Energy cost associated with vortex crossing in superconductors

M.A. Moore
Department of Theoretical Physics, University of Manchester,
Manchester, M13 9PL, United Kingdom

N.K. Wilkin
Department of Physics, University of Sheffield,
Sheffield, S3 7RH, United Kingdom.
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Abstract

Starting from the Ginzburg-Landau free energy of a type II superconductor in a magnetic field we estimate the energy associated with two vortices crossing. The calculations are performed by assuming that we are in a part of the phase diagram where the lowest Landau level approximation is valid. We consider only two vortices but with two markedly different sets of boundary conditions: on a sphere and on a plane with quasi-periodic boundary conditions. We find that the answers are very similar suggesting that the energy is localised to the crossing point. The crossing energy is found to be field and temperature dependent – with a value at the experimentally measured melting line of $U_x \approx 7.5kT_m \approx 1.16/c_L^2$, where $c_L$ is the Lindemann melting criterion parameter. The crossing energy is then used with an extension of the Marchetti, Nelson and Cates hydrodynamic theory to suggest an explanation of the recent transport experiments of Safar et al.
I. INTRODUCTION

Thermal fluctuations are widely believed to play an important role in the physics of high temperature superconductors. In this paper we consider a possible manifestation of these fluctuations — that the vortex lines will be able to cross through each other. We begin by estimating the energy associated with such a process starting from the Ginzburg-Landau free energy functional. We then analyse some of the transport measurement data of Safar et al., which has connections with the flux line crossing energy, using a modification of the Marchetti, Nelson and Cates hydrodynamic theory for vortex motion.

The crossing energy calculation has previously been attempted within London theory, an approximation which is valid when a typical vortex separation is much greater than the vortex core size, and by considering just two vortices in a fixed background. However, London theory has an unsatisfactory feature in that it requires a cut-off to be introduced at the length scale of the core radius. This is a difficulty as for crossing the cores of the vortices need to overlap. We shall instead provide an estimate of the crossing energy of two vortices using Ginzburg-Landau (GL) theory, and the LLL (lowest Landau level) approximation. Due to numerical difficulties our system is also restricted to two vortices, but with two very different choices of backgrounds: we have them moving on a sphere, and also on a plane with quasi-periodic boundary conditions. In the planar case we consider a unit cell commensurate with a triangular lattice ground state. We then calculate the energy difference with respect to the perfect vortex lattice. The results of these calculations are similar, suggesting that the extra energy of two crossing vortices is localized to the crossing region.

II. REVIEW OF LANDAU-GINZBURG THEORY RESULTS

To fix notations, we briefly describe anisotropic Landau-Ginzburg theory for a superconductor, where $\psi$, the wavefunction is our spatially dependent order parameter. For a fuller explanation and justification see [9].

We start with the free energy functional,

$$F[\psi(r)] = \int d^3 r \left( \alpha(T) |\psi|^2 + \beta \frac{|\psi|^4}{2} + \sum_{\mu=1}^{3} \frac{|(-i\hbar \partial_\mu - 2eA_\mu)\psi|^2}{2m_\mu} \right) + \frac{B^2}{2\mu_0}.$$  (1)

Here $\alpha(T)$ is the temperature-dependent variable, $\beta$ is the coupling constant, and $m_\mu$ is the effective mass. In the cases we consider the masses in the $ab$-plane are taken as equal and are denoted by $m_{ab}$, and the mass in the $c$-direction is written as $m_c$. The temperature dependence of $\alpha(T)$ is taken to be linear, $\alpha(T) = (T - T_c)\alpha'$. We also assume the lowest Landau level (LLL) approximation, which is valid near the $H_{c2}$ line. If we allow the variation in $B$ to be determined by the equation $B = \mu_0 H_0 + (\mu_0 e\hbar)/(m_{ab})|\psi|^2$ (valid near to the $H_{c2}$ boundary) then we can write our temperature variable as $\alpha_H = \alpha + e\mu_0 H\hbar/m_{ab}$. This is zero along the $H_{c2}$ line. A neater variable to work with is $\alpha_T$, which is dimensionless. It is related to $\alpha_H$ by,

$$\alpha_H = \left( \frac{\beta e\mu_0 Hk_B T}{4\pi\hbar^2} \right)^{2/3} \alpha_T.$$  (2)
The temperature dependence of the \( \alpha_T \) variable is such that high temperature is represented by \( \alpha_T \to \infty \), low temperature by \( \alpha_T \to -\infty \) and \( \alpha_T = 0 \) corresponds to being on the \( H_{c2} \) line. The above treatment is valid where the LLL approximation can be trusted which probably requires at the very least that \( H > H_{c2}/f \), where \( f \) = 3 according to Tešanović et al.\(^{10}\). The LLL approximation allows us to write the order parameter as a set of orthonormal basis functions, the form of these functions being determined by the boundary conditions imposed to account for the finite size of the system.

