Surface melting of the vortex lattice

A. De Col1, G.I. Menon2, V.B. Geshkenbein1,3, and G. Blatter1
1Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland
2The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600 113, India and
3L.D. Landau Institute for Theoretical Physics, RAS, 117940 Moscow, Russia
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We discuss the effect of an (ab)-surface on the melting transition of the pancake-vortex lattice in a layered superconductor within a density functional theory approach. Both discontinuous and continuous surface melting are predicted for this system, although the latter scenario occupies the major part of the low-field phase diagram. The formation of a quasi-liquid layer below the bulk melting temperature inhibits the appearance of a superheated solid phase, yielding an asymmetric hysteretic behavior which has been seen in experiments.

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The transition between vortex solid and vortex liquid phases observed in the mixed phase of high-\(T_c\) superconductors has generated renewed interest in the problem of melting. In common with other discontinuous phase transitions, melting should involve the appearance of both metastable undercooled liquid and overheated solid phases. Hence, hysteretic behavior is expected upon cycling through the transition. However, experiments on the layered, high-\(T_c\) superconductor BiSSCO reveal an asymmetric hysteresis, characterized by the appearance of only the supercooled liquid and no overheated solid. Similar behavior is displayed by ordinary crystals, where such asymmetry is understood to be a consequence of surface (pre-) melting: surfaces act as nucleation centers for the liquid, thereby inhibiting the metastable solid above the melting transition. However, such surface melting is not generic and there are experimental systems where the surface remains solid up to the bulk melting transition. In this letter, we study the effects of an (ab)-surface on vortex lattice melting, showing that as the strength of the magnetic field is varied, the same surface may exhibit either ‘surface non-melting’ or ‘surface melting’ behavior. The latter scenario applies to the major part of the low-field phase diagram, in agreement with experiments.

Early studies of simple crystals have focused on the solid phase and have demonstrated that the surface turns unstable before the bulk melts. Going beyond such a stability analysis is a difficult task, as a theory is required which describes both solid and liquid phases in a unified manner. Qualitative insight can be gained from a Landau theory by including the destabilizing effect of the surface: two melting scenarios are found, surface melting \(O_2\) with a continuous- and surface non-melting \(O_1\) with a discontinuous vanishing of the order parameter at the surface. More elaborate \textit{ab initio} calculations reduce the problem to a mean-field order-parameter theory and determine the free energy either as a lattice sum or within a density functional theory (DFT) exploiting liquid-state correlations.

The vortex matter in Bi- and Tl- based high-\(T_c\) superconductors is characterized by an extreme anisotropy: pancake-vortices confined to superconducting layers exhibit repulsive logarithmic interactions within the planes and weakly attractive inter-layer interactions extending over many layers (see, e.g. Ref. 2; we ignore here a weak Josephson coupling between the layers). These anisotropic properties inspire the use of a substrate-mean-field theory describing the vortex system in terms of two-dimensional lattices of pancake-vortices subject to a substrate potential generated by the mean action of the vortices residing in other layers. The bulk melting line is known by interpolating between the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature \(T_{\text{BKT}} \lesssim T_c\) of the individual layers at zero external field and the two-dimensional vortex-lattice melting temperature \(T_{\text{m}} \approx T_c\) at high magnetic fields, see Fig. 1. We use the classical DFT of freezing and exploit the anisotropic properties of the system with its natural separation of liquid-state correlations into in-
plane and out-of-plane components. As a result, we obtain a reliable and analytically tractable order-parameter theory which allows us to study (ab)-surface melting. We find two regimes within the $B$-$T$ phase diagram: for low and high magnetic fields $B$ the surface order parameter undergoes a finite, although reduced, jump $(O_1)$ at the bulk melting temperature, whereas for intermediate values of $B$, stray magnetic fields destabilize the layers close to the surface, leading to the surface melting scenario $(O_2)$.

We sketch the derivation of pancake-vortex interactions in a semi-infinite superconductor filling the half-space $z \geq 0$. These interactions are mediated by currents set up by the vortices via the Lorentz force (here, $d$ is the layer separation, $\lambda$ the London penetration depth, and $\Phi_0$ the flux unit): each vortex generates a current density $j = -(e/4\pi \lambda^2)\partial (\Phi_0/2\pi \lambda) \vec{\nabla} \vec{\varphi} + \vec{A}$ which acts on another vortex core with a transverse force $\mathbf{F} = \partial \Phi_0/\partial x \, z/j/c$. For a co-planar pair of pancake-vortices the current density is driven by the phase gradient $\vec{\nabla} \vec{\varphi} = -\vec{n}_z \times \vec{R}/R^2$ and the force $\propto 1/R$ produces a long-range logarithmic repulsion $V_{z,z'}(R) \approx -2\varepsilon_0\ln(R/\varepsilon)$; this potential corresponds to that of a one-component charged plasma (OCP) with charge $e^2 \rightarrow 2\varepsilon_0 $ and $\varepsilon_0 = (\Phi_0/4\pi \lambda)^2$ the vortex line energy. The interaction between two pancake-vortices residing in different layers derives from the vector potential $\vec{A}$: calculating the field associated with a pancake vortex in a semi-infinite geometry and integrating the Lorentz force provides the potential

