Vortex Clustering: The Origin of the Second Peak in the Magnetisation Loops of Type Two Superconductors

[Short title: Vortex Clustering]

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Abstract

We study vortex clustering in type II Superconductors. We demonstrate that the “second peak” observed in magnetisation loops may be a dynamical effect associated with a density driven instability of the vortex system. At the microscopic level the instability shows up as the clustering of individual vortices at (rare) preferential regions of the pinning potential. In the limit of quasi-static ramping the instability is related to a phase transition in the equilibrium vortex system.
When the external magnetic field penetrates a type II superconductor, magnetic vortex lines appear inside the bulk of the sample. These vortex lines are repulsive and quantised each carrying a multiple $q$ of the magnetic flux quantum $\phi_0$. The energy per unit length of a vortex line is proportional to $q^2$ and accordingly one typically expects to have configurations with well separated single quantised vortex lines [1]. We show below, however, that dynamical vortex clustering may become very important: vortices form inhomogeneous spatial structures which become relevant for the evolution of the system. This clustering may for instance cause the “second peak” observed in magnetisation loops and strongly affects the structure of the vortex system, magnetic relaxation, and the distribution of the local magnetic induction as measured in $\mu$ spin-relaxation experiments. The understanding of structural properties of vortices, underlying the presence of the “second peak”, is one of the central issues of current research in superconductivity, and is related to fundamental aspects of vortex matter ranging from dynamical behaviour to phase transitions. (see eg. [2, 3]).

In a superconducting sample in the presence of an external magnetic field, vortex lines penetrating from the surface into the bulk may be trapped on pinning centres [1, 4] leading to a spatially inhomogeneous vortex distribution and to a net magnetisation of the sample. As the external field is increased the vortex lines are squeezed together and therefore interact more strongly. Such a strong interaction will counteract the pinning forces and thus one expects, as in fact is usually observed, the magnetisation to decrease with increasing external field once vortices have fully penetrated the sample.

However, upon further increase of the external field the magnetisation is often observed to increase again [5]. This behaviour leads to the so-called fishtail structure in the magnetisation data for YBCO or the arrowhead structure in equivalent data for BISCCO samples [6, 7]. A similar peak structure has also been observed in low temperature superconductors [8]. The second peak is one of the most important unsolved problems in vortex physics. It has been seen as a signature of a phase transition in the vortex system and its...
explanation has often been attempted by focusing on collective aspects of pinning or relaxation effects related to the sweeping of the field. Here we present evidence that dynamical effects are of crucial importance for the second peak, nevertheless the mechanism inducing the peak is, in the quasi-static limit, related to a density driven phase transition in the vortex system.

In Fig. 1 we show for reference an example of half magnetisation loops in YBCO for a set of different temperatures. One sees how the maximum of the second peak moves to higher magnetic fields as the temperature is decreased. This suggests that the mechanism behind the increase in the magnetisation occurring after the first peak must also be active at zero-temperature. We demonstrate below that the origin of the second peak may be related to the possible grouping of vortices at favourable regions in the random pinning potential, leading to large local fluctuations in the vortex density. This “clustering” can occur in superconductors for which the ratio, $\kappa = \lambda/\xi$, between the magnetic penetration depth $\lambda$ and the coherence length $\xi$ is not too small (from our Molecular Dynamics simulations we expect roughly $\kappa > 10$). The clustering is a dynamical effect induced by the ramping of the external field, as is done in magnetisation experiments. As vortices entering (or leaving) the sample approach another vortex trapped at a position in the pinning potential three possibilities can occur. Firstly, the trapped vortex may be pushed ahead if the vortex-vortex repulsion is strong enough. Secondly, the approaching vortex may move around the trapped vortex. Or, if the trapped vortex is pinned by a force stronger than the maximum vortex-vortex repulsion, the approaching vortex may move into the favourable position in the pinning landscape in the immediate vicinity of the already trapped vortex. In this way the clustering may significantly enhance the effect of the rare strong pinning regions in an otherwise weak pinning background.

