Quantum physics of kinks of dislocations

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We study the physics of kinks of dislocation; their possible wavelike properties and energetics. We discuss their Bose-Einstein condensation and the possible connection with results in recent torsional oscillator experiments. The possible connection with our recent proposal of grain-boundary roughening in this system is clarified.

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I. INTRODUCTION

Since the discovery of an increase in torsional oscillator (TO) frequency in solid ^{4}He at around 200 mK,[1] there have been renewed interests in its low-temperature physical properties. Much recent focus is on the role played by defects in this system.[2–8] For example, it is suggested that large-angle grain boundaries can exhibit superfluid behavior.[4,8] Dislocation cores are found to exhibit superfluid behavior.[6,9]

To study the physical properties in the solid phase, it is important to understand the nature of the elementary excitations. One such type of excitations is phonons. Defects such as dislocations can also form in the solid phase. Dislocations are linelike objects. Their motion is through the motion of kinks whereas phonons do not carry mass currents, defects can.

If the temperature is low enough, the motion of defects can exhibit wavelike behavior. Quantum vacancy waves were discussed in the context of three-dimensional (3D) solid He.[10–13] In this paper we study the physics of kink waves; their Bose-Einstein condensation and discuss their possible connection with the experimental results. The possibility that kinks of dislocations may play a role has previously been raised by de Gennes.[14] Our calculation is very different from his, however.

Kink waves differ from vacancy waves in a very important aspect. The location of the kink can be at any place along the dislocation. Vacancies are located by the position of the missing particle and can only be at discrete lattice sites. Thus the calculation of properties of vacancy waves involve tunneling between these states[13] and is different from the calculation presented below. We have recently studied dislocation waves in a two-dimensional (2D) electron solid and their effect on quantum melting.[15] The work reported here is motivated by those studies.

We find that even though there is an elastic-energy cost to create a kink, there are two quantum contributions which lowers the energy and results in a finite density of the kinks even at zero temperature. There is a long-range strain-induced interaction between kinks on different dislocations. As a result the dispersion in the "perpendicular" direction is proportional to the first power of the wave vector $k_\perp$. Fluctuations are suppressed. The 3D mean-field Bose Einstein condensation (BEC) temperature T_c of the kinks can be quite high.

The BEC of the kinks makes possible dissipationless movement of the dislocation lines. The motion of a dislocation corresponds in part to a circular motion of many He4 atoms, each by a different amount. An estimate of the fraction of He4 atoms can be obtained by weighting with respect to the strains. With this the corresponding "superfluid fraction" due to the motion of the dislocation lines is consistent with current experimental results in TO experiments. The dislocation motion does not produce any net linear motion of the atoms and thus will not generate any direct superflow.

Recently Day and Beamish (DB) (Ref. 3) found a change in the shear modulus with the same temperature dependence as that for the decoupling in TOs. They ascribe this to a change in the mobility of dislocations. In our picture, this increase in mobility as temperature is increased is not directly related to the BEC of the kinks but is due to a different phenomenon, for example, the grain-boundary roughening transition involving fluctuation of the dislocation lines perpendicular to the Burger's vector.[16] This increased movement of the dislocation lines creates a large phase fluctuation and interrupts the BEC of the kinks. The experimental transition observed in the TO experiments is related to this grain-boundary roughening transition. The actual BEC transition, which would have occurred at a higher temperature, cannot be observed. Our view of the effect of impurities is similar to the conventional view, that they affect the mobility of the dislocation lines. For example, we find that the grain-boundary roughening transition temperature is very sensitive to the magnitude of the dislocation core energy and have speculated that He3 impurities may change its value.[16] We now describe our results in detail.

II. ELASTIC DISTORTION DUE TO A KINK

We first discuss the elastic distortion of the solid due to the presence of a kink in the dislocation. The elastic distortion $\mathbf{u}(r)$ due to a dislocation along the z direction with its core at (c_x, c_y, z) has been much discussed in the past.[17] u is determined by the condition of local equilibrium subjected to the constraint that the line integral of the displacement field around the core is equal to the Burger's vector. The distortion of the lattice due to a core given by a trajectory $[c_x(z), c_y(z), z]$ can be obtained from its "elastic equation." For the case with the Burger's vector in the x direction we get

$$\nabla^2\mathbf{u} + \nabla\nabla\cdot\mathbf{u}/(1-2\sigma) = -b\mathbf{e}_y\delta[r_\perp - c(z)], \qquad (1)$$

where σ is the Poisson's ratio of the solid and $\mathbf{e}_y$ is a unit vector in the y direction. We shall solve the elastic equation

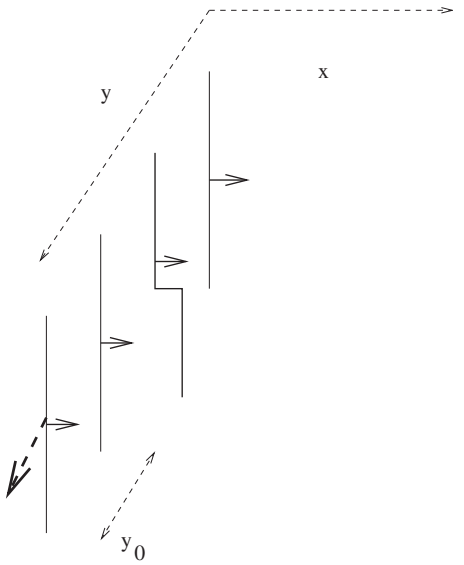

FIG. 1. Schematic of a grain boundary. The solid arrows indicate the directions of the Burger's vector and the kink of dislocations. The dashed arrow indicates the direction of the movement of dislocation for the roughening transition.