$$V_{z,z'}(R) = -\varepsilon_0 d^2 \int_0^\infty dK \frac{J_0(KR)}{\lambda^2 K^2} \times [f_{z-z'}(K) + \beta(K)f_{z+z'}(K)]$$

with $f_z(K) = \exp(-K|z|)$, $K_+ = \sqrt{K^2 + \lambda^2}$, and $\beta(K) = (K_+ - K)/(K_+ + K)$. The bulk term $f_{z-z'}$ is augmented by a stray-field term $f_{z+z'}$ relevant within a distance $\lambda$ from the surface. For small in-plane distances $R \ll \lambda$, the contribution of the stray-field term can be neglected and we recover the bulk expression $V_{z,z'}(R) \approx \varepsilon_0 d(\partial R/\lambda^2)[R/(R + 4|z - z'|)]$. For a large separation $R \gg \lambda$, the surface term is relevant and we obtain

$$V_{z,z'}(R) \approx 2\varepsilon_0 d[\phi_z(z,z') \ln(R/\lambda) + (d/R) e^{-z+z'/\lambda}],$$

where $\phi_z(z,z') = (d/2\lambda)(e^{-z-z'/\lambda} + e^{-(z+z')/\lambda})$ is the fraction of flux trapped in the layer $z'$ generated by a pancake vortex at $z$: a test vortex at $z'$ then effectively experiences a logarithmic attraction from two bulk-type pancake-vortices, the real one at $z$ and a fake mirror vortex with equal sign at $-z$, the latter generated by the stray field. The algebraic repulsion associated with the second term in $V_{z,z'}(R)$ is again due to the stray field and produces a surface softening.

In our investigation of the vortex solid-liquid transition we make use of the classical density functional theory (DFT) [13] which builds on the (grand canonical) free-energy difference $\delta \Omega = \Omega_{\text{sol}} - \Omega_{\text{liq}}$ expressed through the variation $\delta \rho(r) = \rho(r) - \bar{\rho}$ in particle density away from the uniform liquid state density $\bar{\rho}$; for the inhomogeneous and anisotropic vortex matter system, $\delta \rho_z(\mathbf{R}) = \rho_z(\mathbf{R}) - \bar{\rho}$ and $\bar{\rho}$ is the 2D liquid density,

$$\delta \Omega[\rho_z(\mathbf{R})] = \int \frac{d^2 \mathbf{R}}{d} d^2 \mathbf{R} \left[ \frac{\rho_z(\mathbf{R})}{\bar{\rho}} \ln \frac{\rho_z(\mathbf{R})}{\rho_z(\mathbf{R}) - \delta \rho_z(\mathbf{R})} \right],$$

$$= -\frac{1}{2} \int \frac{d^2 \mathbf{R}}{d} d^2 \mathbf{R} \delta \rho_z(\mathbf{R}) \left[ c_{z,z'}(\mathbf{R} - \mathbf{R}') \right] \delta \rho_z(\mathbf{R}').$$

The first two terms describe the entropic contribution of a non-interacting gas, while the last term accounts for the microscopic interactions $V_{z,z'}(R)$ via the direct pair-correlation function $c_{z,z'}(\mathbf{R})$ of the liquid state; in the homogeneous liquid, the (dimensionless) Fourier transform $c_{z,z'}(K) = \langle \rho/\rho \rangle \int d^2 \mathbf{r} c_z(\mathbf{r}) e^{-i\mathbf{K} \cdot \mathbf{r}}$ is related to the static structure factor via $S(k) = 1/[1 - c_{z,z'}(K)]$. The appearance of finite density-modulations $|\delta \rho_z(\mathbf{R})| > 0$ in the solid is a consequence of these correlations. We exploit the anisotropy of the pancake-vortex system and separate $c_{z,z'}(\mathbf{R})$ into in- and out-of-plane parts,

$$c_{z,z'}(\mathbf{R}) = c^{2D}(\mathbf{R}) \delta(z - z') - V_{z,z'}(\mathbf{R})/T,$$

