And quiet flows the supersolid $^4$He

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A superfluid having atomic scale superflow of a hexagonal lattice of vortex and antivortex filaments, described by a single macroscopic wave function is presented as a supersolid. As superfluid $^4$He is pressurized, at a first order transition, rotons (atomic scale current circulation, a vortex loop) not only condense but also expand and fuse into hexagonal or other complex superflow patterns. The vortex core contains an excess density of non-condensate atoms. Further, a Kelvin (m = 0, necklace) mode condenses in the vortex filaments. It results in a 3D atom density wave of hcp symmetry. In our theory, superfluid phase stiffness, rather than atom localization, imitates a solid like rigidity.

Supersolid [1,2] is a quantum crystal that exhibits non classical moment of inertia [3], a type of superfluid response. Decades of efforts [4], following early theoretical suggestions, have culminated in a recent striking observation of non classical moment of inertia, by Kim and Chan [5]. This is yet another jewel in the crown of condensed $^4$He, an elusively simple one component boson system; the deeper one searches and digs, the more surprises are in store. This work has excited a renewed interest [6,7] in the quantum many body theory of supersolid. It is likely to open new directions and find new phenomena in experiments; it also offers a good opportunity to bring the field of cold atom BEC, boson Mott insulators etc., closer to supersolid $^4$He. A correct theoretical understanding of the supersolid phenomena will throw new light into old experimental quantum anomalies in the superfluid-solid helium interface [8], such as crystallization waves, Kapitza resistance etc.

The supersolid predicted by Andreev, Lifshitz [1] and Chester [2] has a reference crystal of localized atoms; large amplitude quantum fluctuations create ground state vacancies or defects which undergo condensation. In our mechanism superfluid is the reference system and solid like rigidity emerges from the superfluid stiffness in a fundamental way. A spatially periodic, atom scale superfluid flow develops spontaneously in the ground state leading to a solid like response, in addition to superfluidity. We call it a roton fusion(ROFU) mechanism, as the atom scale flow pattern arises spontaneously from a condensation and a complex fusion of real rotons (vortex loop of atomic dimensions), as we pressurize superfluid $^4$He. ROFU mechanism is one collective way of releasing the kinetic energy frustration, that is present in a solid with localized atoms. It is a kind of spontaneous generation of staggered Abrikosov vortex lattice, created by hydrostatic pressure. Hydrostatic pressure, a scalar, mimics an internal staggered magnetic field.

Roton minimum of superfluid $^4$He has been viewed [9], for quite some time as a soft mode that drives a superfluid-solid phase transition, as rotons have wave vectors close to the reciprocal lattice vectors of the hcp $^4$He crystal. A new and crucial ingredient in our theory is to use the non-trivial inner structure of roton, an atomic size quantized vortex loop. In our theory rotons do more than condensation; they expand and fuse into ordered vortex and antivortex filaments (atom scale thickness) and lose their identity.

![FIG. 1](image_url)

**FIG. 1.** Figure 1. a) Region of roton minima in the $(k_x, k_y, 0)$ plane. $Q_1$, $Q_2$ and $Q_3$ are Fourier component vectors of the macroscopic condensate wave function $\langle \Psi(r) \rangle$. b) Unit cell of the hexagonal vortex-antivortex array (tubes); it has a 2D atom density wave of hexagonal symmetry c) Kelvin (azimuthal quantum number $m = 0$, necklace) mode with a finite $\pm Q_z$ condenses in the vortex in a staggered fashion. It results in an atom density wave of hcp lattice. Lattice sites (not position of localized atoms) are denoted by shaded circle.

In superfluid $^4$He, nearly 90% of the atoms are outside the zero momentum condensate. These large fraction of atoms with finite momenta appear as spatially uniform quantum fluctuation of the superfluid vacuum. They are part of the vacuum and the ground state is a 100% superfluid. When vortices and antivortices are
spontaneously created in the ground state, a part of the non-condensate fraction gets piled up in the vortex core region, creating a net atom density wave of hcp symmetry. The self consistent potential that maintains this redistribution arises from the underlying superfluid stiffness. In this sense superfluid stiffness gives a solid like rigidity to the 3D atom density wave. A fragile 2\% superfluid condensate (as measured by Kim and Chan), by a complex maneuver of its own flow, orchestrates the 3D atom density wave and a rich 'lattice dynamics'. Periodic superflow leads to a periodic modulation of quantum fluctuation and non condensate component.

In what follows we develop some heuristic pictures, followed by a Bogoliubov theory and then discuss some consequences.