III. DETERMINATION OF THE CROSSING ENERGY

In this section we outline the method used for calculating the crossing of two vortices within the GL framework, and using the LLL approximation. Furthermore our entire system only contains the two crossing vortices. For such a small system there is clearly a risk that the crossing energy will be heavily dependent on the boundary conditions used. Hence we have carried out the calculation with two different kinds of boundary conditions, firstly with the vortices confined to the surface of the sphere and then on a plane filled with unit cells with quasi-periodic boundary conditions. The results of our two calculations yield remarkably similar results — indicating that the crossing energy is relatively insensitive to the presence of the other vortices in the system.

A. On a sphere

We first consider the two vortices moving on a surface of a sphere, a geometry that has been shown to reduce finite size effects in numerical studies of superconductivity\(^{11,12}\) and the quantum Hall effect\(^{13}\). The disadvantage of this approach is that the sphere is not commensurate with the triangular (Abrikosov) lattice ground-state. However, as we will show later, the energy of our ground-state is not very different from that of the triangular lattice.

On a sphere we use the formalism of O’Neill and Moore\(^{12}\). The starting line is the free energy functional given in Eq. (1). We then place a monopole at the center of the sphere, which produces a radial magnetic field, satisfying \( B = 4\pi R^2 = N\Phi_0 \), where \( N \) is the number of vortices, which is two in our case. A choice of vector potential compatible with this condition is:

\[
A_r = A_\theta = 0, \quad A_\phi = BR \tan(\theta/2),
\]

in the usual spherical polar coordinates. The order parameter \( \psi(\theta, \phi) \) can then be expanded as eigenstates of the operator \((-i\hbar \nabla - 2eA)^2/2m_{ab}\).

Within the LLL the orthonormal set can be written as:

\[
\psi(\theta, \phi, h) = \sum_{m=0}^{N} v_m(h) \psi_m(\theta, \phi)
\]

where,

\[
\psi_m(\theta, \phi) = k_m \sin^m(\theta/2) \cos^{N-m}(\theta/2) e^{im\phi},
\]

with \( m = 0, 1...N; \quad k_m = [(N + 1)!/4\pi R^2 m!(N - m)!]^{1/2} \) and \( h \) is the distance along the vortex line and runs from \(-\infty\) to \( \infty \). The zeros of \( \psi \) correspond to the positions of the
vortices at height \( h \). The requirement for ‘crossing’ is that the two zeros lie on top of each other at some value of \( h \). We have calculated the energy associated with the vortices being in their equilibrium configuration at both ends and ‘crossing’ at \( h = 0 \). This has been done by writing down the Euler-Lagrange equations associated with two vortices and then solving with boundary conditions at \( h = 0 \) and \( h = \infty \) compatible with the ‘crossing’ requirement. (Technical details of the calculation can be found in Appendix A.)

To follow the above procedure we need to write the free energy in terms of the coefficients \( v_m \). The general expression becomes:

\[
\frac{F[[v_m]]}{kT_c} = \int_{-\infty}^{\infty} dh \left[ \sum_{m=0}^{2} \frac{\hbar^2}{2m_c} | \frac{\partial v_m}{\partial h} |^2 + \alpha_H |v_m|^2 \right] + \frac{\beta B}{\Phi_0} \sum_{m,n,p,r=0}^N W(m+p,m,n) v_m v_p v^*_n v^*_r \delta_{m+p,n+r}, \tag{5}
\]

where

\[
W(m+p,m,n) = \frac{2(N+1)^2}{N(2N+1)} \frac{f(m+p,m,n)}{f(2N,m,n)} \frac{f(2N-m-p,N-m+N-n)}{f(2N,N)}
\]

and

\[
f(x,y,z) = x!/[y!z!(x-y)!(x-z)!]^1/2 + 2x+2. \tag{6}
\]

