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Dislocations and the critical endpoint of the melting line of vortex line lattices

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We develop a theory for dislocation-mediated structural transitions in the vortex lattice which allows for a unified description of phase transitions between the three phases, the elastic vortex glass, the amorphous vortex glass, and the vortex liquid, in terms of a free-energy functional for the dislocation density. In the presence of point defects, the existence of a *critical endpoint* of the first-order melting line at high magnetic fields, which has been recently observed experimentally, is explained.

Since the pioneering work[1] where the first-order flux-line lattice (FLL) melting into an entangled vortex liquid (VL) was established, there has been a continuous development of our views of the vortex lattice phase diagram in high-T_c superconductors.[2] Weak point disorder was shown to drive the vortex lattice into a vortex glass (VG) state with zero linear resistivity.[3–5] Observations of hysteretic resistivity switching and magnetization measurements[6] have supported the first-order melting of very clean lattices. A crossover from the first-order melting at low magnetic fields to a continuous VG-VL transition has been related to the structural transition within the vortex solid which is described[8–10] as a topological transition between the low-field *elastic* VG,[7] free from topological defects[7,11,12] and maintaining quasi long-range translational order,[13,7] and the high field *amorphous* VG, where disorder generates proliferation of dislocations.[11,12] A simple picture of the vortex phase diagram has emerged where the three generic phases — VL, the high-field amorphous VG, and the low-field, low-temperature quasilattice or Bragg glass (BrG) (Ref. 7) — are governed by the three basic energies: the energy of thermal fluctuations, pinning, and elastic energies. The transition lines are determined by matching of any of the two basic energies, and the match of all three energies marks the tricritical point where the first-order melting terminates.[9] While this simplistic picture is supported by observations on $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), it fails to describe the $YBa_2Cu_3O_{7-\delta}$ (YBCO) phase diagram (see Fig. 1) where the endpoint of the first-order melting line appears to be separated from the point where topological transition and melting line merge.[14]

In this paper we present an explanation for the existence of a critical endpoint of the first-order melting line in the presence of point disorder. Our argumentation is based on a unified description of the vortex lattice phases. We demonstrate that all phase transitions between vortex lattice phases can be described as *dislocation mediated* by deriving the free energy for an ensemble of directed dislocations as a function of the dislocation density in the presence of thermal *and* disorder. Each of the experimentally observed phases is characterized by its inherent *dislocation density* or, equivalently, by the characteristic dislocation spacing R_D. The elastic VG is dislocation-free and has $R_D=\infty$. The VL can be viewed as a vortex array saturated with dislocations such that $R_D\sim a$, and in the amorphous VG, $R_D\sim R_a$, where R_a is the so-called positional correlation length on which typical vortex displacements are of the order of the lattice spacing a.[2] Within our approach each phase corresponds to one of the *local* minima in the dislocation ensemble free energy, and dislocation densities in these minima represent the *equilibrium* dislocation densities in the corresponding phases. The global minimum corresponds to the thermodynamically stable phase under the given conditions, phase transitions occur when two local minima exchange their role as global minimum. This mechanism for the transitions enables us to *derive* Lindemann-criteria both for the locations of the thermal melting line and for the disorder-induced instability line of the BrG. Furthermore, the characteristic scale set by the mean distance between free dislocations offers a natural explanation of the critical endpoint of the first-order melting line: While at low magnetic fields $R_a \gg a$ and the amorphous VG appears to contain significantly less dislocations than the VL, at higher field where $R_a=a$ the two phases become thermodynamically *equivalent* and the first-order melting line has to terminate.

Before addressing effects of disorder we need to revisit the dislocation-mediated thermal melting of the FLL.[15] A free energy for the dislocation degrees of freedom governing phase transitions is derived from vortex lattice elasticity theory. Dislocations in the FLL can be of both screw or edge type, but in either case they are confined to the gliding plane spanned by their Burger's vector **b** and the magnetic field.[15] The single dislocation energy consists of the core energy E_c

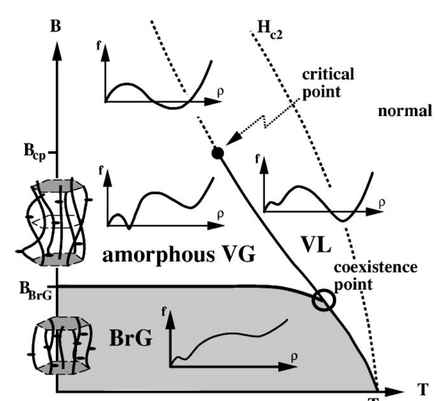

FIG. 1. Schematic phase diagram of YBCO. Insets show typical free energy densities f of a dislocation ensemble as function of the dislocation density ρ.

