Quenched Dislocation Enhanced Supersolid Ordering

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I show using Landau theory that quenched dislocations can facilitate the supersolid (SS) to normal solid (NS) transition, making it possible for the transition to occur even if it does not in a dislocation-free crystal. I make detailed predictions for the dependence of the SS to NS transition temperature \( T_c(L) \), superfluid density and dislocation spacing \( L \), all of which can be tested against experiments. The results should also be applicable to an enormous variety of other systems, including, e.g., ferromagnets.

Recent reports\cite{1} of supersolidity - a crystal exhibiting “off-diagonal long-range order” (ODLRO) \( 2, 3 \) in solid \( ^4 \)He raise many questions. First, quantum Monte Carlo simulations\cite{4} find no supersolid phase. Second, the temperature \( T \) dependence\cite{1} of the superfluid density \( \rho_s(T) \) in the supersol (SS) differs from that in the superfluid (SF), contradicting theory\cite{3}. Third, no specific heat anomaly is seen at the SS to NS transition.

In this paper, I propose a resolution of these puzzles. Since, depending on the material, either local compression or local dilation increase the local transition temperature \( T_c(\vec{r}) \)\cite{5}, and since edge dislocations have regions of both types near their cores\cite{6}, these defects induce, in all materials, regions of elevated \( T_c \), as first noted for superconductors\cite{7}. ODLRO therefore happens at higher temperatures on the tangled network of quenched dislocations in \( ^4 \)He crystals than in the bulk, as in superconductors\cite{2, 5}. ODLRO is defined by eqn. (6).

Specifically, the DGT\cite{5} model with quenched dislocations implies the following scenario: as temperature \( T \) decreases below what I’ll call the “condensation” temperature \( T_{cond} \), which is always \( > T_{c, clean} \), the transition temperature of the clean (i.e., dislocationless) lattice, each dislocation line in a tangled network of them nucleates a cylindrical supersolid “tube” tangent to it. The radius of these tubes grows with decreasing temperature.

We can think of places where dislocations cross, making supersolid tubes overlap, as the “sites” of a random lattice. The sections of tube between these “sites” act as ferromagnetic “bonds”. The typical length of these bonds is \( L \), the mean dislocation spacing, which grows with annealing; \( L \rightarrow \infty \) for a clean crystal. This random lattice does not develop macroscopic supersolidity (or undergo any phase transition) at \( T_{cond} \), because the sites lack long-range phase coherence near \( T_{cond} \). However, as temperature is lowered further, such coherence inevitably develops at \( T = T_c(L) \), with \( T_{cond} > T_c(L) > T_{c, clean} \). Indeed, if condensation occurs, long-range order always develops (i.e., \( T_c(L) > 0 \)), even if the clean system never orders! This ordering at \( T_c(L) \) is the SS to NS transition.

This picture is very similar to Shevchenko’s\cite{8}.

Figure 1 plots the superfluid density \( \rho_s(T) \). When \( T_c^{clean} > 0 \), near \( T_c(L) \),

\[
\rho_s(T, L) = \frac{A}{L^\nu} \left( 1 - \frac{T}{T_c(L)} \right)^\nu ,
\]

where \( \nu \approx 2/3 \) is the 3dXY correlation length exponent\cite{10}, \( \chi = 2(1-\nu) \approx \frac{1}{2} \), \( A \) and \( T_0 \) are independent of \( L \), \( a \) is a lattice constant, and

\[
T_c(L) = T_c^{clean} + T_0 \left( \frac{a}{L} \right)^{1-\nu}, \quad T_c^{clean} > 0 ,
\]

When temperature \( T \) is lowered into the range

\[
\delta T(L) \ll T - T_c^{clean} \ll T_c(L) - T_c^{clean},
\]

where \( \delta T(L) \propto \frac{1}{L} \),

\[
\rho_s(T, L) = A \left( \frac{T - T_c^{clean}}{L^2} \right)^{\nu-2} \propto (T - T_c^{clean})^{-\frac{4}{3}} ,
\]

