

# Defect-induced melting of vortices in high- $T_c$ superconductors: A model based on continuum elasticity theory

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We set up a melting model for vortex lattices in high-temperature superconductors based on the continuum elasticity theory. The model is Gaussian and includes defect fluctuations by means of a discrete-valued vortex gauge field. We derive the melting temperature of the lattice and predict the size of the Lindemann number. Our result agrees well with experiments for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ , and with modifications also for  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ . We calculate the jumps in the entropy and the magnetic induction at the melting transition.

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## I. INTRODUCTION

The magnetic flux lattices in high-temperature superconductors can undergo a melting transition as was first suggested by Nelson in 1988.<sup>1,2</sup> Previously, Brezin *et al.*<sup>3</sup> had calculated a first-order liquid-to-solid phase transition by renormalization group methods.<sup>3</sup> Since then detailed properties of this transition have emerged from various theoretical and experimental papers.

Most prominent are computer simulations of the Langevin equation<sup>4</sup> for the dynamics of the vortices, or Monte Carlo simulations of an XY-type model<sup>5</sup> coupled to an external magnetic field. Analytic approaches are based mainly on the Ginzburg-Landau model<sup>6</sup> or on elastic models of the vortex lattice. The simplest estimates for the transition temperature in the vortex lattice came from an adaption of the famous Lindemann criterion of three-dimensional ordinary crystals.<sup>7</sup> In the formulation of Houghton *et al.* and Brandt,<sup>8</sup> the criterion states that the vortex lattice undergoes a melting transition once the mean thermal displacement  $\langle u^2 \rangle^{1/2}$  reaches a certain fraction of the lattice spacing  $a \approx (\Phi_0/B)^{1/2}$ , where  $\Phi_0$  is the flux quantum and  $B$  the magnetic induction. The ratio  $c_L \equiv \langle u^2 \rangle^{1/2}/a$  is the characteristic Lindemann number, which should be independent of  $B$ . Its value is *not* predicted by Lindemann's criterion. It must be extracted from experiments, and is usually found to lie in the range  $c_L \approx 0.1-0.3$ .

The most prominent examples of high-temperature superconductors which exhibit vortex lattice melting are the anisotropic compound  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  (YBCO), and the strongly layered compound  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  (BSCCO). Decoration experiments<sup>9</sup> on BSCCO show the formation of a triangular vortex lattice; neutron scattering on YBCO shows a tilted square lattice of vortices<sup>10</sup> close to the melting region, the latter being favored by the  $d$ -wave symmetry of the order parameter and the anisotropy of the crystal.<sup>11</sup> An explicit calculation of the Lindemann number  $c_L = \langle u^2 \rangle^{1/2}/a$  for YBCO can be found in Ref. 8 and for BSCCO in Ref. 12.

In this paper, we present a theory that is capable of specifying the size of the Lindemann number  $c_L$ , and predicting corrections to the criterion. Our theory is based on a simple Gaussian model which takes into account both lattice elasticity and defect degrees of freedom in the simplest possible way. The relevance of defect fluctuations for the understanding of melting transitions is well known. For ordinary crys-

als, this is textbook material.<sup>7</sup> In the context of vortex melting it was emphasized in Ref. 13. For ordinary crystals, the size of the Lindemann number has been calculated successfully by means of Gaussian lattice models with elastic and defect fluctuations, which clearly display first-order melting transitions in three dimensions and either first-order or a sequence of continuous transitions in two dimensions.

An important quality of these models is that in the first-order case, where fluctuations are small, they lead to a simple universal melting formula determining the melting point in terms of the elastic constants. The universal result is found from a lowest-order approximation, in which one identifies the melting point with the intersection of the high-temperature expansion of the free energy density, dominated by defect fluctuations with the low-temperature expansion dominated by elastic fluctuations. The resulting universal formula for the melting temperature determines also the size of the Lindemann number. Recently, the results of Ref. 7 for square crystals were successfully extended to face-centered and body-centered cubic lattices in three dimensions<sup>14</sup> and also to two-dimensional triangular lattices.<sup>15</sup> A similar intersection criterion was also used for the melting point of vortex lattices in the Abrikosov approximation of the Ginzburg-Landau model<sup>6</sup> useful for YBCO. Here we shall apply our defect model to calculate the melting curves, the entropy jumps, and magnetic induction jumps of the vortex lattices in YBCO and BSCCO. We do not discuss in this work effects on the vortex lattice from other sources than defect fluctuations which can give rise to tricritical points and glass transitions.<sup>16,17</sup> Theoretical work on this subject can be found in Refs. 18–20. There is in principle no problem of adding pinning in our formalism. For simplicity, we shall confine our discussion to the defect mechanism of melting.

