



Simulations of clustering of vortices in superconductors: a possible origin of the second peak

D.K. Jackson, N.A. Lindop¹, Henrik Jeldtoft Jensen^{*}

Department of Mathematics, Imperial College, London SW7 2BZ, UK

Abstract

We describe by use of molecular dynamics simulations how the attraction, at short range, between the vortex cores aids the clustering of vortices. Our simulations suggest that the short range core attraction and ensuing vortex clustering is the mechanism responsible for the second peak in the magnetisation loops of superconductors. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Magnetization; Vortex clustering; Molecular dynamics simulation

1. Introduction

There is still no consensus as to the explanation of the second peak observed in the magnetisation loop of high temperature superconductors and of some low temperature superconductors [1]. Experimentally, one observes that the peak structure in YBCO becomes more pronounced with decreasing temperature. From this, we expect that a zero temperature mechanism must be at the heart of the origin of the peak [2]. This is our motivation for performing zero temperature molecular dynamics simulations.

We have elsewhere briefly presented some of our simulations in a discussion which focusses on the relationship to experiments and more general consequences of the vortex clustering [2]. In the present

paper, we present a more detailed description of our molecular dynamics simulation.

We consider an infinite slab of superconductor in a magnetic field applied parallel to the slab's face. We choose the London limit in so far as we consider discrete flux lines. The energy of interaction between two segments of flux lines is [4],

$$U_{vv}(r) = \frac{\phi_0^2}{2\pi(\lambda')^2\mu_0} \times \left[\frac{e^{-r/\lambda'}}{r} d\vec{l}_1 \cdot d\vec{l}_2 - \frac{e^{-r/\xi'}}{r} |d\vec{l}_1||d\vec{l}_2| \right] \quad (1)$$

where $r = |\vec{r}_1 - \vec{r}_2|$ is the distance between the two segments $d\vec{l}_1$ and $d\vec{l}_2$ located at positions \vec{r}_1 and \vec{r}_2 , respectively. $\lambda' = \lambda/\sqrt{1-b}$ 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} .

^{*} Corresponding author.

E-mail addresses: david@ic.ac.uk (D.K. Jackson), h.jensen@ic.ac.uk (H.J. Jensen).

¹ Present address: Department of Chemistry, University of Edinburgh, Edinburgh EH9 3JJ, UK

For numerical convenience we treat the vortices as straight parallel flux lines so that we can move from a three-dimensional (3-D) to a two-dimensional (2-D) model. The interaction energy per unit length becomes,

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

where K_0 is a modified Bessel function. Brandt [4] has shown this potential to reproduce to a good approximation the elastic properties of a vortex lattice found by Ginzburg–Landau theory and the microscopic theory of Gorkov. Its long-range repulsive component reduces to the London potential at low field. The attractive term is due to a change in the condensation energy with the overlapping of vortex cores.

It is immediately clear by comparing Eqs. (1) and (2) that if clustering is found for the 2-D case clustering will also occur in three dimensions. This is because the repulsive term of the interaction energy in Eq. (1) depends on the relative orientation of the two vortex segments and has a maximum when the segments are parallel — as they are in the 2-D situation. The attractive core-part of the interaction energy does not depend on the orientation and will accordingly be relatively more important for non-parallel vortex lines. Clearly, much future research is needed in order to understand quantitatively the relationship between our model and experiment. For instance, the potential used, Eq. (2), is still only an approximation, though it does incorporate the core attraction.

We note that for a system of evenly distributed vortices the separation of the vortices is well characterised by the average vortex separation $a_0 = \sqrt{\phi_0/B} = 450 \text{ \AA} / \sqrt{B}$ (with the magnetic induction measured in tesla and ϕ_0 denotes the flux quantum). Clearly, at experimentally accessible fields, $a_0 \gg \xi$ since the coherence length, ξ , is typically of, say, 10 to 20 Å. For this reason, simulations have hitherto neglected the second term in Eq. (2) [3]. A homogeneous vortex distribution is expected to arise in field-cooled experiments.

The situation is very different when magnetisation loops are measured. Here, the external field is ramped up and down forcing the vortices to move in and out of the sample. In doing so, the vortices have to push

each other through the pinning potential present inside the superconducting sample. The shortest separation encountered between a vortex being pushed in (or out) of the sample and a vortex trapped at a position in the pinning potential will be determined by the mechanical force balance between the force derived from Eq. (2) and the pinning force. It is easy to estimate that physically realistic pinning forces can be larger than the maximum of the vortex–vortex force. This is a purely two-body argument. In reality, many-body effects will come into play and tend to lower the repulsive vortex force by smoothing.

2. Simulations

We use a deterministic (zero temperature) over damped equation of motion. The pinning potential is constructed by randomly positioning Gaussian-shaped pinning wells of a concentration n_p , amplitude A_p , and range ξ . The amplitude is a fraction of the superconducting condensation energy contained per length in a cylinder of radius ξ .