From Eq. (5) and Eq. (6) we find that the free energy(per unit length in the z-direction for two vortices can be written as:

\[
F = \int_{-\infty}^{\infty} dh \left[ \sum_{i=0}^{2} \frac{\hbar^2}{2m_c} | \frac{\partial v_i}{\partial h} |^2 + \alpha_H |v_i|^2 \right] + \beta B/\Phi_0(0.45|v_0|^4 + 0.3|v_1|^4 + 0.9|v_0|^2v_1|^2 + 0.9|v_0|^2|v_2|^2 + 0.9|v_1|^2|v_2|^2 + 0.3|v_0|^2|v_2|^2 + 0.9|v_1|^2|v_2|^2 + 0.3(v_0v_2v_1^*v_1 + v_0^*v_2^*v_1v_1) \right]. \tag{7}
\]

The first task in evaluating the crossing energy \( \Delta F \), is to find the baseline, the free energy minimum of the ground state of the system. It is easily found by minimisation of Eq. (7) to be \(-\alpha_H^2 \Phi_0/(1.2\beta B)\) per unit length, as compared with the Abrikosov ground-state of \(-\alpha_H^2 \Phi_0/(1.2\beta B)\). Hence we have an effective \( \beta_a = 1.2 \), which is a reasonable approximation to the Abrikosov triangular lattice value of 1.16. This solution corresponds to \( v_0 = \pm c, v_2 = \mp c \), where \( c = \sqrt{\alpha_H \Phi_0/1.2\beta B} \). To find the crossing energy we next write down the Euler-Lagrange equations for the coefficients \( v_i(h) \). Solutions exist for which \( v_1 \equiv 0 \) and in which \( v_0(\infty) = -c \), \( v_0(\infty) = c \), \( v_2(\infty) = c \), \( v_2(\infty) = c \). The crossing point then occurs at \( h = 0 \) when \( v_0 = 0 \), which happens in our notation to be when both vortices are at the south pole of the sphere. (See Appendix A for details.)

The idea was to start from the crossing point and integrate forward numerically along \( h \) to the ground state configurations. Using energy conservation and symmetry arguments at \( h = 0 \) left us with one remaining unknown parameter there. We then varied this parameter until we found a value that allowed us to integrate forward and obtain our equilibrium configuration. Classically this can be thought of as finding the trajectory of a particle that is stationary at the maximum in the potentials at \((c,c)\) to \((c,c)\), which moves as dictated
by the Euler-Lagrange equations. (See Fig. (I) for this potential, and the actual trajectory taken.)

Having found a suitable trajectory, we could numerically integrate along the path to find the difference in energy from the equilibrium state. This left us with a prediction for the crossing energy of:

$$\Delta F = \frac{1.3 | \alpha H |^{3/2} / 2 m_e}{\beta B \sqrt{2 m_e}} = 0.33 | \alpha T |^{3/2} kT. \quad (8)$$

Our procedure could be generalized to handle several vortices. For two vortices, use of symmetry and conservation arguments resulted in only one adjustable parameter, but with three vortices (say) we would have at least a three dimensional space to search. The problem rapidly becomes completely intractable as the number of vortices increases and hence we did not attempt to go beyond two.

**B. On a plane**

Given that we could not easily solve for more than two vortices on a sphere, we instead looked at the same problem under very different boundary conditions. Fortunately we obtain a very similar answer which suggests that the crossing energy is determined mainly by the two vortices which are being crossed. This second set-up was on the plane, using the boundary conditions suggested by Kato and Nagaosa\(^\text{14}\). A rectangular unit cell is chosen with sides commensurate with the formation of a triangular lattice of vortices, in effect forcing the ground-state to be a triangular lattice. The cell also has quasi-periodic boundary conditions such that the same motion of the vortices is carried out in all of the unit cells simultaneously, which at first sight looks rather unrealistic!

Within the LLL, and working in the gauge (0,\(B_x\)) the order parameter can be written as,

$$\psi(x, y, h) = \sum_{n=0}^{N-1} c_n(h) \phi_n(x, y), \quad (9)$$

where the \(\phi_n\) are defined by (see Ref. \(^\text{14}\)):

$$\phi_n(x, y) \equiv \sqrt{\frac{1}{L_y \sqrt{l^2}}} \sum_{m=-\infty}^{\infty} \exp \left[ -i \left( \frac{2 \pi l^2}{L_y} n + mL_x \right) \frac{y}{l^2} - \frac{1}{2l^2} \left( x - \frac{2 \pi l^2}{L_y} n - mL_x \right)^2 \right] \quad (10)$$

and \(l^2 = L_x L_y / (4 \pi)\). \(L_x\) and \(L_y\) are the sides of the cell. The ground state is a triangular lattice if \(\sqrt{3} L_y = L_x\). The periodicity of \(\phi_n\) is such that

$$\phi(x, y + L_y) = \phi(x, y) \quad \text{and} \quad \phi(x + L_x, y) = \phi(x, y) \exp(-i \frac{L_x y}{l^2}). \quad (11)$$