The melting criterion will be derived in Sec. II. The calculation of the melting temperatures, the entropy jumps, and the jumps of magnetic induction for YBCO and BSCCO is carried out in Sec. III.

## II. MELTING CRITERION

Due to the large penetration depth  $\lambda_{ab}$  in the layers in comparison to  $a$  we have to take into account the full non-local elasticity constants when integrating over the Fourier space, as emphasized by Brandt in Ref. 21. For our Gaussian

model, the partition function of the vortex lattice can be split into  $Z=Z_0Z_{\Pi}$  where  $Z_0$  is the partition function of the rigid lattice and  $Z_{\Pi}$  is the thermally fluctuating part calculated via the elastic Hamiltonian plus defects. Due to the translational invariance of the vortex lattice in the direction of the vortices, which we shall take to be the  $z$  axis, we may simply extend the models on square<sup>7</sup> and triangular lattices<sup>15</sup> by a third dimension along the  $z$  axis, which we artificially discretize to have a lattice spacing  $a_3$ , whose value will be fixed later. The elastic energy is

$$E_{\text{el}} = \frac{v}{2} \sum_{\mathbf{x}} (\nabla_i u_i) (c_{11} - 2c_{66}) (\nabla_i u_i) + \frac{1}{2} (\nabla_i u_j + \nabla_j u_i) \times c_{66} (\nabla_i u_j + \nabla_j u_i) + (\nabla_3 u_i) c_{44} (\nabla_3 u_i). \quad (1)$$

The subscripts  $i, j$  have values 1, 2 and  $l, m, n$  have values 1, ..., 3. The vectors  $u_i(\mathbf{x})$  are given by the transverse displacements of the line elements of the vortex lines with coordinate  $\mathbf{x}$ . We have suppressed the spatial arguments of the elasticity parameters, which are really functional matrices  $c_{ij}(\mathbf{x}, \mathbf{x}') \equiv c_{ij}(\mathbf{x} - \mathbf{x}')$ . Their precise forms were calculated by Brandt.<sup>21</sup> The volume of the fundamental cell  $v$  is equal to  $a^2 a_3$  (square) or  $a^2 a_3 \sqrt{3}/2$  (triangular). For a square lattice, the lattice derivatives  $\nabla_i$  in Eq. (1) are given by  $\nabla_{ij} f(\mathbf{x}) = [f(\mathbf{x} + a\mathbf{e}_i) - f(\mathbf{x})]/a$  and  $\nabla_3 f(\mathbf{x}) = [f(\mathbf{x} + a_3\mathbf{e}_3) - f(\mathbf{x})]/a_3$ . For a triangular lattice, the  $xy$  part of the lattice has the link vectors  $\pm a\mathbf{e}_{(m)}$  with  $\mathbf{e}_{(1,3)} = (\cos 2\pi/6, \pm \sin 2\pi/6, 0)$  and  $\mathbf{e}_{(2)} = (-1, 0, 0)$ . The lattice derivatives around a plaquette are defined by  $\nabla_{(1)} f(\mathbf{x}) = [f(\mathbf{x} + a\mathbf{e}_{(1)}) - f(\mathbf{x})]/a$ ,  $\nabla_{(2)} f(\mathbf{x}) = [f(\mathbf{x}) - f(\mathbf{x} - a\mathbf{e}_{(2)})]/a$ ,  $\nabla_{(3)} f(\mathbf{x}) = [f(\mathbf{x} - a\mathbf{e}_{(2)}) - f(\mathbf{x} + a\mathbf{e}_{(1)})]/a$ . From these we define discrete Cartesian lattice derivatives used in the Hamiltonian (1)  $\nabla_{ij} f(\mathbf{x}) = (2/3)\mathbf{e}_{(l)} \nabla_{(l)} f(\mathbf{x})$  and  $\nabla_3 f(\mathbf{x}) = [f(\mathbf{x} + a_3\mathbf{e}_3) - f(\mathbf{x})]/a_3$  transforming like the continuum derivative with respect to the symmetry group of the lattice.<sup>15</sup> Therefore, the Hamiltonian (1) has the full symmetry of the triangular lattice and the correct continuum elastic energy for zero lattice spacing.

