

Quantum plasticity and dislocation-induced supersolidity

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Abstract. - We suggest that below a certain temperature T_k , the free energy for the creation of kinks-antikinks pairs in the dislocation network of solid He^4 becomes negative. The underlying physical mechanism is the related liberation of vacancies which initiate Feynman's permutation cycles in the bulk. Consequently, dislocations should wander and sweep an increasingly larger volume at low temperatures. This phenomenon should lead to a stiffening of the solid below T_k and possibly to the appearance of a non zero superfluid fraction at a second temperature $T_c \leq T_k$.

After a burst of theoretical activity in the early seventies [1–3], the question of supersolidity is again the focus of intense attention since the discovery by Kim and Chan [4, 5] of a non classical moment of inertia in solid He^4 at low enough temperatures. The physical mechanism leading to superfluid flow in these crystals is still unclear; it is actually not even established that there is true superflow. However, some consensus seems to prevail on several aspects of the problems [6]. From a theoretical point of view, there is now agreement that perfect He^4 crystals are *not* supersolids [7, 8], or at least have an extremely small superfluid fraction, much too small to account for experimental findings (see also [10]). Two rather striking features have been emerged from experiments: i) the supersolid critical temperature and the superfluid density are surprisingly large and ii) both depend sensitively on the detailed preparation history of the crystal samples [11] and on the presence of minute fractions of He^3 impurities [4, 5]. The role of superfluid flow within grain boundaries [12], possibly important in some experimental conditions, also seems to be moot since single He^4 crystals still appear to display significant supersolidity [5]. It now looks plausible that dislocations might play an important role. de Gennes [13] has discussed some aspects of the quantum mobility of dislocations, and concluded that kink anti-kink bound states should suppress, rather than enhance, dislocation mobility. There has also been some recent work [14] suggesting that the *core* of dislocations could be superfluid, possibly leading to a (small)

supersolid signal. A phenomenological theory of the role of dislocations can be found in [15]. The aim of this note is to discuss some aspects of the physics of dislocations in a quantum crystal of bosons and suggest that below a certain temperature T_d , the free energy of kink-antikink pairs (in the climb direction) becomes negative, leading to an increasing wandering of dislocations that would form an entangled network similar to a polymer melt. This proliferation of kink-antikink pairs should lead both to an increased stiffness of the solid, and to kink-induced superfluid motion. The ideas put forth here are clearly highly speculative; we nevertheless hope to modestly contribute to the ongoing heated debate on the origin of supersolidity.

Our approach follows Feynman's seminal paper on superfluidity [16], and more recent work by Pollock and Ceperley [17] on the importance of permutation cycles to understand superfluidity. The starting point is the exact path-integral representation of the partition function Z of a bosonic system of N interacting particles as:

$$Z = \frac{1}{N!} \sum_P \int \prod_i d\vec{z}_i \int \mathcal{D}\vec{x}_i(t) \exp S(\{\vec{x}_i(t)\}) \quad (1)$$
$$S = \left[- \int_0^\beta dt \left\{ \sum_i \frac{m}{2\hbar^2} \left(\frac{\partial \vec{x}_i}{\partial t} \right)^2 + \sum_{i < j} V(\vec{x}_i - \vec{x}_j) \right\} \right]$$

where the initial positions of the particles are $\vec{z}_i = \vec{x}_i(0)$'s and the final positions are constrained to be *any permutation* P of the initial configuration. The difficulty is to correctly guess what set of configurations and “trajecto-

ries” dominate this very high dimensional integral. As emphasized by Feynman, although t is the imaginary time, it helps intuition to think of a problem of N classical particles moving in “real” time. At high temperature, $\beta = 1/T$ is small, and the particles do not have much time to move around, so that the main contribution to Z comes from the trivial identity permutation such that $x_i(0) = x_i(\beta)$, $\forall i$; the bosonic nature of the particles is irrelevant. When β increases, more and more permutations can be explored. In a liquid, where motion is relatively easy, Feynman argues that at some temperature the average length of permutations diverges, leading to a superfluid phase transition. The precise connection with superfluidity was worked out by Ceperley and Pollock, who showed using linear response theory and periodic boundary conditions that the superfluid fraction f_s can be exactly written as [17]:

