

## Defective vortex lattices in layered superconductors with point pins at the extreme type-II limit

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The mixed phase of layered superconductors with no magnetic screening is studied through a partial duality analysis of the corresponding frustrated  $XY$  model in the presence of weak random point pins. Isolated layers exhibit a defective vortex lattice at low temperature that is phase coherent. Sufficiently weak Josephson coupling between adjacent layers results in an entangled vortex solid that exhibits weak superconductivity across layers. The corresponding vortex liquid state shows an inverted specific-heat anomaly that we propose accounts for that seen in yttrium barium copper oxide. A three-dimensional vortex lattice with dislocations occurs at stronger coupling. This crossover sheds light on the apparent discrepancy concerning the observation of a vortex-glass phase in recent Monte Carlo simulations of the same  $XY$  model.

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High-temperature superconductors are layered and extremely type-II.<sup>1</sup> This fact led to the suggestion early on that a state with phase-coherent yet decoupled layers is possible.<sup>2</sup> It was later demonstrated, however, that *any* amount of Josephson coupling between layers results in a macroscopic Josephson effect across layers at low temperature.<sup>3</sup> In the presence of external magnetic field perpendicular to the layers, other workers made the analogous proposal that sufficiently weak coupling could lead to a decoupled stack of phase-coherent two-dimensional (2D) vortex lattices.<sup>4,5</sup> Monte Carlo simulations<sup>6</sup> and a partial duality analysis<sup>7,8</sup> of the corresponding frustrated  $XY$  model demonstrate, however, that a highly entangled vortex lattice state with relatively small or no phase coherence across layers does not exist in practice.

The elusive decoupled vortex lattice state may exist at low temperature in the presence of random point pins, however.<sup>9,10</sup> In this paper, we show that this is indeed the case through a partial duality analysis of the corresponding layered  $XY$  model with uniform frustration.<sup>11</sup> We show first that a defective vortex lattice state<sup>5</sup> can exist in isolated layers. It exhibits macroscopic phase coherence in the zero-temperature limit, despite the presence of unbound dislocations that are assumed to be quenched in by the random pins.<sup>12</sup> We next turn on Josephson coupling between adjacent layers and find that weak superconductivity exists across layers at sufficiently high layer anisotropy<sup>11</sup> in the zero-temperature limit. After assuming a continuous 2D ordering transition for each layer in isolation, we then find that an inverted specific heat jump can occur inside of the vortex liquid state at weak coupling. This prediction compares favorably with the recent observations of such a peak in the high-temperature superconductor yttrium barium copper oxide (YBCO).<sup>13</sup>

**2D.** Consider a stack of isolated superconducting layers in a perpendicular external magnetic field. In the absence of Josephson coupling as well as of magnetic screening, the  $XY$  model over the square lattice with uniform frustration provides a qualitatively correct description of the mixed phase in each layer. The corresponding Boltzmann distribution is set by the sum of energy functionals,

$$E_{XY}^{(2)}(l) = - \sum_{\mu=x,y} \sum_{\vec{r}} J_{\mu} \cos[\Delta_{\mu} \phi - A_{\mu}], \quad (1)$$

for the superfluid kinetic energy of each layer  $l$  written in terms of the superconducting phase  $\phi(\vec{r}, l)$ . Here  $\Delta_{\mu} \phi(\vec{r}, l) = \phi(\vec{r} + a\hat{\mu}, l) - \phi(\vec{r}, l)$  and  $\vec{A} = (0, 2\pi f x/a)$  make up the local supercurrent, where  $f$  denotes the concentration of vortices over the square lattice, with lattice constant  $a$ . The local phase rigidity  $J_{\mu}(\vec{r}, l)$  is assumed to be constant over most of the nearest-neighbor links  $(\vec{r}, \vec{r} + a\hat{\mu})$  in layer  $l$ , with the exception of those links in the vicinity of the pinning sites that are located at random. After taking the Villain approximation, which is generally valid at low temperature,<sup>14</sup> a series of standard manipulations then lead to a Coulomb gas ensemble with pins that describes the vortex degrees of freedom on the dual square lattice.<sup>8</sup> The ensemble for each layer  $l$  is weighted by the Boltzmann distribution set by the energy functional

