Coexisting ordinary elasticity and superfluidity in a model of defect-free supersolid

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We present the mechanics of a model of supersolid in the frame of the Gross-Pitaevskii equation at $T = 0K$ that do not require defects nor vacancies. A set of coupled nonlinear partial differential equations plus boundary conditions is derived. The mechanical equilibrium is studied under external constrains as steady rotation or external stress. Our model displays a paradoxical behavior: the existence of a non classical rotational inertia fraction in the limit of small rotation speed and no superflow under small (but finite) stress nor external force. The only matter flow for finite stress is due to plasticity.

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The recent surge of interest in supersolids\textsuperscript{1} makes it important to reach a clearer understanding of the mechanical properties of such materials. In particular why a supersolid behaviour is observed in a rotating experiment, whilst, as in a ordinary solid no constant mass flux is driven by pressure gradient? (see Refs.\textsuperscript{2,3}) In two of us (YP and SR) proposed a fully explicit model of supersolid where many properties can be discussed in details. We thought timely to reconsider this model, in particular with respect to its properties of elasticity coupled to its ability to carry some sort of superflow in the absence of any defect. Although supersolidity is often related to the presence of defects, vacancies and so forth our model introduces an important difference between ordinary (classical) crystals and supersolids: in perfect classical crystals there is an integer number (or a simple fraction) of atoms per unit cell. Therefore the number density and the lattice parameters are not independent. On the contrary, in our model of supersolid, there is no such relation. The lattice parameters and the average density can be changed independently.

This model is based upon the original Gross-Pitaevskii equation (G–P later)\textsuperscript{4} with an integral term with a kernel that can be seen as a two-body potential in a first Born approximation\textsuperscript{1}. This model yields the exact spectrum found long ago by Bogoliubov\textsuperscript{5}, namely a relation between the energy of the elementary excitations and their momentum depending on the two-body potential. In this framework the roton minimum is a precursor of crystallisation. Something predicted in\textsuperscript{6} where the possibility of a linear instability was only considered, although the transition is subcritical-first order\textsuperscript{3}. By increasing the density, crystallization happens through a first order phase transition (see figure\textsuperscript{2}). As shown in\textsuperscript{1} the crystal phase shows a periodic modulation of density in space together with some superfluid-like behaviour under rotation.

The aim of the present letter is to show that, besides this behaviour, the system has also solid-like behaviour, at least under small stress. At larger stress, it flows plastically, the plasticity being facilitated by the eventual presence of defects. We derive the equation of motion for the average density $\langle n \rangle$, the phase $\Phi$ and the displacement $\mathbf{u}$ in the solid. A new propagating mode appears besides the usual longitudinal and transverse phonons in regular crystals. This mode is partly a modulation of the coherent quantum phase, like the phonons in superfluids at zero temperature. We discuss at the end the boundary conditions and how to handle steady rotation and pressure driven flow in this model.

Our starting point is the original G–P equation\textsuperscript{4} for the complex valued wavefunction $\psi(\mathbf{r}, t)$ common to all bosonic particles of mass $m$:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + \psi \int d\mathbf{r}' U(\mathbf{r}' - \mathbf{r})|\psi(\mathbf{r}', t)|^2,$$  \hspace{1cm} (1)

where $U(\cdot)$ is a two body potential depending on the distance. For the numerics we choose a potential $U(|\mathbf{r}|) = U_0 \theta(\alpha - |\mathbf{r}|)$, with $\theta(\cdot)$ Heaviside function.

\textsuperscript{1} This is an exact approximation for the full quantum problem in the van der Waals limit of long range low amplitude potential $U(\mathbf{r}) = \gamma^2 U(\gamma r)$ whenever $\gamma \to 0$. 