The quadratic approximation to the energy (1) is so far only appropriate for the low-temperature classical thermodynamic behavior. It is possible to extend the Hamiltonian at the *quadratic level* in such a way that the range of applicability extends beyond the melting transition. This is possible by the introduction of integer-valued defect gauge fields. We observe that the displacement fields in (1) are restricted to values within the fundamental cell. The defect gauge fields enter to characterize the jumps of the displacement fields across the *Volterra surface*.<sup>7,15</sup> As usual for gauge fields we choose a minimal coupling to the lattice displacements. On account of the three lattice derivatives per fundamental cell and further two dimensions for the displacements there are six independent integer-valued gauge fields per fundamental cell corresponding to the various defect configurations. One can eliminate two of them (we choose the defect fields corresponding to jumps in the  $z$  direction) by relaxing the restriction of the displacement fields to the fundamental cell (elimination of gauge freedom). See the discussion in Ref. 7 for square lattices. A similar consideration was also carried out in Ref. 15 for the two-dimensional triangular lattice

where the elimination of the gauge degrees of freedom is more complicated due to the absence of the  $z$  direction. Finally, we can eliminate one more integer-valued defect field since the elastic energy in (1) depends only on the displacements  $u_i$  via the strain tensor  $\nabla_i u_j + \nabla_j u_i$ .<sup>7</sup> In summary, only three independent integer-valued fields have to be included in (1) to obtain the elastic energy of the vortex lattice including defects. By taking into account the above considerations one can then easily determine the partition function including defects for the square vortex lattice by using the considerations in Ref. 7 and for the triangular ones by using Ref. 15.

By using a Hubbard-Stratonovich decoupling of the quadratic displacement terms in (1), the stress representation<sup>7</sup> of the partition function becomes

$$Z_{\Pi} = \det \left( \frac{c_{66}}{4(c_{11} - c_{66})} \right)^{1/2} \det \left( \frac{1}{2\pi\beta} \right)^{5/2} \prod_{\mathbf{x}} \left( \prod_{i \leq m} \int_{-\infty}^{\infty} d\sigma_{im} \right) \times \left( \prod_m \sum_{n_m(\mathbf{x})=-\infty}^{\infty} \right) \left( \int_{-\infty}^{\infty} \frac{d\mathbf{u}}{a} \right) \exp \left\{ - \sum_{\mathbf{x}} \frac{1}{2\beta} \times \left[ \sum_{i < j} \sigma_{ij}^2 + \frac{1}{2} \sum_i \sigma_{ii}^2 - \left( \sum_i \sigma_{ii} \right) \frac{c_{11} - 2c_{66}}{4(c_{11} - c_{66})} \left( \sum_i \sigma_{ii} \right) + \sum_i \sigma_{i3} \frac{c_{66}}{c_{44}} \sigma_{i3} \right] \right\} \times \exp \left[ 2\pi i \sum_{\mathbf{x}} \left( \sum_{i \leq m} \nabla_m u_i \sigma_{im} + \sum_{i \leq j} D_{ij} \sigma_{ij} \right) \right]. \quad (2)$$

The parameter  $\beta$  is given by  $\beta = v c_{66} / k_B T (2\pi)^2$ .  $\sigma_{ij}$  represent stress fields.<sup>7</sup> The matrix  $D_{ij}(\mathbf{x})$  in Eq. (2) is a discrete-valued local defect matrix composed of integer-valued defect gauge fields  $n_1, n_2, n_3$  for square<sup>7</sup> and triangular vortex lattices<sup>15</sup> as follows:

$$D_{ij}^{\square} = \begin{pmatrix} n_1 & n_3 \\ n_3 & n_2 \end{pmatrix}, \quad (3)$$

$$D_{ij}^{\triangle} = \begin{pmatrix} \frac{1}{2} n_1 & \frac{1}{\sqrt{3}} (n_1 - n_2) + \frac{2}{\sqrt{3}} n_3 \\ \frac{1}{\sqrt{3}} (n_1 - n_2) + \frac{2}{\sqrt{3}} n_3 & -\frac{1}{2} n_1 - n_2 \end{pmatrix}. \quad (4)$$

The vortex gauge fields specify the Volterra surfaces in units of the Burgers vectors. By summing over all  $n_{1,2,3}(\mathbf{x})$ , the partition function  $Z_{\Pi}$  includes all defect fluctuations, dislocations as well as disclinations. There is a constraint for a vortex lattice which does not exist for ordinary three-dimensional lattices. Dislocations in the vortex lattice can be either screw or edge type, but in either case the defect lines are confined in the plane spanned by their Burgers vector and the magnetic field.<sup>13,22</sup> The reason is that the flux lines in a vortex lattice cannot be broken. This results in the constraint  $D_{11} = -D_{22}$  on the defect fields.