For simplicity we here consider straight parallel flux lines at separation $r$ for which
the interaction energy per unit length is

\[ U_{vv}(r) = \frac{\phi_0^2}{2\pi\lambda'^2} [K_0(r/\lambda') - K_0(r/\xi')] , \tag{1} \]

where \( \lambda' = \lambda/\sqrt{1-b} \) and \( \xi' = \xi/\sqrt{2(1-b)} \) are the effective field dependent London penetration depth and coherence length, respectively. \( b = B/B_{c2} \) is the reduced magnetic induction relative to the upper critical induction \( B_{c2} \), and \( K_0 \) is a modified Bessel function.

Vortices can be brought close together because of the attractive second term representing the interaction between the vortex cores. The maximum repulsive force calculated from Eq. (1) is an upper limit for the repulsive force between two vortex lines. The relative tilting and wiggling of vortex lines will lead to a significant decrease in the repulsion (see Eq. [9]). Therefore, we expect the clustering effect to be at least as significant in three dimensions as we demonstrate here the effect to be in two dimensions. In fact clustering of vortices has been directly observed in electron microscopic imaging by Tonomura [10].

In Fig. 2 we show the magnetisation obtained from zero temperature Molecular Dynamics (MD) simulations. The vortex interaction is given by Eq. (1) and it is cut off at half the system size. We use over damped dynamics in a square two dimensional system, with periodic boundary conditions, of sides \( 100\xi \). The external field is ramped by introducing vortices into a central strip with no pins [11]; the magnetisation plot is calculated by considering the average density of vortices and its gradient in the pinned region. Fig. 2 clearly shows that an upturn in the magnetisation occurs as the external field is increased above the penetration field. The increase in the magnetisation coincides with the appearance of vortices clustered within areas of order \( \xi^2 \). It is important to mention that if the second term in Eq. [1] is left out [12], (see dashed line in Fig. 2.), clustering of vortices cannot occur and no significant upturn in the magnetisation is observed in the simulations. At the highest field densities the potential in Eq. (1) loses its validity. This regime is also difficult to handle numerically. Hence we do not study the full half loop in the MD simulations but use below a simplified lattice model to study the increasing as well as the decreasing leg of the magnetisation.
Let us now describe how the clustering of vortices prevents the magnetisation, $M$, from decaying with increasing field. We recall that approximately $M \propto j_c$, where $j_c$ is the critical current density produced by the volume pinning force $F_p = Bj_c$. When a pinning centre becomes occupied by one or more trapped vortices the attractive short range pinning centre is effectively transformed into a longer range repulsive centre. Other vortices approaching this pin will feel a repulsive vortex-vortex force proportional to the number of trapped vortices at a distance $\lambda$ rather than the attractive force of range $\xi$ from the initially “empty” pinning centre. The local pinning strength will fluctuate through the sample with typically a high density of weak pinning centres and only a few sparse local strong regions. Vortices clustered at the few strong pinning regions can then form spatially extended energy barriers which cage other diffusing vortices. We emphasise that this picture is somewhat schematic and that in reality dynamical and collective effects are important. Vortices are moving in an ever changing energy landscape produced by the combined effect of the static spatial pinning potential and the instantaneous metastable configuration of the interacting vortices. The importance of dynamical effects follows from the fact that the detailed form, especially the width, of the magnetisation loops dependence on the ramping rate of the external field. This is the case in experiments (see ref.s in [5, 2, 13]) as well as in our simulations [14].

