

Coexistence of Ordinary Elasticity and Superfluidity in a Model of a Defect-Free Supersolid

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(Received 14 November 2006; published 9 May 2007)

The mechanical behavior of a supersolid is studied in the framework of a fully explicit model derived from the Gross-Pitaevskii equation without assuming any defect or vacancy. A set of coupled nonlinear partial differential equations plus boundary conditions is derived. The conditions of mechanical equilibrium are studied under external constraints such as steady rotation and external stress. Our model explains the experimentally observed paradoxical behavior: a nonclassical rotational inertia fraction in the limit of small rotation speed but a solidlike elastic response to small stress or an external force field.

DOI: 10.1103/PhysRevLett.98.195301

PACS numbers: 67.80.-s

The recent surge of interest in supersolids [1] makes it important to reach a clearer understanding of the mechanical properties of such materials. In particular, why is a supersolid behavior observed in a rotating experiment while, as in ordinary solids, no constant mass flux is driven by a pressure gradient? [1,2]. In Ref. [3] two of us (Y. P. and S. R.) proposed a fully explicit model of a supersolid where many properties can be discussed in detail. We thought it timely to reconsider this model, in particular, with respect to its properties of elasticity coupled to its ability to maintain some kind of superflow in the absence of defects. Although supersolidity is often related to the presence of defects, vacancies, and so forth, our model introduces an important distinction between ordinary (classical) crystals and supersolids: in perfect classical crystals there is either 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 a supersolid there is no such relation: the lattice parameters and the average density can be changed independently. Similar results were already noticed for the crystallization of a quantum liquid [4].

Our model is based on the original Gross-Pitaevskii (GP) equation [5] with an integral kernel that can be viewed as a two-body potential in the first Born approximation [6]. This model yields the exact spectrum found long ago by Bogoliubov [7], namely, a dispersion relation between the energy and momentum of the elementary excitations that depends on the two-body potential. In this framework the roton minimum becomes a precursor of crystallization. A similar behavior was predicted in [4,8]; however, in [8] the possibility of a linear instability was only considered, although the transition is subcritical (first-order) [3,4]. The crystal phase exhibits a periodic density modulation together with a superfluidlike behavior under rotation.

The aim of the present Letter is to show that, besides this behavior, the model system has also solidlike properties, at least under small stress. Under larger stress, it flows plastically, the plasticity being facilitated by the eventual pres-

ence of defects. We derive the equation of motion for the average density n , the phase Φ , and the displacement \mathbf{u} in the solid. A new propagating mode appears in addition to the longitudinal and transverse phonons characteristics of 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 GP equation [5] valid at $T = 0$ for the complex-valued wave function $\psi(\mathbf{r}, t)$ for bosonic particles of mass m :

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

where $U(\mathbf{r})$ is a two-body potential. For the numerics we choose a potential $U(|\mathbf{r}|) = U_0 \theta(a - |\mathbf{r}|)$, where $\theta(x)$ is the Heaviside function. The Lagrangian density for the GP equation (1) reads in polar variables, $\psi = \sqrt{\rho} e^{i\phi}$:

$$\begin{aligned} \mathcal{L} = & -\hbar \rho \frac{\partial \phi}{\partial t} - \frac{\hbar^2}{2m} \left[\rho (\nabla \phi)^2 + \frac{1}{4\rho} (\nabla \rho)^2 \right] \\ & - \frac{1}{2} \rho(\mathbf{r}) \int d\mathbf{r}' U(\mathbf{r}' - \mathbf{r}) \rho(\mathbf{r}'). \end{aligned} \quad (2)$$

The ground state is given by the solution of the nonlinear integro-differential equation for ρ taking the phase field ϕ uniform in space: $\phi = -\mu t/\hbar$, μ constant:

$$\frac{\hbar^2}{4m} \left(\frac{(\nabla \rho)^2}{2\rho^2} - \frac{\nabla^2 \rho}{\rho} \right) + \int U(\mathbf{r}' - \mathbf{r}) \rho(\mathbf{r}') d\mathbf{r}' = \mu. \quad (3)$$