and of the logarithmically diverging contribution from the long-range elastic strains.[16] Accordingly, the dislocation ensemble can be modeled as an array of elastic lines with a long-range Coulomb-like interaction. A single directed dislocation line is parameterized by its displacement field $u_D(z)$ and is described by the Hamiltonian[17]

$$\mathcal{H}_D[u_D]=\int dz\left(E_s+\frac{1}{2}\epsilon_D(\partial_z u_D)^2\right), \quad (1)$$

where the stiffness $\epsilon_D \propto \ln(1/k_z a)$ has a logarithmic dispersion due to the long-range strain field and E_s is the self-energy of a straight dislocation. For thermal melting, the short-wavelength limit, $k_z \sim 1/a$, is relevant. It is convenient to rescale $z=\tilde{z}\frac{1}{2}\sqrt{c_{44}/c_{66}}$ such that dislocation energies become *isotropic* with $\epsilon_D=E_c=c_D Kb^2/4\pi$ ($c_D\approx 1$) and $E_s=E_c+Kb^2/4\pi \ln(L/a)$, where $K=\sqrt{c_{44}c_{66}}$ is the *isotropized elastic constant* (c_{44} and c_{66} are the tilt and shear moduli of the vortex lattice, respectively. L is the system size in the transverse direction). Note that the Peierls barrier W_p and the associated ''kinking'' (Ref. 16) of edge dislocation lines can be neglected near the melting transition. It can be shown that kinks are irrelevant above the temperature $T_k \sim a\sqrt{W_p \epsilon_D}$. Numerically, we find $W_p \lesssim 10^{-4}E_c$, such that T_k is much *lower* than T_m. Therefore, the basic length scale along the magnetic field is solely set by the competition of FL tilt and shear and given by $a_z \approx \sqrt{c_{44}/c_{66}}/2$ ($a_z \approx a$ in the rescaled system). The free energy of a single dislocation can be readily calculated from the partition sum $Z_D=\int \mathcal{D}u_D \exp(-\beta\mathcal{H}_D[u_D])$ by Gaussian functional integration and consists of the core energy, the long-range strains elastic energy, and the entropy term:

$$\frac{F_D(L)}{L_z}=E_c+\frac{Kb^2}{4\pi}\ln\left(\frac{L}{a}\right)-T\frac{1}{2a_z}\ln\left(1+\frac{2\pi T a_z}{\epsilon_D a^2}\right). \quad (2)$$

The spontaneous formation of a single dislocation is prohibited by the logarithmic divergence of its elastic energy which has to be *screened* for a phase transition to occur. One possible mechanism is screening by dislocation *loops* on all length scales as in a second-order 3DXY-type phase transition,[18] the other is a first-order phase transition where an ensemble of *unbound* dislocation lines with *finite* density threads the sample at the transition. Without loss of generality we can consider an ensemble of *directed* dislocation lines in this scenario. In the ensemble of unbound dislocations with a Coulomb-type interaction, the Debye-Hückel screening by *free* dislocations of opposite Burger's vector is by far more effective than the screening by small closed dislocation loops which we therefore neglect in this situation. The effective hard-core repulsion of dislocations with the *same* Burger's vectors, due to the energy penalty for Burger's vectors with $b>a$, also gives rise to screening. We find in the FLL that the planarity constraint favors such a first-order transition.[19] Taking screening into account and an additional entropy cost ($\propto \rho^3$) from the steric repulsion, we derive the following free-energy density for a (topologically neutral) dislocation ensemble of density 2ρ:[20]

$$f(\rho)=2\rho\left(E_c-T\frac{1}{2a_z}\ln\left(1+\frac{2\pi T a_z}{\epsilon_D a^2}\right)\right)+2\rho\frac{Kb^2}{4\pi}0.3\ln\left(\frac{1}{b(T)\,a^2\rho}\right)+\rho^3\frac{\pi^2}{3}\frac{T^2a^2}{\epsilon_D}. \quad (3)$$

$f(\rho)$ can be obtained in a more rigorous manner by mapping dislocations onto a quantum system of 2D Fermions with Coulomb interaction.[21,22] This allows for the systematic calculation of screening effects in Eq. (3) through the Lindhard-Thomas-Fermi theory for Coulomb screening and exchange terms, and leads to a screening parameter $b(T_m)\approx 0.5$. A *first-order melting* following from Eq. (3) occurs at $T_m \approx 1.57 E_c a_z \approx 0.15 K a^3$, which is equivalent to melting according to the Lindemann-criterion with a Lindemann-number $c_L \approx 0.2$; in good agreement with experimental and numerical results. At the melting transition dislocations proliferate with a *high* density $\rho_m \approx 0.2 a^{-2}$, hence the VL is saturated with dislocations.