We now calculate the low-temperature expansion of the partition function  $Z_{\Pi}$  to lowest order, which includes only the

$n_m=0$  term. By carrying out the integration over the displacement fields  $u_i(\mathbf{x})$  in Eq. (2) we obtain, as in Refs. 7 and 15, the leading term in the low-temperature expansion of the free energy

$$Z_{\text{fl}}^{T \rightarrow 0} = \left(\frac{a_3}{a}\right)^{2N} \frac{1}{\det[(2\pi\beta)c_{44}/c_{66}]} \exp\left(-N \sum_{i \in \{1,6\}} l_{ii}\right), \quad (5)$$

where

$$l_{ii} = \frac{1}{2} \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} d^2k dk_3 \ln\left(\frac{c_{ii}a_3^2 K_j^* K_j + a_3^2 K_3^* K_3}{c_{44}}\right). \quad (6)$$

Here  $K_m$  is the eigenvalue of  $i\nabla_m$  and  $N$  is the number of vertices in the lattice. The momentum integrations in (6) run over the Brillouin zone of the vortex lattice whose volume is  $V_{\text{BZ}} = (2\pi)^3/v$ , as indicated by the subscript BZ.

Next we calculate the high-temperature expansion  $Z_{\text{fl}}^{T \rightarrow \infty}$  to lowest order. By carrying out the integration over the displacement fields  $u_i(\mathbf{x})$  in Eq. (2) and further by summing over the defect fields  $n_m$  under the condition  $D_{11} = -D_{22}$  mentioned above, it turns out that the stress fields  $\sigma_{12}$  and  $\sigma_u \equiv \sigma_{11} - \sigma_{22}$  can have only integer numbers. Doing the integrals over the stress fields  $\sigma_{i3}$  and  $\sigma_g \equiv \sigma_{11} + \sigma_{22}$  we obtain, in the lowest-order high-temperature limit, corresponding to  $\sigma_{12}=0$  and  $\sigma_u=0$ ,

$$Z_{\text{fl}}^{T \rightarrow \infty} = \left(\frac{a_3}{a}\right)^{2N} \frac{C^N}{2^N \det[(2\pi\beta)^2 c_{44}/c_{66}]} e^{-Nh} \quad (7)$$

with

$$h = \frac{1}{2} \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} d^2k dk_3 \ln\left(1 + \frac{c_{11} - c_{66} K_j^* K_j}{c_{44} K_3^* K_3}\right). \quad (8)$$

The constant  $C$  has the values  $C_{\square}=1$  for the square vortex lattice and  $C_{\Delta}=\sqrt{3}$  for the triangular one.

In the low-temperature expansion representing the solid phase, defect field configurations  $n_m \neq 0$  correspond to dislocations and disclinations giving finite-temperature corrections to the free energy  $-\ln(Z)/k_B T$ . These corrections are exponentially small with an exponent proportional to  $-\beta$ .<sup>7,15</sup> In contrast to this, corrections to the high-temperature expansion in the fluid phase corresponding to stress configurations  $\sigma_{12} \neq 0$  and  $\sigma_u \neq 0$  of integer values result in temperature corrections to the free energy which are also exponentially small with an exponent proportional to  $-1/\beta$ . The structure of the high- and low-temperature corrections to the partition function is extensively discussed in Refs. 7 and 15 for ordinary crystals, and can be easily transferred to our case of vortex lattices. It was shown in Refs. 7 and 15 for the two-dimensional square and triangular as well as the three-dimensional square crystal that the exponentially vanishing higher-order corrections to the low- and high-temperature expansion of the free energy are negligible in the determination of the transition temperature. This is particularly true for the three-dimensional crystal (see Ref. 7, p. 1082) which we take as a justification to restrict our calculation to lowest order in this paper.

From the partition function (2) with no defects ( $n_m=0$ ) we obtain for the Lindemann number  $c_L = \langle u^2 \rangle^{1/2}/a$  the momentum integral

$$c_L^2 = \frac{a_3^2 k_B T}{a^2 v V_{\text{BZ}}} \int_{\text{BZ}} d^2k dk_3 \frac{1}{c_{44}} \sum_{i=1,6} \frac{1}{\frac{c_{ii}a_3^2}{c_{44}} K_j^* K_j + a_3^2 K_3^* K_3}. \quad (9)$$

This can be simplified by taking into account that  $c_{11}$  is much larger than  $c_{66}, c_{44}$  in the relevant regime.<sup>21,23</sup> As announced, we find the melting temperature from the intersection of low- and high-temperature expansions, obtained by equating  $Z_{\text{fl}}^{T \rightarrow 0} = Z_{\text{fl}}^{T \rightarrow \infty}$ . By taking into account  $\det[a_3^2 \nabla_3^* \nabla_3] = 1$  we obtain  $h, l_{11} \ll l_{66}$ , and further that the  $i=1$  term in Eq. (9) is much smaller than the  $i=6$  term. In the following analytic discussion (but not in the numerical plots) we neglect these small contributions. The temperature of melting is then given by the simple formula

$$\frac{k_B T}{v} \frac{1}{\det^{1/N}[c_{66}]} C = \frac{e^{-l_{66}}}{\pi}, \quad (10)$$

