Stress induced dislocation roughening – phase transition in 1d at finite temperature

D. Aleinikava¹ and A.B. Kuklov¹

¹Department of Engineering Science and Physics, CUNY, Staten Island, NY 10314, USA
(Dated: January 13, 2013)

We present an example of a generically forbidden phase transition in 1d at finite temperature – stress induced and thermally assisted roughening of a superclimbing dislocation in a Peierls potential. We also argue that such roughening is behind the strong suppression of the superflow through solid ⁴He in a narrow temperature range recently observed by Ray and Hallock (Phys.Rev. Lett. 105, 145301 (2010)).

PACS numbers: 67.80.bd, 67.80.dj, 67.80.-s

Strong interest in the supersolid state of matter in free space [1] has been revived by the recent discovery of the torsional oscillator (TO) anomaly in solid ⁴He [2]. While finding no supersolidity in the ideal ⁴He crystal, ab initio quantum Monte Carlo simulations did find that some grain boundaries [3], dislocations [4, 5] or crystal boundaries [6] support low-d superfluidity spatially modulated by the surrounding lattice. In principle, a percolating network of superfluid dislocations [7] could explain the TO anomaly if the dislocation density is 3-4 orders of magnitude higher than it is expected to be in a slowly grown and well annealed crystal. Consistent with such expectation is also a very small rate of the critical superflow through solid ⁴He (occuring presumably along dislocations with superfluid cores) observed in the UMASS-Sandwich experiments [8, 9]. Thus the nature of the TO anomaly in solid ⁴He remains unclear.

In the present work we focus on the very unexpected feature of the UMASS-Sandwich experiment [9] – the strong suppression of the supercritical flow rate \(V_{cr}\) (by about 3-4 times!) and then its recovery in a narrow range of temperatures. Such a feature occurs well below (about 3-4 times!) and then its recovery in a narrow range of temperatures. Such a feature occurs well below (about 3-4 times!) such an instability leads to a first-order phase transition controlled by the dislocation core and, thus creates spontaneous jog-antijog pairs.

Jog-antijog pairs as quantum objects can be created spontaneously by a macroscopically small stress \(\sigma \geq \sigma_c \propto 1/L\) applied to a superclimbing dislocation of length \(L\) – analogous to the creation of kink-antikink pairs along a stressed gliding dislocation [10, 11]. We have found that such an instability leads to a first-order phase transition even at finite temperature \(T\) between two phases of the dislocation – smooth and rough. This transition is in an apparent violation of Landau’s argument "no phase transitions in 1d at finite \(T\)" [12]. However, we argue that the locality of order parameter(s), which is essential for the validity of Landau’s argument, is not present here. Consequently, in a sharp contrast with conventional 1d systems, where any macroscopic characteristic length decreases with increasing \(T\), a typical scale \(L_b\) for the onset of the hysteretic behavior of the superclimbing dislocation increases with \(T\).

The effective description of such a transition invokes a single coarse grained macroscopic degree of freedom – dislocation deformation characterized by an effective mass and a potential energy with two minima. These quantities are scaled as some positive powers of \(L\) even at \(T \neq 0\), so that the amplitude of the transition between the minima decays exponentially as \(L \to \infty\) – very much like \(d > 1\) systems undergoing first-order transition. However, due to the strongly interacting and effectively long-range nature of the rough phase, specifics of such size dependencies cannot be derived analytically, and we have evaluated them numerically.

The model and its Monte-Carlo simulations. Superclimbing dislocation is modeled as a quantum string oriented along the \(x\)-axis and strongly pinned at its both ends \(x = 0, L\) [13]. The string displacement \(y(x, t)\) along the \(y\)-axis depends on the time \(t\) and is measured in units of the inter-atomic spacing \((\approx \text{Burger’s vector})\) with respect to its equilibrium \(y = 0\) (no tilting is considered). The Peierls potential induced by the crystal is taken as \(U_p = - u \rho \cos(2\pi y(x, t))\). The partition function \(Z\) has the form [3, 14]

\[
Z = \int \mathcal{D}y(x, t) \mathcal{D}\rho(x, t) \exp(-S),
\]

