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LETTER TO THE EDITOR

Thermal fluctuations of flux-line positions of high-T_c superconductors

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Abstract. The thermal fluctuations of flux-line positions in an ideal high-T_c oxide superconductor have been studied. We have calculated the ratio $\sqrt{\langle u^2\rangle}/a$ numerically, and justified the latest conjectured analytic expression.

For a strong enough magnetic field, flux lines can penetrate type-II superconductors in the form of flux lines, each flux line carrying a flux $\phi_0 = 2 \times 10^{-7}$ G cm^{-2}. At lower temperatures the flux lines form a regular triangular lattice. At higher temperatures the flux-line positions fluctuate around their equilibrium positions due to thermal disturbance. Thermal fluctuation can be measured by the Lindemann ratio $\alpha = \sqrt{\langle u^2\rangle}/a$ where a is the lattice constant. It has been found that most classical solids melt at $\alpha \simeq 0.1$ and that quantum solids melt at $\alpha \simeq 0.3$. This value for the flux-line lattice was first calculated from local elasticity by Nelson and Seung [1] and in the extreme non-local limit by Moore [2]. Houghton *et al* [3] and Brandt [4] calculated this quantity under the continuum approximation and obtained values which were much larger than Nelson and Seung's result, but comparable to Moore's. (The non-local correction is important in high-T_c superconductors, because at a typical magnetic field of 2 T the average flux-line distance is much smaller than the range of interaction between flux lines. thus the non-local results are more relevant.) The latest formula for $\langle u^2\rangle$ based on the anisotropic London theory in the continuum approximation is given by [6]

$$\langle u^2\rangle = k_B T\left(1/B\phi_0 C_{66}\right)^{1/2}\left[\tfrac{1}{2}B\kappa^2/\left(B_{c2}-B\right)\right]^{1/2}\lambda_c/\lambda_{ab} \tag{1}$$

where $C_{66} = (B^2/4\pi)/8\kappa^2 b$ is the shear modulus and κ is the Ginzburg–Landau parameter, $b = B/B_{c2}$, and λ_c and λ_{ab} are the penetration depth in the c direction and the ab plane respectively. The formula is written as the local result [1], multiplied by a non-local correction factor $[\frac{1}{2}B\kappa^2/(B_{c2}-B)]^{1/2}$, and the anisotropy ratio λ_c/λ_{ab}. The last two factors were actually conjectured from physical argument by Brandt [5] and, to my knowledge, have never been derived.

We calculate here $\langle u^2\rangle$ numerically from the anisotropic London theory to justify the validity of formula (1); the calculation takes into account both the discreteness of flux-line lattices (i.e. beyond the continuum approximation) and the non-locality exactly within the

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anisotropic London theory under the harmonic approximation. Our results were compared with formula (1) and showed very good agreement. The formula gives a result about 10% smaller than the exact result for a large temperature range. We propose that the formula should be multiplied by a factor of 1.25, and in this way it will almost coincide with the exact result from 0 K to about $0.6T_c(H)$; the maximum deviation in this range is less than 2%, which is the upper limit of our calculation error. We now describe our results in detail. The interaction of flux lines of arbitrary shape was given recently by Sudbøand Brandt [7] using a method based on the anisotropic London equations:

$$U = \frac{1}{2}\sum_{m,n}\int \mathrm{d}l_i\,\mathrm{d}l_j\,V_{ij}(\boldsymbol{r}_m - \boldsymbol{r}_n) \tag{2}$$

where

$$V_{ij}(\boldsymbol{r}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}V_{ij}(\boldsymbol{k})\,\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \tag{3}$$

and

$$V_{ij}(\boldsymbol{k}) = \left[1/\left(1+\Lambda_1\boldsymbol{k}^2\right)\right]\left[\delta_{ij} - q_iq_j\Lambda_2/\left(1+\Lambda_1\boldsymbol{k}^2+\Lambda_2\boldsymbol{q}^2\right)\right] \tag{4}$$

where $\boldsymbol{q} = \boldsymbol{k}\times\hat{\boldsymbol{c}}$. In the following we only consider the case where $\boldsymbol{B}\|\hat{\boldsymbol{c}}$.