$$E_{vx}(l) = (2\pi)^2 \sum_{(\vec{R}, \vec{R}')} \delta Q J_0 G^{(2)} \delta Q' + \sum_{\vec{R}} V_p |Q|^2, \quad (2)$$

written in terms of the integer vorticity field  $Q(\vec{R}, l)$  over the sites  $\vec{R}$  of the dual lattice in that layer, and of the fluctuation  $\delta Q = Q - f$ . A logarithmic interaction,  $G^{(2)} = -\nabla^{-2}$ , exists between the vortices, with a strength  $J_0$  equal to the Gaussian phase rigidity. Last,  $V_p(\vec{R}, l)$  is the resulting pinning potential.<sup>8</sup>

We shall next assume that the array of random pins in each layer,  $V_p(\vec{R}, l)$ , quenches in unbound dislocations into the triangular vortex lattice at zero temperature.<sup>12</sup> To check for superconductivity in such a defective 2D vortex lattice, we now compute the macroscopic phase rigidity, which is given by one over the dielectric constant of the 2D Coulomb gas (2).<sup>15</sup>

$$\rho_s^{(2D)}/J_0 = 1 - \lim_{k \rightarrow 0} (2\pi/\eta_{sw}) \langle \delta Q_{\vec{k}} \delta Q_{-\vec{k}} \rangle / k^2 a^2 \mathcal{N}_{\parallel}. \quad (3)$$

Here  $\delta Q_{\vec{k}} = Q_{\vec{k}} - \langle Q_{\vec{k}} \rangle$  is the fluctuation in the Fourier transform of the vorticity in layer  $l$ :  $Q_{\vec{k}} = \sum_{\vec{R}} Q(\vec{R}, l) e^{i\vec{k} \cdot \vec{R}}$ . Also,

$\eta_{sw} = k_B T / 2\pi J_0$  is the spin-wave component of the phase-correlation exponent, and  $N_{\vec{v}}$  denotes the number of points in the square-lattice grid. Now suppose that a given vortex is displaced by  $\vec{\delta u}$  with respect to its location at zero temperature. Conservation of vorticity dictates that its fluctuation is given by  $-\vec{\nabla} \cdot \vec{\delta u}$ . Substitution into Eq. (3) then yields the result

$$\rho_s^{(2D)} / J_0 = 1 - (\eta'_{vx} / \eta_{sw}) \quad (4)$$

for the phase rigidity in terms of the vortex component to the phase-correlation exponent,

$$\eta'_{vx} = \pi \left\langle \left[ \sum_R' \vec{\delta u} \right]^2 \right\rangle / N_{vx} a_{vx}^2. \quad (5)$$

The latter monitors fluctuations of the center of mass of the vortex lattice.<sup>16</sup> Above,  $N_{vx}$  denotes the number of vortices, while  $a_{vx} = a/f^{1/2}$ .

To proceed further, we now express the displacement field as a superposition of *pure* wave and defect components of the triangular vortex lattice:<sup>16</sup>  $\vec{\delta u} = \vec{\delta u}_{wv} + \vec{\delta u}_{df}$ . Notice by Eq. (5) that phase coherence is insensitive to the wave contribution if rigid translations are excluded, since  $\sum \vec{\delta u}_{wv} = 0$  in such case. The former is achieved through bulk pinning,<sup>8</sup> and the latter then follows under periodic boundary conditions. Consider now a single unbound dislocation with Burgers vector  $\vec{b}$  that slides along its glide plane<sup>1</sup> a distance  $\delta R_{df}$  with respect to its location at zero temperature. The relative displacement field  $\vec{\delta u}_{df}$  then corresponds to that of a *pure* dislocation pair of extent  $\delta R_{df}$  that is oriented along its glide plane. After following steps similar to those taken in Ref. 16 for the pristine case, it can be shown that Eq. (5) yields a fluctuation of the center of mass,

$$\eta'_{vx} \approx n_{df} \overline{(\delta R_{df})^2} (b/2a_{vx})^2 \ln R_0 / a_{df}, \quad (6)$$

