Nonclassical Rotational Inertia of a Supersolid

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(Received 16 April 2007; revised manuscript received 16 July 2007; published 24 September 2007)

As proposed by Leggett [Phys. Rev. Lett. **25**, 1543 (1970)], the supersolidity of a crystal is characterized by the nonclassicalical Rotational Inertia (NCRI) property. Using a model of quantum crystal introduced by Josserand, Pomeau, and Rica [Phys. Rev. Lett. **72**, 2426 (1994)], we prove that NCRI occurs. This is done by analyzing the ground state of the aforementioned model, which is related to a sphere packing problem, and then deriving a theoretical formula for the moment of inertia. We infer a lower estimate for the NCRI fraction, which is a landmark of supersolidity.

DOI: 10.1103/PhysRevLett.99.135301 PACS numbers: 67.80.−s

A recent experiment by Kim and Chan [1] allowed them to measure the moment of inertia of solid helium and find that it is lower than its classical value. This property is referred to as nonclassicalical Rotational Inertia (NCRI). This experiment has raised a lot of interest and was interpreted as a landmark of supersolidity, on the basis of a paper by Leggett [2]. In [2], Leggett predicted that the property of nonclassical rotational inertia possessed by superfluid helium is shared by solids and proposed as a definition for the non-classical rotational inertia fraction $\mathrm{NCRIF} = (I_0 - I)/I_0$ where I is the moment of inertia of the crystal under study and I_0 its classical value. One theoretical challenge (see the review paper of Prokof'ev [3]) is to estimate this NCRIF and check that it is nonzero. This is the aim of this Letter, based on a model of quantum crystal, introduced by Josserand, Pomeau, and Rica [4]. In this respect, we derive a key estimate providing the lower bound (8) for the NCRIF. In the literature (see [3,5]), different microscopic mechanisms have been proposed to describe the supersolidity of a crystal, based mainly on the off diagonal long range order property (ODLRO) of the density matrix and Jastrow wave functions. Here, we do not relate directly the NCRI to ODLRO, or the presence of vacancies, but choose another approach to model the solid.

Josserand, Pomeau, and Rica [4] proposed a model of quantum solid: it is based on the fact that the complex valued wave function common to all particles of mass m minimizes the Gross-Pitaevskii energy with an integral term that can be viewed as a 2-body potential in a first Born approximation:

$$\int \frac{\hbar^2}{2m} |\nabla\psi(\boldsymbol{r})|^2 d\boldsymbol{r} + \frac{1}{4} \iint \tilde{U}(\boldsymbol{r}' - \boldsymbol{r}) |\psi(\boldsymbol{r}')|^2 |\psi(\boldsymbol{r})|^2 d\boldsymbol{r} d\boldsymbol{r}'$$

where $\tilde{U}(\cdot)$ is a potential depending on the distance between atoms. The normalization condition is $\nu = \int |\psi|^2/V$ where V is the volume of the region $\mathcal{D}$ occupied by the solid. This model bears an important difference with classical solids, in the sense that in classical solids, there is an integer number of atoms per unit cell, while in this quantum solid model, the average density is a free number, independent of the crystal parameters. Moreover, this model yields a dispersion relation between the energy and momentum of elementary excitations that depends on the two-body potential. The choice of $\tilde{U}$ is made in order to have a roton minimum in this dispersion relation. For instance, one possibility is to take $\tilde{U}(|\boldsymbol{r}|) = U_0\theta(a - |\boldsymbol{r}|)$, with $\theta(.)$ the Heaviside function [4]. We define $g = U_0 \frac{ma^2}{\hbar^2} \nu a^3$ and rescale distances by a so that the rescaled energy E_g is given by

$$\int \frac{1}{2} |\nabla\psi(\boldsymbol{r})|^2 d\boldsymbol{r} + \frac{g}{4} \iint U(\boldsymbol{r}' - \boldsymbol{r}) |\psi(\boldsymbol{r}')|^2 |\psi(\boldsymbol{r})|^2 d\boldsymbol{r} d\boldsymbol{r}' \tag{1}$$

