Theory of the Vortex Matter Transformations in High-T_c Superconductor YBCO

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Flux line lattice in type II superconductors undergoes a transition into a "disordered" phase such as vortex liquid or vortex glass, due to thermal fluctuations and random quenched disorder. We quantitatively describe the competition between the thermal fluctuations and the disorder using the Ginzburg-Landau approach. The following T-H phase diagram of YBCO emerges. There are just two distinct thermodynamical phases, the homogeneous and the crystalline one, separated by a single first order transition line. The line, however, makes a wiggle near the experimentally claimed critical point at 12 T. The "critical point" is reinterpreted as a (noncritical) Kauzmann point in which the latent heat vanishes and the line is parallel to the T axis. The magnetization, the entropy, and the specific heat discontinuities at melting compare well with experiments.

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The H-T phase diagram of a high T_c superconductor is very complex due to the competition between thermal fluctuations (TF) and disorder. At low fields, vortex solid melts into a liquid [1] due to TF. The discontinuity in magnetization [2–4] and in the specific heat [5,6] unambiguously demonstrate that the transition is a first order. Evidence is growing that the solid-glass transition in YBaCuO (YBCO) [7] is also a first order [4,8]. It was suggested [4] that the two first order phase transition lines $H_*(T)$ and $H_m(T)$ join at a multicritical point or that the melting line continues as a second order transition between the putative liquid II and a liquid [6]. However, other experiments are interpreted using a concept of "unified first order transition line" [9]: Only character of the transition evolves from the thermal fluctuation dominated to the disorder dominated one without multicritical points along the line. This single line was demonstrated in anisotropic materials BiSrCaCuO (BSCCO) [10], LaSrCuO [11], and NdCeCuO [8], and was claimed recently in YBCO [12].

Theoretically idealized models such as the frustrated XY model [13,14] or a collection of interacting pointlike objects subject to both the pinning potential and the thermal bath Langevin force were simulated numerically [15,16]. Alternatively, the melting line was located using the phenomenological Lindemann criterion on the solid side either in the framework of the "cage" model [9] or a more sophisticated approach based on the elasticity theory [17,18]. Although both approaches are very useful in more "fluctuating" superconductors such as BSCCO, a problem arises with their application to YBCO close to T_c: Vortices are far from being pointlike and even their cores significantly overlap. As a consequence, the behavior of a dense vortex matter is different from that of a system of pointlike vortices and of the XY model.

In this Letter, we quantitatively study the effects of the competition of thermal fluctuations and disorder in the framework of the anisotropic Ginzburg-Landau (GL) model appropriate precisely in the region of interest for YBCO. It was used successfully to describe the "clean" case [19,20].

The model without disorder is defined by free energy [1]:

$$\int d^3x \frac{\hbar^2}{2m_{ab}} \left| (\nabla - \frac{2\pi i}{\Phi_0} A)\psi \right|^2 + \frac{\hbar^2}{2m_c} |\partial_z \psi|^2 - \alpha T_c (1-t)|\psi|^2 + \frac{\beta}{2}|\psi|^4, \quad (1)$$

where $\Phi_0 = hc/(2e)$, $t = T/T_c$, $\mathbf{A} = (By, 0, 0)$. The model provides a good description of thermal fluctuations as long as $1 - t - b \ll 1$, where $b = H/H_{c2}$. An "applicability line" $1 - t - b \ll 0.2$ is depicted in Fig. 1. The model, however, is highly nontrivial even without disorder and within the lowest Landau level (LLL) approximation [19] in which only the LLL mode is retained and the free energy simplifies (after rescaling):

$$g_{\mathrm{LLL}} = \int d^3x \left[\frac{1}{2}|\partial_z \psi|^2 + a_T |\psi|^2 + \frac{1}{2}|\psi|^4 \right]. \quad (2)$$

