}\exp(ix\cos\phi)d\phi$ is the Bessel function of the first kind. The form of the pertubation (Eq. 13) can be accurately evaluated numerically and is found oscillatory (data not shown). Given the approximative form used in Eq. 12, it is expected valid only when it is small, *i.e.* for r relatively large. In the integral, we can thus consider $k_\perp r$ as large, for the interesting $k_\perp$ values. This allows to use the following asymptotic form of the Bessel function

$$J_0(x) \approx \frac{2\cos(x - \pi/4)}{\sqrt{2\pi x}} \ . \quad (14)$$

Using the asymptotic form of the Bessel function (Eq. 14), the $k_\perp$ integration entering in Eq. 13 can be performed in the complex plane, which gives:

$$\delta\psi(r) \propto g(r) = \frac{\exp(-k_1 r)}{\sqrt{k_o r}}\cos\left(k_o r - \pi/4 + \frac{k_1}{2k_o} + \phi_o\right) \quad (15)$$

with $k_1 = \Omega/c$ and $\tan(\phi_o) = k_1\frac{\tilde{v}'(k_o)}{\tilde{v}(k_o)}$. Thanks to Eq. 15, we can see that the density profile close to the vortex behaves as an oscillatory function of wavelength $2\pi/k_o$ that exponentially tends to zero with a characteristic length scale $1/k_1$. Let us emphasize that the obtained form of the perturbation $\delta\psi(r)$ only depends of $k_o r$, k_1/k_o and an additional phase-shift ϕ_o. In the small Ω limit (i.e. deep minimum), the ratio k_1/k_o is expected small compared to unity. The sign and amplitude of ϕ_o depends on the shape and variation of the perturbation $\tilde{v}(k_o)$. If $\tilde{v}(k_o) \sim -k_o\tilde{v}'(k_o)$ as obtained with a Gaussian function of characteristic spatial extension the atomic size $\sim 1/k_o$,

[1]Doing so, we neglect the influence of the phase, which changes by 2π when turning around the vortex.

$$f''(r)+\frac{f'(r)}{r}+\left(\frac{4}{3}\pi\Lambda-\frac{1}{r^2}\right)f(r)=\Lambda f(r)\int_{r'=0}^{+\infty}\int_{\varphi=0}^{2\pi}\int_{z=-\infty}^{+\infty}\theta\left(\sqrt{r^2+r'^2-2rr'\cos\varphi+z^2}\right)r'f^2(r')dr'd\varphi dz \quad (16)$$

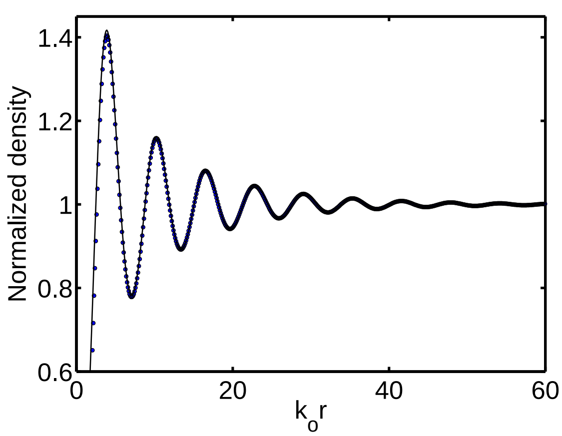

Fig. 1: Comparison between the "equilibrium" density around a vortex (dots) in the Pomeau-Rica model, with the first order approximation Eq. 15 (full line). Eq. 2 is solved *via* a relaxation method. $k_1/k_o = 0.0659$, $\phi_o = -0.177$.

we get a small negative phase-shift. If on the contrary, $\tilde{v}(k_o)$ is small compared to $k_o\tilde{v}'(k_o)$, then ϕ_o can take a significant value, which sign depends on the shape of $\tilde{v}$ around k_o. The corresponding superfluid density profile is $1+2\delta\psi(r)$. We see that the qualitative behavior of the density profile close to a singularity is expected universal, i.e. independent on the precise shape of $\tilde{v}$, only an additional phase-shift is model dependent.

Numerical solution of the Pomeau-Rica equation. – To compare the linear prediction obtained in Eq. 15 with the full rectilinear vortex solution of the Gross-Pitaevskii equation (Eq. 2), we perform a numerical simulation aimed at evaluating the ground-state of Eq. 2 under the constraint that the phase turns of 2π along a line, as it was done in Refs. [4,6,10]. In this axisymmetric geometry, we are thus looking for a order parameter of the form $\psi(\vec{r},t)=f(r)e^{i\varphi}$, where (r,φ,z) is the cylindrical coordinate system. The amplitude $f(r)$ is then given as the solution of the boundary values problem Eq. 16 subject to the conditions $f(0)=0$ and $f(+\infty)=1$.