Now we are in the position to address the effect of a random pinning potential $V_{pin}(\mathbf{r})$, in the presence of which the *dislocation-free* vortex array is collectively pinned and exhibits three different spatial scaling regimes: (i) Small distances where vortex displacements u are smaller than the coherence length ξ and perturbation theory applies.[23] (ii) Intermediate scales where $\xi \lesssim u \lesssim a$ and disorder potentials seen by different FL's are effectively *uncorrelated*. This regime is captured in so-called random manifold (RM) models,[2,7] leading to a roughness $\tilde{G}(\mathbf{r})=\overline{\langle(\mathbf{u}(\mathbf{r})-\mathbf{u}(0))^2\rangle} \simeq a^2(r/R_a)^{2\zeta_{RM}}$, where $\zeta_{RM}\approx 1/5$ for the $d=3$ dimensional RM with two displacement components. The crossover scale to the asymptotic behavior is the *positional correlation length* R_a where the average displacement is of the order of the FL spacing: $u \approx a$. (iii) The asymptotic Bragg glass regime where the a-periodicity of the FL array becomes important for the coupling to the disorder and the array is effectively subject to a *periodic* pinning potential with period a.[13] Here the *logarithmic* roughness $\tilde{G}(\mathbf{r}) \approx (a/\pi)^2 \ln(er/R_a)$, i.e., $\zeta_{BrG}=\mathcal{O}(\log)$[13,7] takes over.

In a disordered system at $T=0$ the mechanism for dislocation proliferation is fundamentally different from the thermal melting discussed before. While thermal melting is governed by the *entropy gain* due to unbinding dislocations pairs, the $T=0$ transition is driven by FLL adjustment to disorder. Disorder distorts the FLL giving rise to significant elastic stresses; dislocation proliferation releases these stresses, and leads to energy gain through the dislocation degrees of freedom. It has been shown in Refs. 11 and 12 that the three-dimensional (3D) BrG phase is *stable* with respect to dislocation formation. As we will show, instabilities arise from the subasymptotic regimes. To handle analytical difficulties and to provide a unified treatment through all scaling regimes, we develop an approach to the 3D problem based on an *effective random stress model* which has the same displacement correlations as the full nonlinear disordered model but allows for a *separation* of dislocation and elastic degrees of freedom. This idea is motivated by the renormalization group (RG) for the two-dimensional (2D) BrG which explicitly shows it renormalizes asymptotically into a random stress model[24] and has been used in Ref. 25 to show the *instability* of the 2D BrG with respect to dislocations.[7,25] For simplicity we consider a *uniaxial* FLL model (in the incompressible limit $c_{11} \gg c_{66}$) which yields the same dislocation energetics as the isotropized two-component model. The Hamiltonian is

$$\mathcal{H}[\mathbf{u}] = \int_{\mathbf{r}} \left\{ \frac{1}{2} K (\nabla u)^2 + \boldsymbol{\sigma} \cdot \nabla u \right\}, \tag{4}$$

where $\boldsymbol{\sigma}(\mathbf{r})$ is the *random stress field* which we assume to be Gaussian distributed with a second moment $\overline{\sigma_i(\mathbf{k})\sigma_j(\mathbf{k}')} = \delta_{ij}\Sigma(k)(2\pi)^3\delta(\mathbf{k}+\mathbf{k}')$ characterized by the function $\Sigma(k)$ in Fourier space. The effective random stresses causing displacements with the same (two point) correlations as those for the RM or BrG regime are

$$\Sigma(k) = \begin{cases} \text{BrG:} & \frac{1}{2} K^2 k^{-1} a^2 \\ \text{RM:} & B_{RM} K^2 k^{-1} a^2 (kR_a)^{-2/5} \end{cases} \tag{5}$$

(the exact crossover determining the numerical constant B_{RM} is nontrivial[26]). The validity of the random stress model is well-established in 2D. Besides, the functional RG treatment of the BrG in $d = 4 - \epsilon$ dimensions shows that displacements asymptotically obey Gaussian statistics up to the first order in ϵ,[27] which can always be modeled by an effective random stress field.