This ground-state solution is periodic in space at large enough densities, in full agreement with our numerical results. It depends only on the dimensionless parameter $\Lambda = U_0 \frac{m a^2}{\hbar^2} n a^3$ [3], where $n = \frac{1}{\Omega} \int \rho(\mathbf{r}) d\mathbf{r}$ is the average number density over the total volume Ω . Although in Ref. [3] we discussed the ground state as a modulation close to a uniform density near the transition, that is, for a finite roton gap, we have observed numerically that the crystal ground state exists over a wider range of densities.

In the limit $\Lambda \gg 1$ the lattice tends to an array of sharp density peaks distant of a , the width of the pulse decreasing as Λ increases.

If $\rho_0(\mathbf{r}|n)$ is a ground-state solution, then $\rho_0(\mathbf{r} - \mathbf{u}|n)$ is also a ground-state solution with the same μ for a constant displacement field \mathbf{u} . The general perturbations around the ground state allow that Φ , \mathbf{u} , and n become fields that vary slowly with space and time. As in Ref. [3], we follow the general method called homogenization [9]. In this method the long-wave behavior of the various parameters and the short-range periodic dependence upon the lattice parameters can be treated separately. The ansatz for density and phase becomes: $\rho = \rho_0(\mathbf{r} - \mathbf{u}(\mathbf{r}, t)|n(\mathbf{r}, t)) + \tilde{\rho}(\mathbf{r} - \mathbf{u}, n, t) + \dots$ and $\phi = \Phi(\mathbf{r}, t) + \tilde{\phi}(\mathbf{r} - \mathbf{u}, n, t) + \dots$, where Φ , \mathbf{u} , and n are slowly varying fields and $\tilde{\phi}$ and $\tilde{\rho}$ are small and rapidly varying periodic functions. Introducing this ansatz into the Lagrangian (2) one gets an effective Lagrangian [10]:

$$\mathcal{L}_{\text{eff}} = -\hbar n \frac{\partial \Phi}{\partial t} - \frac{\hbar^2}{2m} \left[n(\nabla \Phi)^2 - \varrho(n) \left(\nabla \Phi - \frac{m}{\hbar} \frac{D\mathbf{u}}{Dt} \right)^2 \right] - \mathcal{E}(n) - \frac{1}{2} \lambda_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l}, \quad (4)$$

where $\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + \frac{\hbar}{m} \nabla \Phi \cdot \nabla \mathbf{u}$, so that this Lagrangian is Galilean invariant. Furthermore, $\mathcal{E}(n) = \frac{1}{V} \int d\mathbf{r} \left[\frac{\hbar^2}{8m\rho_0} \times (\nabla \rho_0)^2 + \frac{1}{2} \rho_0(\mathbf{r}) \int d\mathbf{r}' U(\mathbf{r}' - \mathbf{r}) \rho_0(\mathbf{r}') \right]$ is an internal energy that comes from an integration over a unit lattice cell (V) of the part of the Lagrangian (2) that depends only on n . Similarly, $\varrho(n)$ and λ_{ijkl} are given by explicit integrals over the unit cell. For $\varrho(n)$, for instance, we introduce the periodic vector field $\mathbf{K}(\mathbf{r})$ that satisfies $\nabla_i \rho_0 + \nabla \cdot (\rho_0 \nabla \mathbf{K}_i) = 0$ which defines the matrix $\varrho_{ij} = \frac{1}{V} \int_V \rho_0(\mathbf{r}) \nabla \mathbf{K}_i \cdot \nabla \mathbf{K}_j d\mathbf{r}$. We restrict ourselves to crystal structures sufficiently symmetric to make this matrix diagonal [$\varrho_{ij} = \varrho(n) \delta_{ij}$]. The quantity $\varrho(n)$ is zero if the crystal modulation is absent and would be very small for a Bose-Einstein condensate with a nonlocal interaction term. The density $\varrho(n) \rightarrow n$ when all the mass is strongly localized at the center of the unit cell. This is presumably the situation for almost all materials in a solid state at low temperature. The large Young's modulus probably results from the small overlap of the wave functions from one site to the next, making ^4He exceptional in this respect. In other words, when $\varrho(n) \rightarrow n$ the supersolid behaves as an ordinary solid. The coefficients λ_{ijkl} appearing in Eq. (4) define the familiar elastic energy of a Hookean solid.