If we substitute the order parameter into Eq. (8), for general \(N\) (number of vortices in the system) we obtain an expression for \(F[\{c_n\}]\). We write this using some auxiliary notation, explained below;
The sum indicated by the symbol $\sum_{I}$ runs over the eight variables $n_{1}, \ldots n_{4}$ and $m_{1}, \ldots m_{4}$, subject to the requirements that

$$n_{1} + n_{2} + N(m_{1} + m_{2}) = n_{3} + n_{4} + N(m_{3} + m_{4}) \quad (13)$$

$$0 \leq n \leq N - 1 \quad \text{and} \quad - M \leq m \leq M \quad (14)$$

The symbols $P$ and $Q$ are defined as

$$P = n_{1} - n_{2} + N(m_{1} - m_{2}) \quad (15)$$

$$Q = n_{3} - n_{4} + N(m_{3} - m_{4}) \quad (16)$$

If we now consider only two vortices and evaluate the sums, we are left with the equation for the free energy in the form:

$$F = \int_{-\infty}^{\infty} dh \sum_{n=0}^{N-1} \left[ \left( \frac{\hbar^2}{2mc} \left| \frac{\partial c_{n}}{\partial h} \right|^2 + \alpha_{H} |c_{n}|^2 \right) + \frac{\beta B}{4\Phi_{0}} \sqrt{\frac{L_{x}N}{L_{y}}} \frac{1}{2M+1} \sum_{I} c_{n_{1},c_{n_{2},c_{n_{3},c_{n_{4}}}}} \exp \left( -\frac{\pi L_{x}}{2N}(P^{2} + Q^{2}) \right) \right]. \quad (12)$$

The ground state energy per unit length is $F = -\alpha_{H}^{2}\Phi_{0}/\beta_{a}\beta B$ with $\beta_{a} = 1.15956$. This is the triangular lattice result, accurate to five decimal places, the error occurring in the evaluation of the sums in $\phi_{n}$. 

We now outline the calculation required to evaluate the crossing energy on the plane, leaving the details for Appendix A2. Symmetry suggests that a suitable place for the zeros of the vortices to be superposed is at the center of the unit cell. To achieve this we imposed the condition,

$$c_{0}(0)\phi_{0} \left( \frac{L_{x}}{2}, \frac{L_{y}}{2} \right) + c_{1}(0)\phi_{1} \left( \frac{L_{x}}{2}, \frac{L_{y}}{2} \right) = 0. \quad (18)$$

The equilibrium configuration can be satisfied with $c_{0}(-\infty) = c$, $c_{1}(-\infty) = -c$, $c_{0}(-\infty) = c$, $c_{1}(-\infty) = c$ where we know $c = \sqrt{\alpha_{H}\Phi_{0}/\beta_{a}\beta B}$ by energy arguments. By imposing ‘energy conservation’, and recognising that we also have ‘angular momentum conservation’, in the dynamical analogue of a particle moving in a potential it is possible to reduce our set of Euler-Lagrange equations again to solving for just one unknown parameter. We can then proceed in a similar manner to the case of the sphere, although in this case we have numerical problems in reaching the equilibrium condition and the energy we evaluate has a residual kinetic energy which is 5% of the maximal kinetic and 2% of the total energy, and hence an error of $\sim$5% on the crossing energy. The final value we calculate is very similar to that for the sphere, Eq. (8),
\[ \Delta F = \frac{1.46 \mid \alpha_H \mid^{3/2} \hbar \Phi_0}{\beta B \sqrt{2m_\epsilon}} = 0.37 \mid \alpha_T \mid^{3/2} kT. \] (19)

It should be remembered when comparing the two calculations of the crossing energy that we already had a 4% difference in the ground-state energies for the different boundary conditions.

IV. CROSSING ANGLE

Previous calculations of the crossing energy within the London regime by Obukhov and Rubinstein and Nelson have considered a mechanism for crossing in which at the crossing point the configuration of the vortices is chosen for simplicity to be that shown in Fig. 2. The crossing angle \( \theta_c \) depends on the anisotropy of the sample, \( \theta_c \simeq \arctan(\sqrt{m_c/m_{ab}}) \), and is 45\(^\circ\) for an isotropic superconductor.