We calculate the free energy of an ensemble of dislocation lines $\mathbf{R}_i(s)$ with the density $\mathbf{b}(\mathbf{r}) = \Sigma_i b \int ds d\mathbf{R}_i/ds$ from the Hamiltonian (4) analogously to.[28] In the random stress model the Hamiltonian *decouples* into the elastic part and a dislocation part:

$$\mathcal{H}_D[\mathbf{b}] = \int_{\mathbf{r}} \int_{\mathbf{r}'} \frac{K}{2} \mathbf{b}_{\mathbf{r}} \cdot \mathbf{b}_{\mathbf{r}'} G_0(\mathbf{r} - \mathbf{r}') + \int_{\mathbf{r}} \mathbf{b}_{\mathbf{r}} \cdot \mathbf{g}_{\mathbf{r}}, \tag{6}$$

where $G_0(\mathbf{r}) = 1/(4\pi r)$ is the 3D Green's function. Here $\mathbf{g}(\mathbf{r})$ is an effective *random potential* for dislocation lines defined by the transversal part of $\boldsymbol{\sigma}$ through $\nabla \times \mathbf{g} = \boldsymbol{\sigma}_T$ [cf. (Ref. 25)]. The energy Eq. (6) contains the long-range elastic energy E_s of dislocations in the first term and in the stochastic second term the disorder energy E_{dis} which allows dislocations to gain energy by optimizing their paths. The dislocation disorder energy is completely determined by the FL displacement correlations through $\overline{g_i(\mathbf{k})g_j(\mathbf{k}')} = \delta_{ij}\frac{1}{2}\Sigma(k)k^{-2}(2\pi)^3\delta(\mathbf{k}+\mathbf{k}')$ in the different regimes given by Eq. (5). For a single directed dislocation line, the Hamiltonian (6) reduces to the problem of a directed elastic line with a logarithmic dispersion in a random potential that is long-range correlated described by Eq.(5). For a directed dislocation of length L_z and confined in the transversal direction to a scale L, the mean-square disorder energy fluctuations are

$$\overline{E_{dis}^2(L_z, L)} \sim \begin{cases} \text{BrG:} & E_c^2 L_z L \\ \text{RM:} & E_c^2 L_z L \left(\frac{L}{R_a} \right)^{2/5}. \end{cases} \tag{7}$$

These expressions give an estimate of the *typical* disorder energy a dislocation line can gain. They neglect *rare fluctuations* in the energy gain from optimally positioning the dislocation in the transversal plane which give logarithmic corrections $\sim \mathcal{O}(\ln L)$.[12] The optimal path of the dislocation is *rough* $u_D \sim L_z^{\zeta_D}$ with an exponent ζ_D. The roughness can be obtained by a Flory argument equating the elastic energy from the deformation $\epsilon_D(L) u_D^2/L$ and the disorder energy $\overline{E_{dis}^2(L_z = L, u_D)}^{1/2}$ on *one* large length scale set by the fluctuation wavelength L. This yields $\zeta_D(BrG) = 1 - \mathcal{O}(\log^{2/3})$ and $\zeta_D(RM) = \frac{15}{13} - \mathcal{O}(\log^{10/13})$, where logarithmic corrections come from the dispersion of the stiffness and rare fluctuations. Since $\zeta_D(BrG) \leq 1$, the BrG is marginally *stable* against penetration of a *single* directed dislocation[11,12] whereas $\zeta_D(RM) > 1$ such that the random manifold is clearly *unstable*. Note that the scaling arguments of Ref. 12 taking into account rare fluctuations give the same result regarding the stability of the BrG phase as our Flory argument.