in Fourier space with $u(r)=\int d\mathbf{p}u(p)\exp(-ip\cdot r)$ and $u(p)=\int d\mathbf{r}u(r)\exp(ip\cdot r)/(2\pi)^3$. The Fourier transform of the displacement u_s of a single straight dislocation where $\mathbf{c}$ is not a function of z is given by

$$\mathbf{u}_s(q_\perp)=[\mathbf{e}_y/q_\perp^2-0.5(1-2\sigma)/(1-\sigma)\mathbf{q}_\perp q_y/q_\perp^4]/(2\pi)^2.$$

We are interested in a dislocation with a kink at $z=c_z$ where $c_x(z)$ changes by a lattice constant a, as is illustrated in Fig. 1. The details of our calculation are described in Appendix A

We find that the displacement is a sum of the bare displacement $\mathbf{u}_0$ of a dislocation with a kink and a correction term $\mathbf{u}_1$,

$$\mathbf{u}=\mathbf{u_0}+\mathbf{u_1}. \tag{2}$$

The "bare" displacement corresponds to that of a dislocation centered at $\mathbf{c}_\perp$ for $z<0$ and at $\mathbf{c}_\perp+a_0\mathbf{e}_x$ for $z>0$, where $u_0(z,r_\perp)=u_s[r_\perp-\mathbf{e}_x\theta(z-c_z)-c_\perp]$,

$$\mathbf{u}_0(q_\perp,z)=\mathbf{u}_s(q_\perp)\exp[iq_\perp\cdot c_\perp(z)], \tag{3}$$

where $\mathbf{u}_0$ by itself does not satisfy Eq. (1). An additional term is required. This is given by

$$\begin{aligned}\mathbf{u}_1(q)=&-i\{\mathbf{e}_z q_\perp\cdot s(q_\perp)+q_z\mathbf{s}(q_\perp)\\&-(1-2\sigma)q_z\mathbf{q}q\cdot\mathbf{s}(q_\perp)/[(1-\sigma)q^2]\}\\&\times\exp(-iq_z c_z)/(2\pi q^2),\end{aligned}$$

$$\mathbf{s}(q)=\mathbf{u}_s(q_\perp)\exp(iq\cdot c_\perp)[\exp(iq_x a_0)-1]. \tag{4}$$

From this the elastic energy of a kink can be computed. Thus

$$E_{kink}^{elas}=\sum_k m\omega_k^2|u(k)|^2/2-E_{dis} \tag{5}$$

is the elastic energy of a kink; $E_{dis}=\Sigma_k m\omega_k^2|u_s(k)|^2/2\propto\log A$ is the strain energy of the straight dislocation, independent of c, We next examine the quantum corrections to the energy of a kink.

III. KINK WAVE

We find that the motion of kinks can be wavelike. Due to the quantum fluctuation in the position of the kink there is a reduction in its energy given by Eq. (10) below. In addition we obtain an estimate of the effective mass [Eq. (11) below] about one tenth the He4 mass. The calculation here is similar to our work on dislocation waves in 2D.[15] We describe this next.

The wave function of the solid with a kink located at position c can be estimated from the ground-state phonon wave function of the perfect solid $|G\rangle$

$$|G\rangle=\prod_k e^{(-b_k|\delta r_k|^2)},$$

where $b_k=m\omega_k/2\hbar$; δr is the deviation of the particles from their equilibrium positions; k stands for the wave vector $\vec{k}$ and polarization λ: $k=(\vec{k},\lambda)$. There has been much studies of phonons in the presence of defects.[18] The frequency of each mode in the continuum is expected to shift by a factor on the order of impurity density. In addition, there may be localized modes. Localized modes have energies in the phonon band-gap region. We are interested in low-energy excitations here and thus shall ignore these high-energy states.

A kink creates static distortions of the lattice $\mathbf{u}_i$ at site i. The wave function for a lattice with static distortion $\mathbf{u}$ is

$$|c\rangle=\prod_k e^{(-b_k'|\delta r_k+u_k^c|^2)}, \tag{6}$$

where $\vec{u}_k$ is the Fourier transform of the static displacement field due to the defect at the origin given by $u_{\vec{k}\lambda}^c=\vec{u}_k^c\cdot\vec{e}_{\vec{k}\lambda}$, $\vec{u}_k^c=\vec{u}_k e^{i\vec{k}\cdot\vec{c}}$; $\vec{e}_{\vec{k}\lambda}$ is the polarization vector of the phonon mode k. b_k' differs from b_k by a factor on the order of $1/N$. We approximate b_k' by b_k in the following.

The approximations used for this wave function are the following: (1) the static displacement field u_k is the one obtained from elasticity theory[17] and is exact only in the long-wavelength limit. (2) This wave function includes the correlations between the particles, which is already much better than a product of one-particle wave functions. Similar to the self-consistent phonon theory, we shall use renormalized phonons and force constants averaged over different interparticle separations in our numerical estimates. Thus some anharmonicity will be included. The details of this are described in Appendix B

In general the classical energy of the defect is a periodic function in the lattice, as is described by the Peierls' potential. We first ignore this periodic potential and incorporate it later on. In the absence of this periodic potential, the system is translationally invariant. It is straightforward to check that the eigenstates of H are just plane-wave states given by $|q\rangle=\Sigma_{c_z}e^{(iqc_z)}|c\rangle$. We find that the energy of this state (Appendix B) is given by

$$E_q=e_z(q_z^2/2w_z-1)/2w_z, \tag{7}$$

where

$$e_z = -m\sum_{k\lambda} \omega_{kl}^2 |i(\nabla_z u_b)_q e_{k\lambda}^b|^2/4, \tag{8}$$

$$w_z = -m\sum_{k\lambda} \omega_{kl} |i(\nabla_z u_b)_q e_{k\lambda}^b|^2/4\hbar. \tag{9}$$

This consists of a constant shift which can be interpreted as a quantum correction to the elastic energy due to the quantum fluctuation in the position of the kink at $q=0$

$$E_{wave} = -e_z/2w_z \tag{10}$$

and a term quadratic in momentum; from which we get an estimate of the effective mass

$$m_z^\star = 2\hbar^2 w_z^2/e_z. \tag{11}$$

We next discuss other contributions that provide for additional lowering of the kink energy.

