Quenched Dislocation Enhanced Supersolid Ordering

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I show using Landau theory that quenched dislocations can facilitate the supersolid to normal solid 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 supersolid to normal solid transition temperature $T_c(L)$, superfluid density $\rho_S(T, L)$, and specific heat $C(T, L)$ on temperature T 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.

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Recent reports [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 [4] find no supersolid (SS) phase. Second, the temperature (T) dependence [1] of the superfluid density $\rho_S(T)$ in the supersolid differs from that in the superfluid (SF), contradicting theory [5]. Third, no specific heat anomaly is seen at the SS to normal solid (NS) transition.

In this Letter, I propose a resolution of these puzzles. Since, depending on the material, *either* local compression *or* local dilation increase the local transition temperature $T_c(\vec{r})$ [5], and since edge dislocations have regions of *both* types near their cores [6], these defects induce, in *all* materials, regions of elevated T_c, as first noted for superconductors [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 [7,8], and can occur even if the clean (dislocationless) lattice remains normal down to $T = 0$.

Specifically, the DGT [5] model with quenched dislocations implies the following scenario: as temperature T decreases below what I will call the "condensation" temperature $T_{\rm cond}$, which is *always* $> T_c^{\rm clean}$, 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; $L \to \infty$ for a clean crystal. This random lattice does *not* develop macroscopic supersolidity (or undergo *any* phase transition) at $T_{\rm cond}$ because the sites lack long-range phase coherence near $T_{\rm cond}$. However, as temperature is lowered further, such coherence *inevitably* develops at $T = T_c(L)$, with $T_{\rm cond} > T_c(L) > T_c^{\rm clean}$. 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 [9].

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

$$\rho_S(T, L) = \frac{A}{L^\chi}\left(1 - \frac{T}{T_c(L)}\right)^\nu, \tag{1}$$

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

$$T_c(L) = T_c^{\rm clean} + T_0\left(\frac{a}{L}\right)^{1/(2-\nu)}, \qquad T_c^{\rm clean} > 0. \tag{2}$$

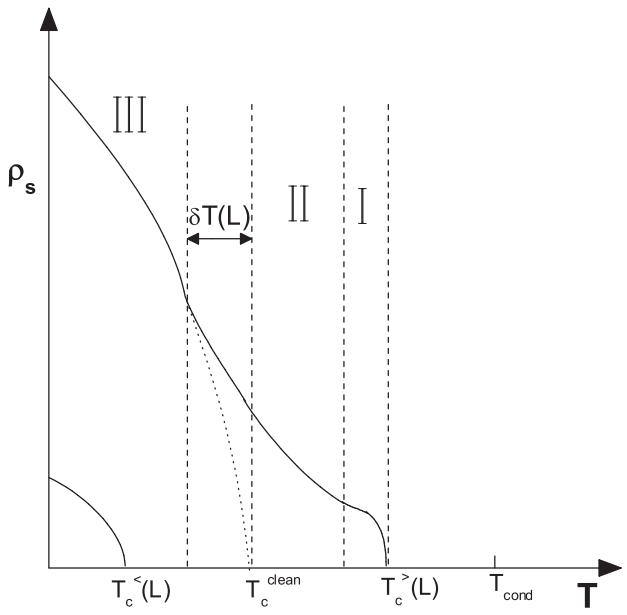

FIG. 1. The superfluid density versus temperature for a dislocated solid in which the clean system *does* (top curve) and *does not* (bottom curve) have a transition. ρ_s obeys Eqs. (1) and (4) in regions (I) and (II), respectively, where (II) is defined by Eq. (3). $T_c(L)$ for the cases $T_c^{\rm clean} >$ and < 0 are, respectively, denoted in this figure by $T_c^>(L)$ and $T_c^<(L)$, and given by Eqs. (2) and (6).

