Underlying Mechanism for the Giant Isochoric Compressibility of Solid ^{4}He: Superclimb of Dislocations

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In the experiment on superfluid transport in solid ^{4}He [Phys. Rev. Lett. **100**, 235301 (2008)], Ray and Hallock observed an anomalously large isochoric compressibility: the supersolid samples demonstrated a significant and apparently spatially uniform response of density and pressure to chemical potential, applied locally through Vycor "electrodes." We propose that the effect is due to superclimb: edge dislocations can climb because of mass transport along superfluid cores. We corroborate the scenario by *ab initio* simulations of an edge dislocation in solid ^{4}He at $T = 0.5$ K. We argue that at low temperature the effect must be suppressed due to a crossover to the smooth dislocation.

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At present, the experimental search for a supersolid in ^{4}He proposed in Refs. [1] focuses mostly on torsional oscillator experiments [2], and on attempts to detect pressure driven nonplastic flow [3]. Direct superflow through solid ^{4}He has been observed only in the experiment by Ray and Hallock [4,5]. The absence of flow at temperatures above $T \approx 0.6$ K is a strong argument against the liquid channels scenario [6,7] and in favor of superfluidity along dislocation cores or grain boundaries. Theoretically, a superfluid dislocation network can manifest itself as a genuine superfluid or be in the Shevchenko state [8], characterized by anomalously low viscosity (due to phase slips) mimicking superfluidity even at relatively high temperatures, $T > 0.1$ K, well above the actual transition determined by the dislocation density.

The "UMass sandwich" setup of Refs. [4,5] differs from the pressure driven cells [3] by feeding superfluid ^{4}He into the crystal through Vycor "electrodes." This means that the chemical potential μ is the physical quantity relevant to the external perturbation applied to the crystal. An insulating (i.e., nonsupersolid) crystal has to be isochorically incompressible: $\chi \equiv (dn/d\mu)_V = 0$; that is, its density n should demonstrate no response to infinitesimal, quasi-static changes of μ [9]. As long as the creation of a vacancy or interstitial is forbidden by finite energy gap, the only way the density of a crystal can react dynamically to a small change in the chemical potential, $\delta\mu$, is by creating or removing crystalline layers. This requires nucleation times exponentially large in $|\delta\mu|^{-1}$. Thus, at temperatures T much smaller than the vacancy or interstitial gaps, χ associated with thermally excited vacancies and interstitials is exponentially small. Consistent with these arguments, all nonsupersolid samples of Refs. [4,5] have $\chi = 0$: two pressure gauges monitoring the solid showed no response to a change in μ by the Vycor electrodes.

Supersolids have no vacancy (interstitial) gap [10] and are thus genuinely isochorically compressible: $\chi \neq 0$. One may argue that χ should scale linearly with the superfluid fraction ρ_s since both are due to zero-point vacancies (interstitials). Given the extremely low value of $\rho_s \lesssim 10^{-5}$ following from estimates based on the observed supercritical flux (see Refs. [4,5] for more details), one does not expect a noticeable χ. However, the observed density or pressure response to μ was by several orders of magnitude larger than expected. We refer to this as the effect of giant isochoric compressibility. Remarkably, the response was apparently spatially homogeneous, since two pressure gauges attached to two ends of the solid typically showed equal variations (but different absolute values; most samples were characterized by a static pressure gradient) [4,5].

In this Letter, we argue that the microscopic phenomenon behind the effect of giant isochoric compressibility is the superclimb of superfluid edge dislocations, that is, climb controlled by superfluid flow along their cores. Our idea is that significant and spatially uniform mass accumulation in the bulk of supersolid ^{4}He is due to the synergy between (i) the presence of a superfluid network capable of delivering ^{4}He atoms from Vycor electrodes to distant bulk regions and (ii) the presence of edge dislocations, whose superclimb is responsible for the density or pressure change.

We corroborate our scenario by *ab initio* simulations showing that edge dislocation with Burgers vector along the hcp C axis has superfluid core (cf. superfluidity in the core of a screw dislocation [11]), and that it can climb in response to $\delta\mu$. We argue that at low T the climb must be suppressed due to a crossover from a rough to a smooth dislocation [12]. This prediction is a manifestation of the structural evolution of dislocations with temperature, and is important for experimental validation of the scenario. While superflow is a necessary condition for superclimb, the dislocation must also have a finite density of jogs to allow for thresholdless climb. Otherwise, a finite gap Δ for creating jogs will protect the dislocation from shifting significantly in response to small $\delta\mu$.

