

Numerical Simulations of Magnetic Vortices in High-Temperature Superconductors

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Abstract

Numerical simulations of magnetic vortices in high-temperature superconductors are discussed. The behaviour of the depinning force as a function of the number of vortices, defects, and the angle of the defects is presented. The structure of pinned and moving vortex systems is also explored. Our simulations show the complex interplay of disorder and interactions in dynamical systems.

Introduction

It is well known that superconductors are materials that below a critical temperature T_c conduct electricity with no resistance. These materials have many potential commercial uses including the most obvious one of zero-loss power transmission and wires with very large current capacity. A possible use of the materials that has already been realized is using the large current carrying capacity to generate large magnetic fields. (See Asimov¹ or Kittel² for a more advanced introduction to superconductivity).

The largest challenge to the usefulness of superconductors is that until quite recently, the materials needed to be cooled to the very low temperatures of liquid helium in order to become superconducting. This meant that superconductors were not a realistic option for non-research uses because the cost and difficulty of keeping them sufficiently cold was prohibitive. Superconducting materials had very interesting physical properties for a scientist to study, but were in no position to challenge the grip of conventional materials on the electronics industry.

However, this appeared about to change in 1986 when the first high-temperature superconductors (materials such as $\text{YBaCu}_2\text{O}_{6-x}$) were discovered³. These materials become superconducting at temperatures above the liquidation temperature of nitrogen. These materials came as a shock to a large part of the academic community, as many thought it was impossible for something to superconduct at such high temperatures. What was even more odd was that these substances were ceramic materials, not something that one would normally consider good conductors, let alone materials that would conduct electricity with zero resistance.

Superconductors do not energetically like to have magnetic field penetrate into the material. Instead, when in the presence of an external magnetic field, they create a current to screen out the magnetic field. This is known as the Meissner effect². Superconductors are grouped into two main classes, type I and type II. Type I superconductors will completely screen out external magnetic fields, until the magnetic field becomes too large for the material to remain superconducting. Type II superconductors are unable

to expel magnetic fields completely, but will instead allow the fields to penetrate at non-superconducting points known as vortex cores above a critical field H_{c1} . A region of swirling electrons around the vortex core screens the rest of the material from the magnetic field lines. This current is called a supercurrent, and the area surrounding the magnetic field line, vortex core and supercurrent is known as a magnetic vortex, in analogy to vortex motion in fluid flow. All known high-temperature superconductors are type II superconductors⁴.

Magnetic vortices are of interest because they destroy resistance free flow⁵. A driving electric field force applied in a direction perpendicular to the magnetic field lines produces a Lorentz force perpendicular to both the magnetic and electric fields. The moving vortex produces a moving magnetic field, which, by applying the right hand rule, will induce an electric field in opposition to the driving field, giving resistance. Thus, when one attempts to use a high-temperature superconductor in the presence of a magnetic field, a resistance in the material is induced.

In practice, in an effort to stop magnetic vortices from moving when a driving current is applied, the material is often bombarded with neutrons or other heavy particles to create columns of non-superconducting defects in the material. The vortices are drawn to the defects to minimize their energy but will become depinned if the driving force is greater than a critical driving force, J_c . However, it has been experimentally determined that the way in which the defects are introduced greatly affects J_c ^{6,7}.

THE MODEL FOR OUR SIMULATIONS

Our simulations focus on vortices in high-temperature superconductors. Magnetic vortices are modeled in our simulations by floppy strings. The strings are modeled as a series of balls each confined to the ab -plane and attached to each other into a chain by springs aligned along the c -axis. The vortices are driven by an externally applied force F_L in a damped environment (with damping constant b) subject to various intrinsic forces. These forces include a repulsive vortex-vortex interaction, a vortex-defect interaction, elastic vortex bending force, and a random thermal force – the magnitude of which is set by the system temperature known as a Langevin

thermal force F_T^s . Each of these forces is derivable by taking derivatives of a corresponding potential. The energy scale is set by $V_v = (\Phi_0 / 4\pi\lambda)^2$, where $\Phi_0 = hc / 2e$ is the magnetic flux quantum and λ is the magnetic penetration depth, our length scale for the simulations. Combining all of the forces on the balls yields the following equation of motion for a ball i :

$$\mathbf{F}_i = \mathbf{F}_L + \mathbf{F}_T - \frac{\partial V_{defect}}{\partial \mathbf{r}_i} - \frac{\partial V_{vortex}}{\partial \mathbf{r}_i} - b\mathbf{v} - k \sum_{l=above,below} [\mathbf{r}_i - \mathbf{r}_l] \quad (1)$$

where $V_{defect,vortex}$ are the vortex-defect and vortex-vortex potentials, respectively.