IV. RENORMALIZATION OF THE ZERO-POINT ENERGY OF THE PHONON FIELD

When a kink is created, the zero-point energy is changed. This zero-point energy change is always negative. The larger the mean-square lattice vibration, the larger this contribution is. At a certain density when the mean-square lattice vibration becomes big enough it can become energetically favorable to create kinks. This idea has been exploited by us in the study of quantum melting of the 2D electron crystal.[15] We generalize this calculation and evaluate this change in the zero-point energy for our case here.

The Hamiltonian of the system is the sum of the kinetic energy and the potential energy $\Sigma_{ij}V(ij)$, where V is the interparticle potential between the He atoms. A kink creates a static displacement u of the lattice positions. The change in the Hamiltonian due to u can be written in a Taylor-series expansion in the difference of the static displacement as, to lowest order in u, $\delta H=\Sigma_{ij}[V(r_{ij}+u_{ij})-V(r_{ij})]=\Sigma_{ij}A(ij)u(ij)$, where $u(ij)=u(R_i)-u(R_j)$. Here $r_{ij}=\delta r_{ij}+R_{ij}$ is the sum of the phonon relative displacement and the equilibrium separation R_{ij} of the corresponding perfect lattice. The kinetic energy is just $\Sigma m(\delta\dot{r})^2/2$ and remains the same as the unperturbed Hamiltonian.

A can be written as a power-series expansion in the phonon coordinates δr. The term $u\delta r\nabla\nabla V$ is zero. $u\nabla\nabla V$ is the elastic force due to the displacement u. This net force is zero because that is how the displacement u of a dislocation with a kink is determined. The lowest-order term is quadratic in δr,

$$\delta H = \sum_{ij} [u_{ij}\delta r_{ij}\delta r_{ij}\nabla\nabla\nabla V(r_{ij})]/4.$$

The first-order correction to the energy, $\langle 0|\delta H|0\rangle$ is zero because u_{ij} changes sign under a parity transformation in the xy plane. The second-order correction to the energy $\Delta E=E_{\rm ZPE}$ is just $\Sigma_i|\langle i|\delta H|0\rangle|^2/(E_0-E_i)$ and can be written as

$$E_{\rm ZPE} = \sum_{kq;l,p=1,3} \hbar/(8m^2N)|e_{lk}e_{p,-k-q}u_q[\bar{V}(k)+\bar{V}(q) + \bar{V}(-q-k)]|^2/\omega_{lk}\omega_{p,-k-q}(\omega_{lk}+\omega_{p,-k-q}), \tag{12}$$

where $\bar{V}(k)=\Sigma_R \exp[i\vec{k}\cdot\vec{R}]\nabla\nabla\nabla V(R)$, e_{kl} is the polarization vector for branch l at momentum k, ω is the phonon frequency. This term is on the order of

$$E_{\rm ZPE} \approx -u^2\langle\delta r^2\rangle^2(V''')^2/\langle\delta r^2\rangle V''.$$

The strain energy of the kink is on the order of

$$E_{elastic} \approx u^2 V''.$$

The ratio of these two energies is given by

$$E_{\rm ZPE}/E_{elastic} \approx -\langle\delta r^2\rangle(V'''/V'')^2.$$

Thus the larger the zero-point vibration, the higher is the magnitude of this ratio.

V. NUMERICAL ESTIMATES

We focus on hcp He4 crystal with a molar volume of 24cc. Our estimates for the energy of the kink is a sum of three terms

$$E_{kink} = E_{kink}^{elas} + E_{wave} + E_{\rm ZPE}, \tag{13}$$

where the three different contributions are given in Eqs. (4), (9), and (11). In this paper, we shall perform simple estimates to demonstrate that E_{kink} can become negative and defer detailed sophisticated more accurate calculations to future work. We think our estimate for the relative magnitude of the different contributions is more accurate than the magnitude of the individual terms.

The calculation of E_{kink} involve estimates of the renormalized phonon frequency and force constants. The He4 system exhibits large zero-point fluctuations with the root-mean-square lattice fluctuation $\delta r_{rms}=\langle(\delta r)^2\rangle^{1/2}$ on the order of $0.27a$.[19] We have obtained our result by averaging V and its derivatives over the distribution of possible interparticle separation. We describe this next.

The average interaction potential $\langle V\rangle$ is, in the self-consistent phonon approximation, given by

$$\langle V(R+\delta r)\rangle = \int d^3 r V(r)\exp\left[-\sum_i (R-r)_i^2/2\langle\delta r_i^2\rangle\right]/N,$$

where $\langle\delta r_i^2\rangle=\hbar/(2MN)\Sigma_{q,\lambda}|\mathbf{e}_{q\lambda,i}|^2(1-\cos q\cdot R)/\omega_{q\lambda}$ is the fluctuation of the relative displacement along the three principle axis (longitudinal and transverse). Here λ is a label for the different phonon branches. Of course δr_i is slightly different from the mean-square displacement given by

$$\delta r_{rms}^2 = \hbar/(2MN)\sum_{q,\lambda} 1/\omega_{q\lambda}. \tag{14}$$

We assume that the transverse relative fluctuation $\langle\delta r_t^2\rangle=(\delta r_{rms})^2/3$ and have used the experimental value of $0.27a$ for the estimate of δr_{rms}. The longitudinal relative displacement is smaller than δr_{rms} because of the repulsion between