\[
S = \int_0^\beta dt \int \left[ i(\rho + n_0)\nabla \phi + \frac{\rho_0}{2} (\nabla \phi)^2 - \frac{1}{2\rho_0}(\rho - y)^2 + \frac{m}{2} ((\nabla^2 y)^2 + V_0^2 (\nabla y)^2) - u \rho \cos(2\pi y(x, t)) - F y(x, t) \right], \tag{2}
\]

where all the variables are periodic in the imaginary time \(t \geq 0\) with the period \(\beta = 1/T\) (units \(\hbar = 1, K_B = 1\); the core density \(\rho\) and the superfluid phase \(\phi\) are canonically conjugate variables, with \(\rho' = \rho - y\) being the local superfluid density; the derivatives \(\nabla \psi\) defined modulo \(2\pi\) (in order to take into account phase-slips); \(n_0, \rho_0\) stand for the average filling factor (we choose \(n_0 = 1\)) and the bare superfluid stiffness, respectively, with the bare speed of...
first sound taken as unity.

The first two terms in Eq. (2) describe the superfluid response of the core [5], and the third term accounts for the superclimb effect [7] — building the dislocation edge so that the core climb \( y \to y \pm 1, \pm 2, \ldots \) becomes possible by delivering matter \( \rho \to \rho \pm 1, \pm 2, \ldots \), respectively, along the core [5]. The dislocation is assumed to be attached to large superfluid reservoirs at both ends, with spatially periodic boundary conditions for the supercurrent.

The terms \( \propto m \) in Eq. (2) account for the elastic response of the string, with \( m \) and \( V_L \) standing for the effective mass of the dislocation core (per \( b \)) and the bare speed of sound, respectively. Since the main source of kinetic energy are supercurrents, we have left out the term \( \approx (\nabla y)^2 \) in Eq. (2). The parameter \( m \) in Eq. (2) is not actually a constant. It contains a contribution from the Coulomb-type interaction potential \( \propto 1/|x| \) between jogs (or kinks, cf. [13]) separated by a distance \( x \) [10]. Accordingly, \( m \) has a logarithmic divergent factor with respect to a wave vector \( q \) so that the core climb \( \mu \to \mu \pm 1, \pm 2, \ldots \) becomes possible by delivering matter \( \rho \to \rho \pm 1, \pm 2, \ldots \), respectively, along the core [5].

The dislocation is assumed to be attached to large superfluid reservoirs at both ends, with spatially periodic boundary conditions for the supercurrent.

The dislocation is assumed to be attached to large superfluid reservoirs at both ends, with spatially periodic boundary conditions for the supercurrent.

In other words, the thermal length \( L \simeq T/\kappa \), where \( \kappa \simeq \chi_2/L \) for the jog-antijog pair creation at \( L \gtrsim 30 \), \( u_P = 3.0 \). Inset: the region of the dip (cf. Fig. 4 of Ref. [6]) showing its shifting with the core [5].

The dislocation is assumed to be attached to large superfluid reservoirs at both ends, with spatially periodic boundary conditions for the supercurrent.

Our main findings presented below are the following: i) a narrow dip in \( \nu_s(T,F) \) vs \( T \) at some macroscopically small \( F = F_c \); ii) periodicity of \( \nu_s(T,F) \) with respect to the bias \( F \); iii) exponential scaling of the dip depth with \( L \); iv) hysteresis developing beyond a certain length \( L_h \) growing with \( T \).

**FIG. 1:** (Color online) Renormalized superfluid stiffness \( \nu_s(T) \) and the velocity \( \nu_s^*(T,F) \) of first sound normalized by their respective low-\( T \) values for different \( F \) (shown on the inset), \( L = 30, \ u_P = 3.0 \). Inset: the region of the dip (cf. Fig. 4 of Ref. [6]) showing its shifting with \( F \).
of the thresholds for creating multiple jog-antijog
shown in Fig. 3. We attribute this to the reaching
ing features we have found is the quasi-periodicity
One of the most strik-
V
κ, R
L
applied bias, provided
Ref.[9] (see Fig.4 there) should recur as a function of the
we predict that the dip in the flow rate observed in
Away from the dip, 
V
is practically insensitive
to 
F
, and the responses 
κ, R
2
become essentially linear
in 
F [14].