The two types of defect configurations that we simulate are the columnar type and the splay type. Columnar defects are orientated along the c -axis and placed randomly in the sample. Splay type defects are orientated at a particular angle θ with respect to the c -axis, and have a randomly generated azimuthal angle. Thus the splayed defects all lie on the cone specified by θ . In both cases the defect force is applied to the vortices on a ball by ball basis with a defect potential given by:

$$V_{defect}(\mathbf{r}) = \begin{cases} -V_D \left[1 - \left(\frac{r}{r_w} \right)^2 \right]^2 & \text{if } r \leq r_w \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

where V_D is the depth of the potential well, and r_w is the radius of the potential well. The shape of the potential was chosen because it goes smoothly to zero at the edge of the defect. Early on, we found that allowing the well depth to be randomly distributed over a range of values did not affect the dynamics of the system. Thus, the defect depth was set to a constant in our simulations, namely, to the interaction energy $V_D = V_v$. The width of the defects was chosen such that the vortices had a large probability of interaction with them when moving through the sample. This is a necessary condition computationally, as it greatly speeds up the equilibration time. The value of the width used was $r_w = \lambda$.

The vortex-vortex interaction V_{vortex} is given by a Hankel function, which we model as an exponentially decaying function

$$V_{vortex}(\mathbf{r}_i) = \sum_{j \neq i} V_v e^{-|\mathbf{r}_i - \mathbf{r}_j|/\lambda} \quad (3)$$

This is an accurate approximation as long as the vortex density is low, which was the case for our simulations.

Simulation Methods

The equation of motion, $F_i = ma_i$, with m the mass of the balls (taken to be an electron mass⁹) and F_i given by Equation (1), was numerically integrated using the 4th-order Runge-Kutta method. The simulation box typically consisted of 40-80 planes of dimension 16λ by 16λ containing up to 50 vortices and 150 defects, with periodic boundary conditions in the ab -plane and free boundary conditions imposed in the c direction. We typically refer to the number of vortices and defects in terms of a matching field $B = B/B_\phi$, where $B = N_{vortices} \Phi_0 / \lambda^2$ and $B_\phi = N_{defects} \Phi_0 / \lambda^2$. The Coulomb interaction was cut off at separations beyond 4λ to speed up the calculation. We run the code for typically tens of thousands of time steps in order to equilibrate our system before performing measurements. The quantities we measure include the average velocity of all the balls making up the vortices as well as the structure factor defined as

$$S(\mathbf{Q}) \propto \sum_{\mathbf{r}_i} e^{i\mathbf{Q} \cdot \mathbf{r}_i} \quad (4)$$

The structure factor S is typically peaked at reciprocal lattice vectors if the vortices are ordered in our sample or consists of a single peak at $\mathbf{Q} = 0$. We measure the velocity in terms of the terminal velocity $v_{TERMINAL} = F_L/b$ and

F_L , as well as all of the other forces in our simulation, are measured in units of $V_v / \lambda = \Phi_0 / 8\pi^2 \lambda^3$. We typically average our results over hundreds of disorder configurations in order to mimic experimental conditions.