for the vortex solid, where  $n_{df}$  denotes the density of unbound dislocations,  $a_{df}$  is the core diameter of a dislocation, and  $R_0$  is an infrared cutoff. Above, the overbar denotes a bulk average. Observe now that both  $\eta_{sw}$  and  $\eta'_{vx}$  vanish linearly with temperature. By Eq. (4), we conclude that the defective 2D vortex lattice shows a positive phase rigidity in the zero-temperature limit at sufficiently dilute concentrations of unbound dislocations,  $n_{df} \rightarrow 0$ . The above is borne out by direct Monte Carlo simulations<sup>17</sup> of the 2D Coulomb gas ensemble (2).

The previous positive result for macroscopic phase coherence [Eq. (4)] in the zero-temperature limit can be confirmed by calculation of generalized phase autocorrelation functions within an isolated layer:  $C_l[q] = \langle \exp[i\sum_{\vec{r}} q(\vec{r}) \phi(\vec{r}, l)] \rangle_0$ . Following a similar calculation in the pristine case,<sup>16</sup> application of the Villain approximation [see Eq. (2) and Ref. 14] yields the form  $C_l[q] = |C_l[q]| \exp[i\sum_{\vec{r}} q(\vec{r}) \phi_0(\vec{r}, l)]$  for these autocorrelations, where  $\phi_0(\vec{r}, l)$  represent the zero-temperature configurations of isolated layers. In the low-temperature regime, phase correlations are then found to decay algebraically as

$$|C_l[q]| = g_0^{n_+} \exp \left[ \eta_{2D} \sum_{(1,2)} q(1) \ln(r_{12}/r_0) q(2) \right] \quad (7)$$

at the asymptotic limit  $r_{12} \rightarrow \infty$ , with a net correlation exponent approximately equal to  $\eta_{2D} \cong \eta_{sw} + \eta'_{vx}$  for small vortex components,  $\eta'_{vx} \ll \eta_{sw}$ . Here,  $g_0 = \rho_s^{(2D)} / J$  is the ratio of the 2D stiffness with its value at zero temperature,  $J$ , while  $n_+$  counts half the number of probes in  $q(\vec{r})$ . Also,  $r_0$  denotes the natural ultraviolet scale.

**3D.** We shall now add a weak Josephson coupling energy  $-J_z \cos(\Delta_z \phi - A_z)$  to all of the vertical links in between adjacent layers of the three-dimensional (3D) XY model. Here,  $J_z = J/\gamma'^2$  is the perpendicular coupling constant, with anisotropy parameter  $\gamma' > 1$ . The layered XY model can be effectively analyzed in the selective high-temperature limit,  $k_B T \gg J_z$ , through a *partial* duality transformation. This leads to a dilute Coulomb gas (CG) ensemble that describes the nature of the Josephson coupling in terms of dual charges that live on the vertical links. Phase correlations across layers can then be computed from the quotient

$$\left\langle \exp \left[ i \sum_{\vec{r}} p(r) \phi(r) \right] \right\rangle = Z_{CG}[p] / Z_{CG}[0] \quad (8)$$

of partition functions for a layered CG ensemble:<sup>11</sup>

$$Z_{CG}[p] = \sum_{\{n_z(r)\}} y_0^{N[n_z]} \prod_l C_l[q_l] e^{-i \sum_{\vec{r}} n_z A_z}, \quad (9)$$

where the dual charge  $n_z(\vec{r}, l)$  is an integer field that lives on links between adjacent layers  $l$  and  $l+1$  located at 2D points  $\vec{r}$ . The ensemble is weighted by a product of phase autocorrelation functions for isolated layers  $l$  probed at the dual charge that accumulates onto that layer:

$$q_l(\vec{r}) = p(\vec{r}, l) + n_z(\vec{r}, l-1) - n_z(\vec{r}, l). \quad (10)$$

It is also weighted by a bare fugacity  $y_0$  that is raised to the power  $N[n_z]$  equal to the total number of dual charges,  $n_z = \pm 1$ . The fugacity is given by  $y_0 = J_z / 2k_B T$  in the selective high-temperature regime,  $J_z \ll k_B T$ , reached at large model anisotropy.