Equation (4) is remarkable because it is fully explicit for a given ground state of the GP model. We conjecture that, because (4) 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 has the same structure at $T = 0$. In a recent Letter, Son [11] derived a Lagrangian of which Eq. (4) is a subclass but with well-

defined coefficients such as $\varrho(n)$, $\mathcal{E}(n)$, and λ_{ijkl} depending on the details of the crystal structure.

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

$$\hbar \frac{\partial \Phi}{\partial t} + \frac{\hbar^2}{2m} \left[(\nabla \Phi)^2 - \varrho'(n) \left(\nabla \Phi - \frac{m}{\hbar} \frac{D\mathbf{u}}{Dt} \right)^2 \right] + \mathcal{E}'(n) + \frac{1}{2} \lambda'_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} = 0 \quad (5)$$

$$m \frac{\partial}{\partial t} \left[\varrho(n) \left(\frac{Du_i}{Dt} - \frac{\hbar}{m} \frac{\partial \Phi}{\partial x_i} \right) \right] - \frac{\partial}{\partial x_j} \left(\lambda_{ijkl} \frac{\partial u_k}{\partial x_l} \right) + \hbar \frac{\partial}{\partial x_k} \left[\varrho \left(\frac{Du_i}{Dt} - \frac{\hbar}{m} \frac{\partial \Phi}{\partial x_i} \right) \frac{\partial \Phi}{\partial x_k} \right] = 0 \quad (6)$$

$$\frac{\partial n}{\partial t} + \frac{\hbar}{m} \nabla \cdot (n \nabla \Phi) - \frac{\hbar}{m} \frac{\partial}{\partial x_k} \left[\varrho(n) (\delta_{ik} - \partial_k u_i) \left(\partial_i \Phi - \frac{m}{\hbar} \frac{Du_i}{Dt} \right) \right] = 0. \quad (7)$$

The last 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 (5)–(7) and the one of Andreev-Lifshitz [12] are almost identical in the zero temperature limit [see Eq. (16) of Ref. [12]], our model has significant differences with theirs. 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 $T = 0$. Therefore, at small finite temperature, our model has a normal component that is a fluid of vanishing density at $T = 0$ in addition to its coherent superfluid and solid part that should change the superfluid density fraction. Following Landau's ideas, this normal fluid is a gas of quasiparticles with a mixed spectrum able to carry momentum while the coherent part (superfluid plus solid) stays at rest.

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

$$\frac{\hbar}{m} \left[n \partial_k \Phi - \varrho (\delta_{ik} - \partial_k u_i) \left(\partial_i \Phi - \frac{m}{\hbar} \frac{Du_i}{Dt} \right) \right] \hat{e}_k = n V_k \hat{e}_k,$$

where V_k is a component of the local speed of the solid wall of the container and \hat{e}_k is normal to it. The displacement field moves with the wall: $\frac{D\mathbf{u}}{Dt} = \mathbf{V}$.