Periodicity vs external bias. One of the most striking
features we have found is the quasi-periodicity
in 
F of 
κ, R
2
as shown in Fig. 2 and in 
V
as shown in Fig. 3. We attribute this to the reaching
of the thresholds for creating multiple jog-antijog
pairs. Thus, the peak (dip) positions are given as

\[ F = F_c(L, n) \approx n F_c(L, 1) \sim n L^{-\gamma}, \quad n = 1, 2, 3, \ldots \]

and we predict that the dip in the flow rate observed in
Ref.[2] (see Fig.4 there) should recur as a function of the
applied bias, provided 
T is kept fixed.

Size dependencies. Transformation between the smooth
(where 
R
1 << 1) and the rough ( 
R
1 \approx 1) states occurs
within an exponentially narrow region \(\delta F\) around 
F_c.
It is given by the tunneling rate \(\sim \exp(-L/L_R)\) < 1
through the macroscopic jog-antijog barrier (cf. the
mechanism for the kink-antikink tunneling, Ref.[11]),
where 
L_R stands for the tunneling length. Thus, as
follows from Eq.[4], the peak value of 
R_2(T, F_c) diverges
with 
L as \(\approx 1/\delta F \sim \exp(L/L_R)\). Fitting 
R_2(T, F_c) by an exponential function, Fig.4
gives 
L_R \approx L_0^{-1}(1 - T/T_R)^{2.3}. Here 
L_0 is the 
T = 0 tunneling length
\(L_0 \approx 1.7\) for 
\uP = 3.0) and 
T_R sets the scale for thermal roughening, i.e. the temperature above which the
density of jog pairs is large even in the limit 
F \rightarrow 0.

T_R is determined by the double energy \(2\Delta \propto \sqrt{u_P}\) of a jog modeled as a Sine-Gordon soliton. We have found
$T_R \propto u_P^4$, $s = 0.5 \pm 0.1$ which is consistent with such an interpretation.

The critical stress $F_c(L, 1)$ has been found to deviate from the $1/L$ dependence (11) at finite $T$. Specifically, $F_c \propto 1/L^{\gamma_c(T)}$ with $\gamma_T > 1$. As $T$ grows, $\gamma_T \rightarrow 1.7$, and $\gamma(T) \rightarrow 1$ in the limit $T \rightarrow 0$. The temperature scale for this variation is set by the Peierls potential amplitude $u_P$ as well. It is natural to attribute the deviation from $\gamma = 1$ to a suppression of the energy gap $\Delta \propto L^{3-\gamma} \rightarrow 0$ at finite $T$.

**Hysteresis.** The resonant-peak type behavior in $R_2$ (and in $\kappa$) turns out to be a precursor for the jump in $R_1$. As seen from Eq. (39), $R_2 \approx F_c dR_1/dF \sim F_c/\delta F$ as $\delta F \rightarrow 0$. The hysteresis emerges when $\delta F$ becomes significantly less than the coexistence region for the smooth and rough states. This conditions sets a typical length $L_h$ above which $(L > L_h)$ hysteresis develops. We have found that $L_h$ grows with $T$ as $L_h \approx L_0(T/T_c)^{\gamma_h} > L_0$, $\gamma_h > 0$ ($\gamma_h \approx 2 - 3$ for $u_P = 1 - 3$). We attribute the energy scale $T_*$ to the tunneling splitting energy through the microscopic jog-antijog barrier so that $T_* \approx T_R$ (11). This feature is clearly due to the collective multi-jog nature of the rough state, and it deviates strongly from the single pair tunneling scenario (11) (see Eq. (39)) where the tunneling rate saturates at some length decreasing as $\propto T^{-3/2}$.

Fig. 5 demonstrates the $L$-dependencies of the "coercivity fields". Along the lower branch of the hysteresis loop (inset in Fig. 5) the dislocation is in the smooth state. Upon increasing $F$, it "jumps" into the rough state at $F \approx F_u$. While "moving" back along the upper branch representing the rough state, the dislocation returns into the smooth state at $F \approx F_L < F_u$. As seen from the main panel of Fig. 5 both fields scale as $F_{u,L} \propto L^{-\gamma_n-L}$, with $\gamma_n \approx 0.4$ and $\gamma_L \approx 2.7$, respectively. The middle straight line corresponds to the extrapolation of the peak position data $F_c \propto L^{-\gamma}$, $n = 1$, $\gamma \approx 1.7$ (for $L < L_h$). Such strong sensitivity to the size $L$ as well as $L_h$ growing with $T$ clearly indicate that the stress-induced roughening is a phase transition at finite $T$ in 1d.