In the absence of Josephson coupling, random point pins lead to zero-temperature phase configurations  $\phi_0(\vec{r}, l)$ , which are completely uncorrelated across layers. At zero parallel field, Eqs. (8) and (9) therefore yield the expressions<sup>18</sup>

$$\overline{\langle \cos \phi_{l,l+1} \rangle} \cong y_0 \sum_1 \overline{C_l(0,1)} \cdot \overline{C_{l+1}^*(0,1)} \quad (11)$$

and

$$\begin{aligned} & \overline{\langle e^{i\phi_{l,l+1}} \rangle^2} \\ & \cong y_0^2 \sum_1 \sum_2 \overline{C_l(0,1) C_l^*(0,2)} \cdot \overline{C_{l+1}(0,2) C_{l+1}^*(0,1)} \end{aligned} \quad (12)$$

for the interlayer ‘‘cosine’’ and the interlayer phase correlation, to lowest order in the fugacity. The overbar represents a

bulk (disorder) average, while  $\phi_{l,l+1}(\vec{r}) = \phi(\vec{r}, l+1) - \phi(\vec{r}, l) - A_z(\vec{r}, l)$  is the gauge-invariant phase difference across adjacent layers. Macroscopic phase coherence shown by each layer in isolation (4) is lost at a transition temperature<sup>17</sup>  $T_g^{(2D)} > 0$ . Only short-range phase correlations on the scale of  $\xi_{2D}$  exist at higher temperature following  $C_l(1,2) = g_0 e^{-r_{12}/\xi_{2D}} e^{i\phi_0(1)} e^{-i\phi_0(2)}$ . By analogy with 2D melting physics,<sup>16,19</sup> the presence of quenched-in unbound dislocations also implies that only short-range phase correlations exist inside of each layer in isolation, on average, at zero temperature. Specifically, we have  $\overline{\exp[i\phi_{l,l+1}^{(0)}(1)] \exp[-i\phi_{l,l+1}^{(0)}(2)]} = e^{-2r_{12}/l_{2D}}$  asymptotically, where  $\phi_{l,l+1}^{(0)}(\vec{r}) = \phi_0(\vec{r}, l+1) - \phi_0(\vec{r}, l) - A_z(\vec{r}, l)$  is the quenched interlayer phase difference, and where  $l_{2D}$  represents a zero-temperature disorder scale set by  $n_{df}$ . Substitution into expression (12) then yields the result  $[\langle e^{i\phi_{l,l+1}} \rangle]^2 \sim [g_0^2 (J/k_B T) (l_{2D} \xi_{2D} / \Lambda_0^2)]^2$  for the interlayer phase correlation inside the critical regime,  $\xi_{2D} \gg l_{2D}$ , where  $\Lambda_0 = \gamma a$  is the Josephson penetration length. This approximate result reaches unity at a crossover field

$$f\gamma_X'^2 \sim g_0^2 (J/k_B T) (l_{2D} \xi_{2D} / a_{vx}^2), \quad (13)$$

in units of the naive decoupling scale  $\Phi_0 / \Lambda_0^2$  that separates 2D from 3D vortex-liquid behavior.<sup>7</sup> Substitution into expression (11) for the interlayer cosine, on the other hand, yields a nondivergent result

$$\overline{\langle \cos \phi_{l,l+1} \rangle} \sim g_0^2 (J/k_B T) [(l_{2D}^{-1} + \xi_{2D}^{-1})^{-1} / \Lambda_0]^2, \quad (14)$$

which is valid in the decoupled vortex liquid that exists at fields much larger than  $f\gamma_X'^2$ . It can be shown<sup>20</sup> that the next-leading-order term for the interlayer cosine (11) is negative, that it diverges just like the leading-order term for the interlayer correlation (12), and that it becomes comparable to its own leading-order term precisely at fields below the 2D-3D crossover scale, Eq. (13). Last, Eq. (14) implies an anomalous interlayer contribution to the specific heat per volume equal to

$$\delta c_v^\perp \cong 2 [1 + (\xi_{2D} / l_{2D})]^{-1} (\partial \ln \xi_{2D}^{-1} / \partial T) e_J, \quad (15)$$