Let us consider small perturbations around a nondeformed ($\mathbf{u} = 0$) and steady ($\nabla \Phi = 0$) state of average density n . The linearized version of (5)–(7) 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 $\varrho(n) \rightarrow 0$ the crystal structure disappears and the phase mode propagates at the usual speed of sound found by Bogoliubov, $c = \sqrt{n\mathcal{E}''(n)/m}$. In

the limit $\varrho(n) \rightarrow n$, that is, whenever the supersolid behaves as a regular solid, the two propagation speeds are $v_1 = \sqrt{c_K^2 + c^2}$ and $v_2 = \sqrt{c_K^2 c^2 / (c_K^2 + c^2) \sqrt{1 - \varrho(n)/n}}$, where c_K is the longitudinal elastic wave speed [13], meaning that the phase mode disappears at the supersolid-solid transition.

As suggested by Leggett [14], an Andronikashvili-type of experiment could manifest a nonclassical rotational inertia (NCRI). Suppose that the wall of the container of volume Ω rotates with uniform angular speed ω . Then for low angular speed the crystal moves rigidly with the container $\dot{\mathbf{u}} = \boldsymbol{\omega} \times \mathbf{r}$ without any elastic deformation. The densities n and $\varrho(n)$ being constant in space, Eq. (7) simplifies to

$$\begin{aligned} \nabla^2 \Phi &= 0 \quad \text{in } \Omega \\ \text{with } \nabla \Phi \cdot \hat{\mathbf{e}} &= (m/\hbar)(\boldsymbol{\omega} \times \mathbf{r}) \cdot \hat{\mathbf{e}} \quad \text{on } \partial\Omega. \end{aligned} \quad (8)$$

Equation (8) has a unique solution [15]. The moment of inertia comes directly from the energy per unit volume of the system: $E = \Phi_t \frac{\delta \mathcal{L}}{\delta \Phi_t} + \mathbf{u}_t \cdot \frac{\delta \mathcal{L}}{\delta \mathbf{u}_t} - \mathcal{L}$. In the rotating case $E = \frac{1}{2} I_{ss} \omega^2$, where I_{ss} is the zz component of the inertia moment: $I_{ss} = m[n - \varrho(n)]I_{pf} + m\varrho(n)I_{rb}$, where $I_{pf} = \int_{\Omega} (\nabla \Phi)^2 d\mathbf{r}$, Φ being a solution of Eq. (8) (ω , m , and \hbar are taken as unity). It depends only on the geometry, as does I_{rb} , corresponding to the rigid-body rotational inertia $I_{rb} = \int_{\Omega} (x^2 + y^2) d\mathbf{r}$, where x and y are orthogonal to the axis of rotation. The relative change of the moment of inertia when the supersolid phase appears is

$$(I_{ss} - I_{rb})/I_{rb} = -[1 - \varrho(n)/n](1 - I_{pf}/I_{rb}), \quad (9)$$

where $I_{rb} = mnI_{rb}$. Because $I_{pf} < I_{rb}$, one has $(I_{ss} - I_{rb})/I_{rb} \leq 0$ as expected and observed experimentally [1]. The NCRI fraction (NCRIF) disappears, as does the phase mode sound speed, when the supersolid becomes an ordinary solid [$\varrho(n) \rightarrow n$].

Within the model presented here it is easy to implement a numerical procedure to demonstrate an NCRI in a 2D system. We first minimize $H - \omega L_z$ for different values of the angular frequency ω , where $H = \frac{\hbar^2}{2m} \int |\nabla \psi|^2 d\mathbf{r} + \frac{1}{2} \times \int U(\mathbf{r}' - \mathbf{r}) |\psi(\mathbf{r}, t)|^2 |\psi(\mathbf{r}', t)|^2 d\mathbf{r} d\mathbf{r}'$ is the energy and $L_z = \frac{i\hbar}{2} \int (\psi^* \mathbf{r} \times \nabla \psi - \psi \mathbf{r} \times \nabla \psi^*) d\mathbf{r}$ the angular momentum. The minimization should be carried out with a fixed total mass: $N = \int |\psi|^2 d\mathbf{r}$. Starting with $\omega = 0$ we find the minimizer and then by increasing ω step by step we follow the evolution of the local minima. We measure a rotational inertia that varies with both ω and nU_0 [see Fig. 1(a)] so that we can numerically define an NCRIF. Figure 1(b) shows this NCRIF in the limit $\omega \rightarrow 0$ as a function of the dimensionless compression $\Lambda = U_0 \frac{m a^2}{\hbar^2} n a^3$. Both curves are in qualitative agreement with recent experiments (see Fig. 3D of Ref. [1(b)] and Fig. 4 of [1(c)]).

