Evaporation of the pancake-vortex lattice in weakly-coupled layered superconductors

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The pancake-vortex lattice in layered superconductors defines a tunable soft matter system with astonishing properties. Among them, the thermodynamic phase transition of vortex-lattice melting and its first-order character is now experimentally well established, but questions remain as to which correlations are lost at the transition. Theoretically, the position of the melting line can be estimated with a Lindemann criterion, but a more detailed description of melting is required to determine the characteristics of the transition. The challenge in defining a theoretical scheme describing vortex-lattice melting follows from the complexity of the vortex system in real superconductors combined with the general lack of exact theories of melting.

In a moderately anisotropic material, such as YBa$_2$Cu$_3$O$_7$, the vortex crystal melts to a line liquid and numerical simulations have treated this in detail. In Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSCCO), however, the coupling between layers is so weak that the layered structure (with spacing $d$) plays a crucial role, and the vortex matter acts as a collection of interacting two-dimensional (2D) vortices, or pancake vortices. Rather than using numerical simulations, we describe here a novel analytic treatment to track the melting line through the $B$-$T$ phase diagram in the extreme anisotropic limit of zero Josephson coupling between layers. In this limit the 3D pancake-vortex lattice (PVL) remains stable at low temperatures due to an attractive electromagnetic interaction between pancake vortices in different layers, with range $\lambda \gg d$ ($\lambda$ is the in-plane penetration depth). Changing the magnetic field tunes the relative importance of this attractive interlayer interaction and the long-range repulsion between vortices in the same layer. At high fields $B \gg B_\lambda = \Phi_0/\lambda^2$, the in-plane interactions dominate and the 3D lattice melts to independent 2D liquids (a pancake-vortex gas) close to the 2D melting temperature $T_{m}^{2D} \approx \varepsilon_0 d/70$ [where $\varepsilon_0 = (\Phi_0/4\pi\lambda)^2$]. At lower fields the interlayer attraction stabilizes the lattice and increases the melting temperature. In the low-field limit of weakly-coupled 1D stacks, the crystal melts below the evaporation transition of an isolated stack of pancake vortices located at the Berezinskii-Kosterlitz-Thouless (BKT) vortex unbinding transition of an isolated layer at $T_{BKT} = \varepsilon_0 d/2 \approx 35T_{m}^{2D}$. The field regime $B \sim B_\lambda$ where the melting line interpolates between the above limits then spans a factor $\sim 35$ in “reduced” temperature $T/\varepsilon_0 d$ (in real superconductors $\varepsilon_0$ vanishes as $T_c$ is approached, and the real temperature ratio $T_{BKT}/T_{m}^{2D}$ will be smaller). Before reaching zero field, the melting line is cut by a competing low-field reentrant transition to a dilute liquid of stacks with exponentially-weak interactions. A Lindemann analysis tells us that at $T \sim \varepsilon_0 d/2$ reentrant melting occurs at a field below $10^{-2}B_\lambda$.

Ignoring reentrance, we have a 3D melting line that interpolates between a 1D stack evaporation (exactly described by 2D BKT theory) and a 2D melting transition usually described by a BKT-type mechanism of dislocation pair unbinding. Both limits are well described by a self-consistent approximation and we here generalise this to all magnetic fields. Our self-consistent method relies on the long range of the inter-layer attractions; each pancake vortex feels the attractive force of pancake vortices in $\sim \lambda/d$ other layers. Therefore the fluctuations in pancake-vortex positions may be averaged, leading to an accurate “mean-field” approach where the 2D lattice in one layer sits in a substrate potential due to the attraction of the vortex stacks in all other layers. With this substrate model we calculate the fluctuations of individual pancake vortices, which in turn smear the substrate potential, and we solve self-consistently. The upper bound in temperature to a self-consistent solution leads to an instability line which we calculate in this paper. We then determine the melting line by comparing the free energy of the 3D PVL to the free energy of a collection of 2D liquids, using numerical results for the 2D system.

