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THERMODYNAMICS AND DYNAMICS OF VORTEX LATTICES IN TYPE-II SUPERCONDUCTORS

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

By

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***

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Solidification of Monocrystalline Si: Equilibrium and Non-equilibrium Models”, Phys.

I. Lukeš, R. Šášik and R. Černý, “Study of Excimer Laser Induced Melting and
Solidification of Si by Time-Resolved Reflectivity Measurements”, Appl. Phys. A 54,


R. Šášik and D. Stroud, “Flux Lattice Melting, Flux Pinning, and Superfluid Density

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CHAPTER I

Introduction

The field of low-temperature physics started in 1908 when H. Kamerlingh Onnes liquefied helium. Soon thereafter [1] he reported a remarkable discovery: the resistance of mercury dropped abruptly to zero when cooled below 4.19 K. This new, "superconducting" state of matter was also found to occur for other elements and compounds. Even more intriguing than transport properties turned out to be the magnetic properties of superconductors. In 1933 [2] it was found that superconductors below the critical temperature $T_c$ exhibit perfect diamagnetism; a phenomenon called the Meissner effect. Perfect diamagnetism means that magnetic flux is completely expelled from the bulk of the sample. This class of materials is now called type-I superconductors.

Type-II superconductors were first envisioned as a theoretical possibility in 1950 by V. L. Ginzburg and L. D. Landau [3]. These materials, when placed in a strong external magnetic field, have negative surface energy. Therefore, instead of screening the applied field out completely, they prefer some form of coexistence of superconductivity and magnetic flux. This is called the mixed state of a type-II superconductor. The exact microscopic arrangement of flux penetration was speculated upon by Lan-
dau to be laminar, in analogy with the so-called intermediate state seen in type-I superconductors of special geometry. The correct description of the mixed state is due to A. A. Abrikosov (1957) [4], who found that magnetic flux penetrates the sample in the form of flux lines which, in the absence of sample inhomogeneities or other disturbances, arrange themselves in a two-dimensional triangular lattice. The point of maximum flux penetration coincides with a zero of the superconducting order parameter $\psi(r)$—some complex, scalar pseudo-wavefunction—around which circulates a microscopic permanent current (supercurrent). These circular currents are called vortices and the flux lattice is sometimes called vortex lattice.

After the initial excitement of the 1960's when type-II superconductors were extensively studied, the theory of type-II superconductivity began to suffer from a lack of experimental stimulation and a lack of technological progress in particular. The highest achieved critical temperature of about 23 K (Nb$_3$Ge) remained unchanged between 1973 and 1986, when a new compound, La$_{1-x}$Ba$_x$CuO$_4$, was discovered by J. G. Bednorz and K. A. Müller [5]. The critical temperature of this material was in excess of 40 K. This and other related compounds based on Y, Bi, or Hg, are collectively called high-$T_c$ superconductors. They are all of type II, they all are layered with layers formed by conducting CuO$_2$, and some have $T_c$ as high as 164 K [6].

Two compounds in particular, YBa$_2$Cu$_3$O$_{7-\delta}$ and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, have been subjected to the most thorough experimental investigation using a variety of techniques. Much to general surprise, early transport measurements showed that when high-$T_c$ superconductors are cooled in a magnetic field of a few Tesla, they do not be-
come superconducting at all. Where one would expect a fairly sharp drop of resistivity upon cooling, there was only a broad resistive shoulder stretching to temperatures well below $T_c$. Even though the resistivity would become small, it was still measurable. This was the first indication that the new materials were not only quantitatively different from the pre-1986 type-II superconductors, but that they were qualitatively different.

The high temperature involved hints that thermal fluctuations might play an important role in their behavior. Indeed, it was suggested by D. R. Nelson in 1988 [7] that the regular Abrikosov lattice of vortices might be destroyed by fluctuations at a temperature well below $T_c$, leaving a large temperature window where a vortex liquid, a novel, dynamically disordered phase, might exist. In agreement with experiment, this phase would be dissipative and ohmic, qualitatively identical to the normal, non-superconducting phase. The existence of the vortex liquid phase has since been confirmed by numerous transport and magnetization measurements. An important property of the vortex liquid is perfect reversibility; the state of the superconductor is entirely specified by a pair of intensive variables $T$ and $H$. In contrast, when the liquid is cooled below the “irreversibility” temperature $T_{irr}(H)$, the state of the system becomes history-dependent, which is macroscopically manifested by irreversible magnetization. Ironically therefore, we have to conclude that the existence of the vortex solid as a thermodynamic phase has not been confirmed.

The above scenario invokes the phenomenon of vortex lattice melting as a true phase transition, which was predicted to be first order. This prediction initiated a
concentrated experimental search for a macroscopic signature of such a transition. A sharp resistivity jump that should occur as the vortex liquid is cooled below the melting temperature $T_m$ was eventually seen by H. Safar et al. in 1992 [8] in very clean YBa$_2$Cu$_3$O$_{7-\delta}$ crystals. Although this piece of evidence is quite suggestive—and quite satisfactory to some—the rest of the community continues to search for an equilibrium signature of this transition: for a material immersed in a temperature and a magnetic-field bath, two such equilibrium quantities are entropy and magnetization. If vortex melting is a first-order transition, there should be a magnetization jump and a corresponding entropy jump across the transition. To date the effort has been focused on the detection of the former, although specific heat measurements have been showing great promise as well. So far the results have been conflicting. High-precision differential torque magnetometry of D. E. Farrell et al. (1995) [9] detects no sign of a magnetization jump in YBa$_2$Cu$_3$O$_{7-\delta}$. On the other hand, SQUID measurements of U. Welp et al. (1996) [10] produced reversible jumps the size that exceeds the sensitivity of a torque magnetometer by a factor of at least 100. The situation is better with Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, where both E. Zeldov et al. (1995) [11] and D. E. Farrell et al. (1995) [12] find comparable magnetization jumps. There is dispute, however, as to whether or not these jumps represent equilibrium bulk properties.

This thesis represents my contribution to understanding of these problems. Vortex lattice melting is a phenomenon which I investigate in both two-dimensional (2D) and three-dimensional (3D) layered systems. In addition, I study superconducting phase coherence of the vortex solid in 2D, and dimensional crossovers within the vortex
solid phase in 3D. I further calculate equilibrium properties of YBa$_2$Cu$_3$O$_{7-\delta}$ such as magnetization and latent heat of vortex melting. The last chapter deals with the formalism necessary to describe non-equilibrium transport properties of high-$T_c$ superconductors at high fields, although no numerical calculations are presented.
CHAPTER I REFERENCES

[1] H. Kamerlingh Onnes, Leiden Comm. 120b, 122b, 124c (1911).
CHAPTER II

Mean-field Theory

2.1 Introduction

In this chapter we will give a new derivation of the Abrikosov triangular lattice. Like Abrikosov [1], we will make the lowest Landau level approximation, and develop a form for the free energy functional which reveals straightforwardly that the ground state of a homogeneous type-II superconductor in a magnetic field is a triangular lattice of vortices.

2.2 Ginzburg-Landau phenomenology

We describe a superconductor using the Ginzburg-Landau (GL) Hamiltonian

\[ H[\psi, A] = \int d^3r \left\{ a(T)|\psi(r)|^2 + \frac{1}{2m^*} \left| (-i\hbar \nabla - \frac{e^*}{c} A) \psi(r) \right|^2 + \right. \\
\left. \frac{b}{2} |\psi(r)|^4 + \frac{1}{8\pi} \left( \nabla \times A - H \right)^2 \right\}, \tag{2.1} \]

where \( T \) is temperature, \( H = H\hat{z} \) is an external magnetic field far away from the superconductor, \( \psi(r) \) is the complex scalar order parameter characterizing the su-
perconducting state, $a(T)$ and $b$ are material-dependent parameters, and $|e^*| = 2e$ is the charge of a Cooper pair. $m^*$ has dimensions of mass, but its numerical value is irrelevant. Integration extends over all space, even if the sample does not. For a two-dimensional type-II superconductor of thickness $d$ and infinite extent in the $xy$ plane, the average flux density inside the superconductor equals the flux density at infinity, $\mathbf{B}(r) \equiv \mathbf{H}$, as demanded by flux conservation. We proceed on the assumption that $\mathbf{B}(r) = \mathbf{H}$ everywhere, thus neglecting the fluctuations of the vector potential entirely. This is a very good approximation for many purposes in the extreme type-II limit. We choose the gauge $\mathbf{A} = H x \hat{y}$ and write eq. 2.1 as

$$\mathcal{H}[\psi] = d \int d^2r \left\{ a(T)|\psi(r)|^2 + \frac{1}{2m^*} \left| \left( -i\hbar \nabla_\perp - \frac{e^*}{c} A \right) \psi(r) \right|^2 + \frac{b}{2} |\psi(r)|^4 \right\}. \quad (2.2)$$

The thermodynamics of the system is defined by the free energy

$$\mathcal{F} = -k_B T \ln Tr_\psi \exp(-\mathcal{H}[\psi]/k_B T). \quad (2.3)$$

The quadratic free-particle Hamiltonian $\mathcal{H}_0 = a(T) + (2m^*)^{-1}(-i\hbar \nabla_\perp - qA/c)^2$ has a discrete spectrum of infinitely degenerate Landau levels. The level spacing is the cyclotron gap $\hbar \omega_c = 2\hbar e |H|/(m^* c)$. We further make the lowest Landau level (LLL) approximation to the free energy, in which the fluctuations of order parameter are confined to the LLL. This renormalized GL-LLL theory is assumed to be exact, provided that fluctuations into all higher Landau have been included in the renormalized coefficients $a(T), m^*$ and $b$. Symbolically, $\mathcal{F} = -k_B T \ln Tr_\psi^0 \exp(-\mathcal{H}/k_B T)$.

The magnetic field sets the unit of length, $\ell = (\phi_0/2\pi |H|)^{1/2}$, where $\phi_0 = h c/2e$ is
the flux quantum. We set \( \psi(\mathbf{r}) \to \left( \frac{b}{\pi} \right)^{1/2} |a(T) + \hbar \omega_c/2|^{-1/2} \psi(\mathbf{r}) \) and obtain

\[
-\frac{\mathcal{H}}{k_B T} = -\frac{1}{T} \int d^2 \mathbf{r} \left\{ \pm |\psi(\mathbf{r})|^2 + \frac{\pi}{2} |\psi(\mathbf{r})|^4 \right\}. \tag{2.4}
\]

Here \( T = \frac{b k_B T}{[\pi d |a(T) + \hbar \omega_c/2|^2]} \) is the dimensionless temperature of the system. The sign on the right-hand side of eq. 2.4 is the same as that of \([a(T) + \hbar \omega_c/2]\). When \( a(T) + \hbar \omega_c/2 > 0 \), the minimum \( \mathcal{H} \) is realized for \( \psi(\mathbf{r}) \equiv 0 \). The superconductor is in the normal state. When \( a(T) + \hbar \omega_c/2 < 0 \), \( \mathcal{H} \) is minimized by a non-trivial \( \psi(\mathbf{r}) \). This is the superconducting state. The boundary \( H_{c2}(T) \) between the normal and the superconducting states is given by the condition \( a(T) + \hbar \omega_c/2 = 0 \), or

\[
H_{c2}(T) = -a(T) \frac{m^* c}{\hbar}. \tag{2.5}
\]

Note that \( H_{c2}(T) \) is linear in temperature as long as \( a(T) \) is linear. Since neither coefficient is directly measurable, the linearity is often simply assumed. Also noteworthy is the fact that \( T \to \infty \) as \( H \to H_{c2}(T) \) from below, which means that the vortex system must be dynamically disordered (fluid) sufficiently close to \( H_{c2}(T) \), even for low-\( T_c \) superconductors.