The simplified model has just one parameter — the (dimensionless) scaled temperature: $a_T \equiv (t + b - 1) \times \sqrt[3]{2/(\mathrm{Gi}\pi^2 b^2 t^2)}$ with the Ginzburg number $\mathrm{Gi} \equiv 32[\pi\lambda^2 T_c \gamma/(\Phi_0^2 \xi)]^2$, $\gamma^2 = m_c/m_{ab}$ the anisotropy parameter, λ the magnetic penetration depth, and ξ the coherence length. The (effective) LLL model is applicable in a surprisingly wide range of fields and temperatures determined by the condition that the relevant excitation energy ε is much smaller than the gap between Landau

levels $\varepsilon_c \equiv 2\hbar eB/(cm_{ab})$. Within the mean field approximation in the liquid $\varepsilon/\varepsilon_c = x$ is a solution of the "gap equation"[21]): $2bx + (1 - t - b) = 2\pi t\sqrt{\mathrm{Gi}b} \times [\sqrt{4x - 2} + \sum_{n=0}^{\infty}(\sqrt{4x + 4n + 2} - \sqrt{4x + 4n - 2} - 1/\sqrt{n + x})]$. The LLL dominance line in Fig. 1 represents a conservative condition $\varepsilon/\varepsilon_c = 1/20$. On the right of the line, the HLL (higher Landau level) TF modes should be considered, while for $b < (1 - t)/13$, HLL in solid becomes important [20]. Apart from the fields smaller than $H_{\mathrm{LLL}} \approx 3$ kG, experimentally observed melting and the solid-glass lines are well within the range of applicability of the LLL approximation.

The disorder is described within the GL approach via a random field W_x with correlator $\overline{W_x W_y} = W\delta(x - y)$ [1], while TF are described by partition function $Z = \int_{\psi^*,\psi} \exp\{-[F + \int_x W_x|\psi_x|^2]/T\}$. Assuming small W, the free energy $-T\ln Z$ is calculated perturbatively to the second order:

$$g = g_{cl} + \int_x W_x\Big\{\langle|\psi_x|^2\rangle - \frac{1}{2T}\int_y W_y[\langle|\psi_x|^2|\psi_y|^2\rangle - \langle|\psi_x|^2\rangle\langle|\psi_y|^2\rangle]\Big\}, \tag{3}$$

where $\langle\,\rangle$ and g_{cl} denote the thermal average and effective free energy of the clean system. Averaging the random field, one obtains in the scaled units $g = g_{cl} - n(t)\Delta g_{\mathrm{dis}}$, where $\Delta g_{\mathrm{dis}} = \frac{1}{2}\int_x[\langle|\psi_x|^4\rangle - \langle|\psi_x|^2\rangle^2]$, and $n(t) \propto W/T$.

Recently, a quantitative theory [20] of TF in "clean" vortex liquids and solids based on the GL model of Eq. (2) was developed and was successfully applied to the fully oxidized $YBa_2Cu_3O_7$ for which the effects of disorder are negligible in whole currently accessible fields range [1,4]. The two loop result for solid in the clean case $g_{\mathrm{sol}} = -a_T^2/(2\beta_A) + 2.85|a_T|^{1/2} + 2.4/a_T$ is sufficiently precise (on the 0.1% level) all the way to melting. We calculated the one loop disorder correction: $\Delta g_{\mathrm{sol}} = 2.14|a_T|^{1/2}$. An explicit expression for $g_{\mathrm{liq}}(a_T)$, obtained using the Borel-Pade resummation of the renormalized high temperature series, is rather bulky and can be found in [20]. The disorder correction in liquid can be obtained by differentiating the "clean" partition function with respect to parameters: $\Delta g_{\mathrm{liq}} = (g_{\mathrm{liq}} - 2a_T g'_{\mathrm{liq}})/3 - (g'_{\mathrm{liq}})^2/2$. These results enable us to find the location of the transition line and calculate discontinuities of various physical quantities across the transition line.