In our calculation it was not necessary to impose the configuration of the vortices at the crossing point, but in the planar case it can be extracted from the solution to the Euler-Lagrange equations. (For the case of the sphere it is difficult to decide how the angles map to those of the flux lines physically crossing.) It should be noted that the lowest energy configuration for the vortices to cross may differ between the London and LLL regimes as in the latter the variation of the \( B \)-field is not included.

On the plane, we know the positions of the zeros at all heights is given by,

\[ c_0(h)\phi_0(X,Y) + c_1(h)\phi_1(X,Y) \equiv 0, \] (20)

where \( c_0(h) \) and \( c_1(h) \) are known from solving the Euler-Lagrange equations. In order to investigate the behaviour of the flux lines near the crossing point we consider deviations \((x, y)\) from the position at \( h = 0 \), \( X = L_x/2, Y = L_y/2 \), by considering the differential of Eq. (20) with respect to \( h \);

\[ \alpha \left( \partial_h c_0 \phi_0 + (\partial_h c_1) \phi_1 + (\partial_h x) \left( c_0 \partial_x \phi_0 + c_1 \partial_x \phi_1 \right) + (\partial_h y) \left( c_0 \partial_y \phi_0 + c_1 \partial_y \phi_1 \right) \right) = 0. \] (21)

We find that at the crossing point \( \alpha = 0.565i \) and that \( \beta = 5.26(x - iy) \) and \( \gamma = -5.26(ix + y) \). Hence solving for the two equations for the real and imaginary parts we find that in the vicinity of the crossing point \( x = y = \sqrt{0.11}h \).

This implies that the vortices save energy on close approach by allowing their core energies to cancel (see Fig. 3). The vortices also approach not along the body diagonal of the unit cell but at 45\(^\circ\) such that there is a twist along the length of the vortices as they approach.

V. COMPARISON WITH LONDON THEORY RESULTS

In order to allow comparison between our results for the crossing energy and the estimates for crossing within the London regime, it is simplest to re-express our crossing energy in terms of the Lindemann melting criteria. This criteria suggests that when the thermally
induced spatial fluctuations in the positions of the flux lines \( \langle u_{th}^2 \rangle \) become of the order of \( c_L^2 a_0^2 \) the lattice will melt. The Lindemann number can be obtained indirectly from neutron scattering and estimates range from 0.1–0.4.

By writing the Lindemann criterion in the form suggested by Moore\cite{16},

\[
\langle u_{th}^2 \rangle \simeq \frac{kT}{4\pi \sqrt{\rho_s c_{66}}} = c_L^2 a_0^2, \quad a_0^2 = \frac{\Phi_0}{B}
\]

and using the formulae for

\[
\rho_s = \frac{|\alpha_H| h^2}{m_c \beta a}, \quad c_{66} = \frac{0.24 |\alpha_H|^2}{\beta^2 \rho_s},
\]

which are determined using elasticity theory\cite{17} we find that \( c_L^2 = 3.13/|\alpha_T|^{3/2} \) for \( |\alpha_T| \) at the melting line. Hence, using the result for \( U_x \approx 0.35 |\alpha_T|^{3/2} kT \), we find that \( U_x/kT \approx 1.1/c_L^2 \) (leading us to estimate \( c_L \sim 0.4 \)). Nelson\cite{3} has estimated in the London regime that

\[
\frac{U_x}{k_B T} \approx 2(\sqrt{2} - 1) \sqrt{\frac{m_{ab}}{m_c} a_0 \ln [k_{ab}]} \left( \frac{\Phi_0}{4\pi \lambda_{ab}} \right)^2 \sim \frac{0.75}{c_L^2},
\]

which is of the same order of magnitude as our LLL estimate. A more recent estimate, also in the London regime, by Carraro and Fisher\cite{7} leads to a result of \( U_x/kT \approx 0.24/c_L^2 \), which is rather lower than our result. There is of course no reason to expect that the results for the crossing energy in the LLL and the London regime to be identical.

VI. DISCUSSION

Having estimated the crossing energy we now consider its relevance within the flux liquid phase of the high temperature superconductors. In order to understand the magnitude of the crossing energy in terms of physical quantities we first estimate its value in terms of \( kT_M \) at the melting line found experimentally by Worthington et al\cite{18} and Safar et al\cite{19}. (Providing we accept that the melting line can be equated with the irreversibility line in magnetisation measurements.) The latest data from Safar et al has been taken in fields up to 16 T. Their results show a first order transition for fields below \( \sim 10 \) T and a continuous transition (which is no longer a melting transition) for larger fields. In order to consider the magnitude of the crossing energy in the vicinity of the transition we need an estimate of \( \alpha_T \).