### 2.3 Extended lowest Landau level states

We denote the dimensions of the integration region by \( L_x, L_y \), and define area \( S = L_x L_y \). The LLL wavefunctions, normalized to \( \delta_{k,k'} \), are

\[
\psi_k(\mathbf{r}) = L_y^{-1/2} \pi^{-1/4} e^{iky} \exp[-(x-k)^2/2]. \tag{2.6}
\]
Any state of the system can be written as a linear combination of the LLL eigenfunctions as \( \psi(r) = \sum_k a_k \psi_k(r) \), where \( a_k \)'s are complex amplitudes and represent the coordinates of the system in the phase space. Equation 2.4 becomes

\[
-\frac{\mathcal{H}}{k_B T} = -\frac{1}{T} \left\{ -\sum_k a_k^* a_k + \frac{\pi}{2} \frac{1}{\sqrt{2\pi} L_y} \sum_k \sum_{q,q'} a_{k+q}^* a_k a_{k+q'}^* a_{k+q+q'} e^{-(r^2+q'^2)/2} \right\}. \tag{2.7}
\]

This Hamiltonian is not yet suitable for our purposes, because states \( \psi_k(r) \) are localized. In order to proceed with the mean-field theory, we introduce a set of extended states \( \psi_k(r) \). Following Bychkov and Rashba \[2\], we define two magnetic translation operators \( \hat{T}_{a_1} \) and \( \hat{T}_{a_2} \) (\( a_1 \equiv (a_{1x}, a_{1y}) \) and \( a_2 \equiv (0, a_{2y}) \)) according to

\[
\hat{T}_{a_i} \psi_k(r) = \exp(-ia_{ix} y) \psi(r + a_i), \tag{2.8}
\]

where \( \psi(r) \) is an arbitrary function. The operators \( \hat{T}_{a_i} \) commute with the free-particle Hamiltonian, and also with each other if \( (a_1 \times a_2) \cdot \hat{z} = 2\pi \). The vectors \( a_i \) define the basis of the magnetic lattice. The vectors \( b_1 = a_2 \times \hat{z} \) and \( b_2 = \hat{z} \times a_1 \) form the basis of the reciprocal lattice. The basis of states common to \( \hat{T}_{a_1}, \hat{T}_{a_2} \) and \( \mathcal{H}_0 \) is

\[
\psi_k(r) = \left( \frac{a_{1x}}{L_x} \right)^{1/2} \sum_l \exp \left\{ ik_x a_{1x} l - \frac{i}{2} a_{1y} a_{1y} l(l+1) \right\} \psi_{k+y=a_{1y}}(r). \tag{2.9}
\]

These states are normalized to \( \delta_{kk'} \) and form a complete set within the LLL of \( \mathcal{H}_0 \) if \( k \) is chosen within the limits of the first Brillouin zone of the reciprocal lattice. They satisfy the "Bloch wave" condition

\[
\hat{T}_{a_i} \psi_k(r) = \exp(ik \cdot a) \psi_k(r). \tag{2.10}
\]

The corresponding new amplitudes are

\[
A_k = \left( \frac{a_{1x}}{L_x} \right)^{1/2} \sum_l \exp \left\{ -ik_x a_{1x} l + \frac{i}{2} a_{1y} a_{1y} l(l+1) \right\} a_{k+y=a_{1y}}. \tag{2.11}
\]
Figure 2.1: Square Abrikosov lattice. $a_1 = (2\pi)^{1/2}(1,0)$ and $a_2 = (2\pi)^{1/2}(0,1)$. Shades of gray correspond to levels of $|\psi(r)|^2$.

Figure 2.2: Triangular Abrikosov lattice. $a_1 = \pi^{1/2}(3^{1/4}, 3^{-1/4})$ and $a_2 = \pi^{1/2}(0, 3^{-1/4}2)$. Shades of gray correspond to levels of $|\psi(r)|^2$. 
Equations 2.9 and 2.11 correspond to writing the order parameter in the form \( \psi(r) = \sum_k \psi_k(r)A_k \), or \( \psi(r) = S/(2\pi)^2 \int_{BZ} d^2k \psi_k(r)A_k \) in the continuum limit. Summation or integration is performed over the Brillouin zone.

The GL-LLL Hamiltonian can now be cast into a particularly appealing form

\[
-\frac{\mathcal{H}}{k_B T} = -\frac{1}{T} S \left\{ -S(0) + \frac{\pi}{2} \int \frac{d^2q}{(2\pi)^2} e^{-q^2/2} |S(q)|^2 \right\}, \tag{2.12}
\]

where we defined thermodynamically intensive quantities

\[
S(q) = \int_{BZ} \frac{d^2k}{(2\pi)^2} e^{iq_k} A_{k+q}^* A_k
\]

for \( q \) arbitrary, not restricted to the Brillouin zone. Unfortunately, integration in eq. 2.12 over unrestricted quasimomentum \( q \) involves "umklapp" processes when quasi-momentum \( k + q \) is equivalent to some \( k' \) from the Brillouin zone. In such a case we need the wraparound relation

\[
A_{k+Q} = A_k \exp \left\{ ik_x Q_y + \frac{i}{2} Q_x Q_y - \frac{i}{2} a_{12} Q_y - i\pi l_1 l_2 \right\}, \tag{2.14}
\]

where \( Q = l_1 b_1 + l_2 b_2 \) is an arbitrary reciprocal-lattice vector. These processes are essential for the formation and stability of the vortex solid phase.

### 2.4 Abrikosov triangular lattice

The mean-field solution of eq. 2.3 rests in replacing the entire sum behind the logarithm with the largest term of this sum. This is the term with the lowest \( \mathcal{H}\psi \): the ground state.
We will look for a ground state among the class of quasi-periodic states $\psi_k(r)$. They satisfy $|\psi_k(r + R)| = |\psi_k(r)|$, where $R$ is an arbitrary lattice vector. To this end we set $A_k = A_\delta_{k,p}$, where $p$ is an arbitrary vector from the BZ. It is clear from eq. 2.12 and 2.13 that the free energy does not depend on $p$; the Hamiltonian is translationally invariant, as it should. With $S(0) = A^2/(2\pi)$ and $|S(q)|^2 = S^2(0)\delta_{q,Q}$, and minimizing with respect to $A$ one obtains

$$\frac{-\mathcal{H}}{k_B T} = \frac{1}{\mathcal{T}} \frac{S}{2\pi} \beta^{-1},$$  \hspace{1cm} (2.15)$$

where

$$\beta = \sum_Q \exp(-Q^2/2)$$  \hspace{1cm} (2.16)
is the famous Abrikosov ratio, $\beta \equiv |\psi(r)|^2/|\psi(r)|^2$. Result 2.16 holds for any lattice of periodicity defined by vectors $a_1$ and $a_2$. It will enable us to find the ground state of the system and avoid guessing, which lead Abrikosov to mistake the square lattice for the ground state.

In order to minimize $\mathcal{H}$ one simply has to find two such vectors $a_1$ and $a_2$, for which $\beta$ is minimum. We will only consider a case in which $|a_1| = |a_2|$ and investigate the dependence of $\beta$ on the angle between these vectors. The result is presented in fig. 2.4. The minimum of $\beta$ is realized when the angle is $60^\circ$, i.e., for a triangular lattice of vortices. In this case $\beta \equiv \beta_A = 1.159595266963\ldots$ is the famous Abrikosov factor which was first found by others [3]. The square lattice has $\beta = 1.180340599016\ldots$ and is unstable to shear, as evidenced by the figure.

As a final remark we note that every state $\psi_k(r)$ (with proper amplitude) is in fact a ground state of the system. States with different $k$'s define Abrikosov vortex lattices related by a uniform translation of zeros (vortex cores) in the $xy$ plane.
CHAPTER II REFERENCES


CHAPTER III

Calculation of the Shear Modulus of a Two-Dimensional Vortex Lattice

3.1 Introduction

It has long been known [1] that two-dimensional (2D) systems can have very unusual phase transitions. For example, the so-called 2D $XY$ or planar model has a continuous phase transition marked by the unbinding of thermally excited vortex-antivortex pairs [2], with a characteristically diverging correlation length, and a universal jump in the spin-wave stiffness (or helicity modulus) [3]. The melting of a 2D elastic solid has characteristics which are less universally agreed upon than those of the 2D $XY$ model. Kosterlitz and Thouless [4] suggested that this melting proceeds by the unbinding of dislocation pairs. Halperin and Nelson [5], and independently Young [6], derived renormalization-group (RG) equations for this phase transition, which they also found to be continuous, provided the fugacity of bound dislocation pairs is small. The dislocation-unbinding transition is characterized by a discontinuous jump in the coupling constant

$$K(T) = \frac{1}{k_BT} \frac{4\mu(\mu + \lambda)}{2\mu + \lambda} a^2,$$  \hspace{1cm} (3.1)
from $16\pi$ to zero on melting. Here $\mu$ is the shear modulus, $\lambda$ is the second of Lamé elastic constants, and $a$ is the crystal lattice constant. These ideas are commonly referred to as the KTBHNY theory [7].

A particularly convenient model system for studying 2D melting is a thin superconducting film placed in a transverse magnetic field. Such a field produces a density of vortices, which may form either a lattice or a fluid-like state. Recently, several workers [8, 9] have used a simple Ginzburg-Landau (GL) model Hamiltonian in the so-called lowest Landau level (LLL) approximation [10] to provide strong numerical evidence in favor of a first-order phase transition in this system, in contrast to the continuous melting proposed by the KTBHNY theory (although no transition at all has been found in Ref. [16] using the same approximation in a spherical geometry). A more recent calculation [12] treats 2D flux lattice melting in the London limit (probably appropriate at lower fields than the LLL approximation) and finds a continuous transition consistent with the KTBHNY picture.

In this chapter we calculate the temperature-dependent shear modulus of a 2D vortex lattice. The behavior of this quantity is of particular interest, because it seems, at first glance, difficult to reconcile the prediction of a universal jump with the reported first-order melting transition. Our basic result is that, despite the first-order transition, the shear modulus is near the suggested universal value at the extrapolated first-order melting temperature of a very large system. At the end of this chapter, we speculate about some possible reasons for this behavior.
3.2 Method of calculation

To calculate the shear modulus $\mu(T)$, we consider a vortex lattice in equilibrium with a thermal reservoir at temperature $T$, and apply an external force which generates a small shear strain in this lattice. If the force does reversible mechanical work $\delta W$ on the lattice, the free energy of the system changes by $\delta F = \delta W$. The isothermal shear modulus is the second derivative of free energy per unit area with respect to the shear angle $\theta$, i.e.,

$$\mu = \frac{1}{S} \left( \frac{\partial^2 F}{\partial \theta^2} \right)_{T, \theta = 0},$$

(3.2)

where $S$ is the sample surface area. We also introduce the shear modulus per vortex $\mu_\phi = (S/N_\phi)\mu$, where $N_\phi$ is the number of vortices in the sample.

We assume that equilibrium properties of a 2D superconductor are described by the GL energy functional

$$\mathcal{H}[\psi] = L_z \int d^2 r \left\{ a(T)|\psi(r)|^2 + \frac{1}{2m^*} \left| \left(-i\hbar \nabla - \frac{qA}{c} \right) \psi(r) \right|^2 + \frac{b}{2} |\psi(r)|^4 \right\},$$

(3.3)

where $\psi(r)$ is the complex order parameter, $r = (x, y)$, $L_z$ is the sample thickness, $|q| = 2e$ is the charge of supercurrent carriers, and $a(T)$, $b$ and $m^*$ are material-dependent parameters. $A = -By\hat{z}$ is the vector potential of a (uniform) magnetic field perpendicular to the sample surface. This is an approximation valid in the extreme-type-II limit ($\kappa \gg 1$), where $\kappa$ is the standard GL parameter.