Results

Our simulations show a clear depinning transition at a critical driving force $F_c \sim 0.075 - 0.1$ where $v = v_{TERMINAL}$ (see Figure 1) as the driving force is increased for a given number of defects and vortices. This transition appears to depend on the ratio of vortices to defects and on the angle of splay of the defects. Vortices that are not pinned to defects will flow in the presence of a driving force. The vortices are confined to flow in small channels, known as channel flow, near the critical force. Clearly in order to prevent vortex

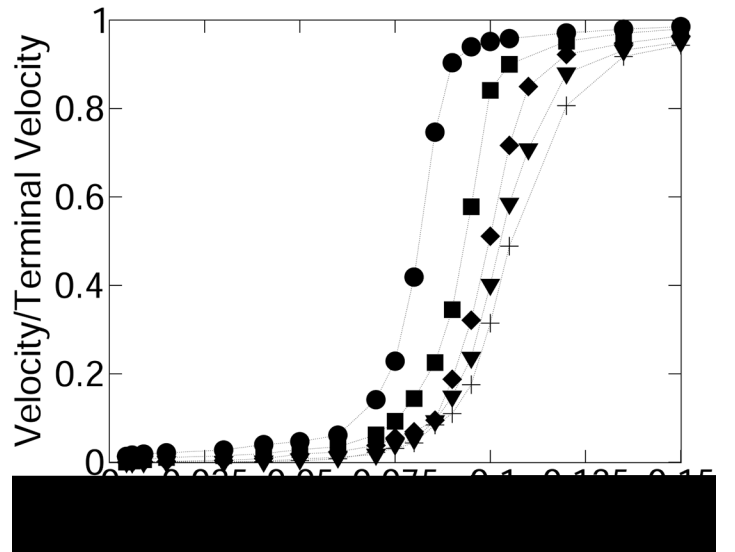


Figure 1 A typical I - V plot. This one shows $B/B_\phi = 0.8$ for columnar disorder as defined in the text. Circles, squares, diamonds, triangles, and crosses correspond to 10, 20, 30, 40, 50 vortices, respectively, in the cell.

motion it is necessary to block these regions of channel flow. As more vortices are added into the system, the interactions between them become more effective at blocking channels of vortex flow, leading to an increase in the critical force for increasing numbers of vortices.

This system displays how complicated the interplay of a system's elements with each other – and with the defects that are present in material – can be. With no defects, the behaviour is completely dominated by the interaction between vortices, as they form a triangular (Abrikosov) lattice in their attempt to move as far apart as possible. Then at low driving forces and with defects, the system is dominated by the attraction of the vortices to the defects, and the system forms a glass. This can be seen in Figure 2 which shows a structure factor peaked only at $\mathbf{Q} = 0$. At higher forces with defects, both the vortex-vortex and the defect-vortex interactions are important as stopping channel flow requires pinned defects to dam off the channels. Interactions between vortices become increasingly important until you reach a point where all of the vortices are freely moving and they once again form a Abrikosov lattice. This is confirmed in Figure 3 which now shows that the structure factor has multiple peaks at the reciprocal lattice vectors of the Abrikosov lattice.

We note that splayed defects are more successful at blocking channel flow as they are going to pin defects not in a straight up and down fashion, but in a manner that offers a larger cross-section against the flow of these

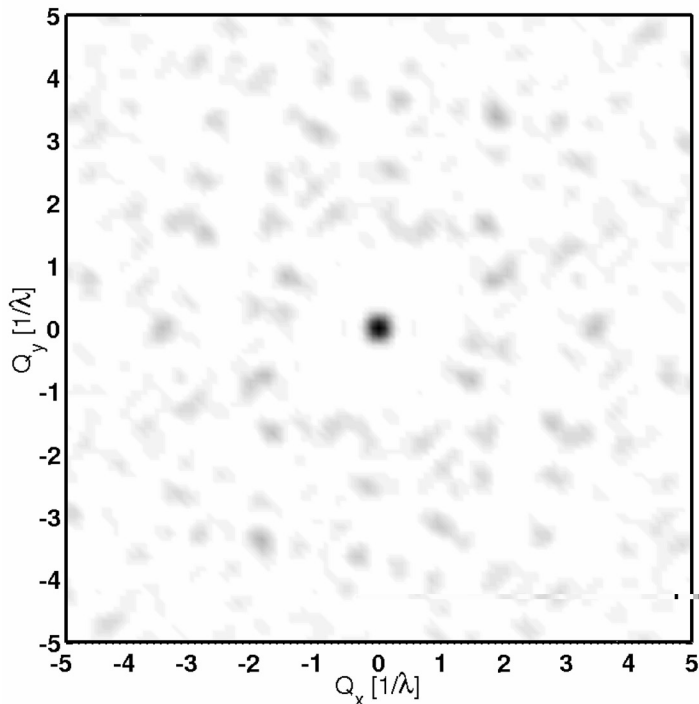


Figure 2 Structure factor for 16 by 16 box with 20 vortices and 20 defects at a low driving force (0.01). The system is disordered because each vortex is pinned to a randomly placed defect.