\hspace{1cm}
The ground state is a solution of equation (11) of the form \( \psi_0(r)e^{-\frac{E_0}{\hbar^2}} \). It is a crystal when \( \psi_0(r) \) is a periodic function such that \( \psi_0(r + q_ia + q_cb + q_dc) = \psi_0(r) \) for \( a,b,c \) arbitrary integers, \( a,b,c \) being vectors defining the elementary lattice cell. This solution is the ground state in the sense that, given an average number density \( n = \frac{1}{M} \int dr|\psi_0|^2 \), \( \Omega \) being the total volume, the lattice parameters and the function \( \psi_0(r) \) make \( E_0 \) the smallest possible. The local density \( n(r,t) \), the displacement field \( u(r,t) \) of the crystal lattice and the slowly varying phase \( \Phi(r,t) \) of \( \psi(t,r) \).

The Lagrangian density for the G–P equation (1) reads in polar coordinates, \( \psi = \sqrt{\rho}e^{i\phi} \):

\[
\mathcal{L} = -\hbar \rho \frac{\partial \phi}{\partial t} - \frac{\hbar^2}{2m} \left( \rho (\nabla \phi)^2 + \frac{1}{4 \rho} (\nabla \rho)^2 \right) - \frac{1}{2} \rho(r) \int dr' U(r' - r) \rho(r').
\]

The ground state is given by the solution of the nonlinear integro-differential equation for \( \rho \) derived by variation of the action taking the phase field \( \phi \) uniform in space: \( \dot{\phi} = -\mu t/\hbar, \mu \) constant, that is a solution of:

\[
-\mu + \frac{\hbar^2}{4m} \left( \frac{(\nabla \rho)^2}{2} - \frac{\nabla^2 \rho}{\rho} \right) + \int dr' U(r' - r) \rho(r') = 0.
\] (2)

This ground state solution, if periodic in space, as we shall assume in full agreement with our numerical results, depends on the dimensionless parameter \( \Lambda = U_0 \rho_0^2 a^3 \Omega^{1/2} \). Although in Ref. 2 we discussed a ground state as a modulation close to an uniform density near the transition, that is for a finite roton gap, we have observed numerically that a crystal ground state exists in a wide range of densities. In the limit \( \Lambda \gg 1 \) the lattice tends to an array of sharp density pulses distant of \( a \), the width of the pulse decreasing like \( \Lambda^{-1/2} \).

Let \( \rho_0(r|n) \) be a ground state solution, then \( \rho_0(r - u|n) \) is also a ground state solution with the same \( \mu \), for a constant displacement field \( u \). The general perturbations around the ground state allow that \( \Phi, u \) and \( n \) become slow varying fields on space and time. As in Ref. 2 we follow the general method called homogenization. This splits cleanly the long-wave behaviour of the various parameters and the short range periodic dependence upon the lattice parameters. Let write the Ansatz for density and phase:

\[
\rho = \rho_0(r - u, n(r,t)) + \tilde{\rho}(r - u, n, t) + \ldots
\]

\[
\phi = \Phi(r,t) + \tilde{\phi}(r - u, n, t) + \ldots
\] (3)

where \( \Phi, u \) and \( n \) are slow varying fields and \( \tilde{\phi} \) and \( \tilde{\rho} \) are small and fast varying periodic functions. Introducing this Ansatz into the Lagrangian (2) one gets an effective Lagrangian made of four kind of terms:

i) As \( n \) changes continuously the periodic solution of the integrodifferential equation (2), say \( \rho_0(r) \), can be considered as a regular function of the Lagrange multiplier \( \mu \) imposing the average density \( n \). Therefore by integrating over an unit cell \( (V) \) of the lattice the Lagrangian from which (2) is derived one obtains an averaged Lagrangian that depends on \( n \) only that writes

\[
-\mathcal{L}_n = \mathcal{E}(n) = \frac{1}{2V} \int dr \rho_0(r) \int U(r' - r) \rho_0(r') dr'.
\] (4)

This yields the simplest case of homogenization.

ii) Similarly, terms mixing the slow varying phase field \( \Phi(r,t) \) and \( \rho_0(r) \) can be averaged directly leading to \( \mathcal{L}_\Phi = -n \left( \hbar \partial_t \Phi + \frac{\hbar^2}{2m} (\nabla \Phi)^2 \right) \) where \( n = \frac{1}{V} \int_V \rho_0(r) dr \).