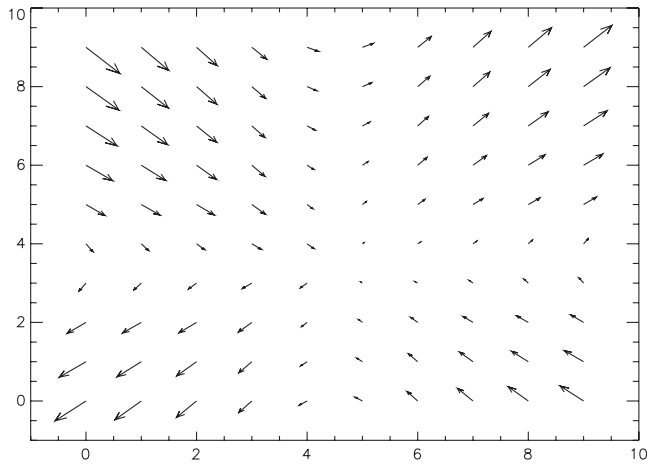

FIG. 2. Schematic of the displacements of the atoms multiplied by the perpendicular radius, $r_\perp \delta u_s(\mathbf{r})$, as the dislocation is moved from $(5,4.5)a_0$ to $(6,4.5)a_0$.

the He atoms. Sophisticated approaches involve introducing Jastrow factors and t matrix corrections. Here we phenomenologically set δr_1^2 to be equal to $\alpha \delta r_{rms}^2/3$ with α less than 1. α is determined from the condition that δr_{rms} as given in Eq. (14) is equal to the experimental value. We found that $\alpha=0.9$

The sum was performed with 20 250 mesh points. With these we found that $E_{kink}^{elas}/k_B=6.8$ K, $E_{wave}/k_B=-3.5$ K, $E_{\mathrm{ZPE}}=-4.5$ K; $m_z^*/m=0.05$. E_{kink}/k_B, the sum of the three contributions, is equal to -1.2 K and is negative. Quantum effects make it energetically favorable to create kinks.

VI. SUPERFLOW

If the temperature is low enough a collection of kinks will form a Bose-Einstein condensate. We expect that the dispersion for the excitation to become linearly proportional to the wave vector in all directions in the long-wavelength limit. This enables movement without damping of the dislocation in the direction along the Burger's vector, as is illustrated by the solid arrows in Fig. 1. Because of the long-range elastic strain caused by a dislocation, the motion of a single dislocation corresponds to the motion of many He4 atoms, each by a different amount. The fraction of He4 atoms moved is much higher than that indicated by the density n_d of the dislocations. An estimate of the fraction of He4 atoms can be obtained by weighting with respect to the strains. We describe this next.

As a single dislocation is moved by a distance δc, the He4 atom a distance $r_\perp$ away from it is moved by an amount on the order $g\delta c$ with $g=a_0/(2\pi r_\perp)$. This is illustrated in Fig. 2 where we show the displacements of the atoms multiplied by the perpendicular radius, $r_\perp \delta u_s(\mathbf{r})$, as the dislocation is moved from $(5,4.5)a_0$ to $(6,4.5)a_0$. Because the experimental system is imperfect there is a length scale L_m over which the displacements from the different dislocations act constructively. This can be due to the dislocation loop size or the mosaic size. The displacement of a He4 atom comes from the sum of displacements from the different dislocations is on the order of $n_d 2\pi \int_0^{L_m} r_\perp dr_\perp g \approx f_0 = n_d L_m a_0$. The effect of the dislocations is not the dimensionless quantity $n_d a_0^2$ but is amplified by a factor of L_m/a_0 because of the long-range nature of the strains.

As a He4 atom is moved in a TO because of the dislocations, its velocity v is reduced by the amount $\delta v = f_0 v$. The kinetic energy of this atom is correspondingly reduced by a fraction $2f_0$. We interpret this as the superfluid fraction observed experimentally. With experimental estimates of[2] $L_m \approx 20$ μm and n_d ranging from[20] 6×10^9 to[21] $10^6/\mathrm{cm}^2$, we get f ranging from 72% to 0.07%. This is within the range on the order of magnitude of the superfluid fraction experimentally observed.

DB (Ref. 3) found a change in the shear modulus with the same temperature dependence as that for the decoupling in TOs. They ascribe this to a change in the mobility of dislocations. We recently studied the roughening of small-angle grain boundaries consisting of arrays of dislocations[16] and found two transitions, corresponding to fluctuations of the dislocations along and perpendicular to the boundaries. These correspond to motion perpendicular and parallel to the Burger's vector.[22]

We interpret the low-temperature grain-boundary roughening transition as corresponding to the one observed by DB. (The higher roughening transition at around 1 K corresponds to the onset of rotational fluctuation in x-ray measurements by Burns *et al.*[2]) After the roughening, phase disorder is introduced and the BEC of the kinks is no more. The actual Bose-Einstein transition is never observed. That fluctuation of the dislocation can destroy phase coherence has been pointed out by Balibar.[23]

For the roughening transition, the direction of motion for this type of fluctuation is indicated by the dotted arrow in Fig. 1 It is perpendicular to the kink motion discussed here and corresponds to a different degree of freedom. When the kinks form a BEC, their dissipationless motion may have an effect on the elasticity constant but presumably the change is less than that caused by the grain-boundary roughening transition.

In the conventional picture of Bogoliubov, the interaction with the condensate changes the single-particle dispersion from quadratic in k to linear in k. We do not know if this will also provide a correction to the shear modulus.

Impurities, such as He3, are found to have a very important effect on the transition. Our view on this is similar to the conventional view that the impurities affect the mobility of the dislocation lines. For example, we find that the lower grain-boundary roughening transition temperature is very sensitive to the magnitude of the dislocation core energy and have speculated that He3 impurities may change its value.[16]

Very little pressure-driven direct superflow was found in this system.[24] As can be seen from Fig. 2 the effect discussed here contains a contribution corresponding to a circular motion but do not contribute to a linear flow. More precisely, for the linear superflow, the quantity of interest is $\langle \delta v \rangle = \int d\mathbf{r}\, \delta \mathbf{v}$. As is mentioned above, the velocity change is proportional to $\delta \mathbf{U}(r) = \Sigma_j \delta c_j \cdot \nabla u(r-c_j)$. If the kinks form a BEC, then we expect δc_j to be the same for different j. For a uniform distribution of dislocations, $\delta \mathbf{U}$ and hence $\delta \mathbf{v}$ changes sign under a parity transformation. Thus $\langle \delta v \rangle$ becomes small.

