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LETTER TO THE EDITOR

Defects in flux lattices and flux creep in high-T_c superconductors

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Abstract. We have estimated the energy of a dislocation loop and found that it exhibits a strong temperature dependence and extrapolates to zero slightly above a temperature which we have previously identified as the melting temperature of the pure lattice. The magnitude of this energy and its dependence on the temperature, the magnetic field and the Landau–Ginzburg parameter all agree reasonably well with experimental estimates for the activation energy in thermally assisted flux flow at low currents. Estimates of the prefactor of the resistivity due to hopping of the flux loop also agree with experimental results. Our result is the first quantitative estimate of the activation energy.

For a strong enough magnetic field, flux lines penetrate type-II superconductors and form a lattice. Anderson and Kim [1] first pointed out that flux creep can occur through collective motion of flux lines. They suggested that in the limit of low current j, the resistivity ρ is thermally activated. Recently Feigelman *et al* [2] furthered understanding of this approach by applying to this problem knowledge gained in the study of random fields [3, 4] and the pinning of charge density waves [5].

These studies assume that the ground state possesses a finite shear modulus, with positional long-range order destroyed by impurities [6, 7]. A different approximation describing the ground state as a vortex glass was proposed by Fisher [8–10]. The dynamics in the possible glass phase were studied by Toner [11]. The descriptions of the ground state as a glass or a solid with no long-range order are not mutually exclusive. The appropriateness depends on the correlation length of the system.

These works have not considered the effect of defects in the flux lattices. Recently Ma and Chui [12] considered a mechanism of flux lattice melting due to spontaneous generation of dislocations. They found that when a single dislocation is created, the vibration free energy of the flux lines decreases by an amount of the order of $\log(A/a)$, where A is the area of the lattice. This decrease cancels the elastic strain energy at some temperature. Thus, creation of a free dislocation becomes favourable and the flux-line lattice will be unstable. They identified this temperature as the melting temperature of the pure lattice and found that the free energy of edge dislocations becomes zero at temperatures that are within 20% of the experimental melting temperatures. Defects such as dislocation loops can be thermally activated and affect flux creep, just like a 'flux bundle' [13–15]. Our melting mechanism suggests that the activation energy will be strongly temperature dependent.

Estimates of the activation energy, U, in flux creep can be extracted by integrating with respect to temperature the experimental quantity [16, 17] $f(T) =$

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$d \ln \rho / dT^{-1} = T^2 d(U/T)/dT$. $U(T, H)$ exhibits a rich dependence on the temperature and the magnetic field. At a fixed magnetic field, as the temperature is increased it *extrapolates to zero* at a temperature below the superconducting temperature. As the magnetic field is increased, the activation energy is decreased. There have not been any previous theories that explain this rich behaviour. Nor were there any quantitative estimates of the activation energy.

In this letter we estimate the energy of dislocation loops in flux lattices and find that it exhibits a strong temperature dependence and extrapolates to zero slightly above a temperature which we previously identified as the melting temperature of the pure lattice. Our results, together with the experimental estimates, are shown in figures 1 and 2 for BSCCO and YBCO. The magnitude of this energy and its dependence on the temperature, magnetic field and the Landau–Ginzburg parameter all agree reasonably well with estimates for the activation energy in flux creep. The experimental curves for U as a function of T exhibit positive curvatures. One of the reasons for the positive curvature comes from the interaction between the dislocation loops, which start interacting with each other when their number becomes large. This interaction will increase the energy to create more defects and thus produces a positive curvature. Because there are uncertainties in the exact experimental values of the parameters that we use, the appearance of agreement with experiment could be enhanced if we had adjusted these parameters accordingly. The discrepency between theory and experiment increases as the magnetic field is decreased and the temperature approaches the superconducting transition temperature. This is reasonable for several reasons. (i) No impurity effects have been included. This effect is especially important when the flux lattice becomes 'soft'. (ii) We have assumed that the coherence length approaches infinity as $(1 - T/T_c)^{-1/2}$. The actual dependence can be different from this close to T_c [18]. (iii) The way we extract the gap from the experimental quantity, f, may be invalid because f exhibits a complicated temperature dependence in this limit. We now describe our results in detail.