$$f_s = \frac{T}{T^*} \frac{N \langle \vec{W}^2 \rangle}{6a^2}; \quad \vec{W} = N^{-1} \sum_i \int_0^\beta dt \frac{\partial \vec{x}_i}{\partial t} \quad (2)$$

where the average is taken over all permutations with the weight defining Z , a is the interatomic spacing (introduced for convenience) and $T^* \equiv \hbar^2/2ma^2$ is the typical kinetic energy of the particles ($a \approx 3\text{\AA}$ and $T^* \approx 1\text{K}$ in solid He^4). Any permutation can be decomposed into cycles. From the above formula, it is clear that only permutations corresponding to system spanning cycles wrapping around the torus can lead to a non zero winding number, W , and hence to a non zero superfluid fraction f_s . The weight of a given cycle involving the *simultaneous* jump of n particles that all move a distance of order a is:

$$p_n \sim \exp\left[-\frac{n\beta m}{2\hbar^2} \left(\frac{a}{\beta}\right)^2 - n\beta\bar{V}\right] = \exp\left[-nm^* \frac{T}{4T^*}\right], \quad (3)$$

where \bar{V} is a typical energy barrier encountered during the motion of each particle and $m^* = m(1 + 4\bar{V}T^*/T^2)$ is the effective mass. In reality the dependence of $m^*(T)$ on temperature is expected to be more complicated. In particular this expression is only valid at high enough temperatures. When $T < (T^*\bar{V})^{1/2}$, quantum tunneling sets in and leads to decrease of the effective value of \bar{V} . At zero temperature one expects a finite effective mass m^* , larger than the bare one m because of interactions (using the previous notation this means that \bar{V} vanishes quadratically with temperature as $T \rightarrow 0$).

Feynman’s insight [16] was to realize that whereas p_n decreases exponentially with n , the number of permutation cycles *increases* exponentially with n , as z^n up to a power-law prefactor in n . If the barrier \bar{V} is small enough compared to T (as in a liquid, where particles can move easily while avoiding each other), the entropy of these cycles dominates whenever $T < T_\lambda \simeq 4T^* \ln z - \bar{V}$, favoring infinite cycles and hence superfluidity. In a solid, however, the energy of the intermediate state is much larger, and is in fact expected to grow *faster* than n due to elastic defor-

mations. Therefore, naively, only finite cycles are expected in a perfect solid, and the superfluid density remains zero.

As has been recognized for a long time, the presence of vacancies can change this. Let us rephrase the argument of Andreev and Lifshitz [1] at finite temperatures, which we will extend later to dislocation kinks. Vacancies in the initial configuration $\{z_i\}$ act as *initiators* of permutation cycles. A neighboring particle can easily hop to the empty site; once this is done (in imaginary time) the next particle can also easily hop, and so on (maybe slightly more collective moves are possible, too). For a path of length n , each particle must dash off to the neighboring empty site in “time” $\sim \beta/n$, while paying an effective potential energy \bar{V} . The extra multiplicative weight associated to the path is now:

$$p_n \sim \exp\left[-n\frac{\beta}{n} \frac{m}{2\hbar^2} \left(\frac{a}{\beta/n}\right)^2 - \beta\bar{V}\right] \equiv p_0 \exp\left[-n^2 \frac{T}{4T^*}\right]. \quad (4)$$