Kim and Chan have discovered non-classical moment of inertia in pressurized solid 4\text{He} ; they observe strong thermal hysteresis, small variation of supersolid transition temperature $T_{ss}$ for a pressures range, 25 to 60 bars, and an anomalous increase of $T_{ss}$ with addition of 3\text{He} impurity. More importantly, the authors indicate that the superfluid response may not be due to zero point vacancies or defects or interfaces. That is, it is likely one is dealing with a solid with integer number of atoms per unit cell and yet exhibiting a superfluid property.

While building our theory we remember that at the superfluid-solid first order transition at $T = 0$, inter 4\text{He} atom distance decreases only by a small, $\sim 3\%$, (a density decrease $\sim 10\%$). This means that locally the quantum solid is no more crowded than the quantum liquid is. Thus any generalized rigidity that emerges on both sides is likely to have the same quantum character, namely some kind of phase stiffness (ODLRO) arising from local coherent number fluctuations. Further, the superfluid solid coexistence line in the P-T plane has nearly zero slope for $T < 0.2$ K indicating that the two phases have the same entropy per mole, according to Clausius-Clapeyron equation $\frac{d\ln P}{dT} = \frac{S_2 - S_1}{V_1 - V_2}$. This means that density of states of low energy bosonic quasi particles is nearly the same for superfluid and supersolid at the coexistence line, indicating a possible deep connection between the stiffness of a superfluid and rigidity of a supersolid.

Now we present a Bogoliubov theory to illustrate our ROFU mechanism. Bogoliubov theory is a mean field theory that works well for weakly interacting bosons. However, for a proper choice two body pseudo potential, it captures qualitative features and some quantitative features, including roton spectrum. The model Hamiltonian is:

$$H = \sum (\epsilon_k - \mu) b^\dagger_k b_k + \frac{1}{\Omega} \sum V(\mathbf{q}) b^\dagger_k b_{k-\mathbf{q}} b^\dagger_{k+\mathbf{q}} b_{k+\mathbf{q}} (1)$$

Here $\epsilon_k = \frac{\hbar^2 k^2}{2M}$ is the kinetic energy of 4\text{He} atoms with mass M, chemical potential $\mu$, created by operators $b^\dagger$'s. $V(\mathbf{q})$ is the two body, effective or pseudo potential and $\Omega$ is the volume of the system.

In the uniform superfluid phase, Bogoliubov theory starts by replacing the zero momentum operator $b_0 \rightarrow n_0 \frac{1}{\Omega} e^{i\phi} N_0 ^\dagger$, a classical expectation value, with $n_0$ as a condensate fraction. The Bogoliubov quasi particle spectrum of the uniform superfluid state has the well known form

$$\hbar \omega_k = \sqrt{\left(\frac{\hbar^2 k^2}{2M}\right)^2 + \left(\frac{\hbar^2 k^2}{2M}\right) 2n_0 V(k)} (2)$$

where $n_0$ is the zero momentum condensate fraction. When the potential $V(k)$ is negative for a range of k, the spectrum has a roton minimum; an example is Brueckner pseudo potential, $V(k) \approx \frac{V_0 \sin ka_0}{ka_0}$, with $a_0 \approx 2.1$A and $V_0 \approx 15$ K.

Landau suggested roton as the first excitation that has associated with it a rotational velocity flow (and hence the name roton). Feynman viewed it as a single atom motion, but dressed by a back flow, the net effect being a quantized vortex loop of atomic dimensions. Recent variational study and wave packet analysis [10] confirms this and shows roton wave packet as a ball of current disturbance, and little density variation.

Within the Bogoliubov theory, the roton minimum (figure 1a) reaches zero energy (become completely soft), $\langle\mathbf{r}\rangle \approx \frac{1}{2m\Omega} \frac{k^2}{\hbar^2}$. This indicates an instability of the uniform superfluid solution. We expect a roton condensation and reorganization of the ground state. A complex current flow associated with a roton, rather than a simple density variation, made us wonder what will be the consequence of a roton condensation. It became clear that a *primary consequence of roton condensation will be formation of a current density wave, not atom density wave*. This resulted in our roton fusion hypothesis. According to this hypothesis the condensed rotons expand and fuse into a hexagonal array of vortices and antivortices. Our hypothesis is naturally influenced by the known hcp structure of solid 4\text{He}.