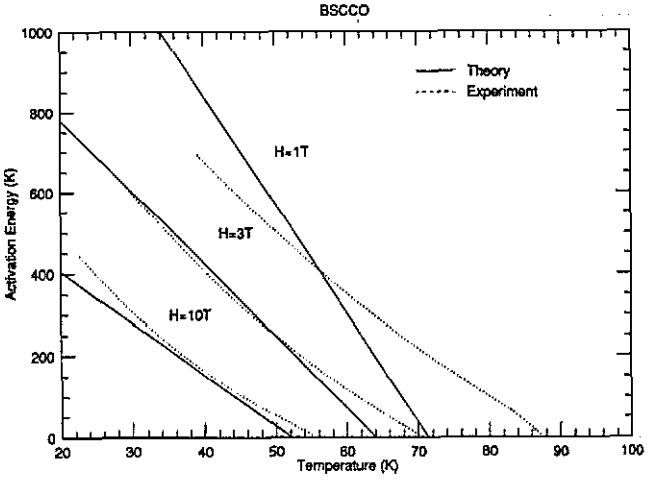

Figure 1. Theoretical estimates of the activation energy (solid lines) and experimental values (dashed lines) of U for BSCCO as a function of temperature at different magnetic field strengths.

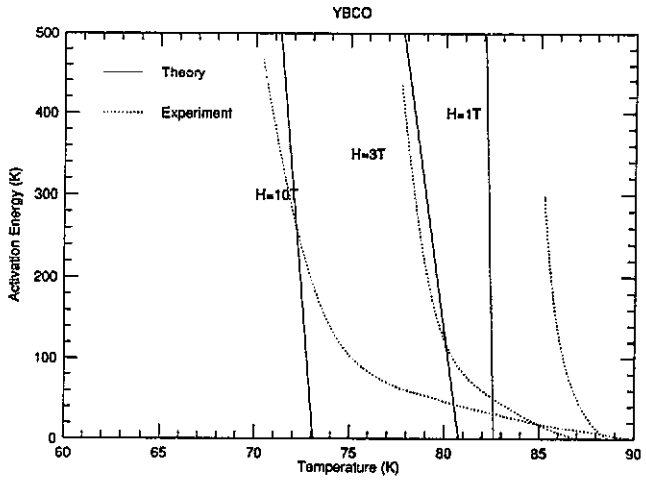

Figure 2. Theoretical estimates of the activation energy (solid lines) and experimental values (dashed lines) of U for YBCO as a function of temperature at different magnetic field strengths.

The interaction energy, W, of flux lines of arbitrary shape was derived recently by Brandt [20] from the London equations in terms of the penetration depths along the ab plane and the z direction, λ_{ab} and λ_z, as:

$$W = \frac{\Phi^2}{8\pi} \sum_{m,n} \int \mathrm{d}l_i \mathrm{d}l_j \tilde{V}_{ij}(\boldsymbol{r}_m - \boldsymbol{r}_n) \tag{1}$$

where

$$\tilde{V}_{ij}(\boldsymbol{r}) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} V_{ij}(\boldsymbol{k}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{2}$$

and

$$V_{ij}(\boldsymbol{k}) = \frac{1}{1+\Lambda_1 k^2} \left(\delta_{ij} - \frac{q_i q_j \Lambda_2}{1+\Lambda_1 k^2 + \Lambda_2 q^2} \right) \tag{3}$$

where $\boldsymbol{q} = \boldsymbol{k} \times \hat{\boldsymbol{c}}$, $\Lambda_1 = \lambda_{ab}^2$, $\Lambda_2 = \lambda_c^2 - \lambda_{ab}^2$. The harmonic energy of vibration, W_0, can be written in terms of the deviations, s, of the flux lines from the lattice positions as

$$W_0 = \frac{1}{2} \sum_{\boldsymbol{k}} \Phi_{\alpha\beta}(\boldsymbol{k}) s_\alpha(-\boldsymbol{k}) s_\beta(\boldsymbol{k}) \tag{4}$$