where  $e_J = \overline{\langle \cos \phi_{l,l+1} \rangle} \cdot J / \Lambda_0^2 d$  is the Josephson energy density and  $d$  denotes the spacing in between adjacent layers. It also notably shows an inverted specific-heat jump that is followed by a tailoff at a temperature  $T_p$  such that  $\xi_{2D}(T_p) \sim l_{2D}$  if  $\xi_{2D}$  diverges faster than  $(T - T_g^{(2D)})^{-1}$ . This approximate result is again valid at high anisotropy,  $\gamma' > \gamma'_X$ , which yields the bound  $l_{2D} < g_0^{-1} (k_B T / J)^{1/2} \Lambda_0$  on the 2D disorder scale by Eq. (13).

The previous analysis clearly demonstrates that a selective high-temperature expansion in powers of the fugacity  $y_0$  necessarily breaks down in the ordered phase,  $T < T_g^{(2D)}$ , where  $\xi_{2D}$  is infinite. At this stage it becomes useful to re-express the layered CG ensemble (9) by replacing  $C_l[q]$  with its magnitude (7), and by compensating this change with the additional replacement of  $A_z(\vec{r}, l)$  with  $-\phi_{l,l+1}^{(0)}(\vec{r})$ . A Hubbard-Stratonovich transformation of the

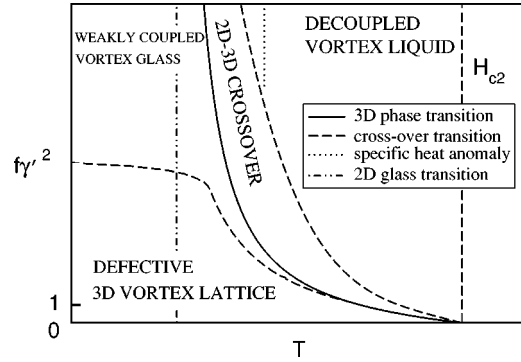


FIG. 1. Shown is the proposed phase diagram assuming weak point pins and a continuous vortex glass phase transition for isolated layers. The concentration of in-plane vortices,  $f$ , is held fixed, and a mean-field temperature dependence,  $J \propto T_{c0} - T$ , is assumed. Monte Carlo simulations of the same XY model studied here find evidence for a second-order transition between the vortex-glass and the vortex-liquid phases (see Ref. 22). When confronted with the first-order decoupling transition that is expected to separate the vortex liquid from the 3D vortex lattice (see Refs. 11 and 23), this implies the existence of a critical end point consistent with experiments on YBCO (Ref. 13) and with other numerical simulations (Ref. 24) of the present XY model. A transition to a 3D vortex lattice without defects is reported in Ref. 25 at  $f\gamma'^2 < 1$ .

CG partition function (9) reveals<sup>21</sup> that it is equivalent to a renormalized Lawrence-Doniach (LD) model with an energy functional that is given by<sup>11</sup>

$$E_{LD} = \rho_s^{(2D)} \int d^2r \sum_l \left[ \frac{1}{2} (\vec{\nabla} \theta_l)^2 - \Lambda_0^{-2} \cos \theta_{l,l+1} \right], \quad (16)$$

where  $\theta_{l,l+1} = \phi_{l,l+1}^{(0)} + \theta_{l+1} - \theta_l$ . A standard thermodynamic analysis<sup>7</sup> then yields that the strength of the local Josephson coupling is given by  $\langle \cos \phi_{l,l+1} \rangle = y_0 + g_0 \langle \cos \theta_{l,l+1} \rangle$ . It can also be shown<sup>11</sup> that phase coherence exists across a macroscopic number of layers, with a corresponding phase rigidity equal to  $\rho_s^\perp / J_z \cong g_0 \langle \cos \theta_{l,l+1} \rangle$ .