To study in detail the change of the effective energetic panorama due to clustering and its consequences for the “second peak” we consider now a schematic model. This approach is close in spirit to similar lattice systems introduced to describe fluxons in superconductors, see e.g. [15]. In particular we study an extension of a *coarse grained* cellular-automaton-like model recently introduced by Bassler and Paczuski (BP) [16]. We consider a simplified version of a many body system with pair interactions given in eq. (1) representing a lattice model of repulsive particles in a pinning potential and in contact with a particle reservoir at a given density. Since our model explicitly allows multiple occupancy of lattice sites up to a value $N_{c2}$, we call it a Restricted Occupancy Model (ROM). We apply Monte Carlo
dynamics and use a Hamiltonian of the form:

\[
\mathcal{H} = \frac{1}{2} \sum_{ij} n_i A_{ij} n_j - \frac{1}{2} \sum_i A_{ii} n_i - \sum_i A^p_i n_i
\]  

(2)

Here \( n_i \in \{0, ..., N_{c2}\} \) is an integer occupancy variable equal to the number of particles on site \( i \). The parameter \( N_{c2} \) plays the role of \( B_{c2} \); it bounds the particle density per site below a critical value (here \( N_{c2} = 27 \)). The first term in eq.(2) represents the repulsive vortex interaction energy. The second term in eq.(2) just normalises the particle self-interaction energy. Here we for simplicity choose the coarse graining length to be of order the zero temperature London penetration length \( \lambda(0) \). This allows us to relate the restriction number \( N_{c2} \) to the upper critical field \( B_{c2} \) in the following way:

\[
N_{c2} = \frac{B_{c2} \lambda(0)^2}{\phi_0}
\]

where \( \phi_0 = \hbar c/2e \) is the magnetic flux quantum. With this choice of coarse graining length it is natural as a first approximation to assume: \( A_{ii} = A_{v} = 1 \), \( A_{ij} = A_{n} \) if \( i \) and \( j \) are nearest neighbours and \( A_{ij} = 0 \) for all other couples of sites. We will below briefly discuss the validity of this approximation of the \( A_{ij} \) matrix. The third term in eq.(2) represents a random pinning potential acting on a fraction \( \rho = 0.5 \) of the lattice sites with \( A^p = 0.5 \) and \( A^p = 0 \) elsewhere. (The same set of interactions is used in the BP model \[16\]). Two opposite sides of our square system \((L = 32^2)\) \[17\] are in contact with a reservoir at a given density \( N_{ext} \). Particles are introduced and escape the system through the reservoir only.

Fig. 3 shows the results of our Monte Carlo simulations of this model. We ramp \( N_{ext} \) and record the magnetisation, \( M = N_{in} - N_{ext} \) (with \( N_{in} = \langle \sum_i n_i \rangle / L^2 \)), as a function of \( N_{ext} \). The ramping of the external reservoir density, \( N_{ext} \), is simply done by increasing it from zero up to some given value (and then decreasing back) by a sequence of small increments, \( \Delta N_0 \). After each increment the system is let to relax for a time \( \tau \) (in unit of Monte Carlo sweeps). This corresponds to a sweep rate of the applied field of \( \gamma = \Delta N_0 / \tau \).

We recorded magnetisation loops for several values of the ratio \( \kappa^* \equiv (\ln A_v/A_n)^{-1} \) which controls the interaction potential. The parameter \( \kappa^* \) is qualitatively similar to \( \kappa = \lambda/\xi \). When \( \kappa^* \) is large enough a definite second peak appears in \( M \). These magnetisation
loops looks qualitatively similar to the experimental loops, though the peak position and amplitude of peaks in Fig. 3 are much more asymmetric than the peaks of the experimental data in Fig. 1. Nevertheless, typically magnetisation loops in other experimental samples and compounds are clearly asymmetric, see e.g. [5, 13]. In fact even Fig. 1 exhibits, on careful inspection, slight asymmetries.