To test our hypothesis we have compared the energy of uniform superfluid state with an off diagonal long range order (ODLRO) ansatz that contains a hexagonal array of vortices and antivortices. After some struggle we found a simple and elegant ansatz - in phase superposition of three plane waves generates the desired vortex structure:

$$\langle\Psi(\mathbf{r})\rangle \equiv \psi_0(\mathbf{r}) \sim n_0 \frac{1}{\sqrt{\Omega}} e^{i\phi} (e^{iQ_1 \cdot \mathbf{r}} + e^{iQ_2 \cdot \mathbf{r}} + e^{iQ_3 \cdot \mathbf{r}}) (3)$$

It also gives a lower energy than the uniform superfluid state, for a choice of $V(k)$. Here $Q_1 = \frac{2\pi}{a}(0,0,0)$, $Q_{2,3} = \frac{2\pi}{a}(\pm 1, \pm 1, \pm 1)$, $Q_1 + Q_2 + Q_3 = 0$, ’a’ is the lattice parameter of the hexagonal lattice. Here, $n_0$ and ’a’ are variational parameters. The above ansatz leads to variation of atom density only in the xy-plane, a 2D atom density wave. This results in a supersolid behaviour
along the x and y directions and superfluid in z-direction - it is an anisotropic supersolid, a type of quantum liquid crystal. Later we will improve it to get a 3D atom density wave of hcp symmetry. We can find more complex flow pattern (braided and knotted vortices) leading to an atom density wave of hcp symmetry using more Q’s etc.

One of the triangular sub lattices of the hexagonal lattice contains vortices and the other antivortices (figure 1b). It is easy to show that equation (3) has asymptotic form

\[ \langle \Psi(\mathbf{r}) \rangle \sim x + iy \quad \text{(vortex),} \quad x - iy \quad \text{(antivortex)} \]  \hspace{1cm} (4)

respectively around the vortex and antivortex filaments of the two sub lattices.

In addition to global U(1) symmetry (overall phase of \( \langle \Psi(\mathbf{r}) \rangle \)) and translational symmetry there is a discrete symmetry breaking arising from P&T violation. That is, another degenerate solution, not connected by a global phase rotation of equation (5) is obtained by the replacement \( Q_j \rightarrow -Q_j \) in equation (3); equivalently, by an interchange of vortices and antivortices.

According to equation (4) the condensate fraction vanishes quadratically as we approach the core of line vortices. Further, the fraction of the total particles condensed in our macroscopic wave function is \( \leq 1 \). Where are the rest of non-condensed particles? In the Bogoliubov theory of uniform superfluid, these are the particles that carry non zero momenta and they appear as a spatially uniform quantum fluctuations of the zero momentum condensate. They influence, for example the superfluid stiffness, through the spectrum; otherwise these finite momentum components are not visible in the low energy dynamics of the irrotational superfluid.

In our ROFU, a spatial density variation of the non-condensate fraction is induced. In particular they appear as extra atom density in the normal core region of our ordered vortices, where the condensate density vanishes. This is somewhat counter intuitive, as one expects a depletion of fluid density at the vortex core. It is known from an early work of Fetter [11] that within Bogoliubov theory, in the vortex core region the local atom density increases compared to the uniform background atom density. This is a remarkable non-local quantum effect, appearing within the Bogoliubov theory, as explained by Fetter.

We elaborate this point further, by comparing a reference Bose Einstein condensed (BEC) state

\[ \Psi_{\text{BEC}} \sim \Pi_i (e^{iQ_1 \cdot \mathbf{r}} + e^{iQ_2 \cdot \mathbf{r}} + e^{iQ_3 \cdot \mathbf{r}}) \]  \hspace{1cm} (5)

with the N-particle projected wave function of Bogoliubov theory for our ROFU solution:

\[ \Psi_N(\mathbf{r}) = \sum_p \chi(\mathbf{r}_{P1}, \mathbf{r}_{P2})\chi(\mathbf{r}_{P3}, \mathbf{r}_{P4})... \chi(\mathbf{r}_{PN-1}, \mathbf{r}_{PN}) \]  \hspace{1cm} (6)

Summation over permutation P symmetrise the wave function. The pair function \( \chi(\mathbf{r}_1, \mathbf{r}_2) \equiv \eta(\mathbf{r}_1, \mathbf{r}_2)\psi_0 \left[ \frac{\mathbf{r}_1 - \mathbf{r}_2}{\mathbf{L}} \right] \). When the pair function \( \eta(\mathbf{r}_1, \mathbf{r}_2) = 1 \), equation (6) becomes the same as BEC (equation 5).

In the BEC state, atom density, by construction, vanishes as we approach the core of the line vortices. In the Bogoliubov wave function, equation (6), the pair function \( \eta \) makes an important difference and creates a pile up of atom density through pushing some of the non-condensate fraction to core regions. The pair function \( \eta \) represents, a repulsive correlation induced between any two particles in the Bogoliubov theory. It shows how pairs of particle are pushed in and out of the condensate by the Bogoliubov process \( \langle b_{Q_1} \rangle \langle b_{Q_2} \rangle b_{k-1}^+ b_{k+Q_1+Q_2} \) etc., in a space dependent fashion.