where  $\det[c_{66}]$  is the determinant of the  $N \times N$  functional matrix  $c_{66}$ . The elastic moduli  $c_{44}$  and  $c_{66}$  at low reduced magnetic fields  $b \equiv B/H_{c2} < 0.25$  can be taken from Brandt's paper<sup>21</sup>

$$c_{66} = \frac{B\phi_0 \zeta}{(8\pi\lambda_{ab})^2}, \quad (11)$$

$$c_{44} = \frac{B^2}{4\pi(1 + \lambda_c^2 k^2 + \lambda_{ab}^2 k_3^2)} + \frac{B\phi_0}{32\pi^2 \lambda_c^2} \ln \frac{1 + 2\lambda_c^2/\langle u \rangle^2 + \lambda_{ab}^2 k_3^2}{1 + \lambda_c^2 K_{\text{BZ}} + \lambda_{ab}^2 k_3^2} + \frac{B\phi_0}{32\pi^2 \lambda_{ab}^4 k_3^2} \ln \frac{1 + \lambda_{ab}^2 k_3^2/(1 + \lambda_{ab}^2 K_{\text{BZ}}^2)}{1 + \lambda_{ab}^2 k_3^2/(1 + 2\lambda_{ab}^2/\langle u \rangle^2)}, \quad (12)$$

where  $\lambda_c$  is the penetration depth in the  $xy$  plane,  $\zeta=1$ , and  $K_{\text{BZ}}$  is the boundary of the circular Brillouin zone  $K_{\text{BZ}}^2 = 4\pi B/\phi_0$ . At high fields ( $b > 0.5$ ),  $c_{66}$  is altered by a factor  $\zeta \approx 0.71(1-b)$ , and the penetration depths in  $c_{66}, c_{44}$  are replaced by  $\tilde{\lambda}^2 = \lambda^2/(1-b)$ , where  $\lambda$  denotes either  $\lambda_{ab}$  or  $\lambda_c$ . In addition, the last two terms in  $c_{44}$  are replaced by  $B\phi_0/16\pi^2 \tilde{\lambda}_c^2$ . For YBCO we have<sup>24</sup>  $\lambda(T) = \lambda(0)[1 - (T/T_c)]^{-1/3}$ ,  $\xi(T) = \xi(0)[1 - (T/T_c)]^{-1/2}$  and for BSCCO  $\lambda(T) = \lambda(0)[1 - (T/T_c)^4]^{-1/2}$ ,  $\xi(T) = \xi(0)[1 - (T/T_c)^4]^{1/2}/[1 - (T/T_c)^2]$ .<sup>25</sup> When calculating  $c_{44}$  in Eq. (12) we have used a momentum cutoff in the two-vortex interaction potential  $k \leq 2/\langle u^2 \rangle^{1/2}$ , and not the inverse of the correlation length  $1/\xi$  as in Ref. 21. The cutoff is due to thermal softening,<sup>7</sup> and becomes relevant for  $\langle u^2 \rangle^{1/2}/\xi \gg 1$ , or equivalently for  $c_L \sqrt{2\pi} \sqrt{H_{c2}(T)/B} \gg 1$ , which is satisfied in the melting regime of BSCCO, but not for YBCO.

It remains to determine the effective lattice spacing  $a_3$  along the vortex lines. An elementary defect in the vortex lattice (arising for example from a crossing of two vortex strings) occurs over a typical length scale in the  $z$  direction determined from the condition that the sum of elastic displacement energy and the energy required to stretch the line

against the line tension is minimal. It is the elastic energy of this smallest defect that has to be taken into account in our model. The energy of an ensemble of dislocations is determined by the interplay of elastic energy of small displacements and integer-valued defect fields. The relevant part of the free energy is given by the discretized free energy  $-\ln(Z_0 Z_{\Pi}) k_B T$  [Eq. (2)] in which  $a_3$  is equal to the above length scale in the  $z$  direction. To determine this, we insert the variational ansatz for the transverse displacement field  $u_i = \delta_{i,1} A_0 \exp[-2|z|/a_3]$  into the continuum version (in the  $z$  direction) of the elastic energy (1) and approximate  $-\nabla_z^2 \approx \langle K^2 \rangle \approx K_{BZ}^2/4$  in  $E_{el}$  and  $K^2 \approx \langle K^2 \rangle \approx K_{BZ}^2/2$  in the elastic constants, where the average  $\langle \dots \rangle$  was taken with respect to a circular Brillouin zone. The optimal length scale  $a_3$  is chosen such that  $E_{el}$  is minimal for a fixed amplitude  $A_0 \approx a$  corresponding to a typical defect elongation.