In order to calculate thermal averages, following [8] and [9], the order parameter is expanded in an orthogonal set of wave functions drawn from the lowest band of the Hamiltonian $(2m^*)^{-1}(-i\hbar \nabla - qA/c)^2$, known as lowest Landau levels (LLL's). These
states are labeled with a continuous index \( k \), and are degenerate with an eigenvalue \( \hbar \omega_c/2 = \hbar eB/(m^*c) \). By making this approximation we assume that fluctuations in higher LL channels either can be neglected or have already been included in a suitably renormalized coefficient \( a(T) \) [10]. The LLL approximation is valid for fields \( B \) near the upper critical field \( H_{c2}(T) \) defined by \( a(T) + \hbar \omega_c/2 = 0 \). We now write

\[
\psi(r) = \left( \frac{\sqrt{3}a_H^2(T)}{4\ell^2} \right)^{1/4} \sum_k c_k e^{ikx} \exp \left[ - (y - k\ell)^2/2\ell^2 \right],
\]

where \( a_H(T) \equiv a(T)[1 - B/H_{c2}(T)] \), and \( \ell = (|q|B/\hbar c)^{-1/2} \) is the magnetic length. Further we will only consider the superconducting region, \( a_H(T) < 0 \).

With periodic boundary conditions along the \( x \)-axis so that \( \psi(x, y) = \psi(x + L_x, y) \), \( k \) assumes values \( k_m = 2\pi m/L_x \), where \( m \) is an integer. We adopt the concise notation \( c_m \equiv c_{km} \). If there are \( N_\phi \) independent amplitudes, the set \( \{c_m\} \) with \( m = 0 \ldots N_\phi - 1 \) describes a state \( \psi(r) \) with \( N_\phi \) zeroes (i.e., vortex cores). A quasi-periodicity along the \( y \)-axis of the form \( |\psi(x, y)| = |\psi(x, y + L_y)| \) is achieved by allowing \( m \) to span all integer values, but with the constraint \( c_m = c_m' \) for all \( m = m' \mod N_\phi \). Evidently, \( L_y = N_\phi \times 2\pi\ell^2/L_x \).

In the unstrained ground state [13, 14], the vortices form a triangular lattice with a nearest-neighbor distance \( \ell_0 = (4\pi/\sqrt{3})^{1/2}\ell \). One way of generating the ground state is to choose \( L_x/\ell_0 = n_x \) to be an integer. The only non-zero amplitudes then are \( c_{(2p+1)n_x} = i c_{2pn_x} = i(2/\beta_A)^{1/2} \), where \( p \) is an arbitrary integer and \( \beta_A = 1.159595 \ldots \) is the Abrikosov ratio\(^1\). The ground state energy is \( \mathcal{H}^{MF} = -k_B T g^2(T) N_\phi / \beta_A \).

The thermodynamics of the system is given by the free energy

\(^1\) Coefficients \( c_m \) for all ground states have been found in Chapter II.
\[ F = -k_B T \ln \int \Pi_m \, dc_m \, dc_m^* \exp(-\mathcal{H}([c_m])/(k_B T)), \]

where

\[ \frac{-\mathcal{H}([c_m])}{k_B T} = -g^2(T) \left\{ -n_x \sum_m |c_m|^2 + n_x^{3/2} \sum_{m,m',n,n'} c_{m+n}^* c_{m+n'} c_{m+n+n'}^* c_{m+n+n'} e^{-\sqrt{3} \pi (n^2+n'^2)/2n_x^2} \right\}. \] (3.5)

This form makes clear that the system is described by a single intensive variable [10] \( g(T) = a_H (\pi \ell^2 L_z/k_B T)^{1/2} \). In eq. 3.5, \( 1/g^2 \) appears as the dimensionless temperature and is the natural variable of the problem: \( 1/g^2 = 0 \) corresponds to \( T = 0 \) K, and \( 1/g^2 = +\infty \) marks the mean-field transition at \( T_c(B) \).

Within this representation, we turn now to an explicit expression for the shear modulus. First, eq. 3.2 can be written as

\[ \mu_\phi = \frac{1}{N_\phi} \left[ \left( \frac{\partial^2 \mathcal{H}}{\partial \theta^2} \right) - \frac{1}{k_B T} \left( \frac{\partial \mathcal{H}}{\partial \theta} \right)^2 \right]_{\theta=0}, \] (3.6)

where the brackets denote thermal averaging in the canonical ensemble. Thus, it remains to determine the dependence of \( \mathcal{H} \) on the shear angle \( \theta \).

A uniform shear such that \( |\psi(x, y)| = |\psi(x+\theta L_z, y+L_y)| \) (see Fig. 3.2) is generated by imposing the condition \( c_m \to c_m \exp[-i \sqrt{3} \pi m^2 \theta/(2n_x^2)] \). Direct differentiation of \( \mathcal{H} \) in this state and taking the limit \( \theta \to 0 \) leads to

\[ \mu_\phi = \frac{k_B T g^2(T)}{N_\phi} \times \]

\[ \left\{ -\frac{3^{5/4} \pi^2}{2^3 \sqrt{3 \pi}} \sum_{m,m',n,n'} \mathbb{R}\{c_m c_{m+n}^* c_{m+n'}^* c_{m+n+n'}^* \left( \frac{nn'}{2n_x^2} \right)^2 e^{-\sqrt{3} \pi n^2+n'^2/2n_x^2} \} - g^2 \left( \frac{3^{3/2} \pi^2}{2^5} \left( \sum_{m,m',n,n'} \mathbb{R}\{c_m c_{m+n}^* c_{m+n'}^* c_{m+n+n'}^* \left( \frac{nn'}{2n_x^2} \right)^2 e^{-\sqrt{3} \pi n^2+n'^2/2n_x^2} \} \right)^2 \right) \right\}. \] (3.7)
Figure 3.1: Ground state of the vortex lattice with $N_{\phi} = 3 \times 4$, subjected to a uniform shear with angle $\theta$ ($\tan \theta = 0.1$). The lines are loci of constant $|\psi(r)|^2$.

Since the vortex lattice in the LLL approximation is incompressible, $\lambda \to +\infty$ and the KTBHNY theory predicts a universal jump for the shear modulus $\mu$ alone.

The mean-field value of the shear modulus, $\mu_{\phi}^{MF}(T) = 0.354 \frac{k_B T g^2(T)}{\mu}$, obtained by evaluating 3.7 in the ground state, can be equivalently written as

$$\mu_{\phi}^{MF}(T) = 0.477 \frac{[H_{2\pi}(T) - B]^2}{8\pi(2\kappa^2)\beta_4^2} L_z.$$ (3.8)

This result is almost identical to that of Labusch and Brandt [15, 16], with two small differences. First, these authors obtain $(2\kappa^2 - 1)$ in the denominator instead of just $(2\kappa^2)$ as we do. This difference occurs because they deal with a 3D system of straight flux lines where the screening magnetic field can be included. It is algebraically
prohibitive to do so in our case, where the order parameter is limited to a thin layer in the $z$-direction, while the magnetic field is not. In any case, the two expressions merge together in the extreme type-II limit $\kappa \to \infty$, which is the case studied here.

Secondly, they obtain a numerical factor, 0.475, which differs slightly from ours. We believe that the difference is real and is caused by a slightly different definition of the shear deformation. Labusch and Brandt assume that the lattice under shear can actually change dimensions, although the surface area $L_x \times L_y$ remains constant. For example, at the largest allowed shear angle, Labusch and Brandt obtain a square flux lattice, whereas the procedure used here generates a vortex lattice with a rectangular unit cell still having an aspect ratio $1 : \sqrt{3}/2$. Our definition seems more relevant to an experiment, in which the vortex lattice in the $y$-direction is limited by the edges of the sample. In either case, the difference is very small.

### 3.3 Results

We have evaluated the shear modulus $\mu(T)$ for this model, using standard MC techniques within the Metropolis algorithm, and initializing the system in its ground state before each run. A single MC move consists of changing a particular amplitude $c_m \to c_m + \Delta c_m$, where $\Delta c_m$ is a random complex number from some $\epsilon$-neighborhood of zero.

Since the modulus is a second derivative calculated in the absence of shear, the calculation can be conveniently done using periodic boundary conditions. In these circumstances, we obtain evidence suggestive of a first order phase transition in the
MC calculation, just as found previously by other workers [8, 9]. In particular, there is a range of temperatures between a lower ("supercooling") limit $T_{sc}$ and an upper ("superheating") limit $T_{sh}$, where the system jumps back and forth between a solid-like and a liquid-like state. These limits seem to be numerically quite well defined, but depend on sample size. The jumps occur typically about once every $10^4$–$10^5$ passes through the entire lattice, for the sample sizes $N_\phi = 120$ and 224 which we consider.

Fig. 3.3 shows the shear modulus $\mu(T)$ plotted in units of the mean-field shear modulus $\mu^{MF}(T)$. The sample cell has dimensions $L_x \times L_y = 10 \ell_0 \times 12(\sqrt{3}/2)\ell_0$ for the smaller system of $N_\phi = 120$ vortices and $L_x \times L_y = 14 \ell_0 \times 16(\sqrt{3}/2)\ell_0$ for the larger system of 224 vortices. Between $T_{sc}$ and $T_{sh}$, $\mu$ is, of course, evaluated by averaging only over the solid-like configurations. These are easily distinguished from the liquid configurations, since the energy among the latter fluctuates around a value $\sim 2\%$ above that of the solid. Among the liquid configurations $\mu$ averages to zero, as expected. For $N_\phi = 120$, $T_{sc}$ and $T_{sh}$ correspond to the values $1/g_{sc}^2 \approx 0.022$, $1/g_{sh}^2 \approx 0.028$. The exact thermodynamic melting transition is not easily determined by this procedure, however. The values of Fig. 3.3 represent averages over about $10^4$–$10^5$ passes through the sample. They show very little dependence on sample size.

In order to compare our results with the predictions of the KTBHNY theory, we rewrite the stability criterion $\lim_{T \to T_c} K(T) \equiv \lim_{T \to T_c} 4\mu(T)\ell_0^2/k_B T = 16\pi$ as

$$\lim_{T \to T_c} \frac{\mu_\phi(T)}{\mu^{MF}_\phi(T)} = \frac{2\sqrt{3}\pi}{0.354} \frac{1}{g^2(T_c)}. \quad (3.9)$$

This is shown as a straight line in Fig. 3.3. Substitution of the mean-field value $\mu^{MF}_\phi(T)$ for $\mu_\phi(T)$ into eq. 3.9 leads to a mean-field estimate for the KTBHNY critical
Figure 3.2: Calculated temperature dependence of the shear modulus $\mu(T)$, in units of the mean-field shear modulus $\mu^{MF}(T)$ for two lattice sizes, $N_\phi = 120$ and 224. Estimated errors are comparable to symbol sizes. The straight line with a slope $2 \cdot 3^{1/2}\pi/0.354$ represents the Kosterlitz-Thouless instability criterion. Arrow labeled “MF” denotes the mean-field instability temperature; arrows labeled “KN” and “HM” denote the thermodynamic melting temperature at infinite size as estimated by Kato and Nagaosa and by Hu and MacDonald. For $N_\phi = 120$, in the temperature range bounded by dotted lines, $0.022 < 1/g^2(T) < 0.028$, both liquid and solid phases can coexist.
value, $g^{MF}(T_c) = -5.54$. This point is marked with an arrow in Fig. 3.3, and clearly lies above the superheating limit, as might be expected from a mean-field theory. On the other hand, for $N_\phi = 120$, the KTBHNY prediction appears to coincide roughly with the supercooling limit, which is the point where a liquid can first be locally stable.

Now the critical temperature, determined as a point at which the energy distribution has two equal-height maxima [21], suffers from large finite-size effects due to the large correlation length in the vortex liquid [8, 9]. Kato and Nagaosa [8] have suggested an extrapolation of the thermodynamic melting temperature for $N_\phi \to \infty$, $g(T_c) = -7.15 \pm 0.10$ or $1/g^2(T_c) = 0.020$. This value does lie very near the temperature at which the instability criterion of Kosterlitz and Thouless is satisfied. Thus, our results for the shear modulus at melting could be consistent with the instability criterion. However, the exact value of $T_c$ at infinite size is still a matter of controversy. This is indicated in Fig. 3.3, where the infinite-size extrapolation of $T_c$ by Kato and Nagaosa [8], and an alternative extrapolation by Hu and MacDonald [9], are denoted by arrows.