Next contributions need to solve the Euler-Lagrange conditions for the fast variables \( \tilde{\phi} \) and \( \tilde{\rho} \). We shall sketch the effective Lagrangian for the phase \( \tilde{\phi} \), leaving for the reader a similar calculation for the deformation part.

iii) The \( \phi \) dependence term of this Lagrangian can be re-written of the form: \( \mathcal{L}_{\tilde{\phi}} = -\frac{\hbar^2}{2m} \int \left( 2 \rho_0 A \cdot \nabla \tilde{\phi} + \rho_0 (\nabla \tilde{\phi})^2 \right) dr \), where \( A = (\nabla \Phi - (\nabla \Phi \cdot \nabla) u - \frac{\mu}{\hbar} \partial_t u) \) (considered as a constant in the unit cell). The Euler-Lagrange condition for \( \mathcal{L}_{\tilde{\phi}} \) reads \( A \cdot \nabla \rho_0 + \nabla \cdot (\rho_0 \nabla \tilde{\phi}) = 0 \). This Poisson-like equation is to be solved within the unit cell of the lattice, for a function \( \tilde{\phi} \) that is periodic with the same period as \( \rho_0 \). The result (that can be expressed as the minimum of a certain Rayleigh-Ritz functional) is linear in \( A \) and can be written as \( \tilde{\phi} = K A_i \), where \( K(r) \) is a vector-valued function of \( r \) that is periodic and satisfies \( \nabla_i \rho_0 + \nabla \cdot (\rho_0 \nabla K_i) = 0 \). Putting the result into the Lagrangian \( \mathcal{L}_{\tilde{\phi}} \) one obtains the relevant contribution for the slowly varying part of the phase: \( \mathcal{L}_{\tilde{\phi}} = \frac{\hbar^2}{2m} \rho_{ij} A_i A_j \) with the positive defined matrix \( \rho_{ij} = \frac{1}{V} \int_V \rho_0(r) \nabla K_i \cdot \nabla K_j dr \). The Lagrange function \( \mathcal{L}_{\tilde{\phi}} \) depends on the slow variables only. We shall restrict ourselves below to crystal structures sufficiently symmetric to make \( \rho_{ij} \) diagonal \( \rho_{ij} = \rho(n) \delta_{ij} \). The quantity \( \rho(n) \) is zero if the crystal modulation is absent and would be
very small for Bose-Einstein condensate with a non local interaction term. \( \varrho(n) \to n \) when all the mass is strongly localized in the center of the cell site with a small overlap in between the different sites. This is presumably the situation of almost all materials in their solid state at low temperature. A large Young modulus is likely a measure of the small overlap of the wave functions from one site to the next, making \(^4\)He exceptional at this respect. In other words when \( \varrho(n) \to n \) the supersolid behaves as a ordinary solid state.

iv) The same method of homogenization works for the long-wave perturbations of gradients of the displacement \( u \) and yields a contribution to the Lagrangian that reads \( \mathcal{L}_u = -\frac{1}{2} \lambda_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} \). The coefficients \( \lambda_{ijkl} \) are given by integrals over the unit cell of various functions defined explicitely. This is the familiar elastic energy of a Hookean solid.

To summarize, the effective Lagrangian reads:

\[
\mathcal{L}_{\text{eff}} = -\hbar n \frac{\partial \Phi}{\partial t} - \frac{\hbar^2}{2m} \left[ (\nabla \Phi)^2 - \varrho'(n) \left( \nabla \Phi - \frac{m \frac{Du}{\hbar \frac{Dt}}}{\hbar} \right)^2 \right] - E(n) - \frac{1}{2} \lambda_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} \tag{5}
\]

where \( \frac{Du}{\hbar \frac{Dt}} = \frac{\partial u}{\partial t} + \frac{\hbar}{m} \nabla \Phi \cdot \nabla u \). This expression is remarkable because it is fully explicit for a given ground state of the G–P model. As one can check this Lagrangian is Galilean invariant.