In fact, the above estimate can be seen as a saddle point calculation where one decomposes the path in hops of duration τ_i such that $\sum_{i=1}^n \tau_i = \beta$, with fixed intermediate positions along the path. The saddle-point corrections add a factor $nC^n(T/T^*)^{3/2}/2\sqrt{\pi}$ to the above naive result, where C is a numerical constant. The above calculation becomes unsuitable at low temperatures when transition between sites becomes instantonic transitions (i.e. localized events along the time axis). It leads to a slightly different expression for p_n and allows one to recover the tight-binding model used by Andreev and Lifshitz (see Appendix). However, in both cases, $\ln p_n \sim -T^*/TG(nT/T^*)$, where $G(u) = G_0 + G_1u + G_2u^2$ for the above “quasi-free” model and $G(u) = u \ln(u/eT)$ for the tight binding (instanton) model (see Appendix for the expression of the transmission coefficient T).

For the vacancy to return to its initial position at time β , the path must be a closed random walk on the crystal lattice. One can define the free-energy F_v for the creation of a single vacancy *around a given site* as:¹

$$F_v \approx E_v - T \ln \left[1 + \sum_{n=2}^{\infty} \Pi_n \right], \quad \Pi_n \simeq \frac{z^n p_n}{(2\pi n)^{3/2}} \quad (5)$$

where E_v is the energy of a localized vacancy, when no permutation is allowed. The extra term $z^n/(2\pi n)^{3/2}$ accounts for the number of random walks returning at the origin after n steps (for large n). Using again a saddle-point approximation for the sum, valid when $T \ll T^*$, we find that it is in both cases dominated by values of n around $n^* = \mu T^*/T \gg 1$ with $\mu = 2 \ln(zC)$ in the quasi-free model and $\mu = zT$ in the instanton model. Noting that $\bar{V}(T \rightarrow 0) = 0$, the limiting behaviours are easily found to be:

$$F_v(T \ll T^*) \approx E_v - \zeta T^*; \quad F_v(T \gg T^*) \approx E_v, \quad (6)$$

¹The full free energy of a single vacancy should clearly include the obvious $-T \ln(V/a^3)$ contribution, corresponding to the choice of the initial site on the permutation cycle.

with $\zeta = \ln^2(zC)$ for the quasi-free model and $\zeta = zT$ for the tight-binding model. The leading correction when $T > 0$ is found to be *positive*, equal to $+3T/2 \ln T^*/T$ for both models, as it should be, since finite temperatures inhibit permutation cycles. The free-energy for the creation a vacancy F_v is therefore lowered at low temperatures. The shape of $F_v - E_v$ as a function of T/T^* , for both models and for different choice of parameters is shown in Fig. 1.² Depending on the value of these parameters, one may find a temperature T_v at which F_v vanishes. When $F_v > 0$, the equilibrium density ϕ_v of vacancies is given obtained by minimizing the total free energy (per unit volume):

$$\mathcal{F} = T\phi_v \left[\ln \left(\frac{\phi_v a^3}{e} \right) - 1 \right] + \phi_v F_v + O(\phi_v^2) \quad (7)$$

This leads to

$$\phi_v^* = \frac{\exp(-F_v/T)}{a^3}, \quad (8)$$

which is vanishingly small at low temperatures. If on the other hand F_v becomes negative, one expects a finite density of vacancies in the system even when $T \rightarrow 0$. This density is now controlled by the vacancy-vacancy interaction [1], which adds a term $A\phi_v^2/2$ to the above expression for \mathcal{F} . When $T_v \ll T^*$, the vacancy density first decreases as the temperature is reduced, but then sharply increases as the temperature approaches T_v . At low temperatures, the density is given by $\phi_v^* \approx |F_v|/A$. When A is small, the proliferation of vacancies might actually lead to a true phase transition to a low density solid phase. The case of kinks discussed below will closely follow the above argument. Note that the decrease of ϕ_v until T_v holds only when F_v decreases faster than linearly with temperature, which is indeed what we finds in our approximate treatments, see Fig. 1. Even when this is not the case, T_v is the characteristic temperature determining the point where vacancy-vacancy interaction becomes crucial in order to limit the density of vacancies (which would otherwise proliferate). Now, for superfluidity to set in, the permutation paths should not end where they where initiated since in this case the winding number W in Eq. (2) above is zero. Paths should rather end on the site where a different vacancy started off. If the end-to-end distance of the path is R , the corresponding weight is modified to:

$$\Pi_n(R) = \Pi_n \exp \left[-\frac{R^2}{2na^2} \right]. \quad (9)$$

It is clear that these paths are exponentially suppressed when $R^2 \gg n^*a^2$. If one wants to see the appearance of a permutation cycle winding around the system and contributing to W , the distance between vacancies should be such that the suppression factor does not preclude the existence of a percolating path of inter-vacancy hops, which

²In a fermionic environment, the free-energy reduction is much weaker, because different permutations interfere destructively. As a rough approximation one may keep only self-retracing paths, which leads to a reduction of μ and ζ in the above formulas.

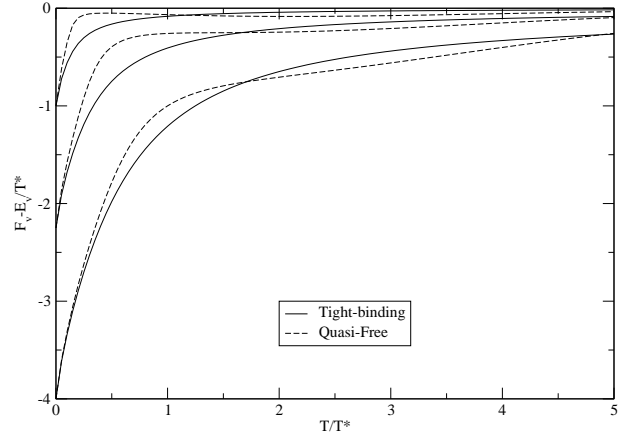


Fig. 1: Evolution with temperature of the excess free-energy $F_v - E_v$ for the creation of a single vacancy, lowered by the surrounding permutations of the bosonic solid, for both models: quasi-free (dashed lines) and tight binding (plain lines). From top to bottom, $\zeta = 1^2, 1.5^2, 2^2$ and $\bar{V} = 0$ for the quasi-free model (this is only reasonable at low enough T/T^*). Axis are in reduced units: T/T^* and F/T^* .

happens below a certain temperature T_c given by:

$$a\sqrt{n^*} \sim a\phi_v^{*-1/3} \longrightarrow T_c \sim \frac{\mu}{2}\phi_v^{*2/3}T^*. \quad (10)$$

The superfluid transition temperature T_c is of the same order of magnitude as the temperature at which a dilute gas of particles of mass m would Bose condense. Below T_c , the superfluid fraction can be estimated using the Ceperley-Pollock formula. The probability that a given atom belongs to a winding chain is $\phi_v^*n^*$, each of which contributes to $\langle W^2 \rangle$ by an amount a^2/N , leading to:

$$f_s \approx \frac{T}{T^*}\phi_v^*\frac{\mu T^*}{2T} \sim \phi_v^*; \quad (11)$$

i.e. the superfluid density is of the order of the vacancy density, which is itself temperature dependent. Due to the large positive value of $F_v(T=0)$ in solid He^4 (around $13K$, see [8]), the density of vacancies is extremely small and vanishes at zero temperature [9]. As a consequence, the condition (10) is never met. No supersolid transition induced by vacancy delocalization is expected and this scenario cannot account for experimental results.