The evaporation at $T_{BKT}$ of a single stack of pancake vortices occurs because each element is only logarithmically bound to the stack: A pancake vortex in a layered superconductor generates supercurrents within each layer, resulting in a pairwise interaction energy.
where \( n \) is the number of layers separating the two vortices, and \( \mathbf{R} \) is the in-plane distance. The form of this interaction for different limits is well documented: the in-plane repulsion is \( V_n(R) = -2\varepsilon_0d \ln(R/L) \) (where \( L \) is the system-size cut off) and the out-of-plane attraction has the large \( R \) limit, \( V_{n\neq 0}(R) = \varepsilon_0d/(\lambda^2) e^{-nd/\lambda} \ln(R/L) \). This implies that the energy to pull a single pancake vortex (of core-size \( \xi \)) from a straight stack is \( 2\varepsilon_0d \ln(R/\xi) \) when \( R \gg \lambda \) and the entropy will unbend the pancake vortices above \( T_{\text{BKT}} \).

This stack evacuation is easily reproduced within a self-consistent substrate model \cite{5}. Here, each pancake vortex is subject to a quadratic potential, but with a strength chosen to match the thermal average \( \langle \cdots \rangle \) of the curvature in the real potential \cite{5}, \( V_n(u_0) = \frac{3}{2}\varepsilon_0d\alpha_0^2 \), where \( u_n \) is the \( n \)-th pancake vortex displacement, and

\[
\alpha_n = \sum_{n\neq 0} \left( \frac{\partial^2 V_n(u_n - u_0)}{\partial u_n^2} \right). \tag{2}
\]

We ignore correlations in the pancake vortex fluctuations and use the identity for Gaussian fluctuations \( \langle \exp[-iK \cdot (u_n - u_0)] \rangle = \exp(-K^2\langle u^2 \rangle/2) \), to give

\[
\alpha_n = -\sum_{n\neq 0} \int \frac{d^2 K}{(2\pi)^2} K_x^2 V_n(K) e^{-K^2(u_n^2/2)}, \tag{3}
\]

where \( V_n(K) = \int d^2 R e^{-iK \cdot R} V_n(R) \). The equipartition theorem for a harmonic potential, \( \langle u^2 \rangle = 2T/\alpha_n \), allows us to solve Eq. (3) self-consistently: for large displacements \( \langle u^2 \rangle \gg \lambda^2 \), the limiting form is \( \alpha_n = \varepsilon_0 d/(\langle u^2 \rangle + 2\lambda^2) \), which has the solution \( \langle u^2 \rangle = 2\lambda^2/[1 - (2T/\varepsilon_0d)] \), diverging at the evaporation temperature \( T_{\text{BKT}} = \varepsilon_0d/2 \).

We now extend this self-consistent analysis to the full 3D system at finite fields. We consider the full 2D fluctuations of the crystal in each layer, sitting on a substrate due to the stacked vortex crystals in the other layers. Before deriving this in detail, we give a quick-and-dirty derivation of evaporation at small fields. Close enough to \( T_{\text{BKT}} \) the instability occurs when \( \lambda^2 \ll \langle u^2 \rangle \ll a_0^2 \), for a vortex density \( n_v = N_0/B = 2/\sqrt{a_0^2} \). In this limit the substrate potential picks up a negative background contribution (see below), \( \alpha_n \approx \varepsilon_0 d/[-2\pi n_v + 1/(\langle u^2 \rangle + 2\lambda^2)] \). Inserting this to the equipartition result gives the quadratic equation in \( \langle u^2 \rangle \), \( \langle u^2 \rangle = (2T/\varepsilon_0d)[2\lambda^2 + \pi^2 n_v(\langle u^2 \rangle)^2] \), which only has solutions below a temperature given by \( (1 - T/T_{\text{BKT}})^2 - 16\pi n_v \lambda^2 = 0 \), and the instability line approaches the zero-field transition in the form

\[
B_n \sim B_\lambda (1 - T/T_{\text{BKT}})^2, \quad T \rightarrow T_{\text{BKT}}. \tag{4}
\]

Note also that this instability occurs when the fluctuations reach the condition \( \langle u^2 \rangle \sim a_0^2 \lambda \). This contrasts with the often used Lindemann criterion for melting at \( \langle u^2 \rangle = c_L^2 a_0^2 \) and corresponds to a field dependent Lindemann number \( c_L \sim (B/B_\lambda)^{1/4} \) [see \cite{3} where a field-dependent \( c_L \) was also found].