where $U(|\boldsymbol{r}|) = \theta(1 - |\boldsymbol{r}|)$ and $\int |\psi|^2 = V$. For small g, the ground state is $|\psi| = 1$, and for large g, computations in [4] indicate the presence of a crystal phase with some supersolidlike behavior under rotation. Moreover, the authors of [4] checked that this model also provides mechanical behaviors typical of solids under small stress. We believe that the model proposed in [4] is not far from a realistic model of solid helium, that is of a dense solid with strongly repulsive interaction. Note that for He, we have $g \sim 25$, and for Ne, $g \sim 100$ [6]. In the large g limit, we will see that the ground state of (1) is a periodic array of peaks. The self interaction of a peak becomes a constant, added to the energy, and independent of the wave function local profile. One could argue that in a mean field model of a real crystal, the interaction has a hard core so that the self interaction is infinite. But in the true physical system of solid helium, a given atom does not interact with itself and thus does not provide any infinite self interaction. This, added to the various properties of the quantum crystal derived in [4], which are in agreement with experimental solid helium, makes us believe that the model provides insight into the understanding of supersolids. The aim of this Letter is to use this model to derive an approximate theoretical value for the reduction of the moment of inertia of a supersolid. The proof is two-fold: on the one hand, we use the specific choice of the interaction potential U to get that for large g, the ground state ψ_g has a periodic density $\rho_g = \psi_g^2$. Moreover, the wave function is localized around sets defined by a sphere packing problem. On the other hand, given this periodic density ρ_g, we use the expression (6) of the NCRIF and the fact that ψ_g is a ground state, hence a solution of some nonlinear Schrödinger equation, to obtain a lower estimate of the NCRIF (7) and (8). Since this second part of the proof only relies on the periodicity of ρ_g and the fact that it is a solution of an equation, it could be used for other models providing a periodic density, for instance that of an optical lattice (with an exterior field creating a periodic density with several atoms per site).

If $\mathcal{D}$ is a solid sample, the sphere packing problem [7,8] provides a number $n(\mathcal{D})$, the largest number of points in $\mathcal{D}$ which are at distance larger than 1 from each other. When this number is large, the optimal location of points is proved [7,8] to be close to a hexagonal lattice in 2D. In 3D, 2 configurations are optimal: body centered cubic close packing and face centered cubic close packing. When g is large, the two terms in (1) are of different order; hence, the ground state ψ_g is very close to a function ψ_0 that is found by minimizing the kinetic energy within the functions that minimize the interaction term, which is dominant. We are going to prove that such a function is supported in sets A_i which are at a distance at least one and whose number is $n(\mathcal{D})$. Thus, the sets A_i are determined by the minimization problem

$$\inf_{A_i,\,\mathrm{dist}(A_i,A_j)>1}\left\{\sum_{i=1}^{n(\mathcal{D})}\lambda_1(A_i)\right\} \qquad (2)$$

where λ_1 is the ground energy of $-\Delta$ in A_i with zero boundary conditions: $\lambda_1(A_i) = \inf_{\int|u|^2=1}\{\int_{A_i}|\nabla u|^2\}$. The expected configuration is illustrated in Fig. 1. The function ψ_0 corresponds to the ground state of $-\Delta$ in each A_i and vanishes outside the A_i's. A ground state of E_g will be very close to ψ_0 in the sets A_i, and exponentially small away from the A_i's, except on a boundary layer.

When the sample is set under rotation Ω about the z axis, the free energy of the system is defined as

$$e(\Omega) = \inf_{\psi}\{E_g(\psi) - \Omega\langle\psi, L_z(\psi)\rangle\} \qquad (3)$$

where $L_z(\psi) = i\mathbf{r}\times\nabla\psi\cdot e_z$ and E_g is the energy defined in (1). When Ω is small, $e(\Omega)$ can be expanded as $e_0 - (1/2)I\Omega^2$ where I is the effective moment of inertia of the system. Leggett [2] suggested as a criterion for superfluidity the existence of a nonclassicalical rotational inertia fraction (NCRIF), defined as $(I_0 - I)/I_0$, where I_0 is the classical moment of inertia of the crystal phase and is equal to $\int|\psi_g|^2r^2$ where ψ_g is a ground state of E_g. The point of this analysis is to find an estimate for the NCRIF, computed numerically in [4], and prove that it is non zero. As can be seen in (6), a good knowledge of ρ_g, the ground state density with no rotation, is needed to estimate NCRIF in (7) and (8).