On the other hand, it is most probable that even single He^4 crystal contains quenched-in dislocations; estimates vary in the range $10^6 - 10^{10} \text{ cm}^{-2}$. This means that the typical distance D between two dislocations is in the range $300 \leq D/a \leq 3 \cdot 10^4$, and the probability ϕ for an atom to be part of a dislocation of the order $\phi \sim 10^{-9} - 10^{-5}$, much smaller than the superfluid fraction $2 \cdot 10^{-3}$ reported for isotropically pure single crystals (1 ppb of He^3 impurities). An important message conveyed by the work of Boninsegni et al. [14] is that dislocation cores can be considered as liquid-like, and permutation cycles are favored *along* the dislocation lines at low temperatures. In-

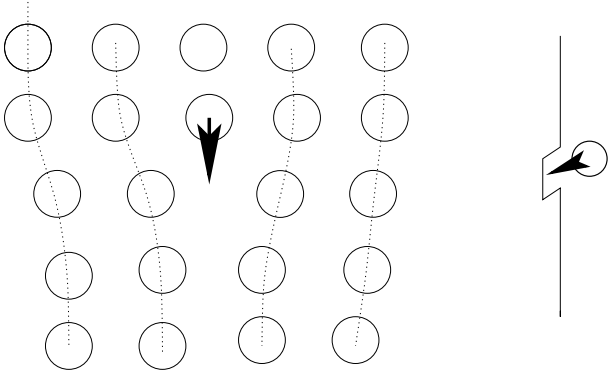


Fig. 2: Left: cartoon of an edge dislocation in the plane perpendicular to the dislocation direction. The creation of a kink-antikink in the climb direction (or jog) corresponds to liberating a vacancy, as indicated by the arrow, which can then initiate a permutation cycle in the direction *transverse* to the dislocation. Right: side view of the same situation.

deed, even classically self-diffusion is enhanced in dislocation cores [21]. Because these lines are one dimensional, however, superfluid coherence is only maintained up to length ℓ such that $\ell \sim aT^*/T$ (see, e.g. [15]).

Now, consider an edge dislocation with a kink-antikink corresponding to one (or several) atom(s) moving in the climb direction (see Fig. 2)³. In effect, this creates a vacancy (or a string of vacancies) which can now act as the starting point of permutation cycles in the direction *transverse* to the dislocation. The creation energy of a kink-antikink pair, E_k , is expected to be appreciably lower than that of a vacancy E_v , since the crystal is already strongly deformed around the dislocation. When temperature goes down, the creation free-energy of the kink-antikink pair is lowered by the permutation cycles initiated around it, and is given by an expression similar to Eq. (6):

$$F_k(T \ll T^*) \approx E_k + \overline{B}(T) - \zeta T^*, \quad (12)$$

where $\overline{B}(T)$ is the effective barrier to unbind the vacancy from the dislocation core, averaged over the relevant vacancy paths and corrected by quantum tunnelling effects. At high temperature it is equal to the binding energy, E_B , between the vacancy and the dislocation core, but is reduced by quantum fluctuations at low temperatures. This effective barrier in fact depends on the typical extension of the paths $R^* \sim a\sqrt{n^*}$ and on the orientation of these paths, since the deformation field around the dislocation contains both compressed and expanded regions [15].

Our scenario relies on the assumption that E_k, \overline{B} are small enough such that $F_k(T)$ becomes negative below a temperature T_k (see Fig 1). Both E_k and \overline{B} should indeed not be larger than a few Kelvins, at least when pressure is not too large. Taking for example $\zeta = 4$, $E_k = 3T^*$, and $\overline{B}(T \rightarrow 0) \approx 0$ leads to $T_k \sim 0.2T^*$ or 200 mK (see Fig.

³These objects are in fact called jogs in the dislocation literature [18] but we will still call them kinks.