Here, we show results from molecular dynamics simulations for a system with periodic boundary conditions of size 70ξ by 70ξ . A slice of the system is left unpinning, and vortices are introduced here to represent ramping of the applied field, an effective computational method first used by Ref. [3]. The rest of the system, representing the superconductor contains the randomly distributed Gaussian pins. The interaction force between the vortices is cut off at half the smaller dimension of the system. This cutoff is made smoothly to avoid false vortex configuration that may result from a sharp cutoff [5].

As a measure of the magnetisation M we use the gradient of the vortex density in the pinned region, i.e., dB/dx . In the case of a linear vortex profile inside the sample (a good approximation at high induction), one has $dB/dx \propto M$. We plot this gradient as function of the average vortex–vortex density in the pinned region, i.e., B . In this way, we do not have to define the external magnetic field.

3. Simulation results

The inclusion of the attractive term in the vortex interaction makes a considerable difference to the

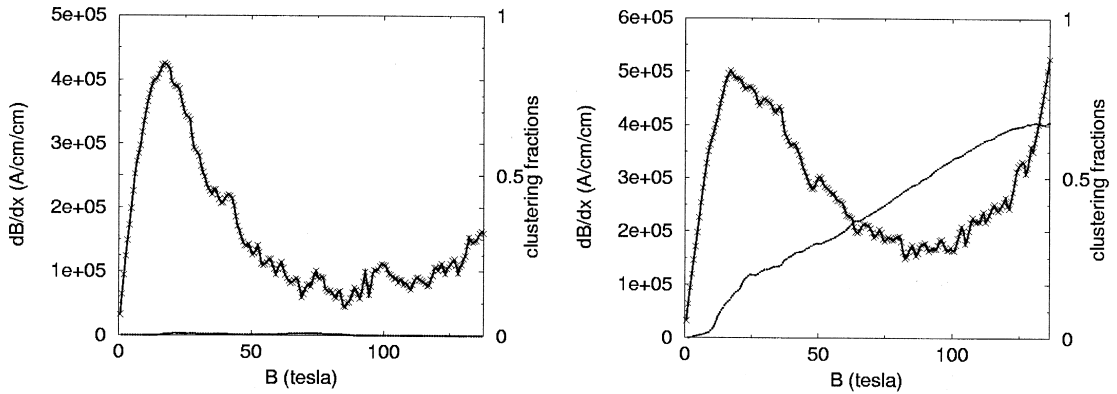


Fig. 1. Magnetisation averaged over four different pinning configurations. On the left is a system with a vortex–vortex interaction containing only a repulsive term, on the right, the attractive term is also used (see Eq. (2)). Solid line is the magnetisation, dashed line is the fraction of vortices within ξ of another vortex. Pin amplitude 0.3 of condensation energy. $\kappa = 70.7$. Fields calculated for $\xi = 15 \text{ \AA}$.

magnetisation loop, most noticeably at high fields (see Fig. 1) The attractive term allows vortices to cluster; a significant fraction of vortices sit within ξ of another vortex, as Fig. 1 shows. The magnetisation results vary between different pinning configurations. However, our computational method limits us to small systems so this ensemble of results is averaged to obtain a result more typical of the macroscopic scale.

4. Conclusion

We conclude that the second peak may require us to consider situations where vortices come close together. In such a situation, the magnetisation *cannot* be described within a framework, say, such as elastic medium theory, which considers long wavelength deformations (possibly with small density of topological defects) and which assume a separation between vortices of order the average separation $a_0 = \sqrt{\phi_0/B}$. The core attraction, which is most often assumed to be of negligible importance, allows for a clustering of vortices at favourable positions in the pinning potential. We expect this clustering to have significant dynamical consequences in magnetic relaxation experiments.

Finally, we remark that the clustering described here is equivalent to large fluctuations in the local superconducting current density.

Acknowledgements

We are grateful to Mario Nicodemi and Garry Perkins for collaboration and discussions. DKJ and NL are grateful to EPSRC and the Imperial College Centre for High Temperature Superconductivity for studentships. HJJ is supported by EPSRC.

References

- [1] L.F. Cohen, H.J. Jensen, Rep. Prog. Phys. 60 (1997) 1581.
- [2] D.K. Jackson, M. Nicodemi, G.K. Perkins, N.A. Lindop, H.J. Jensen, cond-mat/9908454.
- [3] C. Reichardt, C.J. Olson, J. Groth, S. Field, F. Nori, Phys. Rev. B 52 (1995) 10441.
- [4] E.H. Brandt, Phys. Rev. B 34 (1986) 6514.
- [5] H. Fangohr, A. Price, S. Cox, P.A.J. de Groot, G.J. Daniell Efficient methods for handling long-range forces in particle–particle simulations, in press.