where

$$\Phi_{\alpha\beta}(\boldsymbol{k}) = \frac{B^2}{4\pi} \sum_{\boldsymbol{Q}} \left(k_z^2 V_{\alpha\beta}(\boldsymbol{k}+\boldsymbol{Q}) + (\boldsymbol{k}+\boldsymbol{Q})_\alpha (\boldsymbol{k}+\boldsymbol{Q})_\beta V_{zz}(\boldsymbol{k}+\boldsymbol{Q}) - Q_\alpha Q_\beta V_{zz}(\boldsymbol{Q}) \right) \tag{5}$$

and $(\alpha, \beta, \ldots) \in (x, y)$, and $(i, j, \ldots) \in (x, y, z)$. The sum runs over all reciprocal lattice vectors Q.

The free energy of the defect is the sum of the core energy, E_c, the free energy of vibration of the core position F_{vc}, the elastic strain energy E_d, and the free energy change of the lattice vibrations when the dislocation loop is created $F_{dis-vib}$. We discuss each of these terms below.

(i) E_c. We view a dislocation loop as a dislocation pair of finite length. Hill *et al* [21] has considered atomistic models of dislocations in flux lattices but only in the limit of small G–L parameter, κ, without periodic boundary conditions. Fisher *et al* [22] have calculated the core energies of defects in the two-dimensional Coulomb lattice. We follow their procedure to calculate the core energy of the dislocation of the flux lattice here. Since the penetration depth is much larger than the lattice constant, the potential is long range and we have used the Ewald sum technique for its evaluation [24]. A periodic boundary condition is used. We follow Adams and MacDonald [25] and choose the Ewald parameter so that the real-space sum is short-ranged and cylindrical, thus its value can be easily tabulated as a one-dimensional array. The sum over the reciprocal lattice vectors can be factorized into a product of terms involving only a single summation and is thus highly efficient. We start off with an initial configuration determined by the analytic formula for the displacement by dislocations. The system is then relaxed until a minimum energy configuration is reached. Instead of using a simplex method as Fisher *et al* did for the relaxation, we use a quasi-Newton method. The process is speeded up with an analytic formula for the derivative of the potential. We investigated dislocation pairs at different distances and, after correcting for the energy changes due to image interactions, we found that the final results differ from each other by less than 10%. Calculations were done for BSCCO and YBCO with the temperature ranging from 0.1 to 0.8 (in units of T_c) and magnetic fields from 1 to 10 T. We found the final result can be well approximated by the formula $2\gamma C_{66}(k=0)a^2 L/\pi$, where γ is Euler's constant, L is the length of the loop, and C_{66} is the shear modulus and is equal to $(BB_{c2}/4\pi)(1/8\kappa^2)$.

(ii) F_{vc}. The free energy of vibration of the dislocation lines, F_{vc}, is computed from the vibration frequency, ω, of a dislocation pair positioned at $d_{1,2}^{(0)}$ as $F_{vc} = k_B T \sum_{k_z} \ln[1 - \exp(-\hbar\omega_{k_z}/kT)]$. The frequency ω can be obtained from diagonalizing the dynamical matrix

$$D_{ab} = \sum_k \Phi_{\alpha\beta}(k) u_{\alpha a}(-k) u_{\beta b}(k) 2[1 - \cos(k \cdot d_{12}^{(0)})]/M.$$

M is the mass per unit length of the dislocation and can be extracted from that of the flux lines, which has been estimated by Suhl [26]. F_{vc} depends on this mass only in a logarithmic fashion. $u(q)$ is the Fourier transform of the strain tesnsors due to a dislocation [27]. For BSCCO F_{vc} is of the order of -40 K and is insignificant compared with the other terms discussed here (which is of the order of 700 K). For YBCO, the temperature range of interest is close to the superconducting transition temperature T_c and ω approaches zero, in which case F_{vc} needs to be included.