The detailed loop shape depends not only on the choice of $\kappa^*$, as shown in Fig. 3, but also on the value of $N_{c2}$ and the ramping rate, $\gamma$. We find that in the $\gamma \to 0$ limit, the second peak location, is associated with a sharp jump in $M_{eq} \equiv \lim_{\gamma \to 0} M(\gamma)$, corresponding to a true transition [14]. The precise nature of this transition is currently under study. The transition occurs above the melting transition and leads to a significant increase in the effective energy barriers experienced by the diffusing vortices.

Increasing $N_{c2}$ (corresponding to higher values of $B_{c2}$) increases the separation between the first and the second peak. The specific features of the loops do also depend on the ratio between the characteristic relaxation time of the vortex system and the ramping rate, for details see [14, 18]. Quantitative differences between the simulations and experiments are to be expected. One reason is that the interaction strength between vortex lines depends on the magnetic induction and the temperature. As for instance in the London approximation of Eq.(1) through the field and temperature dependence of $\lambda'$ and $\xi'$. This corresponds to a field and temperature dependence of the individual elements of the coupling matrix $A_{ij}$ in Eq.(4). Moreover, the effective vortex screening length, $\lambda'$ (see Eq. 1), increases with increasing magnetic field. This effect implies that non-zero $A_{ij}$ elements between sites of separation larger than nearest neighbour may become relevant as the field is increased. Interestingly, however, the present simple approximation captures the qualitative features of the magnetic properties.

We emphasise that according to the above picture the second peak is a dynamical effect associated with the vortices being forced in and out of the sample. It is linked
to a density driven instability of the vortex system. At the more microscopic level of description used in the Molecular Dynamics simulations the instability shows up as the clustering of individual vortices at (rare) preferential regions of the pinning potential. In the coarse grained description of the considered lattice model the instability is related to an underlying density driven phase transition of the equilibrium system. The instability induces a dramatic change of the effective collective energy landscape encountered by the diffusing vortices. This, in turn, enormously enhances equilibrium times \[14, 18\] and induces the presence of significant more spatial disorder, in strict correspondence with glass formers \[19\].

This clustering or density instability can produce the second peak in the magnetisation loops. It can be thought of as a type of strong plastic deformation, an effect which should be observable in neutron scattering or $\mu$-spin resonance experiments probing the distribution of local magnetic induction.

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Figures Captions

**Fig. 1** An example of magnetisation data and the fishtail effect in a single crystal of YBa2Cu4O8 at temperatures 20K, 50K and 65K. The magnetic moment is measured continuously using a vibrating sample magnetometer while the applied field is ramped from zero to eight Tesla and back to zero at a rate 10mT/sec. The 124 system is neither susceptible to twinning or oxygen inhomogeneity (unlike YBa2Cu3O7-d) indicating that the fishtail effect is intrinsic to the pinning of point-like disorder in the crystal lattice.

**Fig. 2** Magnetisation ($dB/dx$) vs field ($B$) for simulation with $\kappa$ of 67. The external field is ramped by adding one vortex between relaxation intervals of 40 where each time step is a maximum of 0.01. Fields calculated for $\xi$ of 15 Å. Solid line represents the system interacting through Eq. 1 (soft core). The dashed line represents the system interacting through Eq. 1 with last term omitted (hard core). The short-long dashed curve represents the proportion of stacked vortices in the soft core case.

Pinning centres are represented by Gaussian wells of width $\xi$ and of amplitude $0.3\xi^2$ times the condensation energy. In this simulation they can exert a maximum pinning force (at zero external field) of $4 \cdot 10^{10} A/cm^2$ for the $\kappa = 10$ and $8 \cdot 10^8 A/cm^2$ for $\kappa = 100$.

**Fig. 3** The magnetisation, $M$, as a function of the applied field density, $N_{ext}$, in the 2D R.O.M. model for $\kappa^* = 0.43, 0.76, 0.79$. The ramp rate for $N_{ext}$ is $\Delta N_0/\tau = 10^{-3}$. 
Magnetic moment (Am$^2$)

$\mu_0 H$ (Tesla)

Temperature (K):
- 20
- 50
- 65
