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Quantum plasticity and dislocation-induced supersolidity

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Abstract

We suggest that below a certain temperature T_J , the free energy for the creation of jog–antijog 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 deform, elongate and occupy an increasingly larger volume at low temperatures. This phenomenon should lead to a stiffening of the solid below T_J and possibly to the appearance of a non-zero superfluid fraction at a second temperature $T_c \leq T_J$. **To cite this article:** J.-P. Bouchaud, G. Biroli, C. R. Physique 9 (2008).

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Résumé

Plasticité quantique et supersolidité induite par les dislocations. Nous suggérons qu'en dessous d'une certaine température T_J l'énergie libre de créations de paires jogs–antijogs devient négative dans l' He^4 solide. Le mécanisme physique permettant la création de ces paires est la libération de lacunes qui initient les cycles de permutation de Feynman dans la masse du solide. En conséquence, les dislocations devraient se déformer et s'allonger, et de ce fait occuper une fraction volumique de plus en plus importante lorsque la température décroît. Ce phénomène devrait conduire à une rigidification du solide en dessous de T_J et à l'apparition d'une fraction supersolide non nulle en dessous d'une seconde température $T_c \leq T_J$. **Pour citer cet article :** J.-P. Bouchaud, G. Biroli, C. R. Physique 9 (2008).

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After a burst of theoretical activity in the early 1970s [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

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also [10]). Two rather striking features have 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 He³ 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 He⁴ 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 jog–antijog 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 [15]. A phenomenological theory of the role of dislocations can be found in [16]. 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_J , the free energy of jog–antijog pairs (in the climb direction) becomes negative, leading to a proliferation of zero-point dislocations that would form an entangled network similar to a polymer melt. This proliferation should lead both to an increased stiffness of the solid, and to jog-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 [17], and more recent work by Pollock and Ceperley [18] 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:

$$Z = \frac{1}{N!} \sum_P \int \prod_i d\vec{z}_i \int \mathcal{D}\vec{x}_i(t) \exp S(\{\vec{x}_i(t)\})$$

$$S = \left[- \int_0^\beta dt \left\{ \sum_i \frac{m}{2\hbar^2} \left(\frac{\partial \vec{x}_i}{\partial t} \right)^2 + \sum_{i<j} V(\vec{x}_i - \vec{x}_j) \right\} \right] \quad (1)$$

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 “trajectories” 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 [18]:

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

where the average is taken over all permutations with the weight defining Z , a is the interatomic spacing (introduced for convenience) and $T^* \equiv \hbar^2/2ma^2$ ($a \approx 3 \text{ \AA}$ and $T^* \approx 1 \text{ K}$ in solid He⁴). 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 [17] 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 (z is a coordination number). 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 deformations. 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 jogs. 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 A). 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 A 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* as¹:

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

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 behaviors are easily found to be:

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

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):

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

¹ The 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.

² In 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.

This leads to

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

which is vanishingly small at low temperatures. If for some reason F_v becomes negative, one expects a finite density of vacancies in the system even when $T \rightarrow 0$. This density would then be controlled by the vacancy–vacancy interaction [1], which adds a term $A\phi_v^2/2$ to the above expression for \mathcal{F} , with a virial coefficient $A > 0$.³ 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 jogs 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 find 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 were 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 happens below a certain temperature T_c given by:

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

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 He⁴ (around 13 K, 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 He⁴ crystal contains quenched-in dislocations; estimates vary in the range 10^6 – 10^{10} cm⁻². This means that the typical distance D between two dislocations is in the range $300 \leq D/a \leq 3 \times 10^4$, 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 2×10^{-3} reported for isotropically pure single crystals (1 ppb of He³ impurities). An important message conveyed by the work of Boninsegni et al. [14] is that atoms have slightly more space to move within dislocation cores, hence permutation cycles are favored *along* the dislocation lines at low temperatures. Indeed, even classically self-diffusion is enhanced in dislocation cores [23]. 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. [16]).

Now, consider an edge dislocation with a jog–antijog corresponding to one (or several) atom(s) moving in the climb direction (see Fig. 2). 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 jog–antijog

³ When A is negative either higher non-linear terms limit the vacancy density or otherwise the crystal is unstable. In the former case one expects a first order phase transition at zero temperature [1]. The properties of the resulting phase cannot be obtained within a low density vacancy expansion approach.

