Thickness dependence of flux-line-lattice melting in high-T_c superconducting films

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Civale *et al.* have recently measured the irreversibility line of $YBa_2Cu_3O_{7-x}$ (YBCO) films in the magnetic field-temperature plane, $B_{irr}(T)$, as a function of film thickness. We are able to reproduce the observed shift of $B_{irr}(T)$ to lower temperatures as the film thickness is reduced within a model of flux-line-lattice melting without pinning. While pinning must be important, this suggests $B_{irr}(T)$ is at least partly an intrinsic property. The onset of the shift of $B_{irr}(T)$ begins for films thinner than 1000–1500 Å in YBCO. The present model predicts that the onset will begin for films thinner than 100–150 Å in $Bi_2Sr_2CaCu_2O_8$.

I. INTRODUCTION

Flux lines in the high-T_c superconductors (HTSC's) show an intriguing transition[1–7] from reversible to irreversible behavior below T_c. The line $B_{irr}(T)$ in the magnetic field (B) and temperature (T) plane below which the magnetic properties become irreversible lies slightly below $B_{c2}(T)$ in $YBa_2Cu_3O_{7-x}$ (YBCO),[1,2,5] but very significantly below $B_{c2}(T)$ in $Bi_2Sr_2CaCu_2O_8$ (BSCCO).[2,5] The reversible behavior above $B_{irr}(T)$ is generally associated with free motion of the magnetic-flux lines.[1] Below $B_{irr}(T)$ the flux lines (FL's) are pinned by defects, either in a glassy or in a flux-line-lattice (FLL) structure. There are many models of the transition: thermally activated depinning[1,8–11] of the FL's, a glass-to-liquid transition,[12] giant flux creep,[13,14] transition from an entangled to a disentangled FL state through flux cutting,[15–17] and FLL melting.[1,16,18,19] Pinning clearly plays an important role,[1] and there may not be a clear distinction between the models. However, some experimental results[20] suggest that the irreversibility line is measurably independent of the density of defects from sample to sample,[1] so that the transition has some character intrinsic to the material independent of pinning sites.

Recent measurements of $B_{irr}(T)$ in YBCO by Civale, Worthington, and Gupta[21] show an interesting dependence of $B_{irr}(T)$ on the thickness of the sample. For samples 1000 Å and thicker, $B_{irr}(T)$ takes the bulk value. As the thickness is reduced below 1000 Å, $B_{irr}(T)$ moves to lower temperatures. This can be explained within the above models involving pinning. FL's are very effectively pinned by line-planar defects. As the length of the line and/or plane is reduced with reduced thickness, the strength of pinning is reduced and $B_{irr}(T)$ moves to lower temperature. In the vortex glass model,[12] there is a crossover from three- to two-dimensional behavior as film thickness decreases, which moves $B_{irr}(T)$ to lower temperature. However, it is difficult to make these models quantitative.

The purpose of the present paper is to test whether the observed[21] reduction of $B_{irr}(T)$ with film thickness can be reproduced within the FLL "melting" picture without pinning. We determine the magnetic field $B_I(T)$ at which

the FLL becomes mechanically unstable. We identify the instability with "melting" and with $B_{irr}(T)$. We find that the onset of the reduction in $B_{irr}(T)$ begins for films of thickness 1000–1500 Å, in agreement with experiment. The magnitude of the shift to lower T of $B_{irr}(T)$ as thickness is reduced below 1000 Å is also quantitatively reproduced. The actual value of $B_{irr}(T)$ depends sensitively on $B_{c2}(T)$ in the model, and $B_{c2}(T)$ is not accurately known.