When temperature T is lowered into the range

$$\delta T(L) \ll T - T_c^{\text{clean}} \ll T_c(L) - T_c^{\text{clean}}, \tag{3}$$

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

$$\rho_S(T, L) = A' \frac{(T - T_c^{\text{clean}})^{\nu-2}}{L^2} \propto (T - T_c^{\text{clean}})^{-4/3}, \tag{4}$$

and A' an L-independent constant. In the $L \to \infty$ limit, $\delta T(L) \propto \frac{1}{L} \ll T_c(L) - T_c^{\text{clean}} \propto L^{-1/(2-\nu)} \approx L^{-3/4}$, ensuring a large window of validity for Eq. (4). Once $T < T_c^{\text{clean}} - \delta T(L)$, the tubes overlap, the entire volume becomes supersolid, and ρ_s is that of the clean system, completely independent of L, and so obeys

$$\rho_S(T) \propto (T_c^{\text{clean}} - T)^{2/3}. \tag{5}$$

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 Fig. 2, $\rho_s(T)$ data from Chan's group [12] are plotted in the form $\rho_s^{-3/4}$ versus T, which Eq. (4) predicts should give a straight line section, for T satisfying Eq. (3). The data do 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 $(T_c^{\text{clean}} - T)^{-4/3}$ in Eq. (4), and using this ratio to test the predicted L dependence of $\rho_s(T, L)$ and $T_c(L)$ Eqs. (1) and (2).

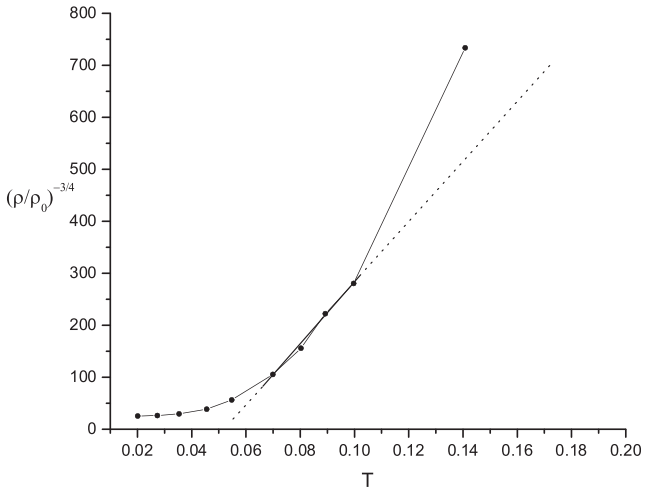

FIG. 2. Superfluid density versus temperature data from Chan's group [12], plotted in the form $\rho_s^{-3/4}$ versus T. The straight segment of this plot predicted by Eq. (4) is indicated by the dashed line.

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

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

where T_0 is another L-independent constant, a result first obtained in Ref. [9], could also be tested by measurements and/or deductions (as described above) of L. Equation (1) still holds near $T_c(L)$, but now with $\chi = 2$. Equations. (4) and (5) never apply, since $T = 0$ intervenes above T_c^{clean}. The lower curve in Fig. 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 nonclassical 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 Fig. 2, suggest $T_c^{\text{clean}} > 0$. In the 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

$$C \propto \frac{|\frac{T}{T_c} - 1|^{-\alpha}}{L^{(4-3\nu)/(2-\nu)}} \propto \frac{|\frac{T}{T_c} - 1|^{-\alpha}}{L^{3/2}}, \qquad T_c^{\text{clean}} < 0 \tag{7}$$

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 will treat elsewhere [18].

I will now outline the derivation of these results. My Hamiltonian is an isotropic [19] version of that of [5]:

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

with

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

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^{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 elastic strain tensor.

Thermal fluctuations in u_{ii} have no effect on the critical properties of the superfluid density and specific heat at the transition [5]; 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 will assume (as usual) that $t_0(T) = \Gamma \frac{(T - T_c^{\text{clean}})}{|T_c^{\text{clean}}|}$, where Γ 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, $u_{ii} = \frac{4\mu}{2\mu+\lambda}\frac{ax}{r_\perp^2} = \frac{4\mu}{2\mu+\lambda}\frac{a\cos\theta}{r_\perp}$ [6], where μ and λ are the Lame elastic constants [19]. Inserting this into Eq. (9) gives

$$t(\vec{r}) = t_0 + \frac{g'\cos\theta}{r_\perp}, \tag{10}$$

where $g' \equiv ga(\frac{4\mu}{2\lambda+\mu})$ [19].