According to the RG calculations of Halperin, Nelson and Young, the shear modulus should have a power-law cusp as $T \to T_c^-$, $K(T) \sim 16\pi/(1 - c|1 - T/T_c|^\nu)$, where $c$ is a non-universal positive constant and $\nu = 0.3696 \ldots$. There is no evidence of such behavior seen in our data, which is further evidence against the continuous transition.

In order to gain further insight into the two coexisting phases, we have examined the structure factor in each one. The instantaneous structure function $S(q) \equiv$
\[ S(q_x, q_y) \text{ is defined by} \]
\[ S(q) = \int d^2r d^2r' |\psi(r)|^2 |\psi(r')|^2 e^{i\mathbf{q}(r-r')}, \tag{3.10} \]
evaluated in a randomly chosen representative of the MC ensemble. The instantaneous structure factor \( I(q) \) is defined as the structure function for a given configuration reduced by the "atomic" structure factor, \( I(q) = S(q)/\exp(-q^2 \ell^2/4) \).

Fig. 3.3 shows \( I(q) \) for \( N_\phi = 120 \) and three different cases: (a) the solid phase at \( 1/g^2(T) = 0.020 \); (b) the superheated solid at \( 1/g^2(T) = 0.026 \); and (c) the liquid at \( 1/g^2(T) = 0.030 \). These Figures clearly confirm the structural identification of the two phases as solid and liquid, and in conjunction with Fig. 3.3 further show that the structural solid is the phase with the non-zero shear modulus. Note also the superheated solid in Fig. 3.3 (b), which shows that the solid structure may be formed at various angles with respect to the coordinate axes. This suggests that the absence of full rotational invariance in this representation, with these boundary conditions, may not prevent the accurate calculation of physical properties.

### 3.4 Discussion

The present results suggest that the shear modulus in a two-dimensional vortex lattice does have a jump from zero to a finite value at the thermodynamic freezing temperature \( T_c \), and that the magnitude of the jump is near the postulated universal value. It is difficult to make a more precise statement, however, because \( T_c \) is significantly size-dependent, while \( \mu(T) \) (cf. Fig. 3.3) is not. Thus, at our largest size
Figure 3.3: Instantaneous structure factor $I(q)$ for a vortex lattice with $N_\phi = 120$ in a state drawn from (a) the solid phase at $1/g^2(T) = 0.020$; (b) the superheated solid at $1/g^2(T) = 0.026$; and (c) the liquid at $1/g^2(T) = 0.030$. Central maxima at $q = 0$ have been eliminated in these plots.
\(N_\phi = 224\), \(\mu(T_c)\) is still slightly smaller than the universal value, but at the value of
\(T_c\) extrapolated to infinite lattice size, it may be equal to this value, or even slightly larger.

If \(\mu(T_c(N_\phi \rightarrow \infty))\) is, in fact, larger than the universal value, this would suggest that the first-order melting may intervene before the continuous melting transition can occur, as in the melting of the 2D Lennard-Jones solid studied by Abraham [18]. Our simulations may also be consistent with an alternative to the KTBHNY scenario, namely, the simultaneous unbinding of dislocations and disclinations at a first-order transition, as proposed by Kleinert [19]. The occurrence of a first-order melting transition presumably also explains the absence of a cusp-like behavior in \(\mu(T)\) just below \(T_c\) in our calculations. On the other hand, since \(\mu\) has a jump close to the universal value, it is clear that this first-order transition is quite weak, and could possibly be made continuous with only a slight change in the Hamiltonian.
Chapter III References


CHAPTER IV

Phase Coherence in Two-dimensional Type-II Superconductors

4.1 Introduction

In type-II superconductors, magnetic field and superconductivity can coexist over a wide region of the $H-T$ phase diagram in the form of the mean-field Abrikosov vortex lattice [1, 2]. This picture is dramatically changed in most of the high-$T_c$ superconductors. Because of the short coherence lengths and layered character of these materials, thermal fluctuations are greatly enhanced in comparison to the low-$T_c$ superconductors reducing the domain of validity of the mean-field description. The fluctuation effects have been the subject of considerable investigation, both experimentally and theoretically.

Of particular relevance in this context is the vortex melting transition in 2D and at high fields. Earlier studies have provided evidence for such a transition far below $T_c(H)$ [3] and indicated that it is weakly first-order [4, 5, 6, 7]. The low-temperature phase has a finite shear modulus, like a conventional solid [6]. However, the vortex solid differs from a conventional atomic solid in one key respect: the vortices
which undergo a liquid-solid transition are not explicitly connected to the correlation functions of the original order parameter field, $\psi(r)$. Because of the highly non-linear relationship between the vortices and $\psi(r)$, it is a formidable theoretical challenge to find such a connection. While this issue obviously does not arise in conventional solids, it is of central importance for the superconducting transition.

In this chapter, we use the numerical Monte Carlo (MC) method to investigate correlations in a 2D vortex solid. We show that in two-dimensional type-II superconductors, the vortex liquid-solid transition is not accompanied by a simultaneous divergence of the phase correlation length. Even in the “vortex solid” phase, despite a finite shear modulus and quasi-long range density correlations, the phase coherence remains short-ranged, with a correlation length of order one magnetic length, in stark contrast to the Abrikosov state, where the phase order is long-ranged.

We also find that, in the solid phase, there is no “Bose condensation”, in the sense that any particular Abrikosov lattice state has zero statistical weight in the thermodynamic limit. The vortex solid phase in two dimensions is therefore best described as a Cooper pair charge density-wave (SCDW) with no superconducting phase order, first described by Tešanović [8].

The possibility of a vortex solid phase with no off-diagonal long-range order (ODLRO) in three-dimensional samples has been suggested by several workers [9, 10, 11]. In the so-called supersolid phase [9, 11], built on a conjectured analogy with $^4$He, the phase order is destroyed by interstitials or vacancies in the vortex line-solid which proliferate the sample at a well-defined temperature. It is not clear what are
the implications of this picture for the GL-LLL theory in 2D and layered systems. The supersolid phase does not exist in 2D which makes the SCDW particularly prominent. Furthermore, defect-free SCDW phases without ODLRO exist in 2D, layered systems and 3D. Moreover, there are phases of the GL-LLL and related theories in all dimensions which are saturated with defects but have a perfect ODLRO. The relationship of the supersolid and SCDW phases remains therefore an open problem [11].

The “phase disordered” nature of the “ordered” solid originates in the form of the Ginzburg-Landau (GL) free energy functional at high fields, where it suffices to consider only fluctuations from the lowest Landau level (LLL). Above $T_{c0}(H)$ the quadratic terms in the GL functional predominate, describing independent fluctuations of all degenerate LLL modes. In 2D, this degeneracy leads to fluctuations with a “zero-dimensional” character. This $D \rightarrow D - 2$ dimensional reduction persists in higher dimensions, suggesting that the Abrikosov (superconducting) transition can occur only for $D = 4$ and above. In support of this conclusion, the high-order perturbative expansion of the 2D GL-LLL theory appears zero-dimensional [12], offering no hint of the Abrikosov transition. However, while the Abrikosov transition is absent for $D = 2$ and 3, there is still a transition induced by quartic coupling of degenerate LLL modes far below $T_{c0}(H)$. This is the SCDW transition unrelated to superconducting phase coherence [3, 8].
4.2 Model

We consider a 2D superconductor of dimensions $L_x \times L_y$ in the $xy$ plane, and thickness $L_z$, placed in a transverse magnetic field $B \equiv B\hat{z}$. The equilibrium properties are described by the GL functional

$$\mathcal{H}[\psi] = L_z \int d^2r \left\{ a(T) |\psi(r)|^2 + \frac{b}{2} |\psi(r)|^4 + \frac{1}{2m^*} \left| \left(-i\hbar \nabla - \frac{qA}{c}\right) \psi(r) \right|^2 \right\}. \quad (4.1)$$

Here $|q| = 2e$ is the charge of the supercurrent carriers, and $a(T), b$, and $m^*$ are material-dependent parameters. We assume that fluctuations from higher LL's can be absorbed into renormalization of coefficients $a(T)$ and $b$. This "renormalized GL-LLL theory" should be quantitatively valid for $H > H_{\Delta}(T)/3$, where $H_{\Delta}(T)$ is the upper critical field defined by $a(T) + \hbar c H_{\Delta}(T)/(m^* c) = 0$. In the transverse gauge $A = -By\hat{x}$, the LLL states are $\phi_k(r) = e^{ikx} \exp[-(y-k\ell^2/2\ell^2)]$, where $\ell = (2eB/\hbar c)^{-1/2}$ is the magnetic length.

We now expand the order parameter as $\psi(r) = \psi_0 \sum_k c_k \phi_k(r)$, where $\psi_0 = [\sqrt{3} a_H(T)/(\beta_A^2 b^2)]^{1/4}$, $a_H(T) = a(T)[1 - B/H_{\Delta}(T)]$, and $\beta_A = 1.159595\ldots$ is the Abrikosov ratio. The thermodynamics of the system is given by the free energy

$$\mathcal{F} = -k_B T \ln \int \prod_k dc_k dc_k^* \exp(-\mathcal{H}\{c_k\})/k_B T$$

where $\mathcal{H}\{c_k\}$ is the GL-LLL energy functional 3.5 expressed in terms of the coefficients $c_k$. The parameter $g(T) \equiv a_H(\pi \ell^2 L_z / b k_B T)^{1/2}$ is the single intensive variable characterizing the 2D LLL system [3]; its inverse square represents the effective dimensionless "temperature".

The ground state of the GL-LLL Hamiltonian is an Abrikosov state with zeros arranged in a triangular lattice, and energy per vortex $\mathcal{H}^{MF} = -k_B T g^2(T)/\beta_A$. Every such lattice with primitive vectors $a_1 = \ell_0 \hat{x}$ and $a_2 = \ell_0 (\hat{x}/2 + \sqrt{3}\hat{y}/2)$, where $\ell_0 =$
$(4\pi/\sqrt{3})^{1/2}\ell$ is the nearest-neighbor vortex distance, corresponds to a state of the original field $\psi(r) \equiv \psi_0\varphi_q(r)$, defined by its non-zero coefficients as $c_p(2\pi/\ell_0) = \exp[i(\pi/2)p^2 - ip(2\pi/\ell_0)q_y\ell^2]$. In this expression $q \equiv (q_x, q_y)$ is a labeling index in the reciprocal space of the magnetic translation group corresponding to a triangular vortex lattice [13] and $p$ is an arbitrary integer. All the equivalent ground states $\psi_0\varphi_q(r)$ are simply translations of the Abrikosov lattice with zeros determined by real-space vectors $r_0 \equiv (x_0, y_0) = (\hat{z} \times q)\ell^2$; one such zero is at $(\ell_0/4 - x_0, (\sqrt{3}/4)\ell_0 - y_0)$, while the others are located at positions displaced from that by translation vectors of the Abrikosov lattice. In order to allow for such a lattice to form without defects in our sample, we choose $L_x = N_x\ell_0$ and $L_y = N_y(\sqrt{3}/2)\ell_0$, where $N_x$ is an integer and $N_y$ is an even integer. The number of flux quanta is then $\phi = N_x \times N_y$. The periodic boundary conditions $\psi(x + L_x, y) = \psi(x, y)$ and $|\psi(x, y)| = |\psi(x, y + L_y)|$ imply that the allowed values of $k$ are integer multiples of $2\pi/L_x$ and that $c_k = c_{k+N_\phi(2\pi/L_x)}$. The corresponding conditions on $r_0$ are that $x_0$ and $y_0$ can only be integer multiples of $\ell_0/N_x$ and $(\sqrt{3}/2)\ell_0/N_x$, respectively. For this reason, there are exactly $N_\phi$ equivalent ground states in this finite lattice [14].