We conjecture that, because this Lagrangian satisfies the symmetries imposed by the underlying physics and because it includes a priori all terms with the right order of magnitude with respect to the derivatives, the general Lagrangian of any supersolid at zero temperature has the same structure. In a recent paper, Son derives a Galilean invariant Lagrangian such that (5) is a sub-class but with well defined coefficients like \( \varrho(n) \), \( E(n) \) and \( \lambda_{ijkl} \) depending on the details of the crystal structure.

The dynamical equations are derived by variation of the action \( \int \mathcal{L} \, d^3r \, dt \) which is seen as a functional of \( n, \Phi \) and \( u \). The variation with respect to \( n, u \) and \( \Phi \) yields (writing \( \varrho'(n) = d\varrho/dn \), etc.):

\[
\hbar \frac{\partial \Phi}{\partial t} + \frac{\hbar^2}{2m} \left[ (\nabla \Phi)^2 - \varrho'(n) \left( \nabla \Phi - \frac{m \frac{Du}{\hbar \frac{Dt}}}{\hbar} \right)^2 \right] + E'(n) + \frac{1}{2} \lambda_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} = 0. \tag{6}
\]

\[
m \frac{\partial}{\partial t} \left[ \varrho(n) \frac{Du_i}{\hbar \frac{Dt}} - \frac{\partial}{\partial x_j} \left( \lambda_{ijkl} \frac{\partial u_k}{\partial x_l} \right) + \hbar \frac{\partial}{\partial x_k} \left( \varrho(n) \frac{\partial u_i}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} \right) \frac{m \frac{Du}{\hbar \frac{Dt}}}{\hbar} \right] = 0. \tag{7}
\]

\[
\frac{m}{\hbar} \frac{\partial}{\partial t} \left[ n \frac{\partial \Phi}{\partial x_k} - \varrho(n) \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} \right) \left( \frac{\partial \Phi}{\partial x_k} - \frac{m \frac{Du}{\hbar \frac{Dt}}}{\hbar} \right) \right] = nV_k \dot{e}_k. \tag{8}
\]

The latter equation reduces to the familiar equation of mass conservation for potential flows whenever \( \varrho(n) = 0 \), namely in the absence of modulation of the ground state. Although our equations of motion (6TS) and the one of Andreev–Lifshitz are almost identical in the zero temperature limit (see eqns. (16) of Ref., our model has significant differences with their. Our solid cannot be considered as the normal component of a two “fluids” system, because it is on the same footing (phase coherent) as the superfluid part at \( T = 0K \). Therefore, at small finite temperature, our model has a normal component that is a fluid of vanishing density at \( T = 0K \), besides its coherent superfluid and solid part and should change the superfluid density fraction. Following Landau’s ideas, this normal fluid is a gas of quasi-particles with the mixed spectrum able to carry momentum whilst the coherent part (superfluid plus solid) stays at rest.

The Euler-Lagrange conditions impose also the boundary conditions for the equations of motion:

\[
\frac{m}{\hbar} \left( n \frac{\partial \Phi}{\partial x_k} - \varrho(n) \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} \right) \left( \frac{\partial \Phi}{\partial x_k} - \frac{m \frac{Du}{\hbar \frac{Dt}}}{\hbar} \right) \right) \dot{e}_k = nV_k \dot{e}_k.
\]

where \( V_k \) is the local speed of the solid wall of the container and \( \dot{e}_k \) is normal to it. The displacement moves with the wall: \( \frac{Du}{\hbar \frac{Dt}} = V \).