It was noted [20] that in a clean system a homogeneous state exists as a metastable overcooled liquid state all the way down to zero temperature. This is of importance since interaction with disorder can convert the metastable state into a stable one. Indeed, generally a homogeneous state gains more than a crystalline state from pinning, since it can easier adjust itself to the topography of the pinning centers. Since at large $|a_T|$, $\Delta g_{\mathrm{liq}} \propto a_T^2$ is larger than $\Delta g_{\mathrm{sol}} \propto |a_T|^{1/2}$, the transition line shifts to lower fields. The equation for the melting line is $d(a_T) \equiv (g_{\mathrm{liq}} - g_{\mathrm{sol}})/(\Delta g_{\mathrm{liq}} - \Delta g_{\mathrm{sol}}) = n(t)$. The universal function $d(a_T)$, plotted in Fig. 2, turns out to be nonmonotonic. Since $n(t)$ is a monotonic function of t, one obtains the transition lines for various n in Fig. 1 by "sweeping" the Fig. 2. A peculiar feature of $d(a_T)$ is that it has a local minimum at $a_T \approx -17.2$ and a local maximum at $a_T \approx -12.1$ (before crossing zero at $a_T \approx -9.5$).

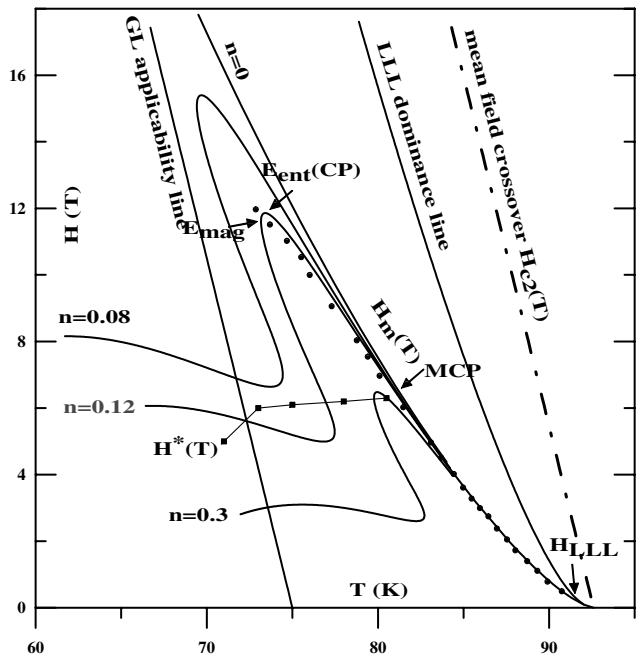

FIG. 1. Theoretical first order transition lines for various degrees of disorder separated between a homogeneous and a crystalline phase of vortex matter. The best fit $n = 0.12$ line is compared with experimental melting line $H_m(T)$ [6] and the solid-vortex glass transition line $H^*(T)$ [4]. Equal entropy and magnetization points are denoted by E_{ent} and E_{mag}. The range of applicability is restricted by the two lines. Very small fields below H_{LLL} are beyond this range.

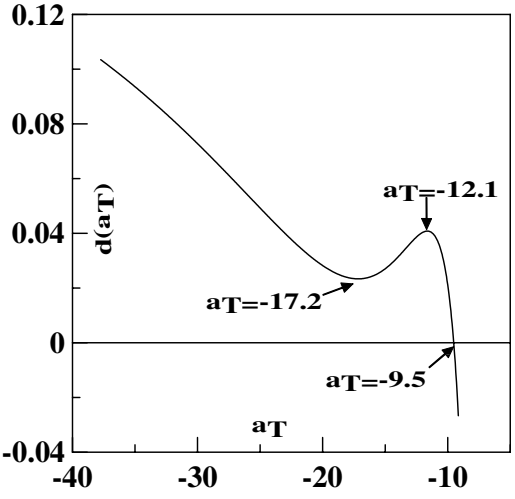

FIG. 2. Nonmonotonic dependence of the disorder function $d(a_T)$ on the LLL scaled temperature a_T.

Therefore between these two points there are three solutions to the melting line equation. As a result, starting from the zero field at T_c, the transition field $H(T)$ reaches a maximum at $E_{\rm ent}$ (point CP in Fig. 1) beyond which the curve sharply turns down (this feature was called "inverse melting" in [10]) and at $E_{\rm mag}$ backwards. Then it reaches a minimum and continues as the solid (Bragg glass)-vortex glass line roughly parallel to the T axis.