The set $\{\varphi_q(r)\}$ is a complete set in the LLL (the Abrikosov basis). Therefore, we can write $\psi(r) = \psi_0 \sum_q c_q\varphi_q(r)$, where the summation is taken over the first Brillouin zone. The Abrikosov vortex lattice phase is characterized by what may be termed Bose condensation of Cooper pairs into one particular $q = q_A$ state. The ensuing "off-diagonal" correlations [15] can be identified, for example, in a gauge-invariant two-point function $\sigma(r, r') = \langle \exp[i\Lambda(r)]\psi(r)\exp[-i\Lambda(r')]\psi^*(r')/\psi_0^2$, where
\[ \nabla A(r) \text{ defines the "pure gauge" piece of } A(r) \text{ and } \langle \cdots \rangle \text{ denotes a thermal average.} \]

It is also useful to define a function
\[ G(s) = N_{\phi}^{-1} \int d^3 r \sigma(r, r + s), \]
which should be most statistically relevant for \( N_{\phi} \to \infty \), in which limit \( \sigma(r, r') \) depends only on the difference between the arguments. We can express \( G(s) \) as [16]
\[
G(x, y) = \frac{1}{N_{\phi}} \left| N_x \sum_k e^{-ikx} \langle c^*_k c^{*}_{k+sy} \rangle \right|. \tag{4.2}
\]

This correlation function when evaluated in any particular Abrikosov state, has a delta-function structure
\[ G(s) = \sum_{n_1, n_2} \delta_{n_1 a_1 + n_2 a_2}. \]

In the 'normal', vortex liquid phase the system is isotropic and homogeneous, \( \langle |\psi(r)|^2 \rangle \) is uniform and \( \langle c_q c_{q'}^* \rangle \propto N_{\phi}^{-1} \delta_{q, q'}. \) In 2D, we expect that this behavior should also persist in the solid phase [17]. For this reason, we expect that continuous spatial symmetries will be preserved in the thermodynamic limit and that \( \langle |\psi(r)|^2 \rangle \) will remain uniform in the vortex solid. Using this assumption to calculate \( \sigma(r, r') \), we obtain
\[
\sigma(r, r') = \left| \sum_q \langle c_q \rangle \varphi_q(r) \varphi_q^*(r') \right| \propto \exp(-|r' - r|^2/4\ell^2). \tag{4.3}
\]

Thus, fluctuations completely destroy phase coherence in a 2D vortex solid. As a consequence, \( G(s) \) should have a Gaussian envelope in the thermodynamic limit. Since this limit is computationally inaccessible, we will investigate \( G(s) \) for several finite \( N_{\phi} \) and look for a tendency towards Gaussian decay in the vortex solid phase.
4.3 Pairing susceptibility

There is another gauge-invariant and unambiguous way to study superconducting phase correlations. Consider the response of a superconductor to an external "field" which couples directly to $\psi(r)$. This response in various LLL 'channels' is measured by a pairing susceptibility matrix,

$$\chi^{sc}_{q,q'} = N_q \langle c_q c_{q'}^* \rangle. \quad (4.4)$$

While this matrix is not gauge invariant, its eigenvalue spectrum is. Define as the "natural basis" the complete set of LLL states $\{\varphi_Q(r)\}$ for which $\chi^{sc}$ is diagonal. In this basis, $\chi^{sc}_{Q,Q'} = N_q n_Q \delta_{Q,Q'}$, and we can use the eigenvalues $n_Q$ to characterize various possible phases of the GL-LLL model. In the 'normal' liquid state, all LLL states are degenerate, i.e., all $n_Q$ are equal and microscopic ($n_Q \sim N^{-1}_\phi$). In the Abrikosov vortex lattice, Cooper pairs condense into one of the states, say $Q = Q_A$, and $n_{Q_A}$ becomes macroscopic (i.e., $N_q n_{Q_A} \to \infty$ for $N_q \to \infty$). Thus, the pairing susceptibility $\chi^{sc}_{Q_A,Q_A}$ diverges in this phase (linearly with $N_q$ if there is ODLRO, sublinearly if there is algebraic order). In contrast, the SCDW state differs from the 'normal' state by spontaneous breaking of the LL degeneracy: $n_Q$ becomes a function of $Q$, reflecting the modulation in $\langle |\psi(r)|^2 \rangle$. However, all $n_Q$'s remain microscopic, ensuring only short-ranged superconducting correlations and a finite pairing susceptibility in all channels. In this sense, the SCDW is more closely related to the 'normal' state than to the Abrikosov state.

In an infinite, strictly 2D system $n_Q$ will be independent of $Q$ even in the SCDW phase [17]. In a finite system, however, $\langle |\psi(r)|^2 \rangle$ will not be uniform in the SCDW
Figure 4.1: Correlation function $G(r)$ for $N_{\phi} = 224$ at $1/g^2 = 0.02$. Darker areas correspond to larger values of $G(r)$. The point $r = 0$ is near the lower left corner.
Figure 4.2: Maxima of $G(r)$ for various system sizes at $1/g^2 = 0.02$, plotted as a function of $r \equiv |r|$. Straight lines are exponential fits $G(r) \sim \exp(-r/\xi)$. Inset: Size dependence of $\xi$.

$n_\mathbf{Q}$ can be directly related to this density modulation through $\sum_\mathbf{Q} n_\mathbf{Q} |\varphi_\mathbf{Q}(r)|^2 \propto \langle |\psi(r)|^2 \rangle$. By monitoring the $n_\mathbf{Q}$’s, in particular their size dependence and relationship to density modulation, we can study the character of phase correlations in the vortex solid.

4.4 Results and discussion

We now turn to our numerical results. The standard MC technique is used, as described in Chapter 3.2. We use $2 \times 10^5 - 5 \times 10^5$ passes through the entire system for
equilibration and between $2 \times 10^5$ and $10^6$ passes for averages, in proportion to the system size, which varies from $N_\phi = 56$ to 440.

Fig. 4.3 shows $G(r)$ for a 2D solid at a temperature $1/g^2 = 0.02$, near but below the melting temperature. Note that, as $|r|$ increases, the contrast diminishes, indicating that the phase order is falling off. The maxima of $G(r)$ form a triangular lattice which reflects positional order of a vortex solid, but the width of individual peaks grows with distance because of thermally induced bulk and shear modes of the solid.

Fig. 4.4 shows maxima of the function $G(r)$ for various system sizes at $1/g^2 = 0.02$, plotted as a function of $r \equiv |r|$ [18]. The straight lines are exponential fits of the form $G(r) \sim \exp(-r/\xi)$. The apparent correlation length has a strong size dependence (inset), fitting very well to the functional form $\xi \propto N_\phi^{-1/2}$. This indicates that, in the thermodynamic limit, phase coherence decays to zero in a faster than exponential manner, consistent with the predicted Gaussian form. We believe that these data conclusively rule out any possibility of a power-law decay. It is now clear that the formation of a vortex solid in 2D cannot be associated with freezing into Abrikosov state, in which there is some form of phase order.

Next, we calculate the largest eigenvalue of the matrix $\langle c_q c_{q'}^\dagger \rangle$, $n_Q$, and the corresponding eigenstate $\varphi_Q(r)$. $n_Q$ has a $\sim N_\phi^{-1}$ size dependence (Fig. 4.4), which also indicates the absence of any form of Bose condensation in the thermodynamic limit. In our finite system the eigenstates $\{\varphi_Q(r)\}$ have the triangular symmetry of the Abrikosov lattice, although there is no a priori reason why the natural basis $\{\varphi_Q(r)\}$ should coincide with the Abrikosov basis in the $N_\phi \to \infty$ limit.
Figure 4.3: The largest eigenvalue $n_q \equiv N^\alpha_{\phi} \chi_{\phi}^{q}$ of the matrix $(c_q c_q^* )$. Inset: Probability distribution $P(\beta_A)$ for the Abrikosov factor.
Further insight can be obtained from the generalized Abrikosov factor $\beta_A[\psi] = \frac{\langle |\psi(r)|^2 \rangle}{\langle |\psi(r)|^2 \rangle^2}$, where the bars indicate volume averages. $\beta_A[\psi]$ measures the "smoothness" of $|\psi(r)|^2$; it is smallest ($\beta_A[\psi] = \beta_A \equiv 1.16$) in the ground state and equals 2 in the completely uncorrelated liquid phase. $\beta_A[\psi]$ plays a role of the many-body interaction in the vortex system and assumes a sharp value in the thermodynamic limit [3]. This is apparent in Fig. 4.4 (inset), where we find $\langle \beta_A \rangle \approx 1.19$ at $1/g^2 = 0.02$. It can also be seen that the Abrikosov vortex lattice configuration with $\beta_A[\psi] = \beta_A$ is completely absent from the thermal ensemble [19]: only those vortex configurations which have $\beta_A[\psi] = 1.19$ contribute to thermal averages in the $N_\phi \to \infty$ limit. Since $\beta_A[\psi] = 1.19$ is even larger than the value 1.18 for the square Abrikosov vortex lattice state, we expect such configurations to be rather disordered, difficult to individually distinguish from configurations contributing to the 'normal', strongly correlated liquid with slightly higher $\beta_A[\psi]$. This point is illustrated in Fig. 4.4.

A randomly selected representative of the thermal ensemble [Fig. 4.4] shows considerable positional disorder. When an average is taken over the full ensemble of such configurations, however, the resulting $\langle |\psi(r)|^2 \rangle$ [cf. Fig. 4(b)] does exhibit a triangular modulation. Fig. 4.4 incidentally confirms that, at this temperature, the system is in the solid phase, consistent with independent shear modulus calculations of the previous chapter.
Figure 4.4: A snapshot of the vortex configuration $|\psi(r)|^2$ for a system of $N_\phi = 120$ vortices equilibrated at $1/g^2 = 0.02$. Dark areas are minima of $|\psi(r)|^2$ (vortex cores).

Figure 4.5: Average density $\langle |\psi(r)|^2 \rangle$, revealing the triangular symmetry of the density modulation.
4.5 Conclusions

In summary, we present clear numerical evidence that the 2D vortex solid is a phase which is quite distinct from the Abrikosov vortex lattice state (except at $1/g^2 = 0$): the phase correlations are short ranged, there is no condensate of Cooper pairs, and the Abrikosov lattice state does not contribute to the statistical ensemble in the thermodynamic limit. Instead, a 2D vortex solid is an example of a charge density-wave of Cooper pairs, a novel phase described in Ref. [8].
CHAPTER IV REFERENCES

[7] J. A. O’Neill and M. A. Moore, Phys. Rev. B 48, 374 (1993) have argued that in 2D there is only a vortex liquid phase and no vortex freezing transition. Their analysis is based on the assumption that the loss of ODLRO will be accompanied by a loss of long-range positional order of the vortices. Our results are inconsistent with this assumption.
[14] This implies a small amount of pinning created by the boundary conditions for finite $N_d$. However, the strength of this pinning potential vanishes in the thermodynamic limit.
[15] Since states $\varphi_Q$ are extended, the phenomenon of Bose condensation, or equivalently, the macroscopic occupation of a single mode, would inevitably induce long-ranged phase coherence (ODLRO) with spatial structure particular to that mode.

[16] Since $\langle \psi(r)\psi^*(r') \rangle$ is not gauge invariant there is some freedom in defining a gauge-invariant two-point correlation function. This freedom has no effect on our results and conclusions (see below).


[18] For small $N_\phi$, the system has some anisotropy produced by the imposed periodic boundary conditions. The data of Fig. 2 were obtained by thermal averaging for vectors $\mathbf{r}$ from the second sextant of the $xy$ plane, where $G(\mathbf{r})$ falls off most rapidly. This plot should still be considered an upper bound to $G(\mathbf{r})$ in an infinite system.

[19] The system is never in a pure $\varphi_\mathbf{q}(\mathbf{r})$ state at this temperature, but is always a mixture of many $\varphi_\mathbf{q}(\mathbf{r})$ states.
CHAPTER V

3D/2D Crossover in Layered High-$T_c$ Superconductors

5.1 Introduction

One of the most striking features of the CuO-based high-$T_c$ superconductors is their extreme anisotropy. In the superconducting state, their coherence length is much larger in the $ab$ plane than in the $c$ direction; in the normal state, they have comparably anisotropic conductivities. For example, the commonly studied hole-doped superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO) is reported to have a mass anisotropy $\gamma \sim 150$, while that of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) is only in the range of 5–7.