1), with a rather modest extension of permutation cycles $R^*(T_k) \sim 3a$: the released vacancies do not travel very far away from the dislocation cores. If the free energy for the creation of kinks indeed become negative below T_k , one should see a proliferation of kinks and anti-kinks in the configurations that contribute most to the partition function Z of the solid⁴. This would lead to a substantial lengthening of the already present dislocations, which start wandering around in the solid, carrying an $O(1)$ density of kinks. Bose statistics of the surrounding atoms favors the extension of the curvilinear length of dislocations. The nature of the resulting quantum dislocation “soup”, i.e. how much dislocations can wander around into the solid and how large are the regions swept by dislocations, is a very complicated problem. The difficulty is to give a correct quantitative treatment of quantum dislocations. We suggest that the limiting factor to a complete delocalization of dislocations is due to the elastic energy. Consider for example a single dislocation. From the reasoning above, it should carry, below T_k an $O(1)$ density of kinks-antikinks pairs. Large fluctuations can only be achieved if kinks and antikinks unpair. However, in this case one has to consider on top of the free energy (12) the elastic interaction energy between kinks and antikinks which disfavors the accumulation of kinks and the corresponding wandering of the dislocation on large length scales. Furthermore dislocations form a network inside the solid. Thus, one also has to consider the elastic energy due to dislocation-dislocation interactions which, again, limits the density of dislocations. Other (shorter-range) interactions between kinks and antikinks could also play an important role.

We propose here an admittedly very naive analysis of this difficult problem. Calling ϕ_d the total density of sites swept by dislocations (per unit volume now), a simple mean-field argument allows one to write the free-energy per unit volume of the dislocation network as:

$$f \approx F_k \phi_d + \frac{1}{2} Y \phi_d^2 \quad (13)$$

where Y is a typical elastic interaction scale, formed with the shear modulus G and the atomic volume a^3 . Since $G a^3 \approx 100\text{K}$, a rough order of magnitude is $Y \sim 50\text{K}$, to within a factor 2. The equilibrium density of dislocations is therefore $\phi_d^* \sim -F_k/Y$. Below T_k there is thus an extra contribution df to the total free energy coming from the dislocation soup and the corresponding proliferation of permutation cycles. Using the above naive estimate, the extra free energy contribution reads, close to T_k : $df \sim -(T_k - T)^2$, leading to a small extra specific heat contribution below T_k . Whether T_k corresponds to a true phase transition where the dislocations network changes nature and forms a kind of “quantum dislocation

⁴There is a remark in de Gennes’ paper [13] where this possibility is mentioned, which he tentatively associates with melting of the solid.

“soup” phase is an open problem. Well below T_k , a reasonable estimate is $F_k \sim -50$ mK, leading to $\phi_d^* \sim 10^{-3}$, a significant increase from the bare estimate $10^{-9} - 10^{-5}$ given above, which assumes that dislocations are essentially straight lines. However, the density of the system, or the Debye-Waller factor, should only change by very small, unmeasurable amounts at T_k , compatible with experimental findings [19]. Since the density of liquid and solid only differ by 10%, we expect the change of density at T_k to be $\sim 10^{-4}$ at most. But the delocalization of dislocations should affect the elastic property of the solid. From the above argument, the density and fluctuations of the “polymer melt” are governed by the repulsive (elastic) interactions between otherwise proliferating and expanding dislocations. When the solid is deformed, the melt must adapt and deform as well. Since the initial state minimizes the free energy, Eq. (13), any shear deformation can only increase the free energy to quadratic order, leading to an increased shear (and bulk) modulus. This might explain the recent results from the Beamish group [20], the anomaly in the sound velocity reported some years ago by Goodkind et al [22] and the elastic resonance frequencies reported in [23]. The elastic region should however significantly narrow down below T_k , giving way to enhanced plasticity effects. We note at this stage that the sudden appearance of a dislocation melt could lead to partial decoupling of the solid in a oscillating pendulum experiment [24], although more careful calculations are needed to see if this is enough to explain the observed NCRI fraction.