The temperature dependence of the disorder strength $n(t)$, as of any parameter in the GL approach, should be derived from a microscopic theory assuming random chemical potential or fitted to experiment. We conjecture (and find to be consistent with the experiments) that the general dependence near T_c is $n(t) = n(1-t)^2/t$ [or $W \propto (1-t)^2$]. The expression approaches the one used at lower temperatures [1] with $n = \gamma\gamma_T^0/(4\pi^2\sqrt{2{\rm Gi}}\xi^3)$. The best fit for the low field part of the experimental melting line $H_m(T)$ of the optimally doped YBCO (data taken from [6], $T_c = 92.6$, $\gamma = 8.3$) gives ${\rm Gi} = 2.0 \times 10^{-4}$, $H_{c2} =$ 190 T, $\kappa = \lambda/\xi = 50$ (consistent with other experiments [4,22]). This part is essentially independent of disorder. The upper part of the melting curve is very sensitive to disorder: Both the length of the "finger" and its slope depend on n. The best fit is $n = 0.12$. This value is of the same order of magnitude as the one obtained phenomenologically using Eq. (3.82) in [1]. We speculate that the low temperature part of the "unified" line corresponds to the solid-vortex glass transition $H^*(T)$ observed in numerous experiments [4,6–8,12] (squares in Fig. 1 [4]). A complicated shape of the "wiggling" line has been recently observed [12].

Magnetization and specific heat of both solid and liquid can be calculated from the above expressions for free energy. Magnetization of liquid along the melting line $H_m(T)$ is larger than that of solid. The magnetization jump is compared in Fig. 3(a) with the SQUID experiments [5] in the range 80–90 K (triangles) and of the torque experiments (stars [3] and circles [4]). One observes that the results of the torque experiments compare surprisingly well above 83 K while the SQUID data a bit lower than theoretical or the torque one. But those of [4] vanish abruptly below 83 K unlike the theory and are inconsistent with the specific heat experiments discussed below [6,22]. We predict that at lower temperatures (somewhat beyond the range investigated experimentally thus far) magnetization reaches its maximum and changes sign at the point $E_{\rm mag}$ (at which magnetization of liquid and solid are equal).

Entropy jump calculated using the Clausius-Clapeyron relation is compared with an experimental one deduced from the spike of the specific heat [6] [triangles in Fig. 3(b)] and an indirect measurement from the magnetization jumps [4] (circles). At high temperatures, the theoretical values are a bit lower than the experimental and both seem to approach a constant at T_c. The theoretical entropy jump and the experimental one of [6] vanish at $E_{\rm ent}$ (Fig. 1) near 75 K. Experimentally, such a point

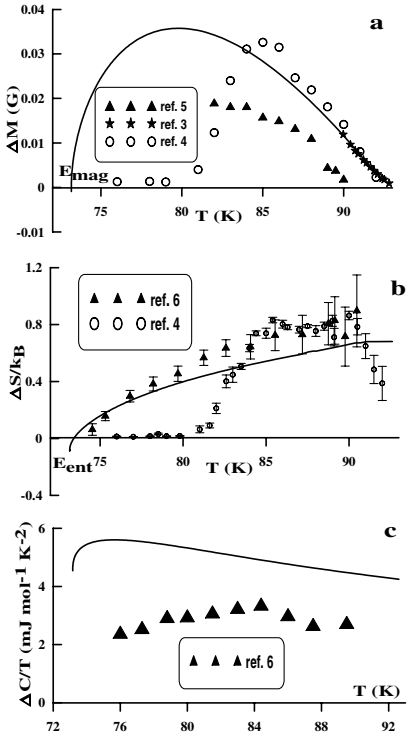

FIG. 3. Discontinuities along the first order transition line in YBCO. Jumps of magnetization, entropy, and specific heat are compared with experiments in (a), (b), and (c), respectively.