### III. APPLICATION TO YBCO AND BSCCO

In the following, we treat first the more isotropic square vortex crystal YBCO ( $a = \sqrt{\phi_0/B}$ ). From  $c_{66}$  and  $c_{44}$  for YBCO, the optimal length scale is given by  $a_3 = 4a\lambda_{ab}/\lambda_c \zeta(1-b)^{1/2}$ . When comparing the melting criterion of the defect model in Eq. (10) with the Lindemann criterion obtained by equating the parameter (9) to a universal number, we obtain identical results when taking into account that the integrand in (9) and in  $l_{66}$  of Eq. (6) receive their main contributions from the region  $k \approx \sqrt{\langle k^2 \rangle} \approx K_{BZ}/\sqrt{2}$ . We can approximate  $k_3 \approx 0$  in this region, resulting in  $a_3^2 c_{66}/a^2 c_{44} \approx 4/\pi$ . With the same approximation in Eqs. (6) and (9) we can perform the integrals numerically. Then we obtain from the melting condition (10) precisely the Lindemann criterion in which the Lindemann number (9) is predicted to be

$$\frac{k_B T_m}{4[c_{44}(K_{BZ}/\sqrt{2}, 0)c_{66}(K_{BZ}/\sqrt{2}, 0)]^{1/2} a^3} \approx c_L^2 \approx (0.18)^2. \quad (13)$$

Denoting the spacing between the  $\text{CuO}_2$  double layers by  $a_s$  we obtain for the entropy jump per double layer and vortex

$$\Delta S_l \approx k_B T_m (\partial/\partial T_m) (a_s/a_3) \ln[Z_{\Pi}^{T \rightarrow \infty}/Z_{\Pi}^{T \rightarrow 0}]. \quad (14)$$

Inserting Eqs. (5) and (7), this becomes

$$\Delta S_l \approx \frac{k_B T_m a_s}{a_3} \frac{\partial}{\partial T_m} \ln \frac{k_B T_m / a^3}{[c_{44}(K_{BZ}/\sqrt{2}, 0)c_{66}(K_{BZ}/\sqrt{2}, 0)]^{1/2}}. \quad (15)$$

Finally, we make use of the Clausius-Clapeyron equation which relates the jump of the entropy density across the melting transition to the jump of the magnetic induction by  $\Delta S_l a_3 / v a_s = -(dH_m/dT) \Delta B / 4\pi$ . Here  $H_m$  is the external magnetic field on the melting line. Combining the Clausius-Clapeyron equation with Eqs. (12) and (15) we obtain, with the abbreviation  $\tau_m \equiv T_m/T_c$ , the following relations near  $T_c$ :

$$B_m(T) \approx \frac{12\zeta}{16^2 \pi^4} \frac{(1 - T/T_c)^{4/3} c_L^4 \phi_0^5}{(k_B T)^2 \lambda_{ab}^2(0) \lambda_c^2(0)},$$

$$\Delta S_l \approx \frac{\sqrt{\zeta} a_s \lambda_c}{6a} \frac{k_B}{\lambda_{ab} (1 - \tau_m)} \approx \frac{2.7}{10^3} \frac{a_s c_L^2 \phi_0^2}{T_c (1 - \tau_m)^{1/3} \lambda_{ab}^2(0)},$$

$$\Delta B \approx \frac{\sqrt{\zeta} \pi}{2a \phi_0} \frac{\lambda_c}{\lambda_{ab}} k_B T_m \approx \frac{2.5 (1 - \tau_m)^{2/3} c_L^2 \phi_0}{10^2 \lambda_{ab}^2(0)}. \quad (16)$$

These results agree with the general scaling results in Ref. 26, with the advantage that here the prefactors are predicted whereas those in Ref. 26 had to be determined by fits to experimental curves (there is only a slight discrepancy because we use a different temperature dependence of the penetration depth).

Next, we calculate the corresponding expressions in the case of the more layered crystal BSCCO [ $a = (2^{1/2}/3^{1/4})\sqrt{\phi_0/B}$ ]. First, we have to determine the dislocation length scale  $a_3$  in this case. For dislocation moves we have  $\langle u^2 \rangle^{1/2} \sim 1/K_{BZ}$ . This means that we can neglect the last two terms of  $c_{44}$  in Eq. (12), coming from the self-energy of the vortex line, when determining  $a_3$ . Remembering this we obtain by a similar procedure as for YBCO the dislocation length scale  $a_3 \approx 4a\sqrt{2}\lambda_{ab}/\lambda_c\sqrt{\pi}$ . From this we find  $a_3^2 c_{66}/a^2 c_{44} \ll 1$ , resulting in  $l_{66} \approx 0$ . By taking into account that  $B\pi^3 \lambda_{ab}^2 / 32 \phi_0 \leq 1$  on the melting line we obtain that  $c_{44}(k, k_3)$  for  $|k_3| < \pi/a_3$  is dominated by the last term in (12). Then we obtain

$$c_{44}(k, k_3) \approx \begin{cases} \frac{B\phi_0}{32\pi^2 \lambda_{ab}^2 (1 + \lambda_{ab}^2 K_{BZ}^2)} & \text{for } k_3 \ll \frac{1}{\lambda_{ab}}, \\ \frac{B\phi_0 \ln(1 + 2B\lambda_{ab}^2/\phi_0 c_L^2)}{32\pi^2 \lambda_{ab}^4 k_3^2} & \text{for } k_3 \gg \frac{1}{\lambda_{ab}}. \end{cases} \quad (17)$$