Finally, we study a gravity- (or pressure-) driven supersolid flow. As earlier suggested by Andreev *et al.* [16], an experiment on an obstacle pulled by gravity in solid helium

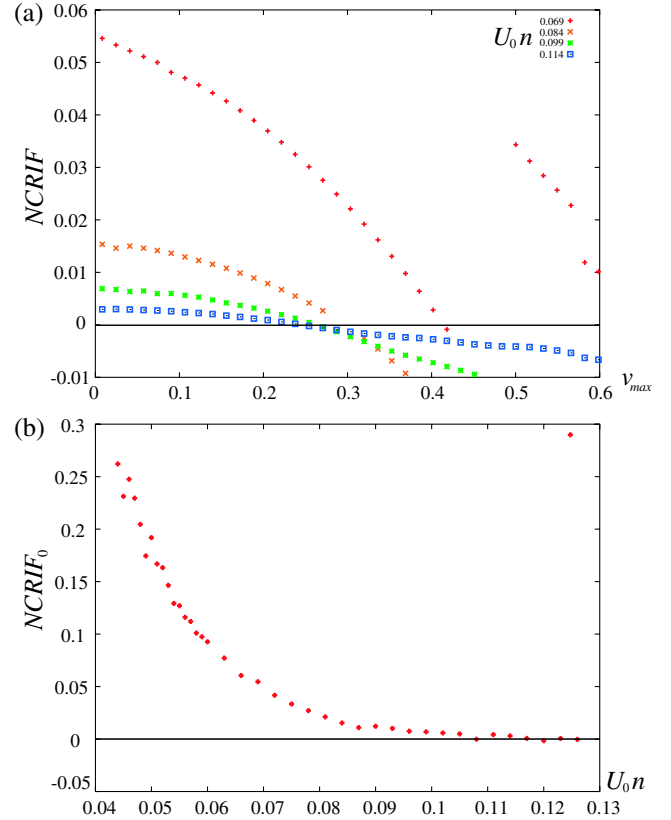


FIG. 1 (color online). We implement a relaxation algorithm in Fourier space with 128×128 modes to find a local minima in a square cell of 96×96 units for different values of $U_0 n$; the potential range is $a = 4.3$. (a) The $\text{NCRIF} \equiv 1 - L'_z(\omega)/\langle I_{rb} \rangle$ vs the local maximum speed $v_{max} = \omega L/\sqrt{2}$ for $nU_0 = 0.069, 0.084, 0.099$, and 0.114 . Here $\langle I_{rb} \rangle$ is the converging inertia moment computed numerically for large nU_0 at $\omega = 0$. Note that the jump in NCRIF for $nU_0 = 0.069$ corresponds to the nucleation of a vortex in the system. (b) NCRIF at $\omega = 0$ as a function of nU_0 . We have verified that (a) and (b) are almost independent of the box size.

could provide a proof of supersolidity. Various versions of this experiment failed to show any motion [2], so a natural question arises: how to reconcile the NCRI experiment of Kim and Chan with the absence of pressure- or gravity-driven flows? Our supersolid model (and it seems also supersolid helium) reacts in different ways under small external constraints such as stress, bulk force, or rotation in order to satisfy the equation of motion and the boundary conditions. For instance, if gravity (or a pressure gradient) is added then the pressure $\mathcal{E}'(n)$ balances the external force mgz in Eq. (5) while the elastic behavior of the solid of Eq. (6) balances the external uniform force per unit volume mng . No $\nabla \Phi$ nor $\dot{\mathbf{u}}$ terms are needed to satisfy the mechanical equilibrium. Moreover, a flow is possible only if the stresses are large enough to display a plastic flow as happens in ordinary solids (this could be different at finite temperature). In [3] we showed that a flow around an obstacle is possible only if defects are created in the crystal, and in this sense we did observe a plastic flow.