The FLL melting or instability model predicts that the onset of reduction in $B_{irr}(T)$ will begin only in much thinner films in BSCCO, for films of thickness 100–150 Å or less. This is a very specific and quantitative prediction which can be tested to verify or refute the model. If the reduction in $B_{irr}(T)$ is controlled predominantly by pinning, the onset thickness dependence would probably be similar in YBCO and BSCCO. The FLL instability is determined here using the self-consistent phonon (SCP) theory[23] of FL lattice dynamics. At a critical temperature, some phonon frequencies in the FLL vanish and the lattice is unstable. We assume nearly straight FL's and map[16] the FLL onto a monolayer of Bose particles having mass $M_B = (\hbar/kT)\tilde{\varepsilon}_1$ and interacting via the potential $V_B = (\hbar/kT)V$. Here $\tilde{\varepsilon}_1$ is the anisotropic stretching constant[16] of a FL, V is the pair interaction[24] between the FL's, T is the temperature of the FLL, and k is Boltzmann's constant. For infinite sample thickness (L) (infinite FLL length), the monolayer of bosons is at zero temperature ($T_B = 0$). The Bose monolayer temperature is related to sample thickness by $T_B = (\hbar/k)L^{-1}$. As L is reduced, the Bose model temperature T_B increases and the FLL becomes less stable. Thus $B_{irr}(T)$ moves to lower real T as L is reduced.

The FLL potential and SCP theory is introduced in Sec. II. The boson analogy and thickness dependence are discussed in Sec. III. The results are presented in Sec. IV.

II. SELF-CONSISTENT PHONON MODEL

We consider a triangular Abrikosov lattice of N nearly straight flux lines in a HTSC with an applied field B parallel to the c axis. As usual, each line has a quantum of flux ϕ_0 and the FLL constant is $a_0 = (2\phi_0/\sqrt{3}B)^{1/2}$. Assuming nearly straight, parallel flux lines, the interac-

tion potential between the lines can be found from London's field equations[24] and is given by

$$V(r) = \left[\frac{\phi_0^2}{2\pi\lambda'^2\mu_0} \right] [K_0(r/\lambda') - K_0(r/\xi')] , \quad (1)$$

where

$$\lambda' = \frac{\lambda(T)}{[1 - B/B_{c2}(T)]^{1/2}} ,$$

$$\xi' = \frac{\xi}{\{2[1 - B/B_{c2}(T)]\}^{1/2}} , \quad (2)$$

$\lambda(T) = \lambda/(1 - t^4)$, and $B_{c2}(T) = B_{c2}(1 - t)$. Here λ is the penetration depth, ξ the usual Ginsburg-Landau coherence length, and $t = T/T_c$ is the reduced temperature. The anisotropy is reflected in the elastic energy per unit length, ε_1, of a FL that is modified by the effective mass ratio:[16]

$$\tilde{\varepsilon}_1 = \left[\frac{M_{xy}}{M_z} \right] \varepsilon_1 . \quad (3)$$

The potential (1), $\tilde{\varepsilon}_1$, and the lattice positions of the FL's is all we need to implement the SCP theory, which has been discussed recently for the FLL.[22] Here we use the self-consistent harmonic (SCH) approximation. In the SCH theory, the frequencies of the phonons along a branch λ are given by

$$\omega_{q\lambda}^2 = \frac{1}{\tilde{\varepsilon}_1} \sum_{\alpha\beta}^{2} \varepsilon_\alpha(q\lambda)\varepsilon_\beta(q\lambda) \sum_j' (1 - e^{-i q \cdot R_{ij}}) \Phi_{\alpha\beta}(ij) , \quad (4)$$

where the $\Phi_{\alpha\beta}$'s are the force constants. If we average those force constants over a Gaussian vibrational distribution of the FL's described by $u = u_i - u_j$, we get

$$\Phi_{\alpha\beta}(ij) = \frac{1}{[(2\pi)^2|\overline{\Lambda}|]^{1/2}}$$

$$\times \int d u \, e^{-u \cdot \overline{\Lambda}^{-1} \cdot u/2} \frac{\partial^2 V(r_{ij})}{\partial u_\alpha \partial u_\beta} . \quad (5)$$

The width of the distribution is given by

$$\Lambda_{\alpha\beta}(ij) = \frac{kT}{N\tilde{\varepsilon}_1} \sum_{q\lambda} (1 - e^{i q \cdot R_{ij}}) \varepsilon_\alpha(q\lambda)\varepsilon_\beta(q\lambda) \frac{1}{\omega_{q\lambda}} . \quad (6)$$