We want to make certain remarks about the nature of ODLRO in our supersolid phase. Our primary order is a long range order in momentum space, an ODLRO. Bosons condense in a single macroscopic wave function \( \psi_0(\mathbf{r}) \) given by equation (5). It has three Fourier coefficients which are not independent: \( \langle b_{Q_1} \rangle = \langle b_{Q_2} \rangle = \langle b_{Q_3} \rangle = n_{Q}^\frac{3}{2} e^{i\phi} \); they have same amplitude and phase.

The spatial variation of atom density implied by our ODLRO should not be thought of as a diagonal long range order (DLRO). A spatial periodic ordering of a small fraction of the non-condensate fraction is induced self consistently in our theory. For example in our Bogoliubov factorization we get an anomalous term such as \( \langle b_{Q_1}^\dagger \rangle \langle b_{Q_2} \rangle b_{k}^\dagger b_{k-1} - Q_1 - Q_2 \). A density wave of wave vector \( Q_1 - Q_2 \) induced by the above term has its origin in single particle condensation. In principle we could generate such an anomalous term through non-vanishing averages such as, \( \sum_k \langle b_{k}^\dagger b_{k+Q_1-Q_2} \rangle \). This will be an independent diagonal long range order (DLRO) parameter.

The solution we have discussed so far, equation (3), has no density variation along z-axis. In real \(^{4}\text{He} \) we expect maximum amount of atom density to be concentrated in the normal core region. Thus it has its natural tendency for local spatial order, arising from short range repulsions. We view this as a Kelvin (azimuthal quanum number \( m = 0 \), necklace or sausage ) mode condenses (figure 1c) at wave vectors \( Q_2 = \pm \frac{2\pi}{a} \) in the vortex filaments. We modify equation (3) and generate a periodic modulation of the vortex core size, along the vortex filament in a staggered fashion:

\[ \langle \Psi(\mathbf{r}) \rangle \sim (x + iy)(1 + \epsilon \cos Q_2 z) \] and
\[ \sim (x - iy)(1 - \epsilon \cos Q_2 z) \]  \hspace{1cm} (7)

close to core of the vortices of the two sub lattices. In view of the short range interaction of the model Hamiltonian, the total energy is reduced further for small \( \epsilon \), another variational parameter. This vortex core modulation leads to an atom density wave of hcp symmetry and a 3D solid like rigidity.
We can choose our model parameters of Hamiltonian (equation 1) such that our hexagonal lattice contains an average of 2 atoms per unit cell or close to it.

From our solution it follows that the superfluid density is mostly concentrated outside the vortex core, which is the interstitial region of the hcp atom density wave (figure 1b and 1c).

So far we have sketched a Bogoliubov theory, a ROFU solution and some key features of the ground state. Our theory is far from rigorous and complete. However, the physical argument for a spontaneous generation of microscopic circulating ground state current is compelling. Bogoliubov (mean field) theory, in view of its non perturbative character is capable of finding possible new phases in dense liquid \(^4\)He.

In what follows we show how our theory qualitatively explains salient features of Kim-Chan’s results. Further, we briefly sketch interesting consequences that also follow; some of them are very unique to our theory.

In our ROFU solution we discussed a 2D solid and a 3D solid. It is likely that as a function of pressure there is a small region in the pressure-temperature diagram where the 2D solid intervenes, as shown in figure 2.

/FIG. 2. Schematic phase diagram for \(^4\)He in the pressure-temperature plane. An intermediate region of anisotropic supersolid (supersolid in x, y directions and superfluid in z-direction) is suggested.

We can qualitatively discuss some features of finite temperature phase transitions that are unique to ROFU solution. Thermally produced vortices in the ROFU condensate will proliferate, depin and melt the underlying vortex lattice. Disappearance of ODLRO will result in a solid of localized atoms. As the process is a melting of a vortex lattice, i) phase transition will be a first order one and ii) small traces of \(^3\)He atoms could help pin the vortices and thereby increase the supersolid-solid transition temperature. Both are consistent with Kim-Chan’s observations. The anomalously low critical velocity, for destruction of the non classical moment of inertia (supersolidity), observed by Kim and Chan is likely to arise from a collective depinning of the ground state vortices from their weak self consistent potential.

A key prediction of our theory is the presence of atom scale circulation. One important consequence of this is on lattice dynamics. The P & T violation in the ground state and the first order dynamics of vortices makes the lattice dynamics different from the classical hcp solid. We get splitting of degeneracies etc.; some of the anomalous modes can be viewed as coupled Kelvin modes. We will discuss them in a future publication.

In summary, our supersolid is a superfluid in disguise with interesting consequences.

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