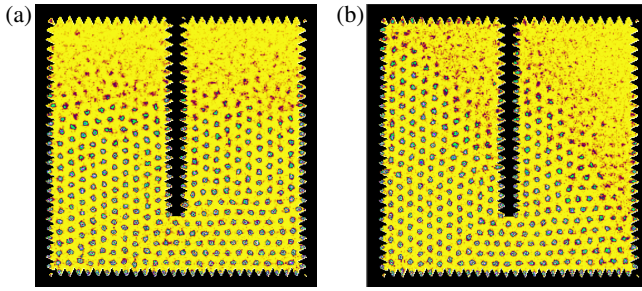


FIG. 2 (color online). The density modulations $|\psi|^2$ (the dark points denote large mass concentration) of a numerical simulation of Eq. (1) with Dirichlet boundary conditions (the boundaries are in black) in a form of a U tube with roughness. We use a Crank-Nicholson scheme that conserves the total 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), and the initial condition is an uniform solution $\psi = 1$ plus small fluctuations. We use the protocol described in the text with $\mathcal{G} = 0.01$ and a tilted angle of 45° . After 2000 time units the system has reached the stationary situation shown in (b), demonstrating that the mass flow is only a transient. See a movie in Ref. [18] for further detail.

However, in the same model we observe a “superfluidlike” behavior under rotation without defects in the crystal structure. In fact, for a small angular rotation the elastic deformations come in at order ω^2 while $\nabla\Phi$ or $\dot{\mathbf{u}}$ are of order ω , and the equations of motion together with the boundary conditions lead to an NCRIF different from zero.

We have carried out a numerical simulation to test for the possibility of a permanent gravity flow for different values of the dimensionless gravity $\mathcal{G} = \frac{m^2 g a^3}{\hbar^2}$. Let us consider a U tube as in Fig. 2. The system is prepared for 500 time units in a good-quality (but not perfect) crystalline state. A vertical gravity of magnitude \mathcal{G} is switched on and the system evolves for 500 more time units up to a new equilibrium [see Fig. 2(a)]. The gravity is then tilted (with the same magnitude) at a given angle. A mass flow is initially observed from one reservoir into the other, but eventually the vessels reach different level [see Fig. 2(b)]. There is some dependence of the transferred mass on \mathcal{G} till $\mathcal{G} \approx 0.0005$ and the mass transfer becomes indistinguishable from fluctuations for $\mathcal{G} < 0.00025$, indicating the existence of a yield stress. The flow is allowed by dislocations and grain boundaries and is a precursor of a microscopic plastic flow as in ordinary solids (e.g., ice), as is probably observed in Ref. [17]. A microscopic yield stress could be defined by the smallest value of the gravity \mathcal{G} such that no dislocations, defects, or grain boundaries appear. In the present model this is $\mathcal{G} < 10^{-4}$.

In conclusion, we have derived a fully explicit model of a supersolid at $T = 0$ that displays either solidlike behavior or superflow depending on the external constraints and on the boundary conditions of the reservoir walls. Our numerical simulations 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.

Finally, the authors thank M.-L. Saboungi and D. Price for critical reading of the manuscript. S. R. acknowledges Anillo de Investigación Act. 15 (Chile).

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 - [18] See EPAPS Document No. E-PRLTAO-98-038718 for a movie of a plastic flow under gravity. For more information on EPAPS, see <http://www.aip.org/pubservs/epaps.html>.