On the other hand, for a circular motion with angular velocity ω, the velocity $\mathbf{v}(\mathbf{r})$ of a particle at position $\mathbf{r}$ is given by $\mathbf{v}=\mathbf{r}\times\omega$. The total kinetic-energy change due to the dislocations is thus given by $\Delta E=m\int d\mathbf{r}\mathbf{v}\cdot\delta\mathbf{v}=m\int d\mathbf{r}\omega\cdot\mathbf{r}\times\partial_{\mathbf{x}}\mathbf{u}\delta c_x$. For example, for a single dislocation $r\times\partial_x u_s=[-5\cos^2(\phi)/4+1.5\cos^2(\phi)\sigma+0.5-\sigma]/(1-\sigma)$. This remains finite after the integration over ϕ is carried out. Because $\mathbf{v}$ also changes sign under a parity transformation, the integral for ΔE remains finite.

We next estimate the Bose-Einstein condensation temperature T_c of the kink waves.

VII. T_c

Our goal is not to estimate the BEC transition temperature T_c very accurately but to show that they can be quite high. As is well known, there is no BEC in one dimension. This comes about because the kinetic-energy cost for the phase fluctuation in the transverse direction is zero. We envision that there is a collection of dislocations with a finite density of kinks on each one. Furthermore there are two types of kinks of opposite "charges," corresponding to movement of the cores in opposite directions.

There has been much studies of the strain-induced interaction between defects in solids.[25] Physically this long-range (1/distance) interaction comes from the elastic-energy difference for kinks at different locations. The kinetic-energy cost for transverse phase fluctuation becomes nonzero when the strain-induced long-range interaction between kinks on different dislocations is taken into account. The problem then becomes a three-dimensional problem.

Shevchenko[26] has considered possible superfluidity of a network of one-dimensional lines and suggests that the relevant length scale for the effect of dislocation on the elasticity of the lattice may be the distance between nodes on a dislocation network. In his model, there is no interaction between the bosons on different lines.

For the different effect discussed here the interaction between kinks is not mediated along the dislocation lines. The interaction is mediated by the disturbance (strain) caused by the kinks on the whole lattice. The model becomes basically three dimensional. Hence the relevant distance is not the distance between nodes of the dislocation network.

More precisely, this elastic interaction between the kinks located at c_i and c_j is given by $\Sigma_{i,j}V(c_i-c_j)$ with $V(c)=\Sigma_q V_q[\cos(q\cdot c)-1]$, where $V_q=m\omega_q^2|u_q|^2=O(1/q^2)$. This interaction provides for a self-energy correction and an effective mass in the transverse direction. The full treatment of this problem is beyond the scope of the present paper. Here we estimate the contribution to lowest order in V. There is no lowest-order direct term because the system is "electrically neutral." The lowest-order exchange term for a state with wave vector $\mathbf{k}$ is given by $E_{ex}(k)=+\Sigma_{k'}V_{k-k'}n(k',T)$, where $n(k',T)$ is the occupation number for state k' at temperature T. This expression differs by a sign from that of the electron gas because the statistics is different. We estimate the magnitude of this contribution by replacing $V(k)$ by $1/k^2$. The details of this is described in Appendix C

We find E_{exch} is a sum of a constant term and k-dependent terms. The constant term is on the order of $E_{elas}na_0/y_0$ (n is the linear kink density) and thus is small. In addition we find the lowest-order k-dependent terms are on the order $E_{elas}a_0k_\perp$ that is proportional to the first power of $k_\perp$ (not $k_\perp^2$) and terms on the order of k_z^2. This result comes from the long-range nature of V. In the low-wavelength limit (small k), the kinetic-energy cost for phase fluctuation is thus much higher than the ordinary case. Because fluctuations are suppressed T_c can indeed be high. Kinks of opposite "polarization" can in principle form a bound pair. We find that not to be likely. We explain this next.

We have numerically computed the strain-induced interaction $V(z)$ between kinks on the same dislocation separated by a distance z and have estimated the smallest possible value E_b of the sum of this and the kinetic energy of confinement, $\hbar^2/(2m_z z^2)$, for different distances z. We find that E_b is less than 0.01 K. Thus at $T=0.1$ K it is not likely that a bound state will occur.

VIII. EXTERNAL PERIODIC POTENTIAL

We next turn our attention to the effect of the Peierls' potential. Peierls argued that a dislocation at position x in a crystal of lattice constant a experiences a periodic potential given by[27]

$$V(x)=\frac{\mu a^2}{2\pi^2}\sum_{n=-\infty}^{\infty}\frac{a^2}{(na-x)^2+a^2}.$$

The Fourier series of this periodic potential can be written as follows:

$$V(x)=V_0+V_1\cos Gx+V_2\cos 2Gx+\cdots,$$

where $V_0=\mu a^2/2\pi$ and $V_p=(\mu a^2/\pi)\exp(-2\pi p)$.

The Peierls potential makes the kink locally stable and we have already assumed that. Here we examine the effect of this potential on the motion of the kink along the dislocation. The motion of a dislocation wave in this periodic potential can be treated in exactly the same way as that of an electron in a periodic crystal. We thus expect band gaps to open up at the zone boundary. For example, the largest gap $V_1=0.0018(\mu a^2/\pi)$ is a small fraction (0.002) of the typical energy we calculated here, the Peierls potential is a small perturbation on the motion of a kink along the dislocation.

IX. DISCUSSION

In this paper we study the physics of kink waves; their Bose-Einstein condensation and discuss their possible connection with the experimental results in recent TO experiments.