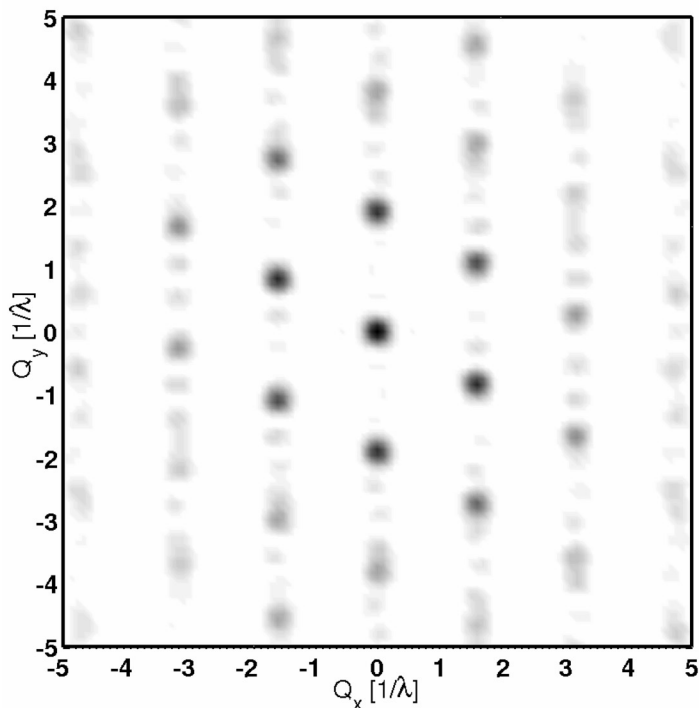


Figure 3 Structure factor for 16 by 16 box with 20 vortices and 20 defects at a large driving force (1.5). The system is ordered because the vortex-vortex interaction is now dominant over the defect interaction.

channels. An optimum J_c is reached when the splay angle balances the ability to block the channels with the energy cost of bending the vortices. In earlier work¹⁰, it was confirmed that an optimal angle exists for the splay angle at approximately 8° (See also Palmer⁴).

Conclusion

We have shown some of the complex dynamics of magnetic vortices in the presence of defects. It was shown that in order to prevent vortex motion, it is useful to block the regions of channel flow by pinning vortices to defects.

Acknowledgements

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References

- ¹Isaac Asimov. *How Did We Find Out About Superconductivity?* Walker. 1988.
- ²Charles Kittel. *Introduction to Solid State Physics*. John Wiley and Sons. 1996. Chapter 12.
- ³J.G. Bednorz and K.A. Müller. "Possible High Tc Superconductivity in the Ba-La-Cu-O System," *Z. Phys. B* (1986) **64**, p. 189.
- ⁴M. Palmer. *Molecular Dynamics Simulations of Vortex Motion in High-Temperature Superconductors*, PhD Thesis. George Washington University. 2000.
- ⁵M.J. Stephen and J. Bardeen. "Viscosity of Type II Superconductors," *Phys. Rev.* (1965) **140**(4A), pp. 1197-1207.
- ⁶George W. Crabtree and David R. Nelson. "Vortex Physics in High-Temperature Superconductors," *Physics Today*. (1997) April.
- ⁷David A. Huse and Matthew P.A. Fisher and Daniel S. Fisher. "Are superconductors really superconducting?" *Nature* (1992) **358**, p. 553.
- ⁸P. Langevin. "On the theory of Brownian Motion," *Comptes Rendus Acad. Sci. Paris* (1908) **146**, pp. 530-533.
- ⁹D.M. Gaitonde and T.V. Ramakrishnan. "Inertial mass of a vortex in cuprate superconductors," *Physical Review B* (1997)
- ¹⁰C.M. Palmer and T.P. Devereaux. "The Role of Splayed Disorder and Channel on the Dynamics of 3D Driven Vortices," *Physica C*. (2000) **341-348**(1-4), pp. 1219-1220.