In the regime of moderate anisotropy, the phase diagram of a clean, type-II superconductor in the magnetic-field/temperature $(H-T)$ plane is believed to be divided into two regimes (in addition to the usual Meissner phase from which flux is excluded). These are the vortex lattice phase, characterized by a three-dimensional (3D) Abrikosov flux lattice, and a fluid phase of melted flux liquid. The latter exists even in the low-$T_c$ superconductors, but is very difficult to observe, because of the low temperatures and relatively long coherence lengths, which conspire to minimize
the thermal fluctuations which are responsible for flux lattice melting.

In the extremely anisotropic limit, which characterizes BSCCO, several workers have raised the possibility of an additional phase [1, 2, 3, 4, 5]. One possibility is the so-called supersolid phase [3, 5], described by Nelson and coworkers [5] as a three-dimensional vortex lattice with a finite density of interstitial flux lines as defects. At low temperatures the interstitials are absent, and the sample can carry infinitesimal currents along the c axis without dissipation. At higher temperatures, if the lattice does not melt first, interstitial vortex lines may permeate the sample in a kind of a delocalized state, in which the lines are not straight but instead, wander in the transverse (ab) direction. In this state, a vortex lattice still exists, with long-range 3D geometrical order, but because the line defects are free to move, they cause dissipation and the sample is not superconducting.

A different, "superconducting charge density wave" (SCDW) phase, which does not involve flux lattice defects, has been proposed for extremely anisotropic layered systems by Tešanović [4]. This phase is characterized by a perfect 3D long-range order in the average local Cooper pair density $\langle |\psi(r)|^2 \rangle$, but no long-range phase coherence in any direction. For small interlayer coupling, this theory predicts that the average modulation of Cooper pair density is weak, so that the predominant vortex fluctuations are in-plane [i.e., two-dimensional (2D)]. The theory of 2D solids then predicts that rms deviations of vortices from their equilibrium positions will be large, and that positional correlations between vortices in different layers will be also weak.
In this chapter, we present strong numerical evidence that an intermediate quasi-2D regime in the solid phase does exist in highly anisotropic high-$T_c$ superconductors. Our method is to carry out Monte Carlo simulations on a Lawrence-Doniach model [6] that we [7, 8] and others [9] have used to treat fluctuations in layered high-$T_c$ superconductors in a high magnetic field. The superconducting order parameter is expanded in products of lowest Landau level states in the $ab$ plane and tight-binding Bloch states in the $c$ direction. The phase diagram is then a universal function of a dimensionless effective temperature $T$ and effective interlayer coupling $\eta$, both of which depend on temperature $T$ and magnetic field $B$. We characterize the vortex lattice by the helicity modulus (superfluid density) $T$ in the $c$ direction, and shear modulus $\mu$ in the $ab$ plane.

For samples as large as 120 flux lines and 10 layers, we find two conventional phases in appropriate regions of the phase diagram. These are a solid phase, characterized by nonzero shear modulus in the $ab$ plane and a nonzero superfluid density (helicity modulus) in the $c$ direction; and a liquid phase, in which both these quantities are zero. Within the solid phase, if the anisotropy is large enough, we recognize two different fluctuation regimes separated by a smooth crossover. In the '3D' solid, found at low temperatures or low fields, the helicity and shear moduli are well approximated by mean-field theory, suggesting that the order-parameter fluctuations are essentially three-dimensional. In the '2D' solid, occurring at moderate fields and temperatures, the helicity modulus deviates significantly from the mean-field result and the shear modulus approaches the value characteristic of a purely 2D system, sug-
gesting 2D order-parameter fluctuations. This ‘2D’ solid regime occurs only in highly anisotropic systems, probably including BSSCO at large enough magnetic fields and temperatures, but not YBCO.

There appears to be no phase transition separating 2D and 3D solids. Instead, the 3D/2D transition is manifested by a smooth crossover of $T$ from nearly mean-field 3D behavior $T \sim \eta$ at large $\eta$, to a 2D, fluctuation-dominated regime $T \sim \eta^2$ at small $\eta$. In the limit $\eta \to 0$ the shear modulus smoothly approaches a finite value characteristic of a purely 2D vortex lattice. At the end of this chapter we discuss the possibility that this dimensional crossover may account for the disappearance of the neutron scattering peaks in BiSr$_2$Ca$_2$CuO$_{8+\delta}$ at high fields.

5.2 Model

Our model has been described in several previous papers [7, 8]. We assume a Ginzburg-Landau (GL) free energy functional appropriate to a layered superconductor, and a GL parameter $\kappa \gg 1$ (extreme type-II limit), so that the local magnetic field $B$ can be approximated by the applied field. With this latter assumption, we can omit the field energy, since it does not fluctuate, and the free energy functional takes the form

$$F[\psi] = d \sum_n \int d^2r \left\{ a(T)|\psi_n(r)|^2 + t|\psi_{n+1}(r) - \psi_n(r)|^2 + \frac{1}{2m_\perp} \left[ \left( -i\hbar \nabla_\perp - \frac{e^*}{c} A \right) \psi_n(r) \right]^2 + \frac{b}{2} |\psi_n(r)|^4 \right\}.$$
Here $\psi_n(r)$ is the complex scalar order parameter in the $n$-th layer, $d$ is the layer thickness, $a(T)$, $m_\perp$, and $b$ are material-dependent parameters, and $|e^*| = 2e$ is the charge of a Cooper pair. $t$ is the strength of the interlayer Josephson coupling and is related to the effective mass anisotropy $\gamma \equiv \sqrt{m_\parallel/m_\perp}$ via [7] $t = \hbar^2/(2\gamma^2 m_\perp s^2)$, where $s$ is the periodicity of the layered structure. We take the applied field $B \parallel z$, i.e., perpendicular to the layers.

By choosing the gauge $A = -By \hat{z}$, we can expand the order parameter in degenerate lowest Landau level (LLL) states of the Hamiltonian $(2m_\perp)^{-1}(-i\hbar \nabla - e^*A/c)^2$ as

$$
\psi_n(r) = (\sqrt{3}a_H(T)/4b^2)^{1/4} \sum_k c_{k,n}e^{ikx} \exp[-(y - k\ell^2)^2/2\ell^2],
$$

where $k$ is the LLL momentum, $\ell = (\hbar c/2eB)^{1/2}$ is the magnetic length, and $a_H(T) \equiv a(T)[1-B/H_{c2}(T)]$. The upper critical field $H_{c2}(T)$ is defined by $a(T)+\hbar eH_{c2}(T)/(m_\perp c) = 0$. The number of independent terms in expansion (2) is the number of vortices in each plane, $N_\phi = N_x \times N_y = L_xL_y/2\pi \ell^2$. $N_x$ represents the number of vortices arranged in each of $N_y$ rows in an ordered triangular ground state commensurate with the sample dimensions $L_x, L_y$. The vortex lattice constant is $\ell_0 = (4\pi/\sqrt{3})^{1/2} \ell$, and we assume $N_z$ layers in the $z$ direction.

The free energy per vortex is $F = -(kB/\phi_0 N_x)\ln \int \prod_{k,n} dc_{k,n}d\psi_{k,n} \exp(-\mathcal{H}/T)$, where

$$
\mathcal{H} = N_x \sum_{k,n} \left\{-|c_{k,n}|^2 + \eta|c_{k,n+1} - c_{k,n}|^2 + 3^{1/2} 2^{-5/2} \sum_{q,q'} c_{k+q,n}^*c_{k+q',n}c_{k+q+q',n}c_{k+q+q',n}e^{-(q^2+q'^2)\ell^2/2} \right\}.
$$

(5.3)
is the dimensionless energy of the system,

\[ \mathcal{T} = \frac{bk_B T}{a_H(T)\pi \ell^2 d} \]  

(5.4)

is the dimensionless effective temperature, and

\[ \eta = \frac{t}{|a_H(T)|} \]  

(5.5)

is the effective interlayer coupling. The entire phase diagram of a layered superconductor in this representation can therefore be characterized in terms of the two parameters \( \mathcal{T} \) and \( \eta \), as has been previously noted by several workers [9, 10].

As discussed in Ref. [7], the parameters of this model can be related to experimental quantities other than the observed melting curve. In particular, if \( a(T') \) is linear,

\[ \mathcal{T} = \frac{2\pi}{\phi_0} \frac{2\kappa^2 k_B}{[H_d(T) - B]^2 d} BT \]  

(5.6)

and

\[ \eta = \frac{\phi_0}{2\pi} \frac{1}{[H_d(T) - B]\gamma^2 s^2} \]  

(5.7)

where \( \phi_0 = hc/2e \) is the flux quantum. In 2D systems (\( \eta = 0 \)), this theory predicts that the melting line is a curve of constant \( \mathcal{T} \). Indeed, it has been experimentally verified that in the high-field regime \( B \) and \( T \) enter only in the combination appearing in the functional form (6) [11], thus demonstrating the validity of this approach in 2D.

With eq. 5.3, \( \mathcal{H} \) is expressed in a form suitable for evaluating various quantities by Monte Carlo (MC) simulations, the coefficients \( c_{k,n} \) being viewed as classical fluctuating variables in a canonical ensemble. We have done calculations on cells of
dimensions $N_x \times N_y \times N_z$ of $7 \times 8 \times 10$ and $10 \times 12 \times 8$, with periodic boundary conditions in all three directions. Several test calculations were done on systems up to four times larger in the $ab$ plane, with no indication of a significant size effect in the averages. We use about $10^4$ passes through the sample for equilibration, and evaluate the MC averages using an additional $5 \times 10^4$ passes. Error estimates are obtained from deviations among averages over shorter time intervals.

We characterize our numerical results by two quantities. The first is the lattice shear modulus $\mu = (\partial^2 \mathcal{F}/\partial \theta^2)_{\theta=0}$, where $\theta$ is the angle of a uniform shear applied to the vortex system in the $ab$ plane. The explicit form for $\mu$ in terms of expansion coefficients $c_k$ in 2D has been given in Chapter III [12]; the generalization to 3D is straightforward. The mean-field value of the shear modulus is $\mu^{MF} = 0.410 k_B T/(\beta A T)$, where $\beta_A = 1.159595...$ is the Abrikosov ratio.

The second characteristic quantity is the component $\mathcal{T} = (\partial^2 \mathcal{F}/\partial A'^2)_{A'=0}$ of the helicity modulus, or superfluid density tensor[13], in the $c$ direction. Here $A'$ represents a constant vector potential added to the existing vector potential $A$, in order to generate a phase twist in the $c$-direction. A finite $\mathcal{T}$ represents a material which is perfectly conducting in the $c$ direction, and hence is an indicator for a material which has entered into the superconducting state. As has been discussed previously [8], the in-plane components of the helicity modulus tensor are zero even in the 3D lattice state of an unpinned defect-free superconductor, because the lattice can slide freely in the absence of pinning. Like $\mu$, $\mathcal{T}$ can be evaluated as an equilibrium quantity; the
result is

$$\Upsilon = \Upsilon^{MF} \frac{1}{N_x N_z} \frac{\beta_A}{2} \left[ \langle N_x \sum_{k,n} \Re \{ c_{k,n} c_{k,n+1}^* \} \rangle - \frac{2\eta}{T} \left( \left\langle N_x \sum_{k,n} \Im \{ c_{k,n} c_{k,n+1}^* \} \right\rangle \right)^2 \right],$$

(5.8)

where $\Upsilon^{MF} = 4\eta k_B T (2\pi s/\phi_0)^2 / (\beta_A T)$ is the mean-field value of the helicity modulus.

5.3 Results and discussion

Fig. 5.2 shows both the helicity modulus $\Upsilon$ and the shear modulus $\mu$, for several different temperatures $T$, as a function of the dimensionless interlayer coupling parameter $\eta$. Both quantities are plotted in units of their respective mean-field values, $\Upsilon^{MF}$ and $\mu^{MF}$. The highest temperature shown, $T = 0.020$, lies just below the melting temperature of a 2D lattice in the thermodynamic limit $T^{2D} \approx 0.022$ [14].