The effect of giant isochoric compressibility is one of the novel properties emerging in the "quantum metallurgy" [13] context. These properties have long been discussed in the past; for example, it was speculated that quantum dislocations should be characterized by "thick" (roughened) cores due to zero-point motion [14]. An important role of quantum roughening of dislocations in the torsional oscillator response has also been proposed in Refs. [15,16]. Superclimb is a quantum analog of classical high-T climb due to thermally activated flux of vacancies toward, away or along the cores (pipe diffusion) [17] which adds (removes) atoms to (from) the extra plane forming the edge dislocation, so that the dislocation core shifts along the extra-plane direction. Obviously, at low T, the activated mass flow is exponentially suppressed and quickly becomes negligible.

Dislocations can also glide which requires no mass influx. In Ref. [12] it was shown that gliding dislocations are smooth at $T = 0$ because Coulomb-type interactions between shape fluctuations [18,19] induce an energy gap $\Delta_{\rm glide}$ with respect to creating a pair of kinks in Peierls potential. Hence, thresholdless glide of a dislocation can effectively occur only at T comparable with $\Delta_{\rm glide}$. This gap is also related to shear modulus stiffening at low T [20]. Similarly, dislocations have a gap Δ for creating a pair of jogs at $T = 0$, which leads to a suppression of climb (and χ) at low T. The values of Δ can be quite different from $\Delta_{\rm glide}$ because the jog-antijog deconfinement couples to fluctuations of the superfluid density leading to an additional mechanism for the gap formation.

Model of climbing superfluid dislocation.—We introduce a coarse-grained description of an edge dislocation with superfluid core oriented along the X axis in terms of the core displacement $y(x, \tau)$ along the Y axis (in the climbing direction), perpendicular to the Burgers vector which is along the Z axis. We assume small gradients and large displacements compared to the lattice spacing. Then, a coarse-grained density variation $\delta n(x, t)$ translates directly into a coarse-grained variations $\delta y(x, t) \propto \delta n(x, t)$. The proportionality coefficient is purely geometrical: adding one atom to the edge results in its displacement by a lattice period in the climb direction $\delta y(x, t) = a'$ and also in a density change $\delta n(x, t) = 1/a$, where a is the length of the unit cell along the core. Thus, $\delta n(x, t) = \xi \delta y(x, t)$ with $\xi \equiv 1/aa'$. This relation implies that for a superfluid dislocation the core displacement δy is the conjugate variable to the superfluid phase φ. The combined coarse-grained low-energy effective action in the imaginary time description reads ($\hbar = 1$)

$$S = \int_0^\beta d\tau \int dx[-i\xi y\dot{\varphi} + (\rho_s/2)(\partial_x\varphi)^2 - \mu\xi y] + S_d, \tag{1}$$

where the purely dislocation part of the action, S_d, is taken in the form of the Granato-Lücke string subject to Peierls potential [19,21]:

$$S_d = \int_0^\beta d\tau \int dx\left[\frac{n_1 v_d^2}{2}(\partial_x y)^2 - u\cos\left(\frac{2\pi y}{a'}\right)\right], \tag{2}$$

with n_1 being the linear mass density of the core, v_d standing for speed of sound along the string determined by shear modulus G: $v_d^2 \approx G/n_1$, and u denoting the strength of Peierls potential. In Eq. (2), the kinetic energy $\propto \dot{y}^2$ is neglected in the low-energy limit under the consideration. Full quantum mechanical description of the system based on calculating the partition function $\int DyD\varphi \exp(-S)$ in line with the approach of Ref. [12] will be presented elsewhere.

Apart from the Peierls term $\propto u$ [not to be confused with the sine-Gordon term where the argument would be $\propto \int^x y(x')dx'$], the quantized action (1) and (2) is a standard harmonic $(1 + 1)$-dimensional action. A renormalization-group analysis, similar to the one given in Ref. [12], shows that, at $T = 0$, the Peierls term has scaling dimension $\dim[u] = 2$ regardless of the parameters of the system, even if the long-range deformation potential forces are ignored. This means that the Peierls barrier is relevant at $T = 0$ and always leads to a finite gap Δ for the climb motion; i.e., the dislocation in its ground state is smooth. Thus, the cosine term can be expanded in powers of y around some equilibrium position $y_m = ma'$, $m = 0, \pm1, \pm2, \ldots$, and the gradient in the action (2) can be ignored in the low-energy limit. This reduces (1) to the standard 1D superfluid action [22]

$$S_1 = \int_0^\beta d\tau \int dx\left[-i\xi y\dot{\varphi} + \frac{\rho_s}{2}(\partial_x\varphi)^2 - \mu\xi y + \frac{g}{2}y^2\right], \tag{3}$$

with $g = u(2\pi)^2/a'^2$. This action describes superfluidity with speed of sound $v_1 = \sqrt{\rho_s g}/\xi \propto \sqrt{\rho_s u}$ with, practically, no climb response to $\delta\mu$: $\delta y = \xi\delta\mu/g$.