Let us look at small perturbations around a nondeformed (\( u = 0 \)) and steady (\( \nabla \Phi = 0 \)) state of average density \( n \). The linearized version of (6TS) shows that the shear waves are decoupled from the compression and phase (Bogoliubov-like) waves. The dispersion relation for the coupled compression and phase waves leads to a simple algebraic equation. In the limit \( \varrho(n) \to 0 \) the crystal structure disappears and the phase mode propagates at the usual speed of sound found by Bogoliubov \( c = \sqrt{\varrho'(n)/(mn)} \). In the limit \( \varrho(n) \to n \), that is whenever the supersolid behaves as a regular solid state, the two propagation speeds are \( (c_K \text{ is the longitudinal elastic wave speed}) \)

\[
m_1 = \sqrt{c_K^2 + c^2}
\]

and \( \varrho = \sqrt{c_K^2 + c^2} \sqrt{1 - \varrho(n)/n} \) meaning that the phase mode disappears at the transition supersolid-solid.

As suggested by Leggett and an Andronikashvili kind of experiment could manifest a non classical rotational inertia (NCRI). Indeed let us suppose that the wall of the container of volume \( \Omega \) rotate with an uniform angular speed \( \omega \).
Then for low angular speed the crystal moves rigidly with the container \( \dot{\mathbf{u}} = \mathbf{\omega} \times \mathbf{r} \) without any elastic deformation. The densities \( n \) and \( \varrho(n) \) being constant in space, equation (8) simplifies into

\[
\nabla^2 \Phi = 0 \text{ in } \Omega \text{ with } \nabla \Phi \cdot \hat{e} = \frac{(m/h)(\mathbf{\omega} \times \mathbf{r}) \cdot \hat{e}}{\mu} \text{ on } \partial \Omega.
\]

This mathematical problem (9) has an unique solution. The moment of inertia comes directly from the energy per unit volume of the system: \( E = \Phi \frac{d\Phi}{dr} + \mathbf{u} \cdot \frac{d^2 \Phi}{dr^2} - \mathcal{L} \). In the rotating case \( E = \frac{1}{2} I_{ss} \omega^2 \) where \( I_{ss} \) is the zz component of the inertia moment : \( I_{ss} = m^2 - \varrho(n) I_{pf} + m \varrho(n) I_{rb} \) with \( I_{pf} = \int_\Omega (\nabla \Phi)^2 d\mathbf{r} \). \( \Phi \) solution of (9), \( m, n \) and \( h \) taken to 1. This number depends on the geometry only, \( I_{rb} \) is also a geometrical factor corresponding to rigid body rotational inertia (xy orthogonal to the axis of rotation) \( I_{rb} = \int_\Omega (x^2 + y^2) d\mathbf{r} \). The relative change of the moment of inertia whenever the supersolid phase appears is (here \( I_{rb} = mn I_{rb} \))

\[
(I_{ss} - I_{rb})/I_{rb} = -(1 - \varrho(n)/n)(1 - I_{pf}/I_{rb})
\]

Because \( I_{pf} < I_{rb} \), one has \( (I_{ss} - I_{rb})/I_{rb} \leq 0 \) as expected and observed experimentally. The NCRIF fraction (NCRIF) disappears, as well as the phase mode sound speed, when the supersolid phase recovers the ordinary solid phase \( (\varrho(n) \rightarrow n) \).

Within the model presented here it is easy to implement a numerical procedure to put in evidence a NCRIF in a 2D system. We shall first minimize \( H - \omega L_z \) for different values of the angular frequency \( \omega \), where \( H = \frac{\hbar^2}{2m} \int |\nabla \psi|^2 d\mathbf{r} + \frac{1}{2} \int U(|\mathbf{r}' - \mathbf{r}|) |\psi(\mathbf{r}, t)|^2 |\psi(\mathbf{r}', t)|^2 d\mathbf{r} d\mathbf{r}' \) is the Hamiltonian and \( L_z = \frac{\hbar^2}{2m} \int (\psi^* \mathbf{r} \times \nabla \psi - \psi \mathbf{r} \times \nabla \psi^*) d\mathbf{r} \) the angular momentum. The minimization should constrain a fixed total mass : \( N = \int |\psi|^2 d\mathbf{r} \). Starting with \( \omega = 0 \) one finds the minimizer and then by increasing \( \omega \) step by step together with the minimization procedure we follow the evolution of the local minima. Figure 1a represents the NCRIF as function of \( \omega \), for different values of \( nU_0 \). We observe a non-zero NCRIF in particular in the limit \( \omega \rightarrow 0 \). Figure 1b shows this limit \( \text{NCRIF}_0 \) as a function of the dimensionless compression \( \Lambda = U_0 \frac{\hbar^2}{2m} \frac{N}{a^3} \). Both curves are in qualitative agreement with recent experiments (see Fig. 3-D of Kim and Chan and the absence of pressure or gravity driven flows?