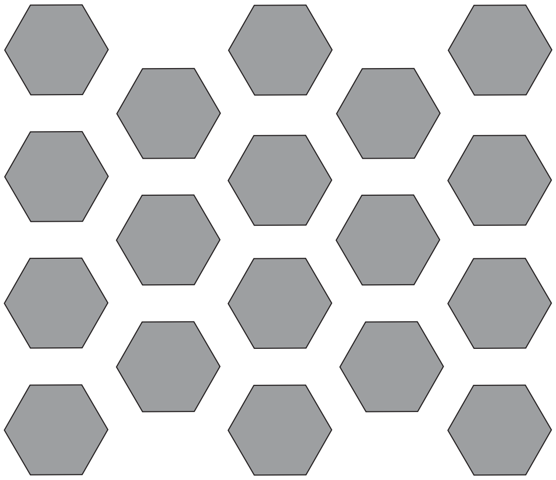

FIG. 1. The expected configuration of sets A_i in 2D.

The Letter is organized as follows: first, we study the ground state of the crystal phase with no rotation and derive (2). Then, we present some more refined computations in the 1D case, and finally we derive estimates for the NCRIF.

Crystal phase with no rotation.—We first describe the minimization of the second term of (1) which provides a class of functions ψ such that $\rho = |\psi|^2$ has mass located in disjoint sets A_i, at a distance at least the range of the potential, which is 1. When one wants to minimize $\int|\nabla\psi|^2$ in this class, this provides a constraint (2) on the shape of the sets A_i that we explain.

We denote by $(U*\rho)(\mathbf{r}) = \int U(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}')d\mathbf{r}'$ and $F(\rho) = \iint U(\mathbf{r}'-\mathbf{r})\rho(\mathbf{r}')\rho(\mathbf{r})d\mathbf{r}d\mathbf{r}'$. Recall that $n(\mathcal{D})$ was defined in the introduction and is related to the sphere packing problem.

Theorem 1.—A measure ρ with $\int\rho = V$ minimizes $F(\rho)$ if and only if there exist $n(\mathcal{D})$ pairwise disjoint sets $A_1, \ldots, A_{n(\mathcal{D})}$, such that

$$\mathrm{dist}\,(A_i, A_j) \geq 1 \quad \text{if} \quad i \neq j, \quad \text{and} \quad \int_{A_i}\rho = \frac{V}{n(\mathcal{D})}. \qquad (4)$$

Moreover, $\min F = V^2/n(\mathcal{D})$.

The proof of this result, which strongly relies on the shape of U, is made in the Appendix. Let us call ρ_0 a ground state of F and ψ_g a ground state of E_g with $\rho_g = \psi_g^2$. Then, $F(\rho_0) \leq F(\rho_g) \leq F(\rho_0) + (1/g)\times \int|\nabla\psi_0|^2 - |\nabla\psi_g|^2$. For g large, we deduce that ρ_g is an almost ground state of F. Among all the possible ρ_0's which are ground states of F, the limit of ψ_g when g is large should be such that $\psi_0 = \sqrt{\rho_0}$ minimizes the kinetic energy $\int|\nabla\psi|^2$ among all ψ such that $\rho = |\psi|^2$ is a ground state of F. This implies that the support of ψ_0 is the union of n connected sets A_i, $1 \leq i \leq n$, which satisfy (2).