With increasing T, thermally excited jogs and kinks render Peierls potential less and less relevant, so that eventually it can be ignored. In this limit, the dislocation becomes rough, that is, similar to a free string [21], and the spatial gradient in Eq. (2) should be taken into account. The effective action (1) then becomes

$$S_2 = \int_0^\beta d\tau \int dx\left[- i\xi y\dot{\varphi} + \frac{\rho_s}{2}(\partial_x\varphi)^2 + \frac{n_1 v_d^2}{2}(\partial_x y)^2 - \mu\xi y\right]. \tag{4}$$

Equation (4) predicts an extremely strong quasistatic climb response: $\partial_x^2\delta y \propto -\delta\mu$ determined by the length of a free dislocation segment L (the crosslinking distance in the network), so that a typical displacement $\delta y \propto L^2 \delta\mu$. This implies that the resulting specific compressibility is independent of the dislocation density $\approx 1/L^2$, provided the network is uniform over the whole sample. Indeed, the added amount of atoms per each "elementary" cube of the side L is $\sim aL\delta y \propto L^3 \delta\mu$. Thus, the added fraction of atoms per unit volume is independent of L.

The superfluid component also demonstrates an anomalous behavior: small oscillations obey

$$\ddot{\varphi} - \eta \partial_x^4 \varphi = 0, \qquad \eta \equiv \frac{\rho_s n_1 v_d^2}{\xi^2}, \tag{5}$$

meaning that the spectrum of superfluid excitations is not soundlike anymore. It is described by a quadratic dispersion $\omega = \sqrt{\eta} q^2$, where q is the momentum along the dislocation line. Here we point out two qualitative predictions of the model (1) and (2): (i) suppression of the climb at $T < \Delta$, and (ii) dramatic softening of superfluid phonons at $T > \Delta$.

Numerical results.—Our *ab initio* Monte Carlo (MC) simulations were based on the worm algorithm [23]. The most important numerical finding is that edge dislocations with Burgers along the hcp axis have superfluid cores in solid ^{4}He. Our example is based on the dislocation with the core along the X axis. Figures 1 and 2 show snapshots of atomic positions in a typical MC configuration, along C axis and along the core. Particles outside the circle, Fig. 2, were pinned to their classical lattice positions and provided boundary conditions for the simulation cell. Since the hcp structure has two atoms in the unit cell, two extra half-planes are involved. For studied dislocation this leads to its splitting into two partials with the fcc fault forming in between [17]. The splitting is so large that the fault does not fit the simulation cell—one of the partials has moved all the way to the cell boundary. A direct simulation of the fcc fault yielded an unmeasurably small (within our accuracy) fault energy <0.1 K/atom, meaning that the splitting (proportional to the inverse of the fault energy) is indeed expected to be as large as $\geq$150–300 Å. Hence, physical properties of both partials are essentially independent from each other.

Under these circumstances we performed extensive simulations of a single partial attached to the fault. The rectangular simulation cell contained from 600 to 3400 particles with periodic boundary conditions along the core. In perpendicular directions a boundary of pinned ^{4}He atoms surrounding a cylinder of radius R provided the necessary boundary conditions for the simulated sample of solid ^{4}He containing the partial dislocation at the center and the fault extending in the positive Y-direction. Depending on R, the number of actually simulated particles varied from 270 to 1700. Superfluid properties were detected by observing winding exchange cycles along the cylinder axis (X axis). The core response to μ has been studied by tracing the position of the maximum $Y(\mu)$ of the columnar superfluid density map in the (Y, Z) plane [24].

The core position exhibited strong continuous response to variations of μ. The slope $dY/d\mu$ was larger in bigger cells indicating that at the simulated temperature $T =$ 0.5 K it is controlled by the image forces provided by the boundary conditions. At fixed μ, the configuration-to-configuration fluctuations of the core position were as large as several unit cells. Remarkably, the exchange-cycle map does not show any visible modulation with the lattice period in the Y direction (while the structure in the Z direction is clearly seen), see Fig. 3, meaning that the core is loosing its crystalline structure locally and the Peierls potential in the climb direction is negligible under the simulated conditions. A systematic numeric study of the Peierls gap effects emerging at much lower temperatures and in larger system sizes remains a major computational challenge.