We find that even though there is an elastic-energy cost to create a kink, there are two quantum contributions which lowers its energy and results in a finite density of the kinks even at zero temperature. The mean-field BEC temperature T_c of the kinks can be quite high because of the long-range elastic interaction between kinks.

In Vycor[28] and other porous media,[29] TO experiments have observed qualitatively and quantitatively the same phenomena as in bulk. The model we propose here relies of the

motion of kinks, and the long-range results of that motion. The fact that the ends of a dislocation line are pinned is immaterial and at no point does the model invoke transport along the dislocation lines. Thus they are also applicable to those situations as well.

The BEC of the kinks makes possible movement of the dislocation lines. Because of the long-range strain caused by dislocations, their motion involves that of many He4 atoms. The corresponding superfluid fraction due to the motion of the dislocation lines is consistent with current experimental results.

We recently studied the roughening of small-angle grain boundaries consisting of arrays of dislocations[16] and found two transitions, corresponding to fluctuations of the dislocations along and perpendicular to the boundaries. The polarization of the kink of interest here corresponds to the glide motion of the dislocation parallel to the Burger's vector. We believe that the lower temperature roughening transition for vibration in the direction orthogonal to the polarization of the kink interrupts the BEC of the kinks.

Aleinikava *et al.*[30] recently studied the dislocation roughening transition and conclude that this cannot happen at zero temperature. They have not included the Casimir term in their consideration.

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APPENDIX A

We write the displacement as a sum of the bare displacement of a dislocation with a kink u_0 and a correction term u_1. The bare displacement corresponds to that of a dislocation centered at $\mathbf{c}_\perp$ for $z<0$ and at $\mathbf{c}_\perp+a_0\mathbf{e}_y$ for $z>0$. $\mathbf{u}=\mathbf{u_0}+\mathbf{u_1}$, where $u_0(z,r_\perp)=u_s[r_\perp-\mathbf{e}_y\theta(z-c_z)-c_\perp]$, u_s is the displacement of a single straight dislocation. We end up with a differential equation for u_1,

$$A\partial_z^2\mathbf{u}_0+B\mathbf{e}_z\partial_z\nabla\cdot u_0+[A\nabla^2+B\nabla\nabla\cdot]u_1=0,$$

where $A=1$ and $B=1/(1-2\sigma)$. Now $\partial_z\nabla\cdot u_0=\delta(z-c_z)\nabla\cdot s(r_\perp)$, $\partial_z^2u_0=\partial_z\delta(z-c_z)s(r_\perp)$, where $s=u_0^+-u_0^-$. We solve for u_1 in Fourier space as follows: $A\nabla^2\mathbf{u}_1+B\nabla\nabla\cdot\mathbf{u}_1=-F$, $F=A\partial_z^2\mathbf{u}_0+B\mathbf{e}_z\partial_z\nabla\cdot u_0=B\delta(z-c_z)\nabla\cdot s(r_\perp)+A\partial_z\delta(z-c_z)s(r_\perp)$, where $s(k_\perp)=u_s(k_\perp)[\exp(ikc_+)-\exp(ikc_-)]$. In Fourier space, $u_1(r)=\int d\mathbf{p}u_1(p)\exp(-ip\cdot r)$, we get

$$Ak^2\mathbf{u_1}(k)+B\mathbf{kk}\cdot\mathbf{u_1}(k)=G.$$

Here

$$G=\int d^3r\exp(ik\cdot r)F/(2\pi)^3=-i\exp(-ik_zc_z)[k_z\mathbf{s}(k_\perp)+\mathbf{e}_zk_\perp\cdot s(k_\perp)]/(2\pi).$$

We next evaluate $\mathbf{u}_1$.

For a matrix $Ak^2+B\mathbf{kk}$, its inverse is $\alpha/k^2+\beta\mathbf{kk}/k^4$ with $\alpha=1/A$, $\beta=-B\alpha/(B+A)=-B/(B+A)/A$. For the elastic equation $\alpha=1$, $\beta=-0.5(1-2\sigma)/(1-\sigma)$,

$$u_1(k)=-i(\mathbf{e}_zk_\perp\cdot s(k_\perp)+k_z\mathbf{s}(k_\perp)-(1-2\sigma)k_z\mathbf{k}k\cdot\mathbf{s}(k_\perp)/[(1-\sigma)k^2])\exp(-ik_zc_z)/(2\pi k^2),$$

Recall that

$$\mathbf{u}_s(q)=[\mathbf{e}_y/q^2-0.5(1-2\sigma)/(1-\sigma)\mathbf{q}q_y/q^4]/(2\pi)^2.$$

Thus

$$\mathbf{u}_0(q)=\mathbf{u}_s(q)\exp[iq\cdot c_\perp(z)].$$

APPENDIX B

The overlap of wave functions corresponding to defects located at positions c and c' is given by

$$\langle c|c'\rangle=\prod_k\int e^{[-b_k(|\delta r_k+u_k^c|^2+|\delta r_k+u_k^{c'}|^2)]}d\delta r_k.$$

This involves Gaussian integrals which can be easily done and we obtain

$$\frac{\langle c|c'\rangle}{\langle c|c\rangle}=\prod_k e^{(-b_k|\delta_k|^2/2)},$$

where $\delta_k=u_k^c-u_k^{c'}=u_k^0[e^{(i\vec{k}\cdot\vec{c})}-e^{(i\vec{k}\cdot\vec{c}')}]$. From now on, we divide, without mentioning it, all quantities by the normalization factor $\langle c|c\rangle$.