where $c^{2D}(\mathbf{R})$ denotes the correlation function of the 2D-OCP as obtained from standard Monte-Carlo simulations [14]. The second term accounts for the weak inter-plane interactions; within lowest-order perturbation theory [14] it is given by the Fourier transform of the out-of-plane interaction $\tilde{V}_{z,z'}(K)/T = -\alpha(K)\tilde{f}_{z-z'}(K) + \beta(K)\tilde{f}_{z+z'}(K)$ with $\alpha(K) = 2\pi \varepsilon_0 d^2 \bar{\rho}/T \lambda^2 K$. We begin with the homogeneous bulk system. Consider the Fourier transforms $\delta \rho_z(\mathbf{K})/\bar{\rho}$ for the density field and $\xi_z(\mathbf{K})$ for the molecular field $\xi_z(\mathbf{K}) = \ln[\rho_z(\mathbf{R})/\bar{\rho}]$; where $\mathbf{K}$ denotes the reciprocal triangular-lattice vectors. For a correlation function $c^{2D}(\mathbf{K})$ decaying rapidly beyond the first reciprocal lattice vector, only the two components need to be retained and we can restrict the Ansatz to the form $\delta \rho_z(\mathbf{R})/\bar{\rho} \approx \eta_z + \mu_z g(\mathbf{R})$ and $\xi_z(\mathbf{R}) \approx \kappa_z + \xi_z g(\mathbf{R})$ with $g(\mathbf{R}) = \sum_{\mathbf{K}_n} e^{i\mathbf{K}_n \cdot \mathbf{R}}$. $G = 4\pi/\sqrt{3} a_s$ (the lattice constant, $a_s^2 = 2\Phi_0/\sqrt{3}B$). Furthermore, $\kappa_z$ and $\xi_z$ are related to $\mu_z$ via [16]

$$\kappa_z = -\Phi(\xi_z), \quad \mu_z = \Phi'(\xi_z)/6,$$
with in-plane correlations $\bar{c}^{2D} \equiv c^{2D}(G)$ and out-of-plane correlations described by the substrate potential $-\bar{c} f(z/d)\bar{f}_z = -2\alpha/d G_z$ with $G_z = \sqrt{G^2 + \lambda^2}$. Note that both $\kappa_z$ and $\xi_z$ have to be understood as functions of the order-parameter $\mu_z$ via (3). The second non-local term in $\delta\omega$ accounts for inhomogeneities of the order-parameter field $\mu_z$ and involves the dispersive ‘elastic coefficient’ $\bar{\alpha} f_{z-z'}$. Here, we neglect the small change in density across the transition described by $\eta_z$; its inclusion involves a more elaborate analysis accounting for the discrete nature of the particles [14].

The bulk melting line $B_m(T)$ is obtained from minimizing the functional $\delta\omega[\mu]$ for a homogeneous order parameter $\mu$. At large values of $B$, the inter-planar interaction is negligible and the melting temperature is given by the solid-liquid transition of the 2D-OCP [13] as described by the free-energy density [5] without substrate potential (termed $\delta\omega^{2D}$). For small $\bar{c}^{2D}$ (large temperatures), $\delta\omega^{2D}(\mu)$ exhibits only the liquid minimum at $\mu_{\text{liq}} = 0$, cf. Fig. [2] Lowering the temperature, the correlator $\bar{c}^{2D}$ increases and $\delta\omega^{2D}(\mu)$ develops a second minimum at a finite value $\mu_c$. At the critical value $\bar{c}^{2D} = \bar{c}_c = 0.856$ the ‘solid’ minimum drops below the ‘liquid’ one and the high-field liquid-solid transition takes place. The comparison with numerical simulations [17] allows us to check the accuracy of our approach: Monte Carlo simulations [17] show that the 2D-OCP freezes at $T^{2D}_{\text{m}} \approx \varepsilon_0 d/70$ where the correlator assumes the value $\bar{c}^{2D} \approx 0.77 < \bar{c}_c$: more sophisticated versions of DFT cure this discrepancy [18].

\begin{align*}
\text{FIG. 2: Top left: direct pair-correlation functions at } & T/\varepsilon_0 d = 0.08 \text{ for the 2D-OCP, } \bar{c}^{2D}(K) \text{ from MC simulations and } \bar{c}^{2D}(K) = c^{2D}(K) + 2\alpha(K)/dK_+ \text{ for the full 3D system at melting (} B = B_m). \text{ Bottom right: Free energy } \delta\omega^{2D}(\mu)/T \text{ for values } \bar{c}^{2D} = 0.80, 0.83, 0.845, 0.856 (= \bar{c}_c \text{ critical value, thick line), 0.87. At melting the order parameter jumps from } \\
\mu_{\text{col}} \approx 0.51 \text{ to } \mu_{\text{liq}} = 0. \end{align*}
at small $\mu_z$ [11]. This equation then admits the exponential solution $A \exp(\sqrt{7}G_z) + B \exp(-\sqrt{7}G_z)$ and inserting this Ansatz back into it the boundary term fixes the ratio $A/B$; as a result, we obtain the boundary condition

$$\left[\mu'/\mu\right]_{z=0} = G_1 (1-\beta)/(1+\beta) = G. \quad (10)$$

The analysis of the boundary value problem [8] with a continuous surface melting (O scenario) with the surface undergoes a discontinuous atomation of this second multi-critical point. In conclusion, we have analyzed surface melting in the pancake-vortex system of layered superconductors and have found both surface-melting (O$_2$) and surface-non-melting (O$_1$) scenarios. The O$_2$ scenario is realized over most of the low-field phase diagram and explains the experimental observation of asymmetric hysteresis [2].

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