The Figure makes dramatically clear that there are two distinct fluctuation regimes within the vortex solid phase. In the first ('3D') regime, the helicity modulus exhibits mean-field behavior, $\Upsilon/\Upsilon^{MF} \sim 1$. As the coupling is decreased at fixed $T$, the helicity modulus crosses over to a '2D' non-mean-field regime, where apparently $\Upsilon/\Upsilon^{MF} \propto \eta$. The cross-over between the '3D' and '2D' regime appears to be smooth, without a phase transition [15], in this disorder-free sample. Near the crossover value of $\eta$, the shear modulus also crosses over from its '3D' behavior to a value obtained in a purely 2D calculation [12].

The results of Fig. 5.2 suggest that in the '2D' solid, the rms deviations of vortices from their equilibrium positions will be large (much larger than just a fraction of the
Figure 5.1: Plot of the scaled helicity modulus $\Upsilon/\Upsilon^{MF}$ and scaled shear modulus $\mu/\mu^{MF}$ vs coupling $\eta$ for various temperatures $T$, for two lattice sizes: $N_x \times N_z = 56 \times 10$ (solid symbols), and $120 \times 8$ (open symbols). $\Upsilon^{MF}$ and $\mu^{MF}$ represent the mean-field helicity and shear moduli. Strictly 2D values of $\mu$ are found for $\eta = 0$. The 3D/2D crossover at a given temperature $T$ is manifested by the crossover from the mean-field behavior $\Upsilon/\Upsilon^{MF} \sim 1$ to $\Upsilon/\Upsilon^{MF} \propto \eta$, and by a crossover of $\mu$ to its 2D value. The lines are guides to the eye.
lattice constant). This also follows from consideration of the purely 2D limit, since in this limit these deviations would diverge logarithmically with sample area. If this is also true in the fluctuation-dominated ‘2D’ regime just described, then a melting theory based on the Lindemann criterion would incorrectly predict melting. Clearly, however, the vortex lattice remains solid in the ‘2D’ regime, since the shear modulus has a finite value. Since the helicity modulus is very small in the ‘2D’ solid, the vortex lattice is very soft in the longitudinal (∥c) direction. The instantaneous positional correlation between vortex “pancakes” in different planes will therefore be weak.

An unusually large vortex displacement in the vortex solid phase has previously been predicted by Moore [16]. Using a harmonic approximation to the GL-LLL energy functional, he finds that the transverse mean-square deviations are given by

$$
\langle \mathbf{u}_{\perp} \cdot \mathbf{u}_{\perp} \rangle = \frac{1}{4\pi} \left( \rho_c c_{66} \right)^{1/2} \frac{k_B T}{\phi_0 (T \mu)^{1/2}},
$$

where $\rho_c = (2\pi s)^{-1} (\phi_0/2\pi)^2 \tilde{T}$ is the $c$ component of the superfluid density tensor, and $c_{66} = (2\pi s)^{-1} \mu$ is the shear modulus of the lattice per unit volume. Evidently, in this approximation, $\langle \mathbf{u}_{\perp} \cdot \mathbf{u}_{\perp} \rangle$ becomes arbitrarily large for sufficiently small $T$. The Lindemann criterion would then predict a spuriously low melting temperature in a regime where the system is known to be a solid (since it has a finite shear modulus).

Besides the ‘3D’ to ‘2D’ crossover, we also observe the usual first-order [9] “melting” transition from the solid phase of either kind into a vortex liquid phase. This transition is characterized by an apparently discontinuous jump of both the helicity and shear moduli to zero as reported previously [8]. The validity of using the disappearance of $T$ as a signature of melting has been confirmed by recent transport
measurements on high-quality single crystals of \((\text{La}_{1-x}\text{Sr}_x)_2\text{CuO}_4\) [17], which find that
the c-axis resistivity becomes finite at the irreversibility line. We can understand this
behavior if the individual planes simultaneously decouple and lose their in-plane crys­
talline structure at the irreversibility line. The liquid phase is characterized by “zero-
dimensional” (‘0D’) order-parameter fluctuations, in which the “pancakes” fluctuate
independently. For values of coupling associated with the ‘2D’ regime \((\eta < 0.001)\),
the melting transition occurs near the strictly 2D melting point \(T^{2D}\). The melting
transition directly from the ‘3D’ vortex solid to a vortex liquid occurs, of course, at
higher temperatures, i. e., \(T > T^{2D}\), because of nonzero values of the coupling \(\eta\).
Because of the first-order nature of the transition [9], and the associated hysteresis,
it is difficult to pinpoint the melting transition numerically with great precision.

In Figs. 5.3a and 5.3b, we sketch the \(B-T\) phase diagram of a BSCCO-like super­
conductor with high anisotropy, and of a moderate-anisotropy YBCO-like supercon­
ductor. Material parameters appropriate to these materials are, for BSCCO, \(\gamma = 150,\)
\(H_{c2}(0) = 440\) kOe, \(T_{c0} = 85\) K, \(\kappa = 100, d = 4\) Å; and for YBCO, \(\gamma = 7,\)
\(H_{c2}(0) = 300\) kOe, \(T_{c0} = 93\) K, \(\kappa = 100, s = 14\) Å, \(d = 8\) Å. Note that eq. 5.7
implies that \(\eta\) for a given material can never be smaller than \((\phi_0/2\pi)/[H_{c2}(0)\gamma^2s^2]\).
Using this condition, and the above parameters, we obtain the remarkably small limit
\(\eta > 0.00014\) for BSCCO, and \(\eta > 0.01\) for YBCO. This estimate makes BSCCO, but
not YBCO, a strong candidate for the ‘2D’ solid state. In YBCO, one would expect
a direct melting from the ‘3D’ vortex solid into the vortex liquid, with no intervening
crossover into a ‘2D’-like region.
It might be objected that, for such extreme anisotropies, our Monte Carlo procedure might not be sensitive enough to detect any effect of the coupling. In rebuttal, we note that, near the crossover $\eta$, the shear modulus already exceeds its 2D value, indicating a clear effect of coupling. Furthermore, the calculated value of $\eta$ at the 3D/2D crossover is consistent with expectations based on a simple argument: The latent heat per vortex for in-plane melting is known to be [14] about 2% of the mean-field condensation energy per vortex, $|H^{MF}| = 1/\beta_A$. On the other hand, it would require an energy of $4\eta/\beta_A$ (per vortex) to entirely decouple the layers. Thus, the unmelted planes should show signs of decoupling without melting only if $4\eta/\beta_A < 0.02/\beta_A$, or $\eta < 0.005$. This value is indeed consistent for our estimate for the 3D/2D crossover.

Finally, we briefly speculate on the possible experimental significance of our results. The dimensional crossover found here suggests a possible explanation for some recent neutron diffraction experiments on BSCCO [18]. In these experiments, the structure factor peaks disappear at magnetic fields above $\sim 600$ G [18]. If such samples were field-cooled in fields $B > B_x$, the system would be taken across our '0D'/2D' melting line (see Fig. 5.3a). Once in the '2D' region of the phase diagram, the individual layers, being very weakly coupled, might freeze out of registry, or into a disordered state, depending on the nature of the random pinning potential. Such a scenario could produce a disordered 2D vortex lattice in every layer, with very little correlation between the layers. The corresponding screening magnetic field would be disordered along the $c$-axis, resulting in the disappearance of the neutron diffraction signal. On the other hand, for cooling in a field $B < B_x$, the vortex
lattice would freeze directly into the '3D' state. In this case, the interlayer coupling is strong enough to make the layers both internally ordered and mutually correlated on some finite length scale, even in the presence of disorder [19]. This would result in well-defined, straight flux lines [21] and a strong neutron diffraction pattern. This pattern should gradually disappear as the field sweeps across $B_x$ into the '2D' solid, as is observed experimentally. It is noteworthy that no such disappearance has been observed in YBCO [20], which has no '2D' region in the $H$-$T$ plane.

Fig. 5.3 suggests another possible explanation for the structure factor disappearance, which does not invoke disorder. If the mean-square displacement is adequately expressed by eq. 5.9, then in the '2D' regime the Debye-Waller factor $\exp(-2W)$ for a structure factor peak with $k\|c$ will be very small, even for the smallest $k$, while in the '3D' solid it should be closer to unity. This might also lead to a disappearance of the structure factor peaks for $k\|c$, as observed.

The crossover from a '3D' to a '2D' solid might have other experimental implications, specifically in regard to the analytic form of the melting curve. In BSCCO, at fields below $B_x$, where the '3D' solid takes over from the '2D' state, the freezing line starts to deviate from its 2D value, leading to a noticeable kink in the freezing line. Indeed, such a kink, or upturn, may have been observed in irreversibility line measurements on BSCCO [22], very near the field where the neutron diffraction peaks vanish ($\sim 600$ G). A similar feature in the melting curve has been observed in artificial NbGe/Ge multilayers with variable anisotropy [23], and in oxygen-depleted samples of YBCO [24]. Deoxygenating YBCO is known to increase the mass anisotropy $\gamma$;
Figure 5.2: (a) Phase diagram of a BSCCO-like material with large anisotropy. Vertical-hatched line: mean-field $H_{c2}$, separating normal region from vortex liquid phase, characterized by '0D' fluctuations. Solid line: melting transition of vortex lattice. Broken line: 2D melting line, $T = T^{2D}$, which nearly coincides with 3D melting transition except at very high and very low fields, where the effective coupling strength $\eta$ is large. $B_x$ denotes the field where the melting line starts to deviate from 2D behavior at low fields. The quasi-'2D' regime within the vortex solid phase is separated from the conventional, nearly mean-field, '3D' vortex solid by a smooth crossover (diagonal hatched area). (b) Phase diagram of a YBCO-like superconductor with moderate anisotropy. Solid, broken, and vertically hatched lines as in (a). In this case, the vortex freezing transition lies well above the 2D melting line, and the vortex liquid freezes directly into the '3D' vortex solid with no intervening quasi-'2D' regime.
so such a kink in the melting line would be expected on the basis of Fig. 5.3(a). In BSCCO the crossover field, which is given implicitly by \( \eta \sim 0.001 \) (see Fig. 5.2), \( T \sim 0.022 \), corresponds to the value \( B_x \sim 550 \) G. Although the LLL approximation is probably not quantitatively reliable at such low fields, the rough agreement with experiment is noteworthy.

The '2D' solid described here differs significantly from the so-called supersolid phase [5]. In the latter, the helicity modulus is identically zero, whereas in the '2D' phase it appears to be finite, if very small for large anisotropy. Furthermore, there is no sharp phase transition between the '2D' and '3D' solids, whereas there should be such a phase transition between the supersolid and true superconducting phase. It is conceivable, however, that the absence of a supersolid phase in our model is due in part to our boundary conditions. With periodic boundary conditions and a commensurate cell size, as in our calculations, interstitial flux lines can only be formed in pairs with line vacancies. Since this process is energetically costly, the crystal melts before it becomes statistically significant. Therefore, it would be useful to carry out this calculation with different boundary conditions which would be compatible with the entrance of unpaired interstitials. On the other hand, the '2D' solid phase closely resembles the so-called SCDW state [4]: it has long-ranged order in density, \( |\psi(r)|^2 \), and an approximately 2D value of the shear modulus. The latter feature suggests that the vortices move diffusively within the planes, with large rms deviations. If the '2D' solid phase is in fact the SCDW phase, it would be expected to have only finite-range phase coherence in the \( ab \) plane, and no macroscopic occupation of a single
LLL mode by the Cooper pairs [25]. If, in addition, the '3D' solid is characterized by macroscopic occupation of a single mode, there is a true 3D/2D phase transition rather than just a crossover. The present work does not conclusively rule out such a possibility, since the helicity modulus would be finite in both phases.