More specific computations in 1D.—In dimension 1 (for N atoms in a cylindrical annulus [2]), that is if $\mathcal{D} = (0, L)$, then $n = n(\mathcal{D}) = [L] + 1$ (if L is not an integer [9]), and the A_i's are intervals $(x_i, x_i + l)$, with $l = L/n - 1 + 1/n$ and $x_i = i(l+1)$. Thus, $\psi_0(x) = \sqrt{(2L/nl)} \sin(\pi(x - x_i)/l)$ if $x \in (x_i, x_{i+1})$ and 0 otherwise (see Fig. 2). Moreover, $E_0(\psi_0) = \pi^2 L/2l^2$. Indeed, the ground state of F provides n sets A_i separated from one another by a distance at least 1. Hence, $A_i \subset [a_i, b_i]$ for all i, and $b_i + 1 \leq a_{i+1}$ for $i = 1, \ldots, n-1$. Then, since (4) implies that $\int_{a_i}^{b_i} |u|^2 = \frac{L}{n}$ for every i, $\int |u'|^2 = \sum_{i=1}^n \int_{a_i}^{b_i} |u'|^2 \geq \sum_{i=1}^n \frac{\pi^2}{(b_i - a_i)^2} \int_{a_i}^{b_i} |u|^2 = \frac{L}{n} \sum_{i=1}^n \frac{\pi^2}{(b_i - a_i)^2}$, with equality if and only if the restriction of u to each interval (a_i, b_i) is a scaled and normalized sine function multiplied by a constant of modulus 1. Moreover, Jensen's inequality implies that $\sum \frac{1}{(b_i - a_i)^2} \geq \frac{n}{[n^{-1} \sum (b_i - a_i)]^2} \geq n/l^2$, with equality if and only if $b_i - a_i = l$ for every i.

One expects a boundary layer around each A_i. In this one-dimensional setting, it is possible to compute it explicitly. In order to do so, we assume that ψ is a dilation of the limit ψ_0, namely $\psi(x) = \sqrt{\frac{2L}{(l+k)n}} \sin(\frac{\pi[x - i(l+1)]}{l+k})$ if $x \in [i(1+l) - k/2, i(1+l) + l + k/2]$, and $\psi = 0$ otherwise. The energy of this trial function is computed explicitly, in the limit of small k: $E_g(\psi) \approx \frac{\pi^2 L}{2(l+k)^2} + \frac{gL^2}{4n} + \frac{g}{4} A(\frac{k}{l+k})^6$, where $A = 13L^2\pi^6/(90n)$. Minimizing this expression with respect to k yields $k = [(2L\pi^2 l^3)/(3A)]^{1/5} g^{-1/5}$. Inserting this into the expression of the energy, we find

$$E_g(\psi) \approx \frac{\pi^2 L}{2l^2} + \frac{gL^2}{4n} - \frac{5}{6}\left(\frac{60L^4\pi^6 n^2}{13 l^{12}}\right)^{1/5} g^{-1/5},$$

as g is large.

The above computation indicates that the boundary layer around each bump of the limit function ψ_0 is of order $g^{-1/5}$ and if x denotes the scaled distance to the boundary, then the matching between ψ_0 and 0 in the boundary layer is described by the solution of $u'' = cx^3 u$. This boundary layer decreases the energy by an amount of order $g^{-1/5}$.

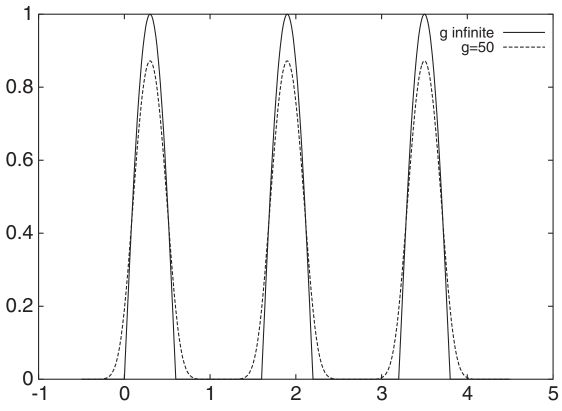

FIG. 2. Ground state of E_g when g is large (dashed line) and its limiting profile ψ_0 (solid line). The bumps are of size l and separated by a distance 1.

Dimension 2 and 3.—There is no complete determination of the A_i's, except that once the sphere packing problem is known to provide a hexagonal lattice, the A_i's are sets whose centers are located on an almost hexagonal lattice. Since minimizing $\lambda_1(A_i)$ over A_i with fixed volume implies that A_i is a ball (see [10]), condition (2) implies that A_i "looks like" a ball to some extent. However, $\lambda_1(A_i)$ is increasing with respect to A_i, which implies that A_i cannot be exactly a ball, but is closer to a hexagon (see Fig. 1).