In order to compute  $\langle \cos \theta_{l,l+1} \rangle$  at low temperature, we must first determine the configuration that optimizes  $E_{LD}$ . Equation (16) implies that it satisfies the field equation

$$-\nabla^2 \theta_l^{(0)} + \Lambda_0^{-2} [\sin \theta_{l-1,l}^{(0)} - \sin \theta_{l,l+1}^{(0)}] = 0. \quad (17)$$

In the weak-coupling limit  $\Lambda_0 \rightarrow \infty$ , we therefore have that  $\theta_l^{(0)}(\vec{r})$  is constant inside each layer. The fact that  $e^{i\phi_0(1)} e^{-i\phi_0(\infty)} = 0$  then implies that  $\cos \theta_{l,l+1} = 0$  at zero temperature in the weak-coupling limit. Indeed, the LD cosine can be calculated perturbatively, where one finds that  $\cos \theta_{l,l+1} \sim (l_{2D} / \Lambda_0)^2 \ln(\Lambda_0 / l_{2D})$  at zero temperature.<sup>10,20</sup> In the opposite limit of weak disorder,  $l_{2D} \rightarrow \infty$ , Eq. (17) yields that  $\sin \theta_{l-1,l}^{(0)} = \sin \theta_{l,l+1}^{(0)}$ , on the other hand. This then implies that  $\cos \theta_{l,l+1}^{(0)} = 1$  in the weak disorder limit. The bulk average  $\cos \theta_{l,l+1}$  at zero temperature must therefore pass between zero and unity at  $\Lambda_0 \sim l_{2D}$ . This condition defines a decoupling crossover field  $f\gamma_D'^2(0) \sim (l_{2D} / a_{vx})^2$  in units of  $\Phi_0 / \Lambda_0^2$ , at which point the reversible magnetization shows a broad diamagnetic peak. By the discussion following Eq.

(16), we conclude that random point pins result in a vortex glass at sufficiently high layer anisotropy,<sup>9,10</sup>  $\Lambda_0 \gg l_{2D}$ , which exhibits weak superconductivity across layers:<sup>11</sup>  $\rho_s^\perp \ll J_z$ .

The results of the above duality method are summarized by the phase diagram displayed in Fig. 1. The present theory notably predicts that an inverted specific heat anomaly (jump followed by a tailoff) occurs at weak coupling in the vortex liquid when the 2D correlation length  $\xi_{2D}$  matches the 2D disorder scale  $l_{2D}$  if  $\xi_{2D}$  diverges faster than  $(T - T_g^{(2D)})^{-1}$  [see Eq. (15)]. Such a feature has, in fact, been observed within the vortex-liquid phase of YBCO.<sup>13</sup> The weight of the latter peak is about  $\Delta e_{\text{exp}} \cong 6 \text{ mJ/cm}^3$ , while the peak shown by Eq. (15) has a weight  $\Delta e_J = (\Phi_0^2/16\pi^3\lambda_L^2\Lambda_0^2)\Delta\langle\cos\phi_{l,l+1}\rangle$ . Equating these and using values of  $\lambda_L \cong 140 \text{ nm}$  and  $\Lambda_0 \cong 7 \text{ nm}$  for the penetration depths in YBCO (Ref. 1) yields a 10% jump in the cosine.

Last, although recent Monte Carlo simulations of the same XY model studied here do indeed find evidence for a

phase-coherent vortex glass at<sup>24</sup>  $f\gamma'^2=16$  and at<sup>22</sup>  $f\gamma'^2=8$ , another one<sup>26</sup> using  $f\gamma'^2=2$  does not. We believe that the zero-temperature crossover shown in Fig. 1 between an entangled vortex glass and a 3D vortex lattice containing dislocations is the origin of this discrepancy.

In conclusion, a duality analysis of the XY model finds that random point pins<sup>9,10</sup> drive a crossover transition in the zero-temperature limit between defective vortex lattices that show strong vs weak superconductivity across layers as a function of the Josephson coupling.<sup>11</sup> We further propose that the inverted specific heat anomaly observed recently inside of the vortex-liquid phase of YBCO does not signal a phase transition,<sup>13</sup> but rather is due to the thermodynamic resonance found here, Eq. (15). Recent Monte Carlo simulations of the same XY model studied here also find a noncritical specific-heat anomaly in the vortex-liquid phase (see Ref. 27).

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