By using these values we obtain by numerical integration of (9)

$$c_L^2 \approx \frac{k_B T_m \times 0.36}{a^3 \sqrt{c_{66}(K_{BZ}/\sqrt{2}, 0)c_{44}(K_{BZ}/\sqrt{2}, 0)}} + \frac{k_B T_m a_3 \times 1.60}{a^4 c_{44}(K_{BZ}/\sqrt{2}, 1/a_3)}$$

$$\approx \frac{k_B T_m \lambda_{ab}^2 \times 138}{\phi_0^2 a} \sqrt{1 + \lambda_{ab}^2 K_{BZ}^2} + \frac{k_B T_m \lambda_{ab}^2 \lambda_c^2 \times 137}{\phi_0^2 a^3 \ln(1/c_L^2)} \frac{\lambda_{ab}}{\lambda_c}. \quad (18)$$

The first term comes from the integration region  $|k_3| < 1/\lambda_{ab}$ , the second from the region  $1/\lambda_{ab} < |k_3| < \pi/a_3$  in Eq. (9).

From our melting criterion (10) and the Clausius-Clapeyron equation [where  $dH_m/dT \approx dB_m/dT$  because  $B_m(T) \geq H_{c1}(T)$  (Ref. 27)], we obtain for BSCCO

$$B_m(T) \approx \frac{1}{192} \frac{1}{\sqrt{3}\pi^7} \frac{[1 - (T/T_c)^4]^2}{\lambda_{ac}^2(0) \lambda_c^2(0)} \frac{\phi_0^5}{(k_B T)^2},$$

$$\Delta S_l \approx \frac{\sqrt{\pi} a_s k_B}{4\sqrt{2}a} \frac{\lambda_c}{\lambda_{ab}} \frac{1 + 3\tau_m^4}{1 - \tau_m^4} \approx \frac{2.9 a_s (1 + 3\tau_m^4) \phi_0^2}{10^4 T_m \lambda_{ab}^2(0)},$$

$$\Delta B \approx \frac{\pi^{3/2}}{2\sqrt{2}a} \frac{\lambda_c}{\lambda_{ab}} k_B T_m \approx \frac{1.8 (1 - \tau_m^4) \phi_0}{10^3 \lambda_{ab}^2(0)}. \quad (19)$$

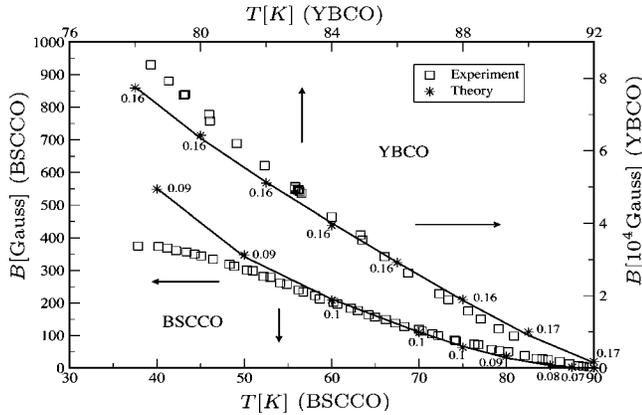


FIG. 1. Melting curve  $B=B_m(T)$  for YBCO and BSCCO. The experimental values are from Ref. 28 for YBCO and Ref. 27 for BSCCO. The numbers on the theoretical melting curves are the Lindemann numbers  $c_L$  calculated from Eq. (9).

Parameter values for optimally doped YBCO (BSCCO) are given by<sup>24</sup>  $\lambda_{ab}(0) \approx 1186 \text{ \AA}$  ( $\lambda_{ab}(0) \approx 2300 \text{ \AA}$ ),  $\xi_{ab}(0) \approx 15 \text{ \AA}$  ( $\xi_{ab}(0) \approx 30 \text{ \AA}$ ),  $\text{CuO}_2$  double-layer spacing  $a_s = 12 \text{ \AA}$  ( $a_s = 14 \text{ \AA}$ ),  $T_c = 92.7 \text{ K}$  ( $T_c = 90 \text{ K}$ ) and the anisotropy parameter  $\gamma = \lambda_c / \lambda_{ab} \approx 5$  ( $\gamma \approx 200$ ).