A precise treatment that can be used at all fields must include the elastic distortions of the lattice within each layer. Within the self-consistent harmonic approximation (SCHA) plus substrate model the average energy cost for these distortions is given by a quadratic form, integrated over all 2D modes in the Brillouin zone, \( H^B[u^0] = \int_{BZ} d^2 K u_0^0(\mathbf{K}) \Phi^{ij}(\mathbf{K}) u_0^j(\mathbf{K}) \)

\[
\Phi^{ij}(\mathbf{K}) = n_v \sum_{\mathbf{R}_n} \left[ (1 - \epsilon_i^R \mathbf{K} \cdot \mathbf{R}_n) \partial_i \partial_j V_n + \sum_{n\neq 0} \partial_i \partial_j V_n \right], \tag{5}
\]

with \( \mathbf{R}_n \) and \( Q_\mu \) the real and reciprocal lattice vectors and \( f_{ij}(Q) = Q_i Q_j (4\pi^2 Q^2 e^{-Q^2a_0^2}/2) \). The first two terms in (5) are the 2D-elasticity and the last is the contribution from the substrate. Again, we have ignored correlations in displacements \( \langle u_n^m(\mathbf{R}_n) u_j^j(\mathbf{R}_\nu) \rangle \approx \delta_{\mu\nu} \delta_{mn} \delta_{ij} \langle u^2 \rangle/2 \) in the last line. Note that the \( Q_\mu \) term is cancelled by the \( Q_\mu = 0 \) part of the second 2D-elastic term. This is a reflection of the long range divergences in the 2D system with log (Coulomb) interactions, which do not exist for the 3D system of stacks where the circulation currents are screened beyond \( \lambda \).

The elastic matrix decomposes to transverse \( \delta_{ij} - K_i K_j \) and \( \Phi^{ij}(\mathbf{K}) = c_{66}(\mathbf{K}) K^2 + n_v \alpha_6 \) and longitudinal \( K_i K_j \) and \( \Phi^{ij}(\mathbf{K}) = c_{11}(\mathbf{K}) K^2 + n_v \alpha_{11} \) projections, where \( c_{66} \) and \( c_{11} \) are the dispersive shear and compression moduli, and \( \alpha_6 \) is the substrate strength,

\[
\alpha_6 = 2\pi \varepsilon_0 d n_v \sum_{Q_\mu} \frac{e^{-Q_\mu^2\langle u^2 \rangle/2}}{1 + \lambda^2 Q_\mu^2}. \tag{6}
\]

The \( \langle u^2 \rangle \rightarrow 0 \) limit of \( c_{66} \) and \( c_{11} \) recovers the usual form for the elasticity of a 2D vortex lattice [4], with a shear modulus \( c_{66}^0 = n_v \varepsilon_0 d/4 \) and a diverging compression modulus \( c_{11}^0(K) = 4\pi \varepsilon_0 d n_v^2 / K^2 \) at small \( K \). A finite \( \langle u^2 \rangle \) softens these moduli, although the diverging compression modulus remains. To solve self-consistently for \( \langle u^2 \rangle \) we use the equipartition result with the substrate,

\[
\langle u^2 \rangle = \int_{BZ} \frac{d^2 K}{(2\pi)^2} \left[ \frac{T}{c_{66}(\mathbf{K}) K^2 + n_v \alpha_6} + \frac{T}{c_{11}(\mathbf{K}) K^2 + n_v \alpha_{11}} \right] \approx \frac{T}{4\pi c_{66}} \ln \left( 1 + \frac{c_{66} K_0^2}{n_v A_0} \right) + \frac{T}{4\pi c_{11}(K_0^2) + A_0}, \tag{7}
\]