FIG. 1: The superfluid density versus temperature for a dislocated solid in which the clean system does (top curve) and does not (bottom curve) have a transition. \( \rho_s \) obeys eqns. (1) and (3) in region (I) and (II) respectively, where (II) is defined by eqn. (3). \( T_c(L) \) for the cases \( T_c^{clean} > 0 \) and \( < 0 \) are, respectively, denoted in this figure by \( T_c^{\geq}(L) \) and \( T_c^{\leq}(L) \), and given by eqns. (2) and (4).
and $A'$ is an $L$-independent constant. In the $L \to \infty$ limit, $\delta T(L) \propto \frac{1}{L} \leq T_c(L) - T_c^{\text{clean}} \propto L^{-\frac{3}{4}} \approx L^{-\frac{3}{4}}$, ensuring a large window of validity for eqn. (4). Once $T < T_c^{\text{clean}} - \delta T(L)$, the tubes overlap, the entire volume becomes supersolid, and $\rho_s$ is that of the clean system, completely independent of $L$, and so obeys

$$\rho_s(T) \propto (T_c^{\text{clean}} - T)^{\frac{3}{4}}. \quad (5)$$

Note that the high temperature ($T > T_c^{\text{clean}} - \delta T(L)$) behavior of $\rho_s(T,L)$ is strongly sample and annealing dependent (because $L$-dependent), but the low-temperature ($T < T_c^{\text{clean}} - \delta T(L)$) behavior is sample and annealing independent, and identical to that of a clean sample.

Precisely such behavior was recently reported [11]. In figure 2, $\rho_s(T)$ data from Chan’s group [12] is plotted in the form $\rho_s^{-\frac{3}{4}}$ versus $T$, which Eqn. (4) predicts should give a straight line section, for $T$ satisfying eqn. (3). The data does indeed show such a straight section, although it is fairly short, and the error bars in this region are large. More accurate measurements of $\rho_s(T)$, and of the dislocation spacing $L$ (by, e.g., ultrasonic velocity and attenuation measurements [13]) are clearly needed. Alternatively, one could deduce the ratio of $L$’s in different samples by comparing the coefficients of $(T_c^{\text{clean}} - T)^{-\frac{3}{4}}$ in eqn. (4), and using this ratio to test the predicted $L$ dependence of $\rho_s(T,L)$ and $T_c(L)$ eqns. (1) and (2).

![Figure 2](image.png)

**FIG. 2:** Superfluid density versus temperature data from Chan’s group [12], plotted in the form $\rho_s^{-\frac{3}{4}}$ versus $T$. The straight segment of this plot predicted by Eqn. (4) is indicated by the dashed line.

If the clean system does not order, which I’ll refer to as $T_c^{\text{clean}} < 0$, $T_c(L)$ vanishes as $L \to \infty$:

$$T_c(L) = T_0 \frac{a}{L}, \quad T_c^{\text{clean}} < 0, \quad (6)$$

where $T_0$ is another $L$-independent constant, a result ref. [4], could also be tested by measurements and/or deductions (as described above) of $L$. Eqn. (4) still holds near $T_c(L)$, but now with $\chi = 2$. Eqns (4) and (5) never apply, since $T = 0$ intervenes above $T_c^{\text{clean}}$. The lower curve in Figure 1 plots $\rho_s(T)$ in this case.

The experimental situation is currently unclear. The $T_c^{\text{clean}} < 0$ scenario is supported by recent experiments [14], showing non-classical rotational inertia in unannealed $^4$He crystals, but none after annealing. On the other hand, Chan’s recent experiments [11], as discussed above and in figure (2), suggest $T_c^{\text{clean}} > 0$. In these experiments of ref. [11], single crystals still show supersolidity, suggesting that dislocations, rather than grain boundaries, are the responsible defects.

Also suggestive are simulations [15] which see supersolid order near screw dislocations. Although screw dislocations do not, in the DGT model, couple to supersolid order, higher order terms allow such coupling [16].

The absence of a specific heat anomaly in some experiments can be explained in this picture. For the case $T_c^{\text{clean}} < 0$, the specific heat near $T_c(L)$ is given by:

$$C \propto \frac{|\frac{T}{T_c^{\text{clean}}} - 1|^{-\alpha}}{L^{\frac{3}{2}}}, \quad T_c^{\text{clean}} < 0 \quad (7)$$

where $\alpha = -0.0127$ is the specific heat exponent of the 3d XY model [10]. Clearly, the $|T - T_c|^{-\alpha}$ singularity vanishes as dislocation density $\to 0$ ($L \to \infty$), and so should be seen only in dirty samples, not clean ones.