(iii) E_d. For an edge dislocation pair a distance R apart, the elastic dislocation energy is equal to $C_{66}(k=0)(1+\sigma)a^2 L \log(R/a)/4\pi$, where R is the separation between the dislocations and L is its length, and σ is Poisson's ratio and is approximately 1. We are interested in the smallest activation energy. Thus R should be the smallest value so that elastic description of it remains valid. Numerical calculations

[22, 23] suggest that $R/a = 3$. There is some uncertainty as to the exact experimental value of κ. We shall follow [33] and use the value of 90 for BSCCO and 50 for YBCO.

(iv) $F_{\text{dis-vib}}$. The calculation by Ma and Chui for the change in the free energy of flux lattice vibrations due to a single dislocation can be generalized to a dislocation pair. Because the potential $\tilde{V}$ in (2) is slowly varying in space, higher-order anharmonic corrections are small [28, 29]; we consider the lowest-order coupling between the dislocation and the vibrations of the flux lines as

$$W_1 = \frac{1}{2}\sum_{k} \Psi_{\alpha\beta l\gamma}(k,q)s_\alpha(-k-q/2)s_\beta(k+q/2)u'_{l\gamma}(q) \tag{6}$$

where Ψ are derivatives of the interline potential V.

The free-energy change of the system, $F_{\text{vib-dis}}$, is $\ln(\langle\exp(-W_1/kT)\rangle)$, where the angular brackets denotes an average with respect to W_0; i.e. $\langle f\rangle = \sum_{\{s\}}\exp(-W_0/kT)f$. This can in principle be calculated exactly. However, the only term that is of the order of the log of the area comes from the second-order cumulant term, $F_{\text{vib-dis}} = -[\langle W_1^2\rangle - \langle W_1\rangle^2]/2kT + \ldots$; $\langle W_1\rangle = 0$ because the system is in equilibrium. The Fourier transform of the strain tensor of a dislocation pair is related to that of a single dislocation by $u' = u(\exp(iqR) - 1)$. Our previous calculation for a single dislocation can be generalized trivially to the present case. Previously $F_{\text{vib-dis}} = -k_B T\Delta W \log(L/a)/4\pi$, for some coefficient ΔW. Now $F_{\text{vib-dis}} = k_B T\Delta W \log(R/a)/2\pi$.

Finally, we turn our attention to the effective length of the dislocation pairs. We can describe the configuration of a dislocation by specifying the two-dimensional position of its core as a function of the distance z, $d(z)$. For dislocation pairs whose core positions are described by $d_{1(2)}$, the energy is given by

$$W' = \sum_{ij} b_i b_j \int \mathrm{d}^2q\,\mathrm{d}k_z\,\mathrm{d}z_1\mathrm{d}z_2\,(q_iq_j/q^2 - \delta_{ij})C_{66}^2/\omega_s(q,k_z)$$
$$\times\,[\cos(q\cdot(d_1(z_1) - d_2(z_2)) + k_z(z_1 - z_2)) - 1].$$

Here ω_s is the shear mode eigenvalue of the dynamical matrix Φ. $\omega_s \approx C_{66}q^2 + C_{44}(q,k_z)k_z^2$. Subdø and Brandt [20] have recently considered the elastic constant C_{44} at a transverse momentum $q = 0$. For a transverse vector $q > 1/\Lambda_2$, the magnitude of C_{44} is much reduced because $V_{\alpha\beta}$ in (3) is much smaller. In that case, $C_{44} \approx 1/\Lambda_2 q^2$. To obtain an estimate, we approximate C_{44} by $C_{44}(q,k_z) = R^2/\pi^2\Lambda_2$. U can be written as for an isotropic elastic medium if one makes the change of variables $C_{66}k_z'^2 = k_z^2C_{44}$ and $z_i' = z_i(C_{66}/C_{44})^{0.5}$. For an isotropic dislocation loop, one expects the height to be comparable to the separation. In the present case, the effective length is changed to $(C_{44}/C_{66})^{0.5}$. This quantity (in units of the flux lattice constant) is of the order of 1 for BSCCO and 5 for YBCO. These are the lengths used in figures 1 and 2. The magnitude of 5 for YBCO is consistent with recent experimental results of the 'irreversibility temperature' as a function of film thickness [30]. At a field strength of 7 T, the transition temperature exhibits a strong dependence on film thickness until the thickness reaches 1000 Å, i.e. of the order of five lattice spacings (200 Å).