where in the last line we have used the small \( K \) limits for \( c_{66} \) and \( c_{11} \) and the circular-Brillouin-zone approximation with \( K_0 \approx \sqrt{4\pi}/a_0 \). Note how the substrate potential cuts off the log divergence for the 2D shear fluctuations.
The self-consistent Eqs. (1) and (2) determine \( \langle u^2 \rangle \). Above a temperature \( T_u \) there are no solutions, giving an upper bound to the melting transition. However, in [15] it was shown that the SCHA underestimates the degree of anharmonic thermal softening of a 2D lattice because of the neglect of odd terms in the anharmonicity. Such cubic anharmonicities are included in the two-vertex-SCHA [17] giving results which compare well to numerical simulations. In Fig. 1 we show the instability line in the B-T phase diagram using the two-vertex-SCHA. The line interpolates between \( T_{\text{BKT}} \) at small fields and \( T_{\text{2D}} \) at high fields. Also shown is the significant thermal softening of both \( c_{66} \) and \( \alpha_s \) at \( B = B_\lambda \) with the resulting anharmonic contributions (beyond linear in \( T \)) for \( \langle u^2 \rangle \).

For melting transitions it is often difficult to accurately determine the free energy of the liquid. We can make progress for PVL melting, as the liquid state behaves to a good approximation as uncoupled 2D liquids in each layer. The free energy of a 2D liquid with log-interactions can be extracted from numerical simulations [10]. A crucial ingredient is that the free energy is known exactly [17] at one special temperature \( T = \varepsilon_0d \). For the solid we calculate the free energy of a 2D crystal on a self-consistent substrate. We must be careful to take the same normalization in both phases: as in [17] we normalize with respect to the ideal gas of \( N \) pancakes, \( Z(H = 0) = 1 \), and define the partition function,

\[
Z = \frac{1}{N!} \int \prod_i \left( \frac{R_i}{c} \right) d^2R_i e^{-H[R_i]/T},
\]

fixing the free energy, measured from the ideal gas, as \( F = -T \ln Z \). We write \( H = H_{\text{2D}} + H_s \) where \( H_{\text{2D}} = (N/2)[\sum_{\mu \neq 0} V_0(R_\mu) - n_s \int d^2R V_0(R)] \) and \( H_s = (N/2) \left[ \sum_{\mu \neq 0} V_n(R_\mu) + n_s \int d^2R V_0(R) \right] \) are the 2D interaction term and substrate energy respectively [18].

In the solid, the free energy of harmonic fluctuations is straightforward to calculate. The right-hand side of the inequality \( F \leq F^h + (H - H^h) \) is minimized by the SCHA (see [15]) where \( H^h \) is defined by (1). The harmonic free energy of 2D fluctuations is

\[
F^h = -\frac{NT}{2\pi v} \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} \left[ \ln \left( \frac{\pi T n_s}{\varepsilon_0(c_{66} K^2 + n_s \alpha_s)} \right) \right]
\]

\[+ \ln \left( \frac{\pi T n_s}{\varepsilon_0(c_{11} K^2 + n_s \alpha_s)} \right) \].

The correction part of the variational free energy has contributions from \( H_{\text{2D}} \) and \( H_s \). Ignoring the small anharmonic part of the 2D energy, the difference \( (H_{\text{2D}} - H^h) \) is just the ground state energy (which is not included in \( H^h \)). In [17] the energy for a 2D lattice of log-interacting particles is found to be \( E_{\text{2D}}^0 = 0.749N\varepsilon_0d \). The substrate energy correction, \( E_s = (H_s - H^h) \), is

\[
E_s = -N \left[ 2\pi n_0 \varepsilon_0d \sum_{Q_\mu \neq 0} \frac{e^{-Q_\mu^2/2}}{Q_\mu^2(1 + \lambda^2Q_\mu^2)} + \frac{1}{2} \alpha_s \langle u^2 \rangle \right],
\]

and the sum \( F^h + E_{\text{2D}}^0 + E_s \) is the variational free energy.