We next calculate the overlap integral $\langle c|H|c'\rangle$ of the renormalized harmonic Hamiltonian between defects located at c and c'. This is equal to

$$\begin{aligned}\langle c|H|c'\rangle&=\prod_k\int d\delta r_ke^{-b_k|\delta r_k+u_k^{c'}|^2}\\&\times\left(\sum_q\frac{P_q^2}{2m}+m\omega_q^2\delta r_q^2/2\right)e^{-b_k|\delta r_k+u_k^c|^2}\\&=\langle c|c'\rangle\left[E_0+\sum_k\frac{1}{2}m\omega_k^2(|u_k^c|^2+Re(u_k^c\delta_k^*)\right]=\langle c|c'\rangle\\&\times[E_0+E_{dis}+E_{kink}^{elas}+E_{cc'}]\,,\end{aligned}\tag{B1}$$

where $E_0=\Sigma_k\hbar\omega_k/2$ is the zero-point energy of the phonon field. $E_{dis}=\Sigma_km\omega_k^2|u_s(k)|^2/2\propto\log A$ is the strain energy of the straight dislocation, independent of c,

$$E_{kink}^{elas}=\sum_k m\omega_k^2|u(k)|^2/2-E_{dis}\tag{B2}$$

is the elastic energy of a kink; $E_{cc'}=\Sigma_km\omega_k^2|u(k)|^2\{\cos[k(c-c')]-1\}/2$. The contributions of E_0 and E_{dis} must of course be subtracted. The above expression is symmetric in c and c'. In general the classical energy of the defect is a periodic function in the lattice, as is described by the Peierls' potential. We first ignore this periodic potential and incorporate it later on. In the absence of this periodic potential, the system is translationally invariant. It is straightforward to check that the eigenstates of H are just plane-wave states given by $|q\rangle=\Sigma_{c_z}e^{(iqc_z)}|c\rangle$. The energy of these states is given by

$$E_q = \frac{\langle q|H|q\rangle}{\langle q|q\rangle} = \frac{\sum_c \langle 0|H|c\rangle e^{(iqc_z)}}{\sum_c \langle 0|c\rangle e^{(iqc_z)}},$$

$$\ln\langle 0|c\rangle = -\sum_k b_k |u(k)|^2 (1-\cos kc). \tag{B3}$$

The overlap integral dies off rapidly as c is increased. We thus use a small c expansion and obtain

$$\ln\langle 0|c\rangle = -0.5\sum_k b_k |u(k)|^2 (kc)^2.$$

Substituting the expression for b_k, we get

$$\ln\langle 0|c_z\rangle = -w_z c_z^2,$$

$$w_z = -m\sum_{k\lambda} \omega_{kl} |i(\nabla_z u_b)_q e^b_{k\lambda}|^2/4\hbar \tag{B4}$$

is on the order of the inverse mean-square quantum lattice vibration and measures the quantum fluctuation in the position of the kink. In the same way

$$E_{0c} = -e_z c_z^2,$$

$$e_z = -m\sum_{k\lambda} \omega_{kl}^2 |i(\nabla_z u_b)_q e^b_{k\lambda}|^2/4. \tag{B5}$$

E_q is thus given by

$$E_q = \frac{\sum_c -e_z c_z^2 \exp[-(w_z c_z^2 + iq_z c_z)]}{\sum_c \exp[-(w_z c_z^2 + iq_z c_z)]}. \tag{B6}$$

The denominator and the energy are finally given by

$$D = \left[\frac{\pi}{w_z}\right]^{(1/2)} e^{(-q_z^2/4w_z)},$$

$$E_q = e_z(q_z^2/2w_z - 1)/2w_z. \tag{B7}$$

APPENDIX C

We provide the numerical details of the calculation of the lowest-order exchange term for the self-energy for a state with wave vector **k** here. Now $E_{ex}(k) = +\Sigma_{k'} V_{k-k'} n(k',T)$, where $n(k',T)$ is the occupation number for state k' at temperature T. We expect $n = 1/[e^{(\hbar k_z^2/m_z - \mu)/k_B T} - 1]$. For one dimensional, μ is negative and finite, or the integral that determines the number of particle diverges. Thus for small k_z, n is a constant. n starts to decrease for $k_z > K$ where $\hbar^2 K^2/2m_z = k_B T$. Thus in the integral we set the upper limit of the k_z' integration as K and replace n by a constant. As is explained above, we estimate E_{exch} as $E_{elas} aI$ where $I = \int d^3k' n(k_z')/|k - k'|^2$. We are mainly interested in the dependence of this energy on $k_\perp$ and thus set $k_z = 0$ for simplicity.

Hence $I \approx n\int dk_\perp'^2 \int_0^K dk_z'/[k_z'^2 + (k_\perp - k_\perp')^2] \approx n\int dk_\perp'^2 \tan^{-1}(K/|k_\perp - k_\perp'|)/|k_\perp - k_\perp'|$. For the present problem, K is larger than 1 (ten times the interatomic spacing) whereas $k' < \pi/L$ where L is the interdislocation spacing. Thus $\tan^{-1}(K/|k-k') \approx \pi/2$. Hence $I \approx n(\pi/2)\int_0^{\pi/L} d^2k' \Sigma_{lm} 4\pi/(2l+1) Y_{lm}*(k) Y_{lm}(k') k_<^l/k_>^{l+1}$.

Only the $m=0$ term contributes. Also $\theta = \pi/2$. Hence there are no contributions from $l=1$. We get $I \approx n(\pi/2)\int_0^{\pi/L} d^2k' (1/k_> + 5/12 k_<^2/k_>^3)$, $I \approx n\pi^2 \int_0^k k'dk' (1/k + 5/12 k'^2/k^3) + \int_k^{\pi/L} k'dk' (1/k' + 5/12 k^2/k'^3)$, $I \approx n\pi^2[(k/2 + 5/48k) + (\pi/L - k) - 5/12 k^2 (L/\pi - 1/k)]$,

$$I \approx n\pi^2[k/48 + \pi/L + O(k^2)]. \tag{C1}$$

If $k_x \neq 0$, the integral of interest becomes

$$I' \approx n\int dk_\perp'^2 \int_0^K dk_z'/[(k_z' - k_z)^2 + (k_\perp - k_\perp')^2]$$
$$\approx n\int dk_\perp'^2 \{\tan^{-1}[(K - k_z)/|k_\perp - k_\perp'|]$$
$$+ \tan^{-1}[(K + k_z)/|k_\perp - k_\perp'|]\}/|k_\perp - k_\perp'|.$$