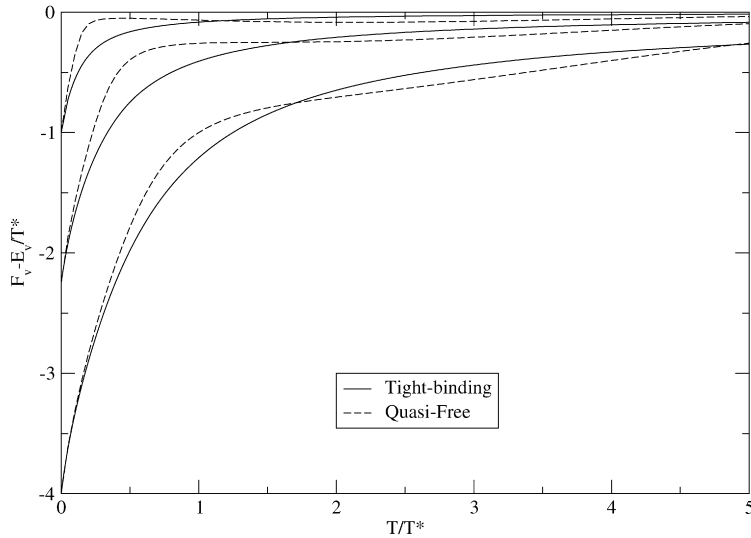


Fig. 1. Evolution with temperature of the excess free-energy $F_v - E_v$ for the creation of a single vacancy, lowered by the surrounding permutations of the bosonic solid, for both models: quasi-free (dashed lines) and tight binding (plain lines). From top to bottom, $\zeta = 1^2, 1.5^2, 2^2$ and $\bar{V}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

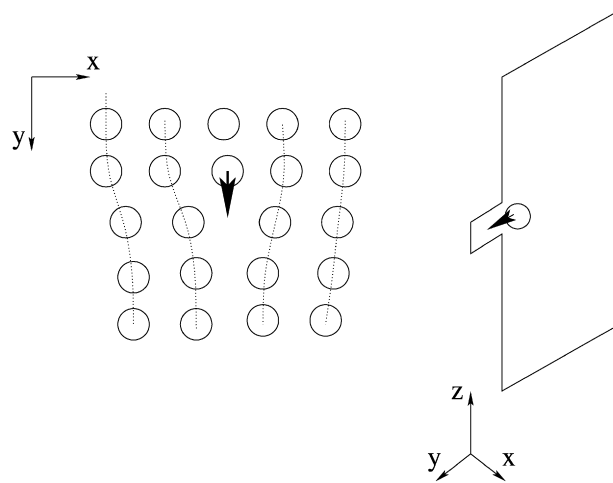


Fig. 2. Left: cartoon of an edge dislocation in the plane perpendicular to the dislocation direction. The creation of a jog–antijog in the climb direction corresponds to liberating a vacancy, as indicated by the arrow on the moving atom. Right: side view of the same situation: the dislocation is indicated as the vertical black line, and the jog–antijog is created by the same moving atom carrying the arrow.

pair, E_J , 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 jog–antijog pair is lowered by the permutation cycles initiated around it, and is given by an expression similar to Eq. (6), which at low temperatures reads:

$$F_J(T \ll T^*) \approx E_J + \bar{B}(T) - \zeta T^* \tag{12}$$

where $\bar{B}(T)$ is the effective barrier to unbind the vacancy from the dislocation core, averaged over the relevant vacancy paths and corrected by quantum tunneling effects. At high temperature it is equal to the full binding energy, E_B , needed to free the vacancy from the dislocation core. It is somewhat reduced at low temperatures, since the effective

barrier depends on the typical extension of the paths $R^* \sim a\sqrt{n^*}$ away from the core.⁴ It also depends on the detailed geometry of these paths, since the deformation field around the dislocation contains both compressed and expanded regions [16]. Therefore, we expect that the dominant vacancy paths will be strongly anisotropic around the dislocations as to reduce the effective barrier $\bar{B}(T)$.

Our scenario relies on the assumption that E_J , \bar{B} are small enough such that $F_J(T)$ becomes negative below a temperature T_J (see Fig. 1). Both E_J and \bar{B} should indeed not be larger than a few Kelvins, at least when pressure is not too large. Taking for example $\zeta = 4$, $E_J = 3T^*$, and $\bar{B}(T \rightarrow 0) \approx 0$ leads to $T_J \sim 0.2T^*$ or 200 mK (see Fig. 1), with a rather modest extension of permutation cycles $R^*(T_J) \sim 3a$: the released vacancies do not travel very far away from the dislocation cores. If the free energy for the creation of jogs indeed becomes negative below T_J , one should see a proliferation of jogs and antijogs in the configurations that contribute most to the partition function Z of the solid.^{5,6} 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 jogs. 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 be elongated and, consequently, how large is the volume occupied 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.⁷ Consider for example a single dislocation. From the reasoning above, it should carry, below T_J an $O(1)$ density of jogs–antijogs pairs. Large fluctuations can only be achieved if jogs and antijogs unpair. However, in this case one has to consider on top of the free energy (12) the elastic interaction energy between jogs and antijogs which disfavors the accumulation of jogs and the corresponding deformation 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 jogs and antijogs 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 traversed 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:

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

where Y is a typical elastic interaction scale, formed with the shear modulus G and the atomic volume a^3 . Since $G a^3 \approx 100$ K, a rough order of magnitude is $Y \sim 50$ K, to within a factor 2. The equilibrium density of dislocations is now only limited by interactions and is given by $\phi_d^* \sim -F_J/Y$, *independently* of the initial density of dislocations. Below T_J there is thus an extra contribution df to the total free energy coming from the dislocation soup and the corresponding proliferation of permutation cycles, leading to a small extra specific heat contribution below T_J . Whether T_J corresponds to a crossover or to a true phase transition where zero-point dislocations proliferate and form a quantum dislocation melt phase is an open problem. A plausible range of zero temperature jog creation energy is $F_J \sim -5 \rightarrow -50$ mK. This leads to $\phi_d^* \sim 10^{-4} \rightarrow 10^{-3}$, a very large increase from the bare estimate 10^{-9} – 10^{-5} given above (and which assumes that dislocations are essentially straight lines). However, even for such a large value of ϕ_d^* , the density of the system or the Debye–Waller factor should only change by very small, unmeasurable amounts at T_J , compatible with experimental findings [21]. Since the density of liquid and solid only differ by 10%, we expect the change of density at T_J 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.

⁴ As suggested by the very recent results of [31], vacancies are expected to form a bound state with the dislocation. In this case R^* first grows when lowering the temperature but then saturate at a finite value. Since we expect a value for R^* which is quite small in the temperature range we are interested in $R^*(T_J) \sim 3a$, the precise determination of the temperature evolution of R^* is not essential for our argumentation.

⁵ There is a remark in de Gennes’ paper [13] where this possibility is mentioned, which he tentatively associates with melting of the solid.

⁶ Note that we focused on jog–antijog pairs on edge dislocations. Depending on the type of dislocation more general group of defects may play the role of seeds for vacancy creation [19]. Our arguments can be extended straightforwardly to these cases too.

⁷ Due to long-range elastic deformations, a single dislocation should actually be *flat* at zero temperatures as a simple generalization of [20] would suggest.

This might explain the recent results from the Beamish group [22], the anomaly in the sound velocity reported some years ago by Goodkind et al. [24] and the elastic resonance frequencies reported in [25]. The elastic region should however significantly narrow down below T_J , 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 [26], 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 find superfluidity along screw dislocations at low temperatures and assume that superfluid order establishes along our (coiled) edge dislocations. Using the jog 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 jog-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 jog would move very easily along the dislocation to match the incoming permutation path). The condition for macroscopic superfluidity therefore reads:

$$\phi_d^* \times (\pi R^2 \ell) > 1 \quad \rightarrow \quad T < T_c = T^* \sqrt{\mu\pi\phi_d^*/2} \sim 30 \rightarrow 100 \text{ mK} \quad (14)$$

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 jog):

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

which is compatible with recent data on single crystals with 1 ppb 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 when $\phi_d^* = 10^{-3}$. On the other hand, He^3 impurities might also change the density of quenched-in dislocations and reduce the bare energy of a jog–antijog E_J , so that the overall influence of He^3 on supersolidity could be rather complex.

What about *solid* He^3 ? The delocalization of vacancies at low temperatures, and therefore the lowering of the jog–antijog creation energy, may also occur in this case. However, the effect is much weaker for fermions and T_J is expected to be much smaller than in He^4 (see footnote 2). Jogs should proliferate more easily in spin polarized than in unpolarized 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 [29]). More experiments on the elastic properties of solid He^3 would be welcome, but unpublished results from the Beamish group seem to indicate a similar elastic anomaly in He^3 as well, although the interpretation given is different.

Let us summarize the main features of our scenario. Around a temperature T_J , jogs proliferate. The underlying physical mechanism is the related liberation of vacancies that can lower their kinetic energy by delocalizing around the dislocation line. As a consequence the dislocations form a quantum dislocation melt 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 in the elastic properties of the system around T_J . This could explain the shear modulus anomaly recently reported by Day and Beamish [22] and other elastic anomalies, perhaps even a partial decoupling of the solid in a oscillating pendulum experiment. If $T_c < T_J$, 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 jog-energy can be increased substantially by increasing the pressure, one should see a complete suppression of both elastic anomalies and supersolidity when $E_J(P) > \zeta(P)T^*$. On the other hand, one

should also take into account how the initial concentration of dislocations changes upon increasing the pressure. The mechanism 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 [27]. 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 [28]. 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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Note added

Very recently, L. Pollet et al. posted a preprint [arXiv:0805.3713] [31] where the role of shear stress on the creation energy of vacancies is studied numerically. These authors find that beyond a certain shear stress this energy becomes negative, and speculate that the shear stresses present around dislocations might be enough for vacancies to appear spontaneously. Although different in the details, this scenario is quite similar to the one discussed above.

Appendix A

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 [30] $K = T^* g \exp(-S_0)$, 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, $(\beta K)^n / n!$ [30]. 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 $F_v(T = 0) = E_v - 6T^*T$.

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