The iteration of those equations is done until a stationary value is reached for the phonon frequencies. If some frequencies go to zero, the FLL is not stable and is considered as melted.[22]

III. BOSON ANALOGY AND THICKNESS DEPENDENCE

The SCP study of FLL dynamics described before[22] did not take into account the effect of the thickness of the sample. It was assumed that this thickness was infinite. The role of the thickness can be readily seen via the two-dimensional (2D) boson analogy[16] to the FLL. The partition function of the FLL is[16]

$$Z = \sum_{N=0}^{\infty} \frac{1}{N!} \int \mathcal{D} r_1(z) \cdots \int \mathcal{D} r_N(z) e^{-F/kT} , \quad (7)$$

in which the FLL free energy is

$$\frac{F}{kT} = \frac{1}{kT} \int_0^L dz \left[\frac{1}{2}\tilde{\varepsilon}_1 \sum_i \left[\frac{dr_i}{dz} \right]^2 + \frac{1}{2}\sum_{i,j}' V[r_i(z) - r_j(z)] \right] . \quad (8)$$

The integration is along the length L of the FL's (along z) and $r_i(z)$ is the FL position in the x,y plane at height z. The first term in (8) is the energy associated with stretching the FL's. The partition function for N bosons of mass M_B interacting via potential V_B confined to the x,y plane in the path-integral representation is given by (7) with F/kT replaced by

$$\frac{S}{\hbar} = \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[\frac{1}{2}M_B \sum_i \left[\frac{dr_i}{d\tau} \right]^2 + \frac{1}{2}\sum_{i,j}' V_B[r_i(\tau) - r_j(\tau)] \right] . \quad (9)$$

Clearly, the two partition functions are the same if $M_B = (\hbar/kT)\tilde{\varepsilon}_1$, $V_B = (\hbar/kT)V$, and $L = \beta\hbar = \hbar/kT_B$, where T_B is the temperature of the bosons. Thus we may incorporate the thickness dependence of the FLL dynamics by varying the boson model temperature T_B via the relation

$$\frac{\hbar}{kT_B} = L , \quad (10)$$

where L is the thickness of the HTSC sample. The temperature dependence enters the two-dimensional boson model via the usual Bose thermal factor $n(\omega)$ and can be taken into account here by changing (6) to

$$\Lambda_{\alpha\beta}(T_B) = \Lambda_{\alpha\beta}(T_B = 0)\coth \left[\frac{\hbar\omega_{q\lambda}}{2kT_B} \right] . \quad (11)$$

For the FLL this term becomes

$$\Lambda_{\alpha\beta}(L) = \Lambda_{\alpha\beta}(L = \infty)\coth \left[\frac{\omega_{q\lambda}L}{2} \right] . \quad (12)$$

When the FLL temperature T is increased, the boson mass $M_B = \hbar\tilde{\varepsilon}_1/kT$ and potential $V_B = \hbar V/kT$ are reduced. Eventually, the weakened potential can no longer confine the light bosons and the FLL becomes unstable. When L is reduced, the temperature T_B of the bosons is increased. When $kT_B \simeq \hbar\omega_{q\lambda}$, we expect thermal vibration to be important (onset of thickness dependence) and, as T_B is increased, the FLL to be less stable for a given B and T.

IV. RESULTS

The FLL model described in Secs. II and III depends on the parameters T_c, $\kappa = \lambda/\xi$, M_z/M_{xy}, and the upper critical field $B_{c2}(0)$. To characterize YBCO we have

chosen[8,25,26] $T_c = 87.2$ K, $\kappa = 50$, $M_z/M_{xy} = 25$, and $B_{c2}(0) = 44$ T. The resulting instability lines of the FLL in the B and T plane for YBCO are shown in the upper half of Fig. 1. The FLL is stable to the left of the lines. Clearly, the stability line moves to lower temperatures as the thickness of the YBCO sample is reduced. In the lower half of Fig. 1, we have reproduced the $B_{irr}(T)$ observed by Civale et al.[20]