The ideas developed here are applicable to, e.g., ferromagnets [17], which I’ll treat elsewhere [18].

I’ll now outline the derivation of these results. My Hamiltonian is an isotropic [19] version of that of [2]:

$$H = \int d^3r \left[ \frac{t(\vec{r})}{2} |\psi|^2 + \frac{u}{4} |\psi|^4 + \frac{c}{2} |\nabla \psi|^2 \right] \quad (8)$$

with

$$t(\vec{r}) = t_0 + g u_{ii}(\vec{r}). \quad (9)$$

Here, $t_0(T)$ is a decreasing function of temperature $T$ satisfying $t_0(T_c^{\text{clean}}) = t_c^{\text{clean}} < 0$, where $t_c^{\text{clean}}$ is the value of $t_0$ at the transition in the clean system, $u$ and $c$ are constants, and $u_{ii}$ is the trace of the strain tensor.

Thermal fluctuations in $u_{ii}$ have no effect on the critical properties of the superfluid density and specific heat at the transition [2]: I will henceforth ignore them, and focus only on strains due to quenched dislocations.

The clean model will not have a $NS \to SS$ transition if $T_c^{\text{clean}} < 0$. When $T_c^{\text{clean}} > 0$, I’ll assume (as usual) that $t_0(T) = \Gamma (T - T_c^{\text{clean}}) / |T_c^{\text{clean}}|$, where $\Gamma$ is a constant, near $T = T_c^{\text{clean}}$. For a straight edge dislocation running along the $z$-axis with Burgers vector $\vec{a}$ along the $y$-axis, $u_{ii} = \frac{4u}{2\mu + \lambda} \frac{a \cos \theta}{r_\perp}$, where $\mu$ and $\lambda$ are the Lame elastic constants [19]. Inserting this into eqn. (9) gives

$$t(\vec{r}) = t_0 + \frac{g' \cos \theta}{r_\perp} \quad , \quad (10)$$
where $g' \equiv ga\left(\frac{\nu}{2\pi T}\right)$ \[10\].

Naively, the system is supersolid in those regions where $t(\vec{r}) < 0$. Actually, the mean field transition occurs when the minimum energy $\psi(\vec{r})$ first becomes non-zero. The temperature at which this occurs is $T_{\text{cond}}$.

The Euler-LaGrange equation for eqn. \[8\] is

$$\nabla^2 \psi = \frac{t(\vec{r})}{c} \psi + \frac{u}{c} \psi^3 . \quad (11)$$

As noted in \[7\], this equation first has non-trivial ($\psi \neq 0$) solutions when $t_0$ drops below a critical value $t_{\text{cond}} = \frac{2mE_0}{\hbar^2}$, where $E_0$ is the quantum mechanical ground state energy of a particle of mass $m$ moving in the 2d dipole potential $V(\vec{r}) = -\frac{a}{2m} r^2$ with $p \equiv \frac{\hbar^2}{2m}$. Variational treatments \[7, 20\], show that $E_0 = -\gamma \frac{m^2}{\hbar^2}$ where $0.24 < \gamma < 2$. So a single dislocation line will, in mean field theory, order once $t_0 < t_{\text{cond}} = \frac{2mE_0}{\hbar^2 c}$. Using $t_0 = \Gamma \left(\frac{T-T_{\text{cond}}}{T_{\text{clean}}}\right)$, this implies $T_{\text{cond}} = T_{\text{clean}} + \frac{2m^2}{\hbar^2} \left(\frac{T_{\text{clean}}}{T_{\text{cond}}}\right) > T_{\text{clean}}$, and $T_{\text{cond}} > 0$, even if $T_{\text{clean}} < 0$, if $\frac{2m^2}{\hbar^2} > 1$. Hence, condensation onto dislocations can happen, even when the clean system does not order.

However, a one-dimensional system like a single dislocation line cannot order. To order, these 1d “tubes” must cross-link into a three-dimensional network. The typical tube length is $L$, the inter-dislocation distance.