From previous work\cite{2} we have a crude estimate of \( \alpha_T \sim -8 \) based on the melting line shown in the Worthington et al\cite{18} data. The latter data is taken in the region now associated with the first order transition but the value of \( \alpha_T \) should not change appreciably with increasing field. An alternative estimate\cite{21} from the analysis of theoretical specific heat data suggests \( \alpha_T \sim -7 \), although their argument is somewhat suspect\cite{20}. If we believe in this magnitude of \( \alpha_T \) then we have \( U_x/kT \approx 7.5 \) (for \( |\alpha_T| = 8 \)) in the region of the phase diagram being investigated.

Previously Marchetti, Nelson and Cates\cite{2,3,4} have shown using a hydrodynamic theory that the effects of a twin boundary or similar pinning surface whose normal is perpendicular to the field act over a characteristic length \( \delta_{ab} \), when the magnetic field is in the c-direction.
This characteristic length is effectively the distance between line crossing events in the ab-plane. Cates found that $\delta_{ab} \approx a_0 \exp[U_x/(2kT)]$, where $a_0$ is the spacing between vortex lines. By extending Cates argument we now deduce the length scale $\delta_c$, relevant for velocity gradients varying along the field direction, which we believe to be the important length scale in the transport measurements of Safar et al. The length $\delta_{ab}$ is the typical transverse distance between crossing events, and can be written as

$$\delta_{ab}^2 = \frac{l_p^2 \delta_c}{l_p} \, \text{(25)}$$

where this is just a ‘random walk’ of $\delta_c/l_p$ steps. $l_p$ is a persistence length, as described by Cates, and is related to $l_c$, the distance along a flux line which one has to travel before encountering another flux line by $l_c l_p = a_0^2$. The resulting distance between crossing events in the c-direction is now given by:

$$\delta_c \approx l_c e^{U_x/(kT)} \, \text{(26)}$$

It is clear that when $\delta_c$ becomes equal to the thickness of the sample (or larger) then the vortex motion at the top face of the sample will be strongly correlated with that at the bottom face of the sample. Experimentally the degree of correlation between the motion of vortices at the top and bottom surfaces of the sample has been measured by Safar et al. on YBCO crystals and has been analysed by Huse and Majumdar. The experimental set-up involves applying a magnetic field along the c-axis and then injecting a transport current in the top a-b plane along the a-axis. The voltages in the top and bottom faces are then measured and the maximum field temperature combinations above which $V_{\text{top}} = V_{\text{bot}}$ are recorded. If the vortices are not readily able to cross through each other then the voltages on the two faces due to the Lorentz force induced on the top surface should be the same. However, once $\delta_c = L$, the size of the sample, line crossing will allow the vortices to remain pinned on the bottom face whilst they continue to move due to the Lorentz force on the top face. The mechanism for this procedure can be seen in Fig. Initially, the flux line labeled ‘A-B’ is in front of the line ‘C-D’ and the top of line ‘A’ is subject to the Lorentz force exerted by the transport current. However, line ‘C-D’ is pinned along its entire length and is unmoved by the Lorentz force. If crossing is energetically favourable then when end ‘A’ encounters end ‘C’ the two lines will cut and re-combine as ‘A-D’ and ‘C-B’ resulting in a net movement of vortices, and hence a voltage in the top surface. There is no net flux line movement and hence no voltage in the bottom surface.

Using the results from Safar et al. and our value of the crossing energy we find that $\delta_c = 2.5 l_e \exp[U_x/(kT)]$ is a good fit to the data for the $L = 30 \mu m$ sample. The value for $l_e$ was estimated by assuming that the persistence length $l_p$ would be of the order of the spacing between the Cu-O planes in YBCO. Considering that $l_e$ is only an order of magnitude estimate, this mechanism is a possible explanation of the results. We also find that for a given magnetic field the point at which $V_{\text{top}} = V_{\text{bot}}$ decreases, with increasing thickness of sample. This is in qualitative agreement with experimental data at 1 T. However, the quantitative comparison is poor, which is not surprising as 1 T is outside the expected region of validity of the LLL approximation.

Clearly, this is a first estimate of the crossing energy, and a more complete calculation will consider a larger number of vortices, as well as allowing for fluctuations of the vortices.
This calculation has also indicated that the length scales in the problem are of the order of the Cu-O layer spacing indicating that an investigation of crossing within a layered structure is called for, rather than as here just within the continuum GL theory.