Using the non-local potential θ of Pomeau and Rica [5], we can perform analtytically the integration over z and φ using the Elliptic integrals of the first $\mathcal{F}(k)=\int_0^1\frac{dt}{\sqrt{1-k^2t^2}\sqrt{1-t^2}}$ and second $\mathcal{E}(k)=\int_0^1\frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}}dt$ kind. We can show then that the RHS of Eq. 16 is given by, for $r\leq 1$

$$8f(r)\Lambda\int_{r'=0}^{1-r}\sqrt{1-(r-r')^2}\,\mathcal{E}\left(\sqrt{\frac{4rr'}{1-(r-r')^2}}\right)r'f^2(r')dr'$$

$$+8f(r)\Lambda\int_{1-r}^{1+r}\sqrt{rr'}\left[2\mathcal{E}\left(b\right)-(a+1)\mathcal{F}(b)\right]r'f^2(r')dr'$$

and for $r\geq 1$

$$8f(r)\Lambda\int_{r-1}^{r+1}\sqrt{rr'}\left[2\mathcal{E}\left(b\right)-(a+1)\mathcal{F}(b)\right]r'f^2(r')dr'\ ,$$

where $a=\frac{r^2+r'^2-1}{2rr'}$, $b=\frac{\sqrt{2}}{2}\sqrt{1-a}$. To numerically solve Eq. 16, we use a relaxation method [11]. The Laplacian is furthermore estimated using a joint Crank-Nicolson and Gauss-Seidel algorithms [11] to ensure numerical stability. Starting with the uniform amplitude $f(r)=1$, the relaxation method converges towards the "equilibrium" distribution $f(r)$ that solves Eq. 16.

In figure (1), we compare this approximation with the "exact" solution of the Pomeau-Rica model, for $\Lambda=40$, obtained with a relaxation method. That is, we compare this solution with $1+\alpha g(r)$, using the approximative form of the pertubation (Eq. 15), α and ϕ_o being fitted for the best agreement. The parameter $\Lambda=40$, for which $k_o\approx 5.40$, is close to the "spinodal" value $\Lambda_s\simeq 43.43$, for which $\Omega=0$. As it can be seen in Fig. 1, the first order approximation (solid line) almost perfectly fits the "equilibrium" density (dots). The value of k_1/k_o is here $k_1/k_o=0.0659$. The value obtained for ϕ_o is $\phi_o=-0.177$.

Melting pressure Helium. – In order to be closer to real superfluids, and to estimate to what extent the above ideas can apply to experimental systems, we consider now a more elaborate model. It has been used in a series of papers by Berloff and Roberts [6], to which we refer for details. Apart from a larger number of parameters in tayloring the two-body interaction potential, it differs from the Gross-Pitaevskii approach by taking into account three-body interactions. Altogether, it allows to adapt the dispersion relation, both qualitatively and quantitatively, to that of the real superfluid of interest.

In this model, the Shrödinger equation 1 is changed to:

$$i\hbar\partial_t\psi(\vec{r},t)=-\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t)-\mu\psi(\vec{r},t)$$
$$+\psi(\vec{r},t)\left(\int d^3\vec{r}'\,\mathcal{U}(\vec{r}-\vec{r}')|\psi(\vec{r}',t)|^2+W|\psi(\vec{r},t)|^4\right) \quad (17)$$

where the three-body potential is treated as local, with intensity W.

Defining $a=\hbar/\sqrt{2m\mu}$, the same transformation than above, $\vec{r}\to a\vec{r}$, $\psi\to\sqrt{n}\psi$, $t\to(2ma^2/\hbar)t$, yields:

$$-i\partial_t\psi(\vec{r},t)=\Delta\psi(\vec{r},t)+\psi(\vec{r},t)\left(1-\chi|\psi(\vec{r},t)|^4\right)$$
$$-\psi(\vec{r},t)\left(\int d^3\vec{r}'\,U(|\vec{r}-\vec{r}'|)|\psi(\vec{r}',t)|^2\right) \quad (18)$$