On length scales $\gg$ the tube radius $a_c(t)$, but $\ll L$, the only important variable is “Goldstone mode”; i.e., the phase $\theta(\vec{r})$ of $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\theta(\vec{r})}$. In the tube between crosslink sites $i$ and $j$, these long length scales, depends only on distance $s$ along the tube. This leads to a 1d Hamiltonian for this tube:

$$H_{1d}(\{\theta(s)\}) = K_{1d}(T) \int_0^L (\partial_s \theta)^2 ds . \quad (12)$$

From this, I can obtain an effective Hamiltonian $H_{\text{eff}}(\theta_i, \theta_j)$ coupling the $\theta$’s on sites $i$ and $j$ by integrating out the $\theta$’s along the tube:

$$e^{-\beta H_{\text{eff}}(\theta_i, \theta_j)} = \sum_{n=-\infty}^{\infty} \int_{\pi n} D\theta(s) e^{-\beta H_{1d}(\{\theta(s)\})}$$

where the functional integral $\int_{\pi n} D\theta(s)$ on the right hand side is taken with $\theta(s)$ satisfying the boundary conditions $\theta(0) = \theta_i$, $\theta(L) = \theta_j + 2\pi n$, where the summation integer $n$ in eqn. \[13\] reflects the $2\pi$ periodicity in $\theta$.

Each of the functional integrals $\int_{\pi n} D\theta(s)$ in eqn. \[13\] can most easily be done by rewriting $\theta(s)$ as follows:

$$\theta(s) = \theta_i + \left(\frac{\theta_j - \theta_i + 2\pi n}{L}\right) s + \delta \theta(s) , \quad (14)$$

where the new integration variable $\delta \theta(s)$ satisfies the boundary conditions $\delta \theta(0) = \delta \theta(L) = 0$. This gives

$$e^{-\beta H_{\text{eff}}(\theta_i, \theta_j)} = \sum_{n=-\infty}^{\infty} e^{-\frac{\beta K_{1d}}{2}(\theta_j - \theta_i + 2\pi n)^2} \times \int D\delta \theta(s) e^{-\beta K_{1d} \int_0^L ds (\nabla \delta \theta(s))^2} . \quad (15)$$

The $\int D\delta \theta$ in eqn. \[15\] is independent of $\theta_i$, $\theta_j$ and $n$ (since the boundary conditions on $\delta \theta$ are), and so is only an overall multiplicative constant in $e^{-\beta H_{\text{eff}}(\theta_i, \theta_j)}$, which only adds an irrelevant constant $C$ to $H_{\text{eff}}(\theta_i, \theta_j)$. Hence, $H_{\text{eff}}(\theta_i, \theta_j)$ becomes a “periodic Gaussian” \[21\].

Adding up $H_{\text{eff}}(\theta_i, \theta_j)$ for all of the bonds gives a model for all of the “sites” (cross links of tubes):

$$H_{\text{eff}}(\{\theta_i\}) = \sum_{\text{bonds}} V_c(\theta_i - \theta_j ; J) . \quad (18)$$

Although these couplings $J$ will be random, due to the random bond lengths of the tubes, such “random $T_c$” disorder is irrelevant in the RG\[22\], and can be ignored.

This Villain model \[13\] orders at a temperature $T_c = O(J/k_B)$; I will now use this to determine $T_c(L)$. Consider first $T_{\text{clean}} < 0$. In this case, provided $T_{\text{cond}} \geq 0$, so that $K_{1d}(T) \neq 0$, we can, for $L \to \infty$, estimate $T_c$ by replacing $K_{1d}(T)$ in eqn. \[17\] with its finite, non-zero, $T = 0$ value $K_{1d}(T = 0) \equiv K_0$. This gives eqn. \[9\] with $T_0 = K_0 k_B$. Note that taking $K_{1d}(T) \to K_0$ in eqn. \[17\] is valid since $T_c(L \to \infty) \to 0$.

For the case $T_{\text{clean}} > 0$, the radii $a_c(T)$ of the tubes of supersolid diverge as $T \to T_{\text{clean}}$. To see this, note that the locus on which this circle passing through the origin, centered on the negative (positive) $y$-axis of radius $a_c(T) = \frac{gt'}{2(t_0 - t_c)} . \quad (19)$

Inside this circle, $t(\vec{r}_0) < 0$, so, naively, this boundary \[10\] defines the supersolid tube. As $T \to T_{\text{clean}}$ from above, $t_0 \to t_c$ and so $a_c(T)$ diverges: $a_c(T) \propto \frac{1}{t_0 - t_c}$.