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 nonzero. The temperature at which this occurs is $T_{\rm cond}$.

The Euler-LaGrange equation for Eq. (8) is

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

As noted in [7], this equation first has nontrivial ($\psi \neq 0$) solutions when t_0 drops below a critical value $t_{\rm cond} \equiv -\frac{2mE_0}{\hbar^2}$, where E_0 is the quantum mechanical ground state energy of a particle of mass m moving in the 2D dipole potential $V(\vec{r}) = -\frac{p\cos\theta}{2mr_\perp}$ with $p \equiv \frac{\hbar^2 g'}{2mc}$. Variational treatments [7,20] show that $E_0 = -\gamma\frac{mp^2}{\hbar^2}$, where $0.24 < \gamma < 2$. So a single dislocation line will, in mean field theory, order once $t_0 < t_{\rm cond} = \frac{\gamma g'^2}{2c}$. Using $t_0 = \Gamma(\frac{T-T_c^{\rm clean}}{|T_c^{\rm clean}|})$, this implies $T_{\rm cond} = T_c^{\rm clean} + \frac{\gamma g'^2}{2\Gamma c}|T_c^{\rm clean}| > T_c^{\rm clean}$, and $T_{\rm cond} > 0$, even if $T_c^{\rm clean} < 0$, if $\frac{\gamma g'^2}{2\Gamma c} > 1$. 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 interdislocation distance.

On length scales much greater than the tube radius $a_c(t)$, but $\lesssim L$, the only important variable is "Goldstone mode"; i.e., the phase $\theta(\vec{r})$ of $\psi(\vec{r}) \equiv |\psi(\vec{r})|e^{i\theta(\vec{r})}$. In the tube between cross-link sites i and j, θ, on these long length scales, depends only on distance s along the tube. This leads to a 1D Hamiltonian for this tube:

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

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

$$e^{-\beta H_{\rm eff}(\theta_i,\theta_j)} = \sum_{n=-\infty}^{\infty}\int_n D\theta(s)e^{-\beta H_{\rm 1D}(\{\theta(s)\})}, \tag{13}$$

where the functional integral $\int_n D\theta(s)$ 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 Eq. (13) reflects the 2π periodicity in θ.

Each of the functional integrals $\int_n D\theta(s)$ in Eq. (13) can most easily be done by rewriting $\theta(s)$ as follows:

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

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

$$e^{-\beta H_{\rm eff}(\theta_i,\theta_j)} = \sum_{n=-\infty}^{\infty} e^{-\beta(K_{\rm 1D}/L)(\theta_i-\theta_j+2\pi n)^2} \times \int D\delta\theta(s)e^{-\beta K_{\rm 1D}\int_0^L ds(\partial_s\delta\theta(s))^2}. \tag{15}$$

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

$$H_{\rm eff}(\theta_i, \theta_j) = V_v(\theta_i - \theta_j; J) = -k_BT\ln\left(\sum_{n=-\infty}^{\infty} e^{-(J/k_BT)(\theta_i-\theta_j+2\pi n)^2}\right) + C, \tag{16}$$

with the "Villain" coupling

$$J \equiv \frac{K_{\rm 1D}}{L}. \tag{17}$$

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

$$H_{\rm eff}(\{\theta_i\}) = \sum_{\rm bonds} V_v(\theta_i - \theta_j; J). \tag{18}$$

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 renormalization group sense[22], and can be ignored.

This Villain model (18) orders at a temperature $T_c = O(J/k_B)$; I will now use this to determine $T_c(L)$.