A ground state ψ_g of E_g is close to ψ_0 in the A_i's and small in between. We need to understand better the smallness of ψ_g. The Euler-Lagrange equation satisfied is $-\Delta\psi_g + gW(x)\psi_g = 0$, where $W(x) = U * |\psi_g|^2 - \lambda_g$, and λ_g is the chemical potential. The shape of U and the mass constraint on ψ_g imply that $1 \leq \max|W| \leq 2$. Thus, the Harnack inequality [11] applied to the equation for ψ_g yields

$$\inf \psi_g \geq 2gC_d e^{(-\sqrt{2gT})} \max \psi_g, \tag{5}$$

for some constant C_d [12], where T is the size of the period of ρ_g and is of order 1. This estimate is used below in order to estimate the NCRIF.

In the limit of very large g, the function ψ_g is exponentially small: the potential W is almost equal to $W_0 = U * \rho_0 - \lambda_0$, which vanishes in each A_i and is positive in between. Using appropriate comparison solutions, it is possible to prove the estimate $|\psi_g(x)| \leq \exp(-\delta\sqrt{g a_\delta})$, for any x such that $\mathrm{dist}(x, A_i) > \delta$. The constant a_δ is the minimal value of W in this region, and is of order $\delta^{(d+5)/2}$, where d is the dimension. The density is thus exponentially small between the A_i's. However, in the experiments, $g \sim 25$, so that it is not large to the point of having tiny density.

Small rotation.—When the sample is set under rotation Ω about the z axis, the free energy of the system is defined by (3) and E_g is the energy defined in (1). We assume that the ground state ψ of (3) is of the form $\psi(x) = \sqrt{\rho_g(x)} e^{i\Omega S(x)}$ for small Ω, where $\psi_g = \sqrt{\rho_g}$ is a ground state of E_g, that is for $\Omega = 0$. This is equivalent to expanding the phase in terms of Ω and assume that the first order variation in the phase is not sensitive to the variations in density in terms of Ω. Then, the phase S should minimize $\int \rho_g |\nabla S - \mathbf{e}_z \times \mathbf{r}|^2$ among all possible test functions. This provides an expansion of $e(\Omega)$ for small Ω and hence a value for I which allows to compute

$$\mathrm{NCRIF} = \frac{\inf_S \int \rho_g |\nabla S - \mathbf{e}_z \times \mathbf{r}|^2}{\int \rho_g r^2}. \tag{6}$$

Two limiting cases are easily identifiable: when $\rho_g = 1$ (i.e., when g is small), this ratio is 1, and when ρ_g is periodic and has all its mass localized in the center of the cell, this ratio tends to 0. For intermediate values of g, the wave function is localized in A_i, with tails in between the sets which are small, but not too small. Then, (6) implies

$$\text{NCRIF} \geq \frac{\inf \rho_g}{\max \rho_g} \frac{\inf\limits_{S} \int |\boldsymbol{\nabla} S - \mathbf{e}_z \times \mathbf{r}|^2}{\int r^2} = \frac{\inf \rho_g}{\max \rho_g}. \quad (7)$$

The last equality is due to the fact that $\inf_S \int |\boldsymbol{\nabla} S - \mathbf{e}_z \times \mathbf{r}|^2$ is achieved for $\boldsymbol{\nabla} S = \mathbf{0}$. Note that this estimate is a mere consequence of (6) and not of the shape of ρ_g. The ratio $\max \rho_g / \inf \rho_g$ was estimated above (5). We thus have

$$\text{NCRIF} \geq 4g^2 C_d^2 e^{-2\sqrt{2g}T}. \quad (8)$$

Since $\sqrt{g}$ is of order 5, this implies that NCRIF $\neq 0$ for the experimental values.

In the very large g limit, (8) is not so good, but in this case, we may replace ρ_g by ρ_0 in (6). Moreover, in each A_i, we can define local coordinates $\mathbf{r}_i$ with respect to a point in A_i whose coordinate is $\mathbf{x}_i$. Then, $\mathbf{r} = \mathbf{r}_i + \mathbf{x}_i$ and the phase S can be defined as a local phase S_i in each A_i through $\boldsymbol{\nabla} S = \boldsymbol{\nabla} S_i + \mathbf{x}_i^{\perp}$ where $\mathbf{x}_i^{\perp} = \mathbf{e}_z \times \mathbf{x}_i$. We thus have

$$\text{NCRIF} \approx \frac{\sum_{i=1}^{n(\mathcal{D})} \inf\limits_{S_i} \int_{A_i} \rho_0 |\boldsymbol{\nabla} S_i - \mathbf{e}_z \times \mathbf{r}_i|^2}{\int \rho_0 r^2}.$$