In view of the 3D/2D crossover found here, it might be of interest to investigate the complementary possibility of a 0D/1D crossover. The '1D' phase would correspond to a state with a finite helicity modulus and a zero shear modulus, i.e., a line liquid phase. This phase has been reported to occur in both weakly frustrated isotropic and highly anisotropic 3D XY models [26]. In the LLL model, such a phase might be expected for large values of $\eta$. In most realistic layered superconductors, this region lies close to the mean-field $H_{c2}$. This fact would make the '1D' regime quite difficult to observe experimentally.

5.4 Conclusions

In conclusion, we have found strong numerical evidence for a smooth 3D to 2D crossover in highly anisotropic layered superconductors in a magnetic field. In the '3D' regime, both the c-axis helicity modulus and the shear modulus are well approximated by their mean-field values. In the '2D' regime, the shear modulus has a characteristic 2D value, and the helicity modulus is fluctuation-dominated, varying roughly as the square of the effective interlayer coupling. In highly anisotropic layered superconductors, such as BSCCO, much of the lattice portion of the phase diagram may lie in this quasi-2D regime. We speculate that the 3D to 2D crossover may
be responsible for the disappearance of neutron diffraction peaks in BSCCO above \(\sim 600\) G.
CHAPTER V REFERENCES

[15] This is consistent with the expectation that $\eta$, no matter how small, is a relevant parameter which will always produce finite $T$ in the vortex solid phase.
CHAPTER VI

First-Order Vortex Lattice Melting and Magnetization of YBa$_2$Cu$_3$O$_{7-\delta}$

6.1 Introduction

As we explained in some detail in Chapter II, the mean-field theory recognizes two distinct states of a type-II superconductor: normal, where $\psi(r) = 0$, and superconducting, where $\psi(r) \neq 0$. In the $H-T$ plane these states are separated by the upper critical field line $H_{c2}(T)$, which is usually linear in $T$. In the superconducting state the vortices are arranged in a triangular lattice (fig. 6.1). Magnetization of a superconductor near $H_{c2}(T)$ is given by the Abrikosov formula [1]

$$M(H, T) = \begin{cases} -(4\pi \beta_A)^{-1}[H_{c2}(T) - H]/(2\kappa^2 - 1) & H < H_{c2}(T) \\ 0 & H > H_{c2}(T), \end{cases}$$

(6.1)

where $\beta_A \sim 1.16$ is the Abrikosov ratio. If $H_{c2}(T)$ is linear, so is $M(T)$ in the superconducting region. Since magnetization is continuous, the normal-to-superconducting transition is continuous (see fig. 6.1). In principle then one can imagine measuring $M(T)$ for a given applied $H$ and determining the upper critical field $H_{c2}(T)$ from the locus of points where $M(T)$ has a break in slope. This can only be done for
Figure 6.1: Mean-field phase diagram and magnetization of a type-II superconductor. $H_{c2}$ and $T_{c2}$ denote the upper critical field and temperature, $S$ and $N$ denote superconducting and normal regions.

low-$T_c$ type-II superconductors. As we noted in chapter II, the vortex lattice has to be dynamically disordered (melted) sufficiently close to $H_{c2}$. This is undoubtedly true of both low-$T_c$ and high-$T_c$ superconductors, only in the former case the window in the $H$-$T$ plane where the vortex liquid exists can be so small as to be difficult to measure. Not so for high-$T_c$ superconductors. The vortex liquid phase occupies a significant portion of the mean-field superconducting region (fig. 6.1). The normal-to-superconducting transition line is pushed to much lower fields, where it becomes the melting line $H_m(T)$. The presence of the mean-field $H_{c2}$-line is directly manifested only in a smooth crossover of magnetization (and a much broader crossover of resistivity) from normal behavior at high temperatures to superconducting fluctuations-
enhanced behavior at lower temperatures. It is therefore impossible to experimentally establish one of the defining properties of high-\( T_c \) superconductors: their \( H_{c2}(T) \).

The vortex lattice melting transition, in contrast to the mean-field transition, is expected to be first order, since exactly at the melting line there is coexistence of the low-temperature phase of discrete symmetry (solid) and the high-temperature phase of continuous symmetry (liquid). Although the same is true of the mean-field transition, that transition is continuous, because the phases in equilibrium are identical (\( \psi(r) = 0 \) in both).

As for any first-order transition, there will be an entropy jump at melting, with the liquid phase likely having the higher entropy. Since the Gibbs free energy density
\( \mathcal{G} \) for this system in a magnetic field satisfies

\[
\frac{d\mathcal{G}}{dT} = -SdT - \frac{B}{4\pi}dH,
\]

where \( S \) is the entropy density, vortex melting will also involve a corresponding discontinuity of the flux density. The Clausius-Clapeyron equation for this problem is

\[
\frac{\Delta S}{\Delta B} = \frac{1}{4\pi} \frac{dH_m}{dT}.
\]

Since in all experiments so far the slope of the melting line \( dH_m/dT < 0 \), \( \Delta B > 0 \): the liquid has a higher density, as suggested in fig. 6.1.

In this chapter we calculate the magnetization of the most studied high-\( T_c \) material, \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \), including the effects of fluctuations\[2, 3, 4\]. We also calculate the first-order flux-lattice melting curve \( T_m(H) \) and entropy jump at melting for the same material. Both \( M \) and \( T_m(H) \) are in very good agreement with experiment over a range of magnetic fields.

### 6.2 Model

Our approach is to start from a Ginzburg-Landau free energy functional which includes the field energy in the form \[5\]

\[
G[\psi, A] = \int d^2r \left\{ a(T, z)|\psi(r)|^2 + \frac{1}{2m^*} \left| (-i\hbar \nabla - \frac{e^*}{c} A(r)) \psi(r) \right|^2 + \frac{b}{2} |\psi(r)|^4 + \frac{(B - H)^2}{8\pi} \right\}.
\]

Here \( \psi(r) \) is the complex order parameter, \( A(r) \) the vector potential, \( B = \nabla \times A \), \( e^* = 2e \) is the charge of a Cooper pair, \( H \equiv H\hat{z} \) is the applied magnetic field intensity,
and \( a(T,z) \), \( b \), and \( m^* \) are phenomenological parameters. The periodic \( z \)-dependence of \( a(T,z) \) is introduced to characterize the underlying layered structure. We assume that spatial modulation of \( a(T,z) \), which acts as a potential for Cooper pairs, results in a tight-binding form for \( \psi(r) \) along the \( z \)-axis, thus creating the effective mass anisotropy \( \gamma \). The integral is to be carried out over a fixed sample volume \( V = (\phi_0/H)N_\phi N_z s \), where \( s \) is the periodicity of the layered structure, \( \phi_0 = hc/2e \) is the flux quantum, \( N_\phi \) is the number of flux lines threading the sample, and \( N_z \) is the number of layers. The Gibbs free energy density appropriate to an experiment at fixed \( T \) and \( H \) is

\[
\mathcal{G} = -(k_B T/V) \ln \text{Tr}_{\psi,A} \exp(-G[\psi,A]/k_B T).
\]

(6.5)

We also define free energy 'per flux line per layer' according to \( \mathcal{G}_\phi \equiv (\phi_0 s/H) \mathcal{G} \); internal energy \( G_\phi \) and entropy \( S_\phi \) are defined in the same fashion.

To determine the magnetization, we assume a uniformly fluctuating magnetic induction \( \nabla \times A(r) \equiv B \hat{z} \), so that \( B \) can in principle assume different values in the flux liquid and solid phases. This approximation is most reasonable in the extreme type-II limit (\( \kappa \gg 1 \)) when density correlations among the vortices are well developed and vortices are clearly defined, as expected in the neighborhood of the melting line. In addition, the assumption of uniform \( B \) should be best in the vortex liquid phase, where contributions to the local field \( B(r) \) come from many positionally uncorrelated vortex line segments, as suggested by Brandt [6], but may still be reasonable in the vortex solid phase, even though \( B \) in that phase should develop spatial modulation.

We evaluate the statistical average (2) using the following procedure. First, we ex-
pand the order parameter $\psi(r)$ in a basis which consists of products of lowest Landau level states of the operator $(2m^*)^{-1}(-i\hbar \nabla_L - e^*A/c)^2$ in the $ab$ plane, and Wannier functions from the lowest band of states of the operator $a(T,z) - (2m^*)^{-1}\hbar^2 \partial^2 / \partial z^2$ in the $c$ direction [7]. This leads to an explicit form for all but the last term of the integrand in eq.6.4, in terms of the complex coefficients $c_{k,n}$ of the expansion, corresponding to the $k^{th}$ lowest Landau state in the $n^{th}$ layer [7]. Then the statistical average implied by eq. 6.5 is carried out by a Monte Carlo (MC) procedure, in which the coefficients $c_{k,n}$, and also the average magnetic induction $B$, are considered as fluctuating MC variables. The entire procedure is closely analogous to the “constant pressure” MC ensemble well known in classical fluids [8]. The variables analogous to pressure and volume are $H$ and $B$. The MC step which changes $B$ increases or decreases the area of the $ab$ plane at constant vortex number.

Within this approach, the mean-field approximation to (2) is specified by a pair $\psi(r)$ and $B$, for which $G$ is minimum [5]. In the normal state ($H > H_{c2}(T)$) this is achieved for $\psi(r) = 0$ and $B = H$. In the mixed state, ($H < H_{c2}(T)$), the corresponding minimum is attained for a triangular lattice of straight vortex lines and magnetization

$$M \equiv \frac{B - H}{4\pi} = \frac{H - H_{c2}(T)}{4\pi(2\kappa^2\beta_A - 1)},$$  \hspace{1cm} (6.6)$$

In the limit $\kappa \gg 1$ studied here, this formula becomes identical to the original Abrikosov result 6.1, which has $4\pi(2\kappa^2-1)\beta_A$ in the denominator. Thus our approach and approximations are indeed correct at the mean-field level in this limit. The corresponding mean-field free energy density is $G^{MF} = -(8\pi)^{-1}[H_{c2}(T) - H]^2/(2\kappa^2\beta_A - 1)$. 

In order to execute the MC calculation for YBa$_2$Cu$_3$O$_{7-\delta}$, we use the following set of parameters: $T_{c0} = 93$ K, $dH_{c2}(T)/dT = -1.8 \times 10^4$ Oe/K, $s = 11.4$ Å, $\gamma = 5$, and $\kappa = 52$. Although there is some experimental evidence that $\kappa$ varies with magnetic field [9], we neglect this field-dependence here. In most of our calculations, we have considered a cell containing $N_\phi = 10^2$ vortices and $N_z = 10$ layers. Our results are based typically on $2-3 \times 10^5$ MC passes through the entire sample following $\sim 2 \times 10^4$ MC passes for equilibration.

6.3 Results and discussion

Fig. 6.2 shows the calculated magnetization $M(T)$ of YBa$_2$Cu$_3$O$_{7-\delta}$ as a function of temperature $T$ at three different values of $H$. The mean-field predictions are shown for comparison. There is no sign of a true phase transition at the mean-field transition temperature $T_{c2}(H)$, since $(\partial M/\partial T)_H$ is continuous at that point. Instead, there is an apparently first-order melting transition at a lower temperature $T_m(H)$, as signaled by a weak discontinuity in the magnetization curves (denoted by arrows in the Figure). The melting curve $T_m(H)$ inferred from this discontinuity is shown in the inset to Fig. 6.2; it is in good agreement with experiment.

The general behavior of $M(H,T)$ agrees very well with experiment [12]. For example, the calculated second derivative $(\partial^2 M/\partial T^2)_H$ is negative throughout the vortex liquid phase, in accord with recent measurements based on a differential torque technique [13]. A second-degree polynomial fit to our magnetization results just above the melting temperature $T_m$ yields $(\partial^2 M/\partial T^2)_H = (-0.0038 \pm 0.002) \text{ emu cm}^{-3} \text{K}^{-2}$.
Figure 6.3: Calculated magnetization $M(T)$ of YBa$_2$Cu$_3$O$_{7-\delta}$ at $H = 10$ kOe, 20 kOe, and 50 kOe. Dashed lines represent the mean-field solution (3). Solid lines are spline curves connecting the calculated points. Arrows denote melting temperatures $T