In fact, our supersolid model (and it seems that supersolid helium too) reacts in different ways under a small external constrain such as stress, bulk force or rotation in order to satisfies the equation of motion and the boundary conditions. For instance, if gravity (or pressure gradient) is added then the pressure \( \mathcal{E}'(n) \) balances the external “hydrostatic” pressure \( mgz \) in equation (10) while the elastic behavior of the solid of equation (7) balances the external uniform force per unit volume \( m \mathbf{g} \). No \( \nabla \Phi \) nor \( \dot{\mathbf{u}} \) are needed to satisfy the mechanical equilibria. Moreover, a flow is possible only if the stresses are large enough to display a plastic flow as it happens in ordinary solids. In [1] we showed that a flow around an obstacle is possible only if defects are created in the crystal, in this sense we did observe a
plastic flow, however in the same model we observe a “superfluid-like” behaviour under rotation without defects in the crystal structure. Indeed for a small angular rotation the elastic deformations come to order $\omega^2$ while $\nabla \Phi$ or $\dot{u}$ are of order $\omega$, the equations of motion together with the boundary conditions leads to a NCRIF different from zero.

We have realized a numerical simulation to test the possibility of a permanent gravity flow for different values of the dimensionless gravity $G = \frac{m^2a^3}{\hbar^2}$. Let us consider an U-tube as in Fig. 2. The system is prepared for 500 time units into a good quality (but not perfect) crystalline state. A vertical gravity of magnitude $G$ is switched-on and the system evolves for 500 time units more up to a new equilibrium state (see Fig. 2-a). The gravity is then tilted (with the same magnitude) at a given angle. A mass flow is observed at the begining from one reservoir into the other, but both vessels do not reach the same level eventually (see Fig. 2-b). There is some dependence of the transferred mass on $G$ till $G \approx 0.0005$ and the mass transfer becomes negligible from fluctuations for $G < 0.00025$ indicating the existence of a yield-stress. The flow is allowed by dislocations and grain boundaries and it is a precursor of a microscopic plastic flow as in ordinary solids (e.g. ice) and as it is probably observed in Ref. 14. A microscopic yield-stress could be defined by the smallest gravity $G$ such that no dislocations, defects nor grain boundaries appear. In the present model this is for $G < 10^{-4}$.

Fig. 2. We plot the density modulations $|\psi|^2$ (the dark points means a large mass concentration) of a numerical Simulation of eqn. (1) with Dirichlet boundary conditions with the shape of an u-tube as in the figure. We use a Crank-Nicholson scheme that conserves the total energy and mass. The mesh size is $dx = 1$, the nonlocal interaction parameters are chosen as $U_0 = 0.01$ and $a = 8$ (physical constants $\hbar$ and $m$ are 1), finally the initial condition is an uniform solution $\psi = 1$ plus small fluctuations. One gets a crystalline state after 500 units time; then a vertical gravity of magnitude $G = 0.01$ is switched-on, and the system evolves for 500 time unites up to $a$. Then gravity orientation is tilted in $45^\circ$. After 2000 time units the system evolves to a stationary situation $b$ showing that the mass flow is only a transient.

In conclusion, we have shown a fully explicit model of supersolid that display either solid-like behavior or superflow depending on the external constrain and on the boundary conditions on the reservoir wall. Our numerical simulations clearly show that, within the same model a nonclassical rotational inertia is observed as well a regular elastic response to external stress or forces without any flow of matter as in experiments $^{1,2}$.

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