From Fig. 1 we see that the model FLL becomes unstable at significantly lower temperatures (smaller t) than the observed irreversibility line. The model instability line is very sensitive to $B_{c2}(0)$. In Fig. 2 we compare the instability lines for $B_{c2}(0) = 44$ and 100 T. Clearly, the instability line moves to higher temperatures when $B_{c2}(0)$ is increased. At a given t, the field at which the FLL becomes unstable scales nearly linearly with $B_{c2}(0)$ [i.e., depends largely on $b = B/B_{c2}(0)$]. Since $B_{c2}(0)$ is not known, $B_{c2}(0)$ might be adjusted to fit the observed instability line to $B_{irr}(T)$. We have not attempted to do this since pinning must play a significant role which is not included here. Also, the present interaction $V(r)$ in (1), which we have used throughout, is not applicable to films at low B ($B \leq 0.5$ T), as discussed below.

FIG. 2. Dependence of FLL melting line in YBCO on $B_{c2}(0)$; lines for $B_{c2}(0) = 44$ and 100 T are shown.

In the upper half of Fig. 3, we show the instability temperature at $B = 7$ T, $T_I(7T)$, divided by T_c as a function of sample thickness in YBCO using $B_{c2}(0) = 44$ T. Both the thickness ($L \simeq 1000$ Å) at which $T_I(7T)/T_c$ begins to depend on thickness (onset thickness) and the relative drop in $T_I(7T)/T_c$ with thickness agree well with the observed values shown in the bottom half of Fig. 3. This agreement suggests that irreversibility is at least in part
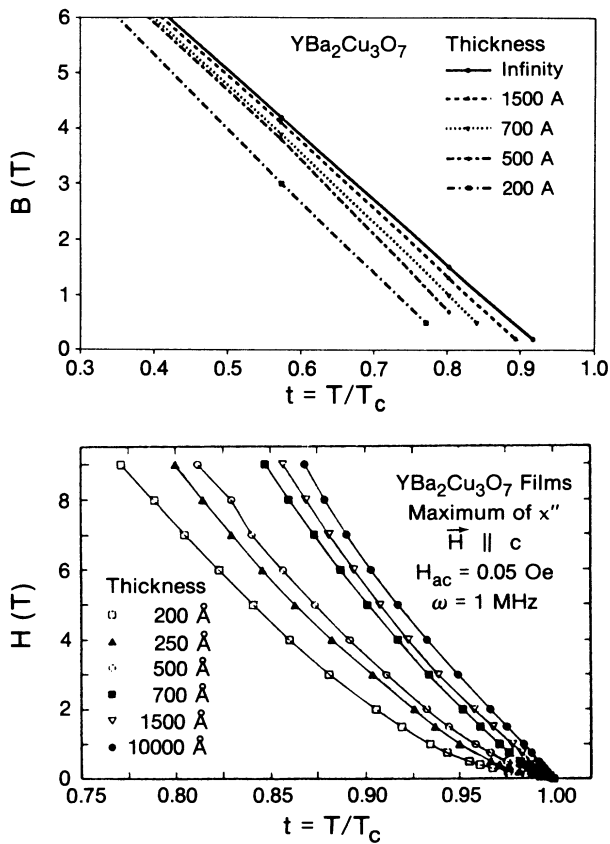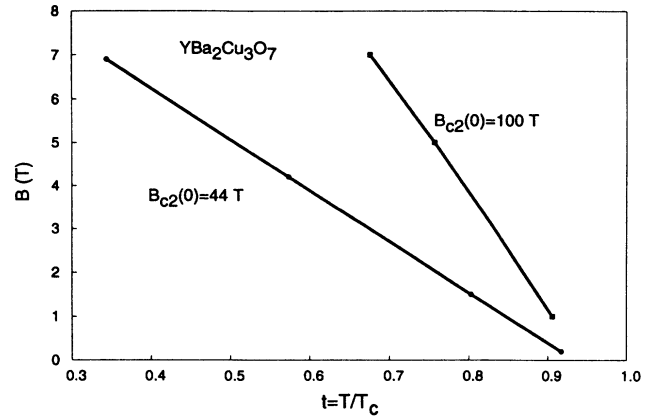