Of course, this argument ignores the $\nabla^2 \psi$ term in eqn. \[11\]. However, since $a_c(T) \to \infty$ as $T \to T_{\text{clean}}$, $\psi$ varies slowly in space, and we can neglect the $\nabla^2 \psi$ term in eqn. \[11\] and simply balance the other two terms.

We can include fluctuations in this “local equilibration” approximation simply by replacing the local superfluid density $\rho_s(\vec{r})$ by its value in a uniform system whose value of $t$ equals the local $t(\vec{r})$, provided $a_c(T) >> \xi(T) \propto (T - T_{\text{clean}})^{-\nu}$, where $\xi(T)$ and $\nu \approx \frac{1}{2}$ are the correlation length and its critical exponent in the clean system.
Since $\nu < 1$, $a_s(T)$ eqn. [19] is indeed $>> \xi(t)$ as $T \rightarrow T^\text{clean}_c$ from above. This implies that the local superfluid density $\rho_s(\vec{r})$ for $T$ near, but slightly above, $T^\text{clean}_c$, is

$$\rho_s(\vec{r}) = B(t_c - t(\vec{r}))^\nu,$$  \hspace{1cm} (20)$$

where $B$ is a constant, and I’ve used the Josephson relation $\rho_s \propto \xi^{-1}$ [23]. This $\rho_s$ acts as the 3 - d “spin-wave stiffness” for the phase $\theta(\vec{r})$; that is,

$$H_{3d} = \frac{1}{2} \int d^3 r K_{\text{local}}(\vec{r}) \left| \nabla \theta \right|^2,$$  \hspace{1cm} (21)$$

with $K_{\text{local}}(\vec{r}) = \hbar^2 \rho_{s(\vec{r})}$. In the case of a straight edge dislocation, taking $t(\vec{r})$ from eqn. [10], $\rho_s(\vec{r})$ by eqn. [20] and $\theta(\vec{r})$ to vary only with distance $s$ along the dislocation line, the 1d spin wave stiffness $K_{1d}$ becomes:

$$K_{1d} = \frac{\hbar^2}{m} \int d^2 r_\perp \rho_{s(\vec{r}_\perp)}.$$  \hspace{1cm} (22)$$

Since $\delta T$ is constant on circles of fixed radius $a$, passing through the origin, with their centers on the $x$-axis, and is given by: $t_\perp(\vec{r}_\perp) = \frac{a}{2} - t_0$, I’ll change variables of integration to $\delta s = \delta t_0 - a$. The area of the interval $[a, a + da]$ is the difference $2\pi a da$ between the areas of the corresponding circles, so I can rewrite eqn. [22] as

$$K_{1d}(T) = \frac{\pi B \hbar^2}{m^2} \int_0^{\infty} \left( \frac{p}{2a^2} - \delta t_0 \right)^\nu da$$

where $\delta t_0 \equiv t_0 - t_c$, and $C(x) \equiv \left( \frac{1.184x}{x^2 + 1} \right)^2$ for $\nu = 2/3$.

Since $\delta t_0 \propto T - T^\text{clean}_c$ eqn. [23] implies that $K_{1d}(T) \propto (T - T^\text{clean}_c)^{\nu - 2}$. Using this $K_{1d}(T)$ in my earlier expression [17] for $J$, and then equating the result to $\kappa_B T$, gives eqn. [2] for $T_c(L)$.

As $T$ drops further, eventually $J(T, L)$ will be $> k_B T$. This is guaranteed to happen, since $T$ can get within roughly $\delta T(L) \propto \frac{1}{L}$ of $T^\text{clean}_c$ before eqn. [23] breaks down. Since $K_{1d}(T^\text{clean}_c + \delta T(L)) \propto L^{2-\nu}$; $J(T_c^\text{clean}_c + \delta T(L)) = \frac{K_{1d}}{\kappa_B} \propto L^{1-\nu} \rightarrow \infty$ as $L \rightarrow \infty$, since $\nu < 1$. In this limit, the phase order on the “sites” of the dislocation network is nearly perfect, and the standard relationship between the macroscopic (as opposed to the local) $\rho_s$ and 3d spin wave stiffness implies:

$$\rho_s(T, L) = J(T, L)/L \times O\left( \frac{m^2}{\hbar^2} \right)$$  \hspace{1cm} (24)$$

which, using [17] for $J(T, L)$, implies eqn. [1].

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