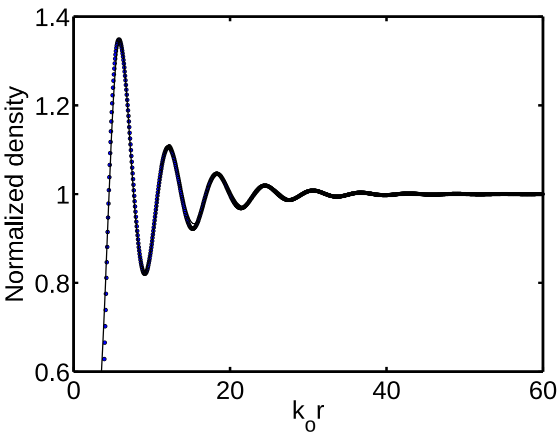

Fig. 2: Comparison between the "equilibrium" density around a vortex (dots) in the Roberts model Eq. 18, with the first order approximation Eq. 15 (full line). Eq. 18 is solved *via* a relaxation method. $k_1/k_o = 0.1144$, $\phi_o = 0.91$.

The reduced potential U is taken as (for convenience, we keep the same notations as [6]):

$$U(r) = (\alpha + \beta A^2 r^2 + \delta A^4 r^4) e^{-A^2 r^2} + \eta e^{-B^2 r^2} \ . \quad (19)$$

The dispersion relation is then given by:

$$\omega^2 = k^4 + 4k^2 \chi + 2k^2 \tilde{U}(k) \quad (20)$$

where $\tilde{U}(k)$ is the Fourier transform of $U(\vec{r})$.

The choice $A = 1.3282$, $B = 0.1992$, $\alpha = 11.5881$, $\beta = -28.48$, $\delta = 7.723$, $\eta = 0.003775$, $\chi = 3.5$, gives good agreement with the experimental dispersion curve at low temperature, at a pressure close to the melting one [12]. In particular, we obtain good values not only of the roton minimum and its curvature, but also of the velocity of sound and the "maxon" energy.

Similar numerical investigations of the density profile near a vortex as the ones done for the Pomeau-Rica case (Eq. 16) can be performed. In this case, the RHS of Eq. 16 can be analytically computed using Bessel functions (see Ref. [6] for details). The comparison between the "equilibrium" density and our first order approximation Eq. 15 is shown in figure 2. Again, the agreement is very good, the discrepancy being visible only close to the second minimum. The value of k_1/k_o is here 0.1144. However, the value of ϕ_o is $\phi_o = 0.91$. Correspondingly, the hollow core of the vortex, that is the radius on which the density is nearly zero, is much wider with this model than with the Pomeau-Rica one. This quantitative phase-shift can be explained using a perturbation potential $\tilde{v}$ that is close to 0 around k_o.

Discussion and Conclusion. – We have shown that the density profile of the superfluid close to a singularity is expected universal when the roton gap Ω is small. We have derived an explicit form of this behavior (Eq. 15) using a linear treatment of the Gross-Pitaevskii equation. We have emphasized that only the additional phase-shift ϕ_o depends on the precise shape of the model. The linear prediction compares well with numerical simulation of the ground state of the Pomeau-Rica and Berloff-Roberts models in presence of a vortex.

The existence and the development of these density oscillations can have important and interesting practical consequences. We already noted that the above approach can be convenient even for stable superfluid Helium, close to the melting pressure. Metastable overpresurized Helium has already been obtained within nanopores [13], or transciently, with acoustic oscillations [14]. Many attempts aimed at obtaining metastable superfluid molecular hydrogen [15], and estimations give good hope for a next future [16]. Finally, even cold atomic gases seem able to realize strongly interacting bose fluids [17].

The consequences of the density oscillations can be numerous, and we list below only a few of them:

1. With a vortex ring, of radius $R < 1/k_1$, density oscillations can interact in the center, yielding to oscillations in the R dependence of the energy E of the vortex. Could it give rise to minima in $E(R)$, that is metastable stationary defects?

2. The amplitude of the density oscillations decreases as $\exp(-k_1 r)/\sqrt{r}$. As the corresponding energy goes with the square of this amplitude, it results in a term proportionnal to $1/k_1$ in the vortex energy. Close to the spinodal point ($k_1 = 0$), this term increases very rapidly with the pressure. Vortices should then be expelled from high pressure zones.

3. These density oscillations are reminiscent of Friedel oscillations of electronic density in metals, responsible for RKKY interactions between magnetic impurities, themselves at the origin of spin glasses [18]. We could wonder whether the density oscillations in dense superfluids could give rise to a glass phase. The existence of such a glass phase in Helium has been suggested for interpreting recent experiments [13].

Furthermore, the independance of the vortex structure *versus* any fluid properties other than the roton ones justify the use of simplified models for evaluating effects in real superfluids. This can give access to phenomena at a scale hardly accessible to experiments. On the other hand, very precise measurements of roton properties are essentials for the reliability of these studies.

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