Now $K \gg |k_\perp - k_\perp'|$. We thus expect $\tan^{-1}((K-k_z)/|k_\perp - k_\perp'|) \approx \pi/2 + \epsilon$ with ϵ small. Since $\tan(\pi/2 + \epsilon) \approx \cot\epsilon \approx 1/\epsilon$. Thus $\epsilon \approx |k_\perp - k_\perp'|/(K - k_z) \approx |k_\perp - k_\perp'|(1 + k_z/K + k_z^2/2K^2)/K$ The term linear in k_z in the integral I' cancels out. Thus no term linear in k_z is created.

[1] E. Kim and M. W. H. Chan, Science **305**, 1941 (2004).
[2] C. A. Burns, N. Mulders, L. Lurio, M. H. W. Chan, A. Said, C. N. Kodituwakku, and P. M. Platzman, Phys. Rev. B **78**, 224305 (2008).
[3] J. Day and J. Beamish, Nature (London) **450**, 853 (2007); Y. Mukharsky, A. Penzev, and E. Varoquaux, Phys. Rev. B **80**, 140504 (2009); X. Rojas, C. Pantalei, H. J. Maris, and S. Balibar, J. Low Temp. Phys. **158**, 478 (2010); J. Day, O. Syshchenko, and J. Beamish, Phys. Rev. Lett. **104**, 075302 (2010); O. Syshchenko, J. Day, and J. Beamish, *ibid.* **104**, 195301 (2010).
[4] S. Sasaki, R. Ishiguro, F. Caupin, H. J. Maris, and S. Balibar, Science **313**, 1098 (2006).
[5] Ann Sophie C. Rittner and J. D. Reppy, Phys. Rev. Lett. **98**, 175302 (2007).
[6] M. Boninsegni, A. B. Kuklov, L. Pollet, N. V. Prokofev, B. V. Svistunov, and M. Troyer, Phys. Rev. Lett. **99**, 035301 (2007).
[7] J. Toner, Phys. Rev. Lett. **100**, 035302 (2008).
[8] L. Pollet, M. Boninsegni, A. B. Kuklov, N. V. Prokofev, B. V. Svistunov, and M. Troyer, Phys. Rev. Lett. **98**, 135301 (2007).
[9] S. G. Soyler, A. B. Kuklov, L. Pollet, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. Lett. **103**, 175301 (2009).
[10] J. H. Hetherington, Phys. Rev. **176**, 231 (1968).
[11] R. A. Guyer, J. Low Temp. Phys. **8**, 427 (1972).
[12] D. S. Greywall, Phys. Rev. B **16**, 1291 (1977).
[13] M. Roger, Phys. Rev. B **30**, 6432 (1984); see also M. Roger, J. H. Hetherington, and J. M. Delrieu, Rev. Mod. Phys. **55**, 1 (1983); M. Roger, Phys. Rev. Lett. **64**, 297 (1990).
[14] P.-G. de Gennes, C. R. Phys. **7**, 561 (2006).
[15] *Physics of the Electron Solid*, edited by S. T. Chui (International

Press, Cambridge, Massachusetts, 1994), Chap. 1.
[16] S. T. Chui, EPL **87**, 66001 (2009).
[17] L. D. Landau and E. M. Lifschitz, *Theory of Elasticity* (Pergamon Press, Oxford, 1986), p. 130.
[18] See, for example, W. Harrison, *Solid State Physics* (Dover, New York, 1972).
[19] C. A. Burns and E. D. Isaacs, Phys. Rev. B **55**, 5767 (1997).
[20] Y. Hiki and F. Tsuruoka, Phys. Lett. **56A**, 484 (1976).
[21] I. Iwasa, K. Araki, and H. Suzuki, J. Phys. Soc. Jpn. **46**, 1119 (1979).
[22] Our calculation suggests large fluctuations happening but does not take into account dynamical constraints. Large-scale motion cannot result from our low-temperature roughening transition as it corresponds to a climb motion of the dislocation perpendicular to the Burger's vector and is difficult.
[23] S. Balibar, Nature (London) **464**, 176 (2010).
[24] J. Day and J. Beamish, J. Low Temp. Phys. **148**, 627 (2007); Phys. Rev. Lett. **96**, 105304 (2006); G. Bonfait, H. Godfrin, and B. Castaing, J. Phys. **50**, 1997 (1989); see also, M. W. Ray and R. B. Hallock, Phys. Rev. B **79**, 224302 (2009), and Ref. 9 above.
[25] See, for example, P. W. Anderson and S. T. Chui, Phys. Rev. B **9**, 3229 (1974), and references therein.
[26] S. I. Shevchenko, Sov. J. Low Temp. Phys. **14**, 553 (1988).
[27] F. R. N. Nabarro, *Theory of Crystal Dislocations* (Oxford University Press, New York, 1967).
[28] E. Kim and M. H. W. Chan, Nature (London) **427**, 225 (2004).
[29] E. Kim and M. H. W. Chan, J. Low Temp. Phys. **138**, 859 (2005); N. Mulders, J. T. West, M. H. W. Chan, C. N. Kodituwakku, C. A. Burns, and L. B. Lurio, Phys. Rev. Lett. **101**, 165303 (2008); A. S. C. Rittner and J. D. Reppy, *ibid.* **101**, 155301 (2008); J. T. West, X. Lin, Z. G. Cheng, and M. H. W. Chan, *ibid.* **102**, 185302 (2009).
[30] D. Aleinikava, E. Dedits, A. B. Kuklov, and D. Schmeltzer, EPL **89**, 46002 (2010).