(called Kauzmann points [23]) was established in BSCCO as a point at which the inverse melting appears [10]. Below this temperature, entropy of the liquid becomes smaller than that of the solid. Note that the equal magnetization point $E_{\rm mag}$ is located at a slightly lower field than the equal entropy point $E_{\rm ent}$. The Kauzmann point observed at a lower temperature in YBCO in [8] is different from $E_{\rm ent}$ since it is a minimum rather than a maximum of magnetic field. It is also located slightly outside the region of applicability of our solution. The point $E_{\rm ent}$ is observed in [12] in which the universal line is continuous.

In addition to the spike, the specific heat jump has also been observed along the melting line $H_m(T)$ [5,6,22]. Theoretically, the jump does not vanish either at $E_{\rm ent}$ or $E_{\rm mag}$, but is rather flat in a wide temperature range. Our results are larger than experimental jumps of [6] by a factor of 1.4 to 2 [Fig. 3(c)]. In many experiments there appears a segment of the second order phase transition continuing the first order melting line beyond a certain point. In [6] it was shown that at that point the specific heat profile shows "rounding." We calculated the specific heat profile above the universal first order transition line. It exhibits a "rounding" feature similar to that displayed in [6] with no sign of the criticality. The height of the peak is roughly of the size of the specific heat jump. We therefore propose not to interpret this feature as an evidence for a second order transition above the first order line.

As seen from fitting the optimal doping YBCO, the disorder parameter n in the cases of interest is very small. However, to address a more delicate question of appearance of the glass transition between liquid and glass claimed in some experiments [4,6] and simulations [14,15], we used a nonperturbative method, the replica trick, combined with the Gaussian variational approximation [24]. Breaking of the replica symmetry signals appearance of the glass transition in static phenomena. Here we summarize the results, leaving details for a longer presentation. The most general hierarchical homogeneous (liquid) ansatz [24] was considered and found that there is no replica symmetry breaking (RSB) solution.

Now we compare our results with other theories starting with models based on the Lindemann criterion [9,17,18]. Near T_c (where effects of disorder are small), the location of the first order transition line $H(T)$ is qualitatively consistent with that found from the Lindemann criterion [1]. In the intermediate region around $E_{\rm ent}$ our results for the melting line are completely different from all the phenomenological models [9,17,18]. In particular, we do not have a critical point assumed in some of them (the two papers in [17] differ on the continuation of the line beyond the critical point in which two first order lines join together). At temperatures below 70 K, the elasticity theory approach based on the London approximation [17,18] (valid beyond the range of applicability of the GL approach) is expected to smoothly interpolate to the GL approach. The advantage of the present approach is that, in addition to location of the transition line, it enables the determination of discontinuities and the calculation of physical quantities away from the transition line.

The comparison with numerical simulations can be made only qualitatively since the disordered GL model has not been simulated. In the XY simulations of [13], a single transition line is parallel to the T axis below certain temperature, while ours is not. In [14] there is, in addition, a slush-liquid transition, while Langevin simulation [15] finds the liquid-glass transition. Their transition criterion, however, is dynamical. Absence of RSB in liquid does not generally imply that this state, especially at low temperatures, does not exhibit "glassy properties" in dynamics. In fact overcooled liquids generally are "glassy." Therefore we propose to consider the glassy properties of the vortex state above the $H^*(T)$ line in the context of the "disordered overcooled" liquids. Recent simulations [16] demonstrate that glassy features in dynamics do not necessarily correspond to the conventional vortex glass scenario. Next we comment on the "vortex loops" scenario for YBCO. The region in which the loops are relevant according to [25] is below $\mathrm{Gi}H_{c2}$, too small to explain the experimental transitions (our fit for $\mathrm{Gi} = 2 \times 10^{-4}$ is much smaller than that assumed in [25]). The LLL is inapplicable in this region (see Fig. 1). In strongly anisotropic materials, a model of the Lawrence-Doniah type is more appropriate [1,26]. We performed a 2D GL calculation and found that in that case there is no "wiggle" of the transition line and speculate that it disappears at a certain value of the anisotropy parameter.

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