In the liquid phase, \( (H_s) \) is very small and we should find the free energy of a 2D liquid. The internal energy \( U_\Gamma \) (with \( \Gamma = 2\varepsilon_0d/T \)) is found from simulations [10],

\[
U_\Gamma = \left( -0.751 + 0.880 \Gamma^{-0.74} - 0.209 \Gamma^{-1.7} \right) N\varepsilon_0d.
\]

From the relation \( F = U + T \partial_\Gamma F \), the excess free energy can be written as \( \Gamma F_{\text{lin}}(\Gamma) = \Gamma_0 F_{\text{lin}}(\Gamma_0) + \int_{\Gamma_0}^{\Gamma} U(\Gamma')d\Gamma' \). We know the value at \( \Gamma_0 = 2 \), where \( F_{\text{lin}}(2) = 0.081\varepsilon_0dN \). so we can integrate (11) to give (with \( t = T/\varepsilon_0d \)),

\[
F_{\text{lin}} = \left( -0.751 - 1.287t + 0.2097t^{0.74} + 0.092t^{-1.7} \right) N\varepsilon_0d.
\]

Using these results we can plot the free energy of both phases and see where they cross; a typical example at \( B = B_\lambda \) is shown in the inset of Fig. 2. Calculating the crossing point numerically at different fields, we find a melting line (see Fig. 2) just below the stability limit of the lattice that approaches zero field at \( T \approx 0.47\varepsilon_0d \).

The jump in slope \( S = -\partial_\Gamma F \) gives a latent heat \( T\Delta S = \Delta U \). In Fig. 2 we plot the entropy jump per pancake vortex as a function of the transition temperature.
At high fields (small $T$) it approaches the value $\Delta s = 0.4 k_B T$, consistent with 2D simulations 15 and simple estimates 16. At low fields ($T \sim 0.55d\lambda$) the latent heat appears to weakly diverge as $T \rightarrow T_{\text{BKT}}$. We understand this as the energy of the liquid is roughly constant, $U(T) \approx U(0)$, while the energy of the solid is dominated by the substrate term, $E_s \sim N_\text{v} d \ln(\lambda/a_0)$ so that the latent heat is $\Delta U \sim -E_s$. This gives an entropy jump per vortex pancake $\Delta s_v = \Delta U/N_T \sim k_B \ln(B_0/B)$. This is of the same form as the entropy difference between an ideal gas, $\Delta s_{\text{gas}} = k_B \ln (a_0^2/\xi^2)$ and the (reduced phase-space) solid $\Delta s_{\text{sol}} = k_B \ln (\langle u^2 \rangle/\xi^2)$ when $\langle u^2 \rangle \sim a_0^2$. We do not include here the $T$ dependence of $\lambda$ in real systems that gives extra terms in the latent heat $\Delta s_{\lambda}$. Doing this, we find that our melting curve of Fig. 2 lies below experimental melting lines 22 for reasonable choices of $\lambda(T)$; this is because the Josephson coupling, neglected in this paper, becomes important as $T_c^0$ is approached 3 and stiffens the vortex lattice. Our results may be recovered in experiments by suppressing the Josephson coupling with a strong in-plane magnetic field.

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**FIG. 2.** The full line in the upper graph shows the melting line $B_m(T)$ of the pancake vortex lattice as calculated by comparing the free energies of the solid and liquid phases. The dashed line is the stability limit $B_m(T)$ of the PVL as shown in Fig. 1. The inset shows the free energy comparison at $B = B_0$. The lower graph gives the entropy jump per pancake vortex $\Delta s_v$. Also shown are the real scales of $T$ and $B$ assuming $\lambda(T) = \lambda(0)/[1 - (T/T_{\text{c}})]^2$, with $\lambda(0) \approx 2000\AA$, $d \approx 15\AA$ and $T_{\text{c}} \approx 100$ K. The low-field reentrant melting line, not shown here, will cut $B_m(T)$ below $10^{-2}B_0$.

Previously, melting of the magnetically coupled PVL has been analyzed numerically 8 and via density functional theory (DFT) of the liquid phase 20. The early simulations in 8 find evidence of melting at $T \approx 0.09d\lambda$ when $B/B_0 \approx 0.2$ (close to our melting line). The DFT gives the stability limit of the liquid and provides results consistent with ours at fields above $0.5B_0$. At lower fields the DFT gives a liquid instability above our melting line, a discrepancy which requires further study.