Assuming that each A_i is the translation of a reference set A_0, the numerator is proportional to $n(\mathcal{D})$ times the infimum of the cell problem, which is always less than V $Vol(A_0)$. Note that this cell problem depends on the volume since the size of A_0 depends on $n(\mathcal{D})$. If V is large, a coarse-grained approximation for ρ_0 yields that $\int \rho_0 r^2 \approx \int r^2 \propto V^{(d+2)/d}$, where d is the dimension bigger than 2. Hence, NCRIF $\leq V^{-d/2} Vol(A_0)$, which tends to 0 in the limit of large V. However, according to Legget [2], the system can be considered as superfluid if NCRIF $\gg 1/N$ (where N is the number of particles equal to νV), where ν is the initial average density (included in our rescaling providing g). In a thermodynamic limit with V large g large, and ν not fixed but large as well, we may still have NCRIF $\gg 1/N$.

Let us point out that this behavior contrasts to the 1D case, where, in the large g asymptotic, the NCRIF is zero: indeed a similar computation yields that it is equal to $L^2/(\int \rho_g \int 1/\rho_g)$ (see also [2]). In the large g case, this tends to 0 since ρ_g tends to ρ_0 which is compactly supported and thus $\int 1/\rho_0 = \infty$.

Conclusion.—We have derived properties on the density of the ground state of a quantum crystal. This has allowed us to estimate the NCRIF and find that the system is supersolid, on the basis of a definition of Leggett [2]. This complements the results of [4] and provides theoretical justification of the non zero NCRIF in the experiments of Kim and Chan [1].

We are very grateful to C. Josserand, Y. Pomeau, and S. Rica for their interest and remarks. We also wish to thank S. Balibar and A. L. Leggett for very fruitful discussions.

Appendix: Proof of Theorem 1. Step 1.—If ρ satisfies (4), we prove that $F(\rho) = V^2/n$. Indeed, for every j, if $x \in A_j$, then $B_x \cap (\cup_{k=1}^{n} A_k) = A_j$, where B_x is the ball of radius 1 centered at x. Since (4) implies that $\rho(\mathcal{D} \setminus \cup A_j) = 0$, we get that if $x \in A_j$, then $\rho(B_x) = \rho(A_j) = V/n$. Since $\cup A_j$ is a set of full ρ measure, we get that $F(\rho) = \int (U * \rho) \times (\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} = \sum \rho^2(A_j) = V^2/n$.

Step 2.—Let ρ be a ground state for F. We can argue by induction that there exist $n = n(\mathcal{D})$ points $x_1, \ldots, x_n$ such that

$$|x_i - x_j| \geq 1 \quad \text{and} \quad U * \rho(x_i) = \inf U * \rho = F(\rho)/V. \quad \text{(A1)}$$

The last equality is in fact the Euler-Lagrange equation. The definition of n implies that if the x_i are any such points, then $\cup B_{x_i} \supset \mathcal{D}$. So that $V \leq \rho(\cup_i B_{x_i}) \leq \sum_i \rho(B_{x_i}) = \sum_i U * \rho(x_i) = \frac{n}{V} F(\rho)$. Thus, $\min F = F(\rho) = V^2/n$.

Step 3.—We have to check that (4) holds. For each x_j, we define $A_j = \{x \in B_{x_j} \cap \operatorname{supp} \rho\}$. Then, by the Euler-Lagrange equation, $U * \rho(x) = V/n$ in A_j; hence, $\rho(A_j) = V/n$. We have that $\rho(\cup A_i) = \sum \rho(A_i)$; hence, $\rho(A_i \cap A_j) = 0$ and if $y_i \in A_i$, then $U * \rho(y_i) = \rho(B_{y_i}) = V/n$. Hence, the points $(\{x_1, \ldots, x_n\} \cup \{y_i\}) \setminus \{x_i\}$ satisfy (A1), and this proves (4).

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