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APPENDIX A: DETAILS OF THE CROSSING ENERGY CALCULATIONS

In this appendix we give a more detailed description of the procedure used to calculate the crossing energy on both the sphere and the plane. The problem we had to solve was essentially a classical mechanics problem of finding a trajectory for a ball to roll from one metastable position on one local maximum to another at the same height, with a set of conditions to control the velocity and position at the central point of the trajectory.

1. On a sphere

The first simplification we used on working on the sphere was to invoke a reduced set of the variables \( \{ v_m \} \). We claimed in §III A that this subset was sufficient to yield the correct solutions — the justification is quite simple although algebraically a little heavy.

We begin with the free energy in terms of the full set of \( \{ v_m \} \), as in Eq. (5), and the order parameter \( \psi \) as defined in Eq. (3). We then express \( \psi \) in terms of spinor variables. In the case of two vortices, \( N=2 \) this is simply:

\[ \psi(\theta, \phi) = A(\cos(\theta/2)e^{-i\phi/2} - i\sin(\theta/2)e^{i\phi/2}) \]

where \( u = \cos(\theta/2)e^{-i\phi/2}, w = \sin(\theta/2)e^{i\phi/2} \) and \( A = re^{i\phi} \) is a complex variable. The positions of the vortices are described by the zeros of \( \psi \) which occur when \( u = u_i \) and \( w = w_i \). Hence we now know the positions of the vortices in terms of the polar angles \( \theta_i \) and \( \phi_i \). By comparison of Eq. (3) and Eq. (A1) we can find the relationship between the \( \{ v_i \} \) and \( A, \{ u_i, w_i \} \) such that we can write Eq. (5) in terms of the spinor variables. A more coordinate-independent variable than the individual positions of the vortices is the separation between them, a measure of which is the scalar product \( n \) of their positions. In terms of the spinor variables \( n \) can be written as:

\[ n = \cos(\theta_1) \cos(\theta_2) + \cos(\phi_1 - \phi_2) \sin(\theta_1) \sin(\theta_2). \]

Inspection of the potential energy written in terms of the spinor variables shows it can easily be re-written in terms of \( n \) and \( r \):

\[ V = \frac{r^2}{4}(3 + n) + \frac{r^4}{160}(39 + 30n + 3n^2). \]  

The kinetic energy is somewhat more complicated. However the terms that cannot be written in terms of \( n \) and \( r \) can be written as sums of squares. Hence they are effectively conserved momenta, whose contribution will be zero when we look for the minimum energy solution. The remaining relevant terms in the kinetic energy are then:

\[ T = \frac{(3 + n)}{4}(\partial_h r)^2 + \frac{r}{4}(\partial_h r) (\partial_h n) + \frac{r^2}{16(1 + n)}(\partial_h n)^2. \]

If we then derive the Euler-Lagrange equations for this new system we find they map back to just the real parts of \( v_0 \) and \( v_2 \). Hence the set of variables we have chosen to work with is sufficient. We should perhaps point out that there is good reason for working with the less intuitive variables \( v_0 \) and \( v_2 \)— the Euler-Lagrange equations are then far simpler.

We are now in a position to calculate the crossing energy. We start by writing down the Euler-Lagrange equations,
\[
\frac{\hbar^2}{2m_c} \partial^2_{r_0} v_0 = v_0 \left( -|\alpha_H| + \frac{\beta B}{\Phi_0} \left( 0.45v_0^2 + 0.3v_0^2 \right) \right)
\]
\[
\frac{\hbar^2}{2m_c} \partial^2_{r_1} v_2 = v_2 \left( -|\alpha_H| + \frac{\beta B}{\Phi_0} \left( 0.45v_2^2 + 0.3v_2^2 \right) \right).
\] (A4)

Then the total energy, \( T + V = \Phi_0|\alpha_H|^2/(1.2\beta B) \), does not vary with \( h \). This is an initial value problem so we need to know the set of \( \{v_0, v_2, \partial_h v_0, \partial_h v_2\} \) at \( h=0 \), where the vortices cross. Examination of the boundary conditions showed that \( v_0 \) was antisymmetric and \( v_2 \) symmetric about \( h=0 \). As a consequence \( v_0 = 0 \) and \( \partial_h v_2 = 0 \) at \( h = 0 \). Then, by conservation of energy, we knew that \( \partial_h v_1 \) is a function of \( v_2 \). Hence we just searched the one parameter space \( v_0 \) until we found a solution of the equations whose end-point was compatible with the ground-state configuration. The value of \( h \) at which the vortices became straight again is \( h \sim 6\hbar/\sqrt{2m_c\alpha_H} \). That is the crossing was completed on a length scale \( l_c \) of the order of the conventional phase correlation length \( \xi_c \), and \( l_c \approx 12\xi_c \), see Fig. 3. In practice this length scale will be of the order of the spacing of the Cu-O planes, indicating the need to go beyond the continuum GL approach of this paper.