Previous calculation with the similar $1/r$ potential [8], as well as our recent Monte Carlo simulation [9], indicates that because of the softness of the potential, the harmonic approximation works well. The harmonic energy U_0 can be written in terms of the deviations u of the flux lines from the ideal lattice positions as

$$U_0 = \frac{1}{2}\sum_{\boldsymbol{k}}\Phi_{\alpha\beta}(\boldsymbol{k})u_\alpha(-\boldsymbol{k})u_\beta(\boldsymbol{k}) \tag{5}$$

with

$$\Phi_{\alpha\beta}(\boldsymbol{k}) = \frac{B^2}{4\pi}\sum_{\boldsymbol{Q}}\Big[k_z^2V_{\alpha\beta}(\boldsymbol{k}+\boldsymbol{Q}) + (\boldsymbol{k}+\boldsymbol{Q})_\alpha(\boldsymbol{k}+\boldsymbol{Q})_\beta V_{zz}(\boldsymbol{k}+\boldsymbol{Q}) - Q_\alpha Q_\beta V_{zz}(\boldsymbol{Q})\Big]. \tag{6}$$

The sum is over all reciprocal lattice vectors $\boldsymbol{Q}$.

Direct evaluation of the summation of $\boldsymbol{Q}$ is impractical because of its very slow convergence; actually, the summation is logarithmically divergent. This divergence originates from the replacement of the normal core part of a flux by a singular line. The summation has to be cut off at $Q_{\max} \simeq 1/\xi$ where ξ is the coherence length that gives the radius of the normal core. The cutting off can be incorporated properly by using a convergence factor $\exp[-2(\boldsymbol{Q}+\boldsymbol{k})^2\xi^2]$ [6]. We have developed a Ewald sum technique to calculate this sum [10], where we transform the sum into two fast-converging series, in real space and reciprocal space, respectively. The elastic matrix can be easily evaluated numerically by taking only a few shells of real space and reciprocal space lattice vectors around the origin.

Thermal fluctuation is given by the mean square $\langle u^2\rangle$ of flux displacement. It can be written in terms of the elastic matrix

$$\langle u^2\rangle = k_BT\int_{-\infty}^{\infty}\frac{\mathrm{d}k_z}{2\pi}\int\int_{\mathrm{BZ}}\frac{\mathrm{d}^2k_\perp}{(2\pi)^2}\,[\Phi_{xx}^{-1}(\boldsymbol{k}) + \Phi_{yy}^{-1}(\boldsymbol{k})]. \tag{7}$$

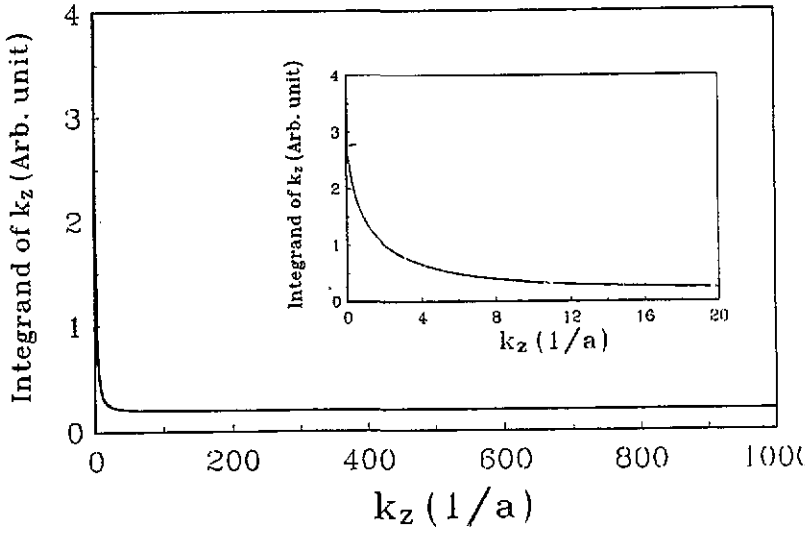

Figure 1. Plot of the integrand of k_z as a function of k_z. Inset: the same plot for small values of k_z.