FIG. 1. FLL melting lines in YBCO for different thicknesses (upper half) compared with the irreversibility lines $B_{irr}(T)$ in YBCO observed by Civale et al. (Ref. 21) for different thicknesses (lower half). The FLL is stable at low B and low T/T_c. Model parameters used are $T_c = 87.2$ K, $\kappa = 50$, $M_z/M_{xy} = 25$, and $B_{c2}(0) = 44$ T.
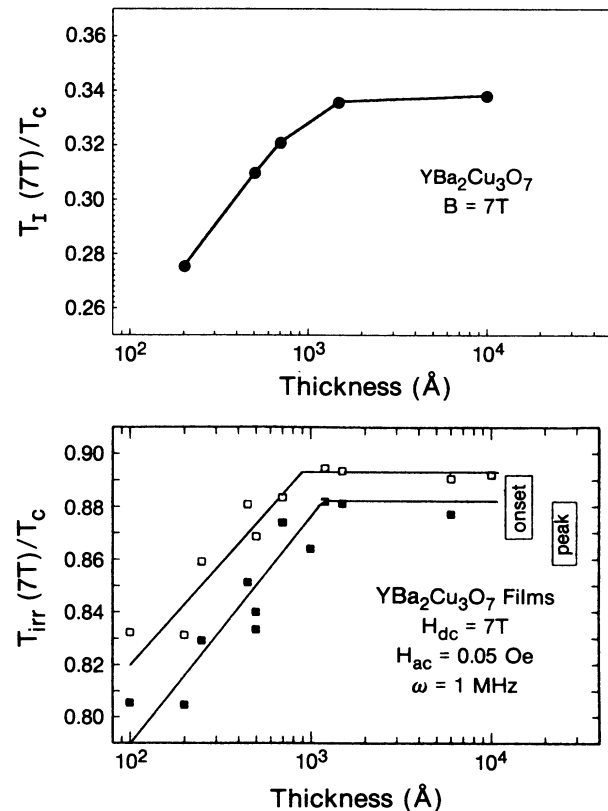

FIG. 3. FLL melting temperature at $B = 7$ T, $T_I(7T)/T_c$, and observed irreversibility temperature at $B = 7$ T, $T_{irr}(7T)/T_c$ (Ref. 21), in YBCO vs thickness.

an intrinsic property of the flux lines in the grains of the material and is not entirely dependent on pinning in the samples studied. We obtained a similar reduction in $T_I(7T)/T_c$ with decreased L in YBCO using $B_{c2}(0)=100$ T. In Fig. 3 the thickness dependence is displayed in a way which is less dependent on the unknown parameter $B_{c2}(0)$.

The FLL model may also be applied to BSCCO for which reasonable parameters are[8,25,26] $T_c=87$ K, $\kappa=95$, and $M_z/M_{xy}=3600$. We again use $B_{c2}(0)=44$ T. The chief difference between BSCCO and YBCO is the effective mass which leads to a smaller $\bar{\epsilon}_1$, a lighter boson mass M_B, and significantly larger phonon frequencies $\omega_{q\lambda}$ in (4). With larger $\omega_{q\lambda}$ in (12), the thickness L must be smaller for the $\coth(\omega_{q\lambda}L/2)$ to differ from unity. This means the onset thickness will be much smaller in BSCCO than in YBCO. In Fig. 4 we show the thickness dependence of the instability in BSCCO. The thickness dependence begins at $L=100-200$ Å^{-1}, a factor of 10 smaller than in YBCO.

The thickness dependence is also less at higher B. If intrinsic FLL melting plays a role in the thickness dependence, then a very different onset thickness is predicted in BSCCO.