To compare to real superconductors our units of field $B_0$ and of temperature $T_0$ must be scaled due to the intrinsic variation in $\lambda(T)$ (diverging at a temperature $T^0_c$). We understand this as the energy of the liquid is roughly constant, $U(T) \approx U(0)$, while the energy of the solid is dominated by the substrate term, $E_s \sim N_\text{v} d \ln(\lambda/a_0)$ so that the latent heat is $\Delta U \sim -E_s$. This gives an entropy jump per vortex pancake $\Delta s_v = \Delta U/N_T \sim k_B \ln(B_0/B)$. This is of the same form as the entropy difference between an ideal gas, $\Delta s_{\text{gas}} = k_B \ln (a_0^2/\xi^2)$ and the (reduced phase-space) solid $\Delta s_{\text{sol}} = k_B \ln (\langle u^2 \rangle/\xi^2)$ when $\langle u^2 \rangle \sim a_0^2$. We do not include here the $T$ dependence of $\lambda$ in real systems that gives extra terms in the latent heat $\Delta s_{\lambda}$. Doing this, we find that our melting curve of Fig. 2 lies below experimental melting lines 22 for reasonable choices of $\lambda(T)$; this is because the Josephson coupling, neglected in this paper, becomes important as $T_c^0$ is approached 3 and stiffens the vortex lattice. Our results may be recovered in experiments by suppressing the Josephson coupling with a strong in-plane magnetic field.

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1. G. Blatter et al., Rev. Mod. Phys. 66, 1125 (1994).
2. E. Zeldov et al., Nature 375, 373 (1995).
3. A. Schilling et al., Nature 382, 791 (1996).
4. D.T. Fuchs et al., Phys. Rev. Lett. 80 4971 (1998).
5. A. Houghton, R.A. Pelcovits, and A. Sudbo, Phys. Rev. B 42, 906 (1990).
6. G. Blatter et al., Phys. Rev. B 54, 72 (1996).
7. R. Šašík and D. Stroud, Phys. Rev. Lett. 75, 2582 (1995); J. Hu and A. MacDonald, Phys. Rev. B 56, 2788 (1997); H. Nordborg and G. Blatter, Phys. Rev. Lett. 79, 1925 (1997); A.E. Koshelev, Phys. Rev. B 56, 11201 (1997); X. Hu, S. Miyashita, and M. Tachiki, Phys. Rev. Lett. 79, 3498 (1997); A.K. Nguyen and A. Sudbo, Phys. Rev. B 58, 2802 (1998); P. Olsson and S. Teitel, Phys. Rev. Lett. 82, 2183 (1999).
8. D. Reefman and H.B. Brom, Physica C 183, 212 (1991).
9. S. Ryu et al., Phys. Rev. Lett. 68, 710 (1992).
10. J.M. Cairol et al., J. Stat. Phys. 28, 325 (1982).
11. J.R. Clem, Phys. Rev. B 43, 7837 (1991); L.N. Bulaevskii, S.V. Meshkov and D. Feinberg, Phys. Rev. B 43, 3728 (1991).
12. V.L. Berezinskii, Sov. Phys. JETP 32, 493 (1971); J.M. Kosterlitz and D.J. Thouless, J. Phys. C 6, 1181 (1973).
13. S.N. Artemenko and A.N. Kruglov, Phys. Lett. A 143, 485 (1990); M.V. Feigelman, V.B. Geshkenbein and A.I. Larkin, Physica C 167, 177 (1990); A. Buzdin and D. Feinberg, J. Phys. (France) 51, 1971 (1990).
14. M.J.W. Dodgson, V.B. Geshkenbein, and G. Blatter, to appear in Physica B.
15. M.J.W. Dodgson et al. (in preparation).
16. E.H. Brandt, J. Low Temp. Phys. 26, 735 (1977).
17. A. Alastuey and B. Jancovici, J. Phys. (France) 51, 1971 (1990).
18. Note that we add and subtract the background energy of the 2D log-system must cancel for 3D stacks.
19. M.J.W. Dodgson et al., Phys. Rev. Lett. 80, 837 (1998).
20. S. Sengupta et al., Phys. Rev. Lett. 67, 3444 (1991); G.I. Menon et al., Phys. Rev. B 54, 16192 (1996); P.S. Cornaglia and C.A. Balseiro, preprint cond-mat/9904183.
21. S.L. Lee et al., Phys. Rev. B 55, 5666 (1997).