The activation energy U is obtained from the experimental quantity f in the following way. Assuming that most of the temperature dependence occurs in the

exponent, f is equal to $T^2 \mathrm{d}(U/T)/\mathrm{d}T$. We integrate this quantity numerically and obtain $U(T) = T\int_{T_0}^{T} f/T^2 + U(T_0)$. For YBCO we take $T_0 = T_c$ and $U(T_c) = 0$. For BSCCO, f exhibits a peak close to T_c and it is not clear if our assumption is valid. There exists a region at low temperature where U seems quite flat [17]. We take that as our starting point in the integration for U. These uncertainties in the way of extracting U will affect the overall magnitude of U, but they will not change the temperature where the activation energy extrapolates to zero, the slope of the temperature dependence, the change as a function of the magnetic field or the dependence on the materials parameters.

To summarize, in this letter we have calculated the magnitude, the temperature and the field dependence of the free energy of dislocation loops. These results exhibit a rich structure and are in reasonable agreement with the experimental estimates of the activation energy from transport measurements. Other point defects may also participate in the transport. We have focused here on dislocation loops because of the connection with possible melting mechanisms. The presence of defects may have other consequences. Marchetti and Nelson [31] have considered the effect of dislocation loops on the bond orientational order.

So far, we have focused on the exponent of the resistivity. It is also possible to estimate the prefactor in the restivity due to the movement of dislocation loops [1]. In the presence of an external current of density J there is a Lorentz force acting on the flux lines. Dislocation loops can move from one flux lattice site to another so that the average hopping distance is the lattice constant a. Associated with this hop there is a net length-movement of all the flux lines that is of the order of a^2 for a dislocation loop of dimension a. Since each line carries a magnetic field of the order of Ba^2, the energy change due to a hop of the loop is thus $U_L = J \times Ba^4$. The loop can hop either along or against the direction of the Lorentz force, so the net hopping rate is thus $\nu_{\mathrm{eff}} = \nu_0 \exp(-U/kT)\sinh(U_L/kT)$, where ν_0 is the attempt frequency. In contrast to the conventional flux bundle argument, U_L is not a strong function of the amount of impurities. When the impurity density is high there will be some dislocation loops that will be situated close to the impurities and U_L, its barrier height against hopping, will be changed. Estimates of U_L have been deduced from the experimental regime in current densities over which linear dependencies on the potential are found [16]. Our result is consistent with this estimate of $U_L \leqslant J \times Ba^4$. The attempt frequency can also be estimated from the formula $\sqrt{normal\ mode\ force\ constant/mass}$. Normal mode force constants have been much discussed recently [20, 32, 33]. We find [34] that the attempt frequency is equal to $2 \times 10^{12}\mathrm{s}^{-1}$ at $B = 1$ T, which is in good agreement with the experimental estimate of $10^{12}\mathrm{s}^{-1}$ [16]. Thus the prefactor of the resistivity, which is equal to $U_L B\nu_0/JkT$, also agrees with the experimental estimate.

A similar picture of melting and finite-temperature transport in two-dimensional quantum systems was recently considered by Chui and Esfarjani [35, 36], who found that the change in zero-point energy of the phonon field when a dislocation is created cancels the elastic strain energy close to the melting temperature. They considered dislocation pairs as charge carriers in a pinned CDW in 2D heterostructures and found the activation energy for transport approaches zero close to the melting point; in reasonable agreement with experimental estimates of the activation energy [37]. The possible connection between flux lattices and two-dimensional quantum systems has been suggested by Nelson and Seung [38], even though this mapping is not accurate quantitatively [19, 33].

We thank R Markiewicz for bringing our attention to the existing experimental data on the activation energy.

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