As noted, we have represented the interaction energy per unit length of two flux lines separated a distance r by $V(r)$ in (1). This is the interaction per unit length between FL's in a bulk sample ignoring effects of the surface on the interaction. We argue that $V(r)$ continues to represent the interaction well in thin films at large B ($B \geq 0.5$ T in YBCO) where the separation between FL's (a_0) is much less than the penetration length λ ($\lambda \gg a_0$). At $B=7$ T, $\lambda \simeq 10a_0$ in YBCO. In this case, within $r \leq \lambda$, some several thousand neighbor shells in the FLL, the interaction is the same in the bulk and in a film independent of the film thickness. The instability in the self-consistent phonon approximation depends on the interaction at short range. Thus the $V(r)$ in (1) represents the FL interaction quite well in films for the purposes of dynamics. As discussed by Pearl,[27] Fetter and Hohen-
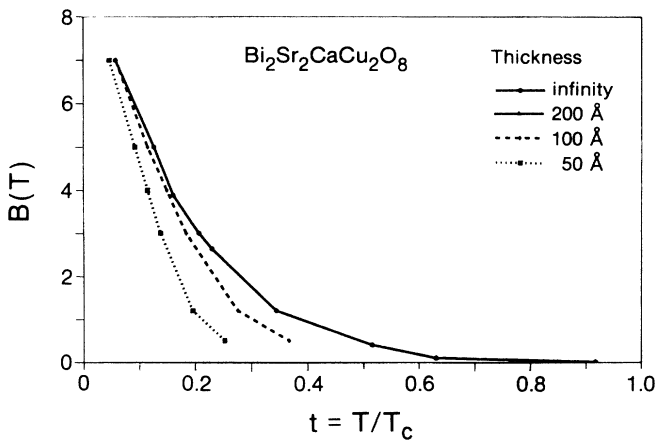
berg,[28] Fetter,[29] and Fisher,[30] surface effects are important if λ is short, or when λ is long and B is small, so that $a_0 \gg \lambda$.

The total interaction between two FL's separated a distance r in a film of thickness $L=d$ using the bulk interaction (1) is

$$v(r)=V(r)d = \left[\frac{\phi_0^2}{2\pi\mu_0\lambda'^2}\right]dK_0\left[\frac{r}{\lambda'}\right]$$
$$\equiv v_0dK_0\left[\frac{r}{\lambda}\right], \tag{13}$$

where we have dropped the cutoff term $K_0(r/\xi)$ and taken $\lambda'=\lambda$. Within the film the magnetic field due to a FL penetrates a distance λ into the superconducting region around the FL. The magnetic field may be said to be "screened out" within a length λ. For a film the magnetic field also escapes through the surface and is "unscreened" in free space. If two FL's interact via both the screened and unscreened fields, the interaction in a film will be different from that in the bulk. However, if λ is long and the separation between the FL's (a_0) is short, then the screened and unscreened interactions will differ little. We show this is the case at large B in the high-T_c materials.

Using the asymptotic limits of K_0, $K_0(x)=\ln(2/x)-\gamma$ for small x and $K_0(x)=(\pi/2x)^{1/2}e^{-x}$ for large x (pp. 375 and 378, Ref. 31), we have, from (13),

$$v(r) \simeq v_0d[\ln(\lambda/r)+\ln2-\gamma], \quad r \lesssim \lambda,$$
$$v(r) \simeq v_0d\left[\frac{\pi\lambda}{2r}\right]^{1/2}e^{-r/\lambda}, \quad r \gg \lambda. \tag{14}$$