2. On a plane

The procedure for calculating the crossing energy on a plane is very similar to that just described for a sphere. Hence we will consider it only briefly. In this case no attempt was made to reduce the set of variables, so we had as our starting point a set of four coupled non-linear Euler-Lagrange equations,

\[
\partial^2_{r_0} r_0 = r_0 \left( 2pr_0^2 + r_1^2 (q + 2s \cos(2\phi_0 - 2\phi_1)) + (\partial_h \phi_0)^2 - 1 \right)
\]
(A5)

\[
\partial^2_{r_1} r_1 = r_1 \left( 2pr_0^2 + r_0^2 (q + 2s \cos(2\phi_0 - 2\phi_1)) + (\partial_h \phi_1)^2 - 1 \right)
\]
(A6)

\[
r_0 \partial^2_{\phi_0} \phi_0 = -2sr_0^2 \sin(2\phi_0 - 2\phi_1) - 2(\partial_h r_0)(\partial_h \phi_0)
\]
(A7)

\[
r_1 \partial^2_{\phi_1} \phi_1 = 2sr_1^2 \sin(2\phi_0 - 2\phi_1) - 2(\partial_h r_1)(\partial_h \phi_1)
\]
(A8)

where \( c_0 = r_0 e^{i\phi_0} \) etc., and \( p, q, s \) are as defined for Eq. (17). Written in this form, we can see by inspection, that as well as conservation of energy we also have conservation of ‘angular momentum’ as \( \partial_h (r_0^2 \partial_h \phi_0 + r_1^2 \partial_h \phi_1) \equiv 0 \). Moreover, because the boundary conditions at \( \pm\infty \) require there to be no kinetic energy, the angular momentum must be equal to zero. So far we have a general set of equations describing the motion of the two vortices within the unit cell, but we need a further constraint to make the vortices cross. Having decided that a suitable place for the vortices to meet would be the center of the unit cell, we find that we need to satisfy the condition, \( c_0(0)\psi_0(L_x/2, L_y/2) + c_1(0)\psi_1(L_x/2, L_y/2) = 0 \). Evaluation of the \( \psi \)’s shows that we require \( r_1 = 0.13165r_0 \) and \( \phi_0 = \phi_1 = 0 \) at \( h = 0 \). In fact the other obvious places for the vortices to cross, \( (\pm L_x/2, 0) \) and \( (0, \pm L_y/2) \) yield equivalent constraints. Through symmetry arguments we find that \( \partial_h c_0 = \partial_h c_1 = 0 \) at \( h = 0 \).

Using all of these facts leaves us again with only one free parameter in our initial conditions. Finding a solution which reached the necessary end-point proved more tricky this time, and we were unable to produce a solution which bettered having 5% of the maximal
kinetic energy (2% of the total energy) in ‘equilibrium’, and correspondingly the equilibrium separation of the vortices is only accurate to 2%. Hence an estimate of the error on the crossing energy of 5% would seem reasonable.
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FIGURES

FIG. 1. Contour plot of the ‘potential’ as described in Eqn. (A2) for the spherical boundary conditions problem. The solution to the Euler-Lagrange equations which corresponds to the vortices crossing is that linking the points ‘A’ and ‘B’, and c is as defined in the text.

FIG. 2. Ansatz configuration for vortices crossing in the London regime used in Ref. 3, where $\gamma = (m_c/m_{ab})^{1/2}$.

FIG. 3. Configuration for vortices crossing within the LLL regime, $l_c$ is the length over which the crossing takes place.

FIG. 4. Possible vortex motion in the Safar et al. experiment. Initially (a) line ‘A-B’ is in front of C-D and subject to a Lorentz force at end ‘A’, and line ‘C-D’ is pinned. Crossing enables end ‘A’ to carry on moving, (b), resulting in a net voltage difference between top and bottom of the sample.

FIG. 5. The functions $v_0(h)$ (antisymmetric) and $v_2(h)$ (symmetric) as calculated by solving the Euler-Lagrange equations. $v_0$ and $v_2$ are in units of ‘$c$’ and $h$ is in units of $h/\sqrt{2m_c\alpha_H}$, the $c$-axis correlation length.