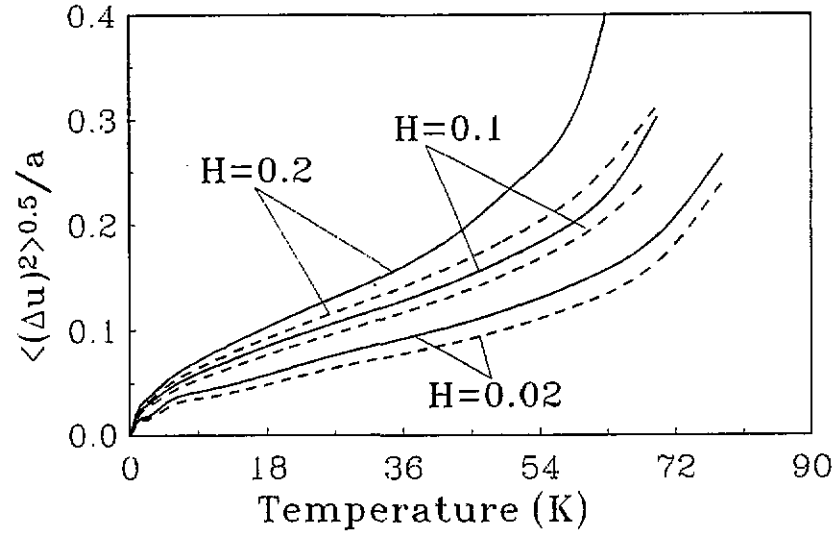

Figure 2. Calculated Lindemann ratio (full curves) and the same quantity from (1) (broken curves) for parameters of YBCO, where $H_{c2}(0) = 22$ T, $\kappa = 100$, $T_c = 87$ K and $M_z/M = 25$; the upper critical field is taken to be $H_{c2}(T) = H_{c2}(0)[1 - (T/T_c)^2]$. The applied magnetic field H (taken to be equal to B in our case) is in units of $H_{c2}(0)$.

The above integration was evaluated in the following way. First, for a given value of k_z, we evaluate the 2D integral of k_x, k_y by dividing $\frac{1}{12}$ of the 2D Brillouin zone (BZ) into 36 triangles; in each triangle, we linearly interpolate $1/\Phi_{xx}^{-1}(\boldsymbol{k})$ and $1/\Phi_{yy}^{-1}(\boldsymbol{k})$ and integrate the interpolated function analytically, then sum over all triangles. (See [11] for a detailed

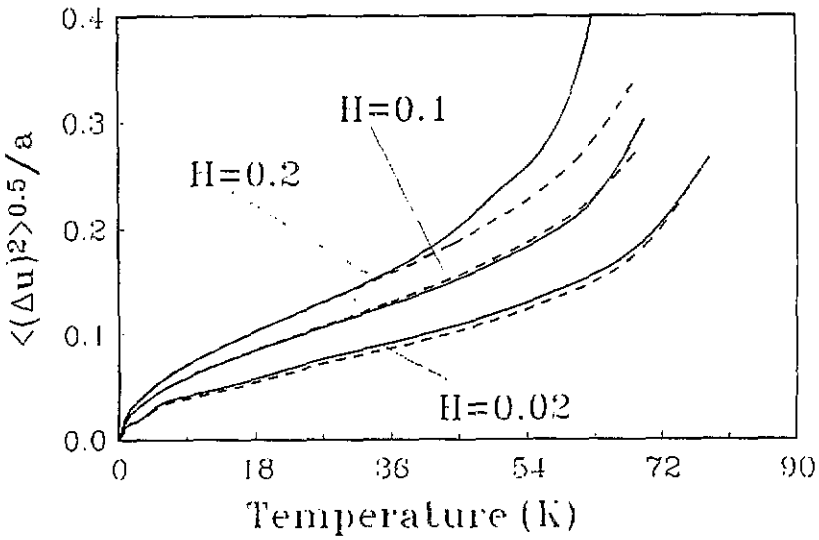

Figure 3. As figure 2 except that $M_z/M = 360$.

discussion of this so-called *simplex integration method.*) The result is a function of k_z at discrete k_z mesh points; it drops quickly for small k_z and tends to a small constant at large k_z (see figure 1 for a typical plot). This implies that the integration over k_z is divergent linearly and that $\langle u^2 \rangle$ is infinite for all temperatures larger than zero. Of course this is not physical; the source of this divergence again originates from the improper treatment of the normal core of flux lines in the London theory. We should cut off the integration over k_z at approximately $1/\xi_c$, where $\xi_c = (M/M_z)\xi$ is the coherence length along the c direction, because the value of the integrand is very small around this cutting point (see figure 1), so the exact cutting position is not important, and we can do this systematically by introducing a convergence factor $\exp(-2k_z^2\xi_c^2)$. Then the integration over k_z was performed by the *spline interpolation method.* We have checked our calculation for one temperature by refining the mesh points in the BZ and double- and triple-k_z mesh points; the estimated relative error of our numerical data is less than 2%. We have performed calculations with parameters characteristic of YBCO and BSCCO. The results are given in figures 2 and 3. We have also plotted in the figures the formula (1). We see that though formula (1) was conjectured via physical arguments, it is quite good and gives results comparable to within about 10% to our exact numerical result. By comparing the two sets of results, we suggest that the formula (1) should be multiplied by a factor of 1.25, which will make it almost exact in the temperature range of interest as pointed out earlier. Figures 4 and 5 give comparisons of formula (1) multiplied by 1.25 with our exact numerical results; the agreement is excellent. We point out here that even though formula (1) was conjectured from the continuum approximation of the anisotropic London theory, it actually exceeds this approximation and is close to the exact result as our calculation indicates. To compare our result with experiment, we have fitted to (1) multiplied by 1.25 the measurements of flux-line lattice melting lines on untwinned single $YBa_2Cu_3O_{7-\delta}$ crystals by Kwok *et al* [12] and similar results by Safar *et al* [13] and Farrell *et al* [14], using the parameters given by [12]; the Lindemann ratio is fitted to 0.11, which is physically reliable and very close to the value for classical melting of solids.