The resonant-type behavior and the hysteresis have also been found in simulations of gliding dislocation network (14). While $L_T$ determines the upper spatial scale for the superclimb, no such restriction exists for the glide, so that the formal limit $L \rightarrow \infty$ can be considered.

**Discussion and conclusions.** The narrow dip in the superflow rate observed in Ref. 3 may have its origin in the stress induced roughening effect of superclimbing dislocations. Specifically, biasing a superfluid dislocation network by macroscopically small overpressure can induce strong suppression of the first sound along the superfluid cores. Such suppression is characterized by the periodicity of the dip in the flow rate, Fig. 5 which can be used as the *experimentum crucis* for the proposed scenario.

We estimate the critical overpressure $\delta p$ in terms of $L$ and a typical jog-antijog energy $2\Delta \approx 0.1k$ (cf. 13) as $\delta p/p \approx 2\Delta h/(LT_D) \sim 10^{-2}h/L$. Measurements of $\delta p$ where the dip recurs can provide crucial information on the nature of the dislocation network – its typical free segment length $L$.

As $T$ is lowered, the opposite condition $L > L_h$ is fulfilled so that the dislocation behavior becomes hysteretic between its smooth and rough states. We believe it is also important to study the hysteresis in the flow rate vs chemical potential (the upper $F_u$ and the lower $F_L$ fields) at different temperatures.

We are grateful to R.B. Hallock, L.P. Pitaevskii, N.V. Prokof’ev, D. Schmeltzer and B.V. Svistunov for useful discussions and comments. This work was supported by the National Science Foundation, grant No.PHY1005527, PSC CUNY, grant No. 63071-0041, by the CUNY HPCC under NSF Grants CNS-0855217 and CNS-0958379.

---

[1] A. Andreev and I. Lifshitz, Sov. Phys. JETP, 29, 1107 (1969); D. J. Thouless, Ann. Phys. 52, 403 (1969); G.V. Chester, Phys. Rev. A, 2, 256 (1970); A.J. Leggett, Phys. Rev. Lett., 25, 1543 (1970).
[2] E. Kim and M. Chan, Nature, 427, 225 (2004); E. Kim and M. Chan, Science, 305, 1941 (2004).
[3] L. Pollet, et. al., Phys. Rev. Lett. 98, 135301 (2007).
[4] M. Boninsegni, et. al., Phys. Rev. Lett. 99, 035301 (2007).
[5] S.G. Söyler, et. al., Phys. Rev. Lett. 103, 175301 (2009).
[6] S. A. Khairallah and D. M. Ceperley, Phys. Rev. Lett. 95, 185301 (2005).
[7] S. I. Shvechenko, Sov. J. Low Temp. Phys. 13, 61 (1987).
[8] M.W. Ray and R.B. Hallock, Phys. Rev. Lett. 100, 235301 (2008); Phys. Rev. B 79, 224302 (2009).
[9] M.W. Ray and R.B. Hallock, Phys.Rev.Lett. 105, 145301 (2010).
[10] Hirth J. P. and Lothe J., *Theory of Dislocations*. McGraw-Hill, 1968.
[11] B.V. Petukhov and V.L. Pokrovksii, Sov. Phys. JETP 36, 336 (1973).
[12] L. D. Landau and E.M. Lifshitz, *Statistical Physics, Part 1: Volume 5. Course of Theoretical Physics*, 3rd Edition, Butterworth-Heinemann, Oxford,2000, p. 537.
[13] A. Granato, K. Luce, J. Appl. Phys. 27, 583 (1956); ibid. 789(1956).
[14] D. Aleinikava, et. al., J. Low Temp. Phys. 162, 464 (2011); arXiv:1006.5228.
[15] D. Aleinikava, et. al., Europhys. Lett., 89 46002 (2010); arXiv:0812.0983.
[16] N.V. Prokof’ev & B.V. Svistunov, Phys. Rev. Lett. 87, 160601 (2001).
[17] F. D. Haldane, Phys. Rev. Lett. 47, 1840(1981).
[18] Yu. Kagan, N. V. Prokofev, and B. V. Svistunov, Phys. Rev. A 61, 045601 (2000).
[19] The peak in $R_2$ and the hysteresis for any studied $L$ vanish at $T \approx T_R$. 