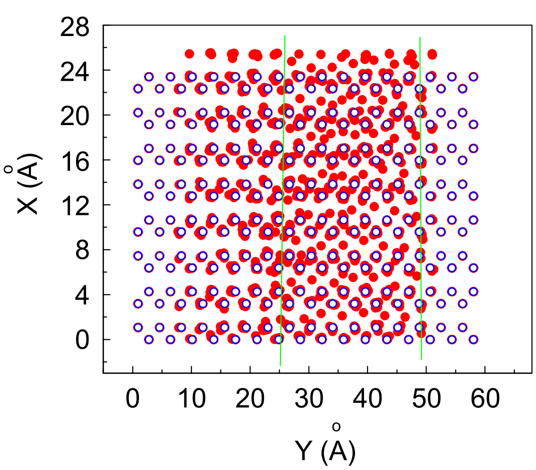

FIG. 1 (color online). Columnar view of a typical MC configuration along the C axis: filled red dots show atomic positions; open blue circles indicate an ideal lattice; vertical solid green lines mark positions of the partial cores. The fcc fault is between these two lines. The superfluidity occurs along the green lines.

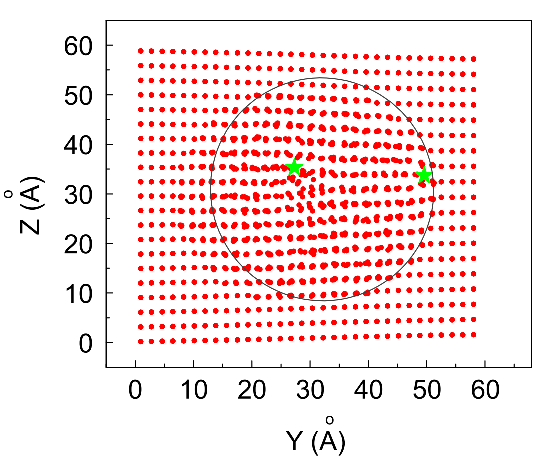

FIG. 2 (color online). Columnar view of the same MC configuration (as in Fig. 1) along the cylinder axis. The circle marks the simulation cell where particle positions have been updated. The superclimb occurs in the "horizontal" plane. Green stars mark positions of the two partials.

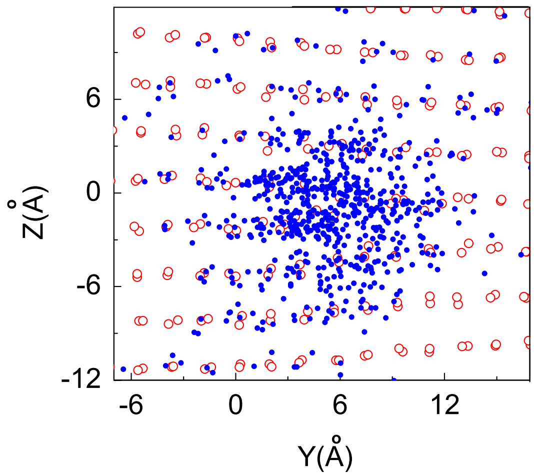

FIG. 3 (color online). A columnar snapshot of atomic positions (open red dots) in the vicinity of the partial core (at the center) superimposed with the map (solid blue dots) of winding exchange cycles responsible for superfluid properties along the core, X axis. Note that (i) the map extends over several unit cells (≈ 3.67 Å), and (ii) it has no visible structure in the Y direction, implying negligibly small Peierls potential for climb at the simulated temperature.

Crucial data can be obtained experimentally with the "UMass sandwich" setup, that potentially allows one to work at T of few tens of mK [25]. Since the quantity of interest is the isochoric compressibility (as a function of T), one can use the superfluid syringe experimental protocol, when both Vycor electrodes are being operated at one and the same chemical potential and are used exclusively to inject atoms into the solid, rather than to induce a dc flow. Such measurements near 400 mK have been already done [26].

Summarizing, we present strong *ab initio* evidence and a coarse-grained analytic description of the edge dislocation climbing in solid ^{4}He, assisted by superfluidity of its core. This phenomenon yields a natural microscopic interpretation for the effect of giant isochoric compressibility accompanying superflow in the experiment by Ray and Hallock [4,5]. Theoretically, we argued that at low T, the superclimb, and, correspondingly, the effect of giant isochoric compressibility, must be suppressed due to a crossover to a smooth dislocation. Experimental observation of the suppression, feasible within the "UMass sandwich" setup, might yield strong support for the proposed scenario bridging "quantum metallurgy" and supersolidity. The superclimb effect can also lead to high mobility of small dislocation loops (with Burgers vectors along C axis) made of one partial surrounding an fcc fault. Such loops could be plenty in real samples (cf. [17]), and implications of their presence are yet to be investigated.

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