Consider first $T_c^{\rm clean} < 0$. In this case, provided $T_{\rm cond} \geq 0$, so that $K_{\rm 1D}(T) \neq 0$, we can, for $L \to \infty$, estimate T_c by replacing $K_{\rm 1D}(T)$ in Eq. (17) with its finite, nonzero, $T = 0$ value $K_{\rm 1D}(T = 0) \equiv K_0$. This gives Eq. (6) with $T_0 = \frac{K_0}{k_B}$. Note that taking $K_{\rm 1D}(T) \to K_0$ in Eq. (17) is valid since $T_c(L \to \infty) \to 0$.

For the case $T_c^{\rm clean} > 0$, the radii $a_c(T)$ of the tubes of supersolid diverge as $T \to T_c^{\rm clean}$. To see this, note that the locus on which $t(\vec{r}_\perp)$ Eq. (10) is equal to t_c is $\cos\theta = \frac{r(t_c-t_0)}{g'}$ which, for $t_0 > t_c$ and $p > (<)0$ is a circle passing through the origin, centered on the negative (positive) x axis of radius

$$a_c(T) = \frac{g'}{2(t_0 - t_c)}. \tag{19}$$

Inside this circle, $t(\vec{r}_\perp) < 0$, so, naively, this boundary (19) defines the supersolid tube. As $T \to T_c^{\rm clean}$ from above, $t_0 \to t_c$ and so $a_c(T)$ diverges: $a_c(T) \propto \frac{1}{T-T_c^{\rm clean}}$. Of course,

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

We can include fluctuations in this "local equilibrium" 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 $a_c(T) \gg \xi(T) \propto (T - T_c^{\text{clean}})^{-\nu}$, where $\xi(T)$ and $\nu \approx \frac{2}{3}$ are the correlation length and its critical exponent in the clean system. Since $\nu < 1$, $a_c(T)$ Eq. (19) is indeed $\gg \xi(t)$ as $T \to T_c^{\text{clean}}$ from above. This implies that the local superfluid density $\rho_s(\vec{r})$ for T near, but slightly above, T_c^{clean}, is

$$\rho_s^{\text{local}}(\vec{r}) = B(t_c - t(\vec{r}))^{\nu}, \tag{20}$$

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

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

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

$$K_{1D} = \frac{\hbar^2}{m^2}\int d^2 r_\perp \rho_s^{\text{local}}(\vec{r}_\perp). \tag{22}$$

Since $t(\vec{r}_\perp)$ is constant on circles of fixed radius a, passing through the origin, with their centers on the x axis, and is given by $t(\vec{r}_\perp) = \frac{p}{2a} - t_0$, I will change variables of integration in Eq. (22) to 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 Eq. (22) as

$$\begin{aligned} K_{1D}(T) &= \frac{\pi B\hbar^2}{m^2}\int_0^{p/2t_0}\left(\frac{p}{2a} - \delta t_0\right)^{\nu} a da \\ &= C\left(\frac{\mu}{\lambda}\right) B\delta t_0^{\nu-2} g^2 a^2 \frac{\hbar^2}{m^2}, \end{aligned} \tag{23}$$

where $\delta t_0 \equiv t_0 - t_c$, and $C(x) \equiv (\frac{3.184x}{2x+1})^2$ for $\nu = 2/3$.

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

As T drops further, eventually $J(T, L)$ will be $\gg k_B T$. This is guaranteed to happen, since T can get within roughly $\delta T(L) \propto \frac{1}{L}$ of T_c^{clean} before Eq. (23) breaks down. Since $K_{1D}(T_c^{\text{clean}} + \delta T(L)) \propto L^{2-\nu}$; $J(T_c^{\text{clean}} + \delta T(L)) = \frac{K_{1D}}{L} \propto L^{1-\nu} \to \infty$ as $L \to \infty$, 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) ρ_s and 3D spin-wave stiffness implies

$$\rho_S(T, L) = J(T, L)/LO\left(\frac{m^2}{\hbar^2}\right), \tag{24}$$

which, using (17) for $J(T, L)$, implies Eq. (4). Standard results for the model (16) and (18) with the T and L-dependent J found above then gives the behaviors of $T_c(C)$, $\rho_s(T)$, and the specific heat $C(T)$ quoted earlier.

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