Pearl[27] and Fetter and Hohenberg[28] have calculated the interaction between FL's in a film. The film character is introduced by solving the Ginzburg-Landau equations assuming the supercurrents J_s are confined to a sheet of zero thickness, $J_s=\delta(z)J_s(r)$. They find a total interaction for a film of thickness $L=d$ of

$$v_F(r)=\frac{\phi_0^2}{2\mu_0\Lambda}\left[H_0\left[\frac{r}{\Lambda}\right]-Y_0\left[\frac{r}{\Lambda}\right]\right], \tag{15}$$

where $\Lambda=2\lambda'^2/d$ is an effective penetration length. For $d \simeq 1000$ Å and $\lambda \simeq 3000$ Å, clearly $\Lambda \simeq 6\lambda_0$. In (15), H_0 is the Struve function (p. 496, Ref. 31) and Y_0 a Bessel function (p. 360, Ref. 31). The limits of these functions are

$$H_0(x)-Y_0(x) \simeq (2/\pi)[x-\ln x+\gamma)],$$

for small x, and $H_0(x)-Y_0(x) \simeq (2/\pi x)$ for large x, so that

$$v_F(r) \simeq v_0d[\ln(\lambda/r)+\ln(2\lambda/d)-\gamma], \quad r \lesssim \lambda,$$
$$v_F(r) \simeq \left[\frac{\phi_0^2}{\pi\mu_0}\right]\frac{1}{r}, \quad r \gg \lambda. \tag{16}$$

These limits and the comparison with the bulk result (14)

FIG. 4. FLL melting lines in BSCCO for different thicknesses. The onset of thickness dependence is at 100–150 Å.

are discussed by Pearl,[27] Fetter and Hohenberg,[28] and Fisher.[30]

Comparing (14) and (16), we see that the interactions are the same for $r \lesssim \lambda$ independent of the thickness—at least the derivatives which determine the dynamics. The leading correction to $K_0(x)$ at small x is $x^2/4$, so that the $r \lesssim \lambda$ limit in (16) represents $V(r)$ quite well out to $r \sim \lambda/2 \sim 5a_0$ for the B fields of interest here. Thus the bulk interaction can be used for films except at very long range. Clearly, the long-range interaction is significantly different and Coulomb like in the film. We expect (16) to apply within a distance λ of the surface in a bulk material, which is comparable to d here.

The instability in the SCP theory used here depends sensitively on the short-range interaction and little on the long-range part. We showed this in an earlier paper[22] by changing the short-range part and noting the sensitivity of the instability temperature T_I to this change. Specifically, the T_I is quite different in the SCH and harmonic approximations. This results from the difference in the "averaged" and "nonaveraged" force constants. This difference is significant for the first few shells only, where $\langle u^2 \rangle$ is comparable to r, the separation between the FL's. Thus, while there is some error, we believe (1) represents the important features of the interaction well at large B.

As discussed by Huse,[32] the difference between (14) and (16) will become important at very low fields, for which $a_0 \gtrsim \lambda$. In YBCO, $a_0 \simeq \lambda$ at $B \simeq 0.05$ T. The present approximation should therefore be valid for $B \gtrsim 0.5$ T. It would be interesting to investigate the FLL dynamics at low B, where surface effects are important and the interaction is Coulomb like. For example, the SCP theory has been used[33] to evaluate the stability of the electron (Wigner) crystal. The SCP theory predicts that the three-dimensional Wigner crystal becomes unstable at $r_s = 180$, where the Lindemann ratio is $\gamma = 0.26$. Simulations by Ceperley and Alder[34] find that the Wigner solid melts at $r_s = 160$, where $\gamma = 0.26$. Some modification of (16) at long range will be needed, either taking account of the finite film thickness or something to simulate a background of uniform charge to "neutralize" the material.[28]

V. SUMMARY

We have evaluated the mechanical stability of the flux-line-lattice assuming nearly straight flux lines and self-consistent harmonic dynamics. Both these assumptions will tend to overestimate the stability of the FLL. The stability also depends on the film thickness, a smaller thickness meaning a higher effective temperature in the corresponding boson model. In YBCO the thickness dependence of the stability line agrees well with that of the irreversibility line as seen from Fig. 3. In Fig. 3 the onset of thickness dependence begins for films of 1000 Å. The mechanical stability model predicts an onset of thickness dependence of 100–150 Å in BSCCO. A measurement of the thickness dependence of $B_{irr}(T)$ in BSCCO would serve as a test of the importance of intrinsic FLL melting in the transition from reversible to irreversible behavior.

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