We now calculate numerically the melting curves, the associated Lindemann parameter  $c_L$ , the entropy and the magnetic induction jumps  $\Delta S_l$  and  $\Delta B$  from the intersection criterion of the full low- and high-temperature expressions (5) and (7) without further approximation. To accomplish this, we use the elastic constant  $c_{11}$  given by Brandt in Ref. 21. The intersection criterion of the low- and high-temperature expansions of the partition function is then at least in the case of BSCCO a complicated integral equation via the dependence of  $c_{44}$  on the Lindemann parameter  $c_L$ . One can solve this integral equation by numerical methods. The results are shown in Figs. 1 and 2.

#### IV. DISCUSSION

Our approximate analytic results (16) and (19) for YBCO and BSCCO turn out to give practically the same curves. For comparison, we show in Figs. 1 and 2 the experimental curves for YBCO of Refs. 28–30 and for BSCCO of Refs. 27 and 31. The good agreement in Fig. 1 with the theoretical curves based on Eq. (13) shows that the Lindemann number is independent of the magnetic field for YBCO for the entire temperature range. For BSCCO the agreement is good for smaller  $B$  fields, but the second term in Eq. (18) introduces some dependence of the Lindemann number on  $B$ , largest near  $B=0$ . There is some disagreement in Fig. 1 at larger  $B$  and in Fig. 2 at small  $B$ . This is not surprising since our vortex lattice model cannot be a good approximation in these regimes. At high  $B$ , the discrepancy comes mainly from Josephson decoupling of the layers,<sup>32</sup> most pronounced for the

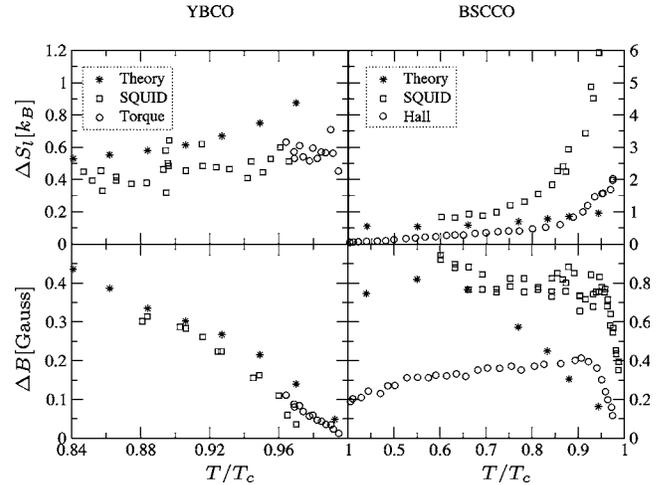


FIG. 2. Entropy jump per double layer per vortex  $\Delta S_l$  (first row) and jump of magnetic induction field  $\Delta B$  (second row) at the melting transition. The experimental values for YBCO are from Ref. 28 for  $\Delta S_l$ , Ref. 29 for  $\Delta B$  by superconducting quantum interference device experiments (SQUID), and Ref. 30 by torque measurements (Torque). The experimental values for BSCCO are from Ref. 31 by SQUID measurements (SQUID) of the magnetic field and Ref. 27 by microscopic Hall sensors (Hall).

strongly anisotropic BSCCO superconductor, which leads also to large pinning effects.<sup>33</sup> We think that this is also the reason for the difference in the curves of Kawasaki *et al.* in Ref. 31 and of Zeldov *et al.* in Ref. 27 shown in Fig. 2. Pinning has the largest influence on the form of the melting curve at high  $B$ ,<sup>34</sup> resulting in a decrease<sup>20</sup> of  $\Delta S_l$  and  $\Delta B$  in the limit of low temperatures shown by the curves of Zeldov *et al.* Near  $B=0$ , our model does not include the increase of the entropy coming from the thermal creation of vortices, in addition to the ones caused by the external magnetic field which form the lattice.<sup>35</sup> Moreover, in YBCO order parameter fluctuations become important,<sup>36</sup> these are ignored here.

Summarizing, we have obtained the melting curve, the entropy, and the magnetic jump from a simple lattice defect model, and derived the Lindemann rule, including the size of the Lindemann number, and corrections to it. The determination of jump quantities over the phase transition cannot be obtained by the simple Lindemann rule. Our curves agree well with the experimental curves for YBCO and BSCCO except at zero and large magnetic fields. The simplicity of the model has allowed us to derive all results via analytic approximations. Our defect model is the simplest extension of the linear elasticity theory of vortex displacements. We have merely added integer-value defect gauge fields which introduce into the elasticity theory the rich physics of other phases of the vortex lattice caused by defect fluctuations, in particular the liquid phase and the associated melting transition.

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