Given the stability of the BrG against spontaneous formation of a *single* dislocation at weak disorder we present a mechanism for the destruction of the topologically ordered BrG phase at increased disorder strengths or magnetic fields. The mechanism is based on the above result that within domains of subasymptotic size $L < R_a$ the FLL is unstable to a spontaneous formation of dislocations. This can indeed lead to the proliferation of infinitely long dislocations in a *weak first-order* phase transition where dislocation elements are laterally confined by a *finite* dislocation density to scales $L < 1/\sqrt{\rho}$. Thus the characteristic dislocation density $\rho_c \sim R_a^{-2}$ at the transition is given just by the crossover scale R_a below which instabilities can occur. The discontinuities in this transition are small and may eventually disappear for weak disorder if the length scale R_a becomes of the order of typical sample dimensions. The random stress model enables us to quantify this idea by estimating typical free-energy *minima* of the dislocation ensemble. The screened long-range elastic energy density and the core energy density for the (neutral) dislocation ensemble with density 2ρ are given by $e_D(\rho) = 2\rho(E_c + (Kb^2/4\pi)\ln(1/a\rho^{1/2}))$ as in Eq. (3) at $T = 0$. Dislocations are confined to a transversal scale $R_D \simeq \rho^{-1/2}$ set by the distance to the next dislocation. The disorder energy gain is optimized against the elastic deformation on each longitudinal scale $L_p \simeq R_D(R_D/R_a)^{-2/15}$ (RM) or $L_p \simeq R_D$ (BrG) *independently*. L_p is the collective pinning length of the dislocation. Using Eq. (7) with $L_z = L_p$ and $L = \rho^{-1/2}$ for the *BRG* regime ($\rho < R_a^{-2}$) and the *RM* regime ($\rho > R_a^{-2}$), we can estimate the corresponding minimal free-energy densities

$$f(\rho) \approx e_D(\rho) - \begin{cases} \text{BrG:} & 2A_{BrG} E_c \rho \\ \text{RM:} & 2A_{RM} \frac{E_c}{a^2} (\rho a^2)^{\frac{13}{15}} \left(\frac{a}{R_a} \right)^{\frac{4}{15}}. \end{cases} \tag{8}$$

The prefactors $A \equiv A_{BrG} \simeq A_{RM}$ are related to B_{RM} and the exact crossover in Eq. (5) and are not known exactly; for $A \approx 8$ (corresponding to $B_{RM} \approx 7$), we obtain good agreement with experiments in estimates below. When both results in Eq. (8) are combined one indeed finds a local minimum in the free-energy density at $\rho = R_a^{-2}$ that characterizes an amorphous VG phase. Over a wide range of magnetic fields the dislocation density in the amorphous VG is much *lower* than in the VL for which we have found $\rho \approx 0.2a^{-2}$ above. The elastic BrG phase loses stability with respect to dislocation proliferation and a transition into an amorphous VG phase if the local minimum at $\rho = R_a^{-2}$ becomes the global free-energy minimum. This occurs via a weak first-order transition above a magnetic field B_{BrG} given by a criterion $R_a/a = C$ with a ''Lindemann-number'' $C = \exp(A-1)$. This is *identical* to the Lindemann criterion obtained in Refs. 11 and 10 and equivalent[10] to the more familiar form $\langle (u(a)-u(0))^2 \rangle = c_L^2 a^2$ (see Ref. 8) with $c_L \approx \exp((1-A)/5) \approx 0.25$ for $A \approx 8$.

So far, we have derived the free energies (3) and (8) and identified *three* possible characteristic minima: (i) The dislocation-free minimum at $\rho = 0$ which is stable in the elastic BrG phase at low T and low H. (ii) The minimum at $\rho \sim a^{-2}$ that becomes stable in the disorder-free case for high T in the VL. (iii) A minimum at $\rho \approx R_a^{-2}$ which is realized in the amorphous VG. Combining our results for the thermal melting and the disorder-induced ''melting,'' we have obtained a qualitative theory for the *entire* phase diagram of the vortex matter.

Moreover, this provides a framework for a natural explanation of the experimentally observed *critical endpoint* of the first-order melting line: At elevated fields the positional correlation length R_a *decreases*[10] and finally reaches $R_a \sim a$ such that the two free-energy minima of the VL and the amorphous VG must *merge*. Both these phases become thermodynamically indistinguishable and have identical *equilibrium* lattice order. Above the critical endpoint there might still exist a *dynamic* transition (or crossover) which involves the thermal depinning of dislocations, similar to the well-known thermal depinning transition of, for example, a single pinned vortex line. The exact location of the critical endpoint, obtained from the condition that the amorphous VG minimum of Eq. (8) moves away from $\rho = R_a^{-2}$ to higher dislocation densities, is determined by the condition $R_a/a = \exp(-\frac{1}{2} + 13A/15)$ (which is again equivalent to a Lindemann criterion, with a slightly larger c_L). This gives an estimate $B_{BrG}/B_{cp} = \exp(-\frac{8}{15}(4A/15-1)) \approx 0.6$ for $A \approx 8$, which is in qualitative agreement with the experiments.[14] B_{BrG} is the instability field of the BrG (see above) and thus the ''coexistence point'' where the topological transition line ends in the first-order melting line and all three phases — elastic BrG, amorphous VG, and VL — can coexist.

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