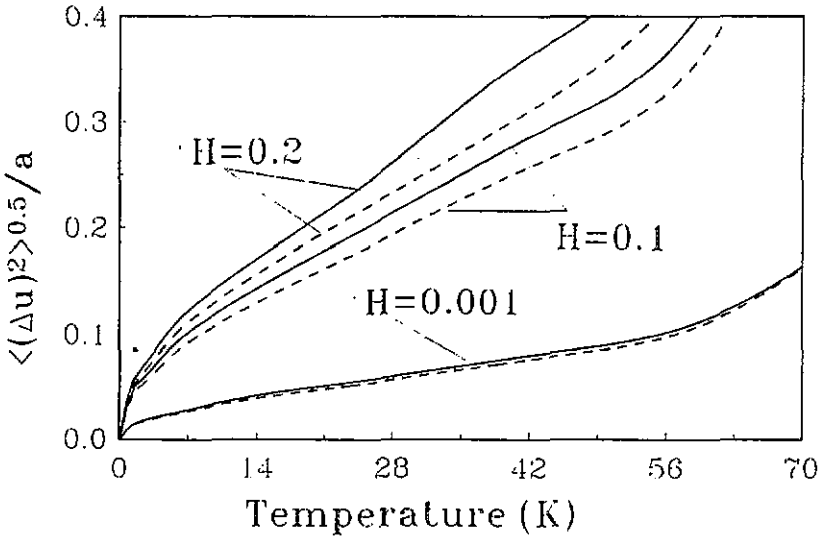

Figure 4. Calculated Lindemann ratio (full curves) and the same quantity from (1) multiplied by 1.25 (broken curves). The parameters are the same as in figure 2. The two curves are almost coincident from $T = 0$ K to $T = 0.6T_c(H)$.

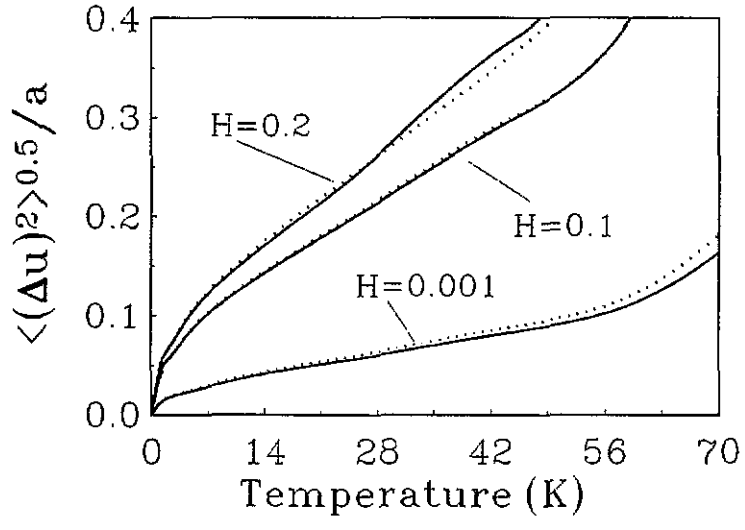

Figure 5. As figure 4 but with the same parameters as figure 3.

To conclude, we have calculated the thermal fluctuations of flux-line positions of high-T_c superconductors exactly, within the anisotropic London theory, and justified the correctness of the analytic formula available. The Lindemann ratio at the flux-line lattice melting point is estimated to be 0.11 by fitting the experimental measurements.

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