Coming back to a possible supersolidity transition, we follow Boninsegni et al. [14] who show that superfluid order establishes along the (coiled) dislocations. Using the kink mechanism above superfluid order can also explore a sausage of radius $R \sim a\sqrt{n^*}$ around the sites swept by dislocations. This can be thought of as a kink-induced proximity effect. Superfluidity propagates from dislocation to dislocation over the whole system only if another dislocation is typically present within a sausage of coherence length $\ell \simeq aT^*/T$ (a kink would move very easily along the dislocation to match the incoming permutation path). The condition for macroscopic superfluidity therefore reads:

$$\phi_d^* \times (\pi R^2 \ell) > 1 \rightarrow T < T_c = T^* \sqrt{\mu \pi \phi_d^* / 2} \sim 100 \text{mK}, \quad (14)$$

which would give the right order of magnitude for the appearance of supersolidity in experiments. Using the Pollock-Ceperley formula, the superfluid density is then given by the “sausage” fraction (each dislocation point can be the source of a permutation cycle up to a fast translation of a kink) :

$$f_s = \frac{T}{T^*} \phi_d^* \frac{\mu T^*}{6T} \sim 3 \cdot 10^{-4}, \quad (15)$$

which is compatible with recent data on single crystals with 1ppb He^3 impurities. Clearly, the above numbers

are only intended to be rough estimates, maybe more significant is our unusual, 2d like scaling prediction $T_c \sim T^* \sqrt{\phi_d^*}$.

An interesting consequence of our scenario is the role of He^3 impurities. Calling φ the fraction of these impurities and assuming that they mostly gather within dislocation cores at low temperatures, one finds that the typical distance between He^3 impurities along dislocations is $d = a\phi_d^*/\varphi$. In Feynman’s picture, it is clear that He^3 are detrimental to superfluidity since any permutation cycle involving an He^3 atom will not contribute to the partition function anymore. One expects that as soon as $d \sim \ell$, the concentration of He^3 becomes noticeable and affects the superfluid density. When $T \sim 10$ mK, our estimate above leads to $\ell/a \sim 100$ and hence $\varphi = 10$ ppm. On the other hand, He^3 impurities might also change the density of quenched-in dislocations and reduce the bare energy of a kink-antikink E_k , so that the overall influence of He^3 on supersolidity could be rather complex.

What about *solid* He^3 ? The delocalisation of vacancies at low temperatures, and therefore the lowering of the kink-antikink creation energy, may also occurs in this case. However, the effect is much weaker for fermions and T_k is expected to be much smaller than in He^4 (see footnote 2). Kinks should proliferate more easily in spin polarised than in unpolarised solid He^3 . Of course, there is no superfluidity in this case (except if vacancies pair up), but there could still be observable elastic anomalies in solid He^3 at low enough temperature and pressure (perhaps also accompanied by a small magnetic susceptibility anomaly due to the formation of spin-polarons around vacancies [27]). More experiments on the elastic properties of solid He^3 would be welcome.

Let us summarize the main features of our scenario. Around a temperature T_k , kinks proliferate and the dislocations form a “quantum dislocation soup” analogous to an entangled polymer melt. Whether the dislocations network undergoes a true phase transition is at this stage an open problem, but one expects a (small) specific heat anomaly and a change the elastic properties of the system around T_k . This could explain the shear modulus anomaly recently reported by Day and Beamish [20] and other elastic anomalies, perhaps even a partial decoupling of the solid in a oscillating pendulum experiment. If $T_c < T_k$, one should see a region with modified shear (and bulk) modulus but only a small superfluid density before supersolidity really sets in at T_c , when permutation cycles hook up different dislocations. Because our mechanism is a hybrid between longitudinal (along dislocation lines) and transverse permutation cycles, small concentration of He^3 impurities may significantly reduce the superfluid density. If the kink-energy can be increased substantially by increasing the pressure, one should see a complete suppression of both elastic anomalies and supersolidity when $E_k(P) > \zeta(P)T^*$. On the other hand, one should also take into account how the initial concentration of dislocations changes upon increasing the pressure. The mecha-

nism for supersolidity proposed in this work may also be relevant in more general cases. Indeed, supersolidity has been obtained not only for single He⁴ crystals but also for He⁴ in porous Vycor [4] and after rapid quenches [25]. In these two latter cases, the underlying solid matrix could be so full of defects that taking the crystal as the reference state and considering its defects such as dislocations may not be relevant. A more sensible reference state might be an amorphous solid [26]. Nevertheless, supersolidity could also arise in this case because of the liberation of vacancies from “soft” preferred regions following a mechanism similar to the one we proposed in this work. Finally, we suggest that the repulsive interaction between superfluid vortices and coiled dislocations could lead to interesting physical effects; we expect shear cycles below T_c to be hysteretic and affect the supersolid properties.

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Appendix. – In the following we present a derivation of the excess free energy for a vacancy in a bosonic crystal, F_v , which makes clear the connection with Andreev and Lifshitz [1]. We consider the contribution to the path integral given by paths in which a vacancy is created in the origin just after $t = 0$, it wanders around and come back at the origin at $t \approx \beta$. We estimate the additional multiplicative weight induced by this process compared to the one in which particles oscillate around crystalline positions. Close to $t = 0$ a vacancy-interstitial pair is formed. The potential energy of this configuration is higher than the initial crystalline one. Once created and at low temperature, vacancies allow the system to gain kinetic energy by moving through the lattice. In order to estimate this effect we note that the crystal with the vacancy-interstitial pair is a local minimum of the potential energy. Moving the vacancy on other lattice sites one obtains new local minima with the same energy (at least if the vacancy is far enough from the interstitial which will happen most of the time at large β). As a consequence the extra weight due to paths in which the vacancy starts at $t \approx 0$ and comes back at the same position at $t \approx \beta$ can be estimated summing over instantons, where each instanton corresponds to the motion of the vacancy to a nearest neighbor lattice site (we neglect for simplicity all other jumps). Each step leads to a factor [28] $K = T^*g \exp(-S_0)$, where S_0 is the value of the action for a single instanton and g is the contribution due to the Gaussian integration around the saddle point. We can write $K = T^*\mathcal{T}$, where \mathcal{T} is the transmission coefficient of the barrier. For large β one

has to sum a dilute gas of instantons. The integration over the instanton positions in time gives, for n instantons, $(\beta K)^n/n!$ [28]. Thus, the weight of a path of n steps on the lattice can be written (for large n):

$$p_n = \frac{C}{\sqrt{2\pi n}} \exp \left[-\frac{T^*G(nT/T^*)}{T} \right], \quad G(u) = u \ln(u/eT) \quad (16)$$

where the constant factor C takes into account the extra contribution due to the creation and annihilation of the interstitial-vacancy pair at $t \approx 0, \beta$. The computation of F_v via the sum over closed paths of length n can be performed by decomposing over paths consisting of n_x forward and n_x backward steps in the x direction (and similarly for the other two directions). The number of closed paths of n steps with n_x, n_y, n_z forward steps in the x, y, z directions, is equal to $n!/(n_x!^2 n_y!^2 n_z!^2) \delta_{n, 2n_x+2n_y+2n_z}$ (for simplicity we focus on a cubic lattice). Introducing into the sum the identity $f(n)^2 = \int_0^{2\pi} d\theta / (2\pi) \sum_{n'=0}^{\infty} e^{-i\theta(n-n')} f(n) f(n')$ and summing over all n s variable one finds the familiar result:

$$F_v = E_v - 3T \ln \left(\int_0^{2\pi} \frac{d\theta}{2\pi} \exp(2\beta K \cos(\theta)) \right) \quad (17)$$

Up to proportionality constants, this is exactly what one would have obtained for a particle (vacancy) in a tight binding model at temperature T . This computation allows one to show how vacancies can lead to quasi-particle excitations and bridges the gap between our approach and the one of Andreev and Lifshitz [1] who analyzed the $T = 0$ case starting directly from a tight binding model. Note that $F_v(T = 0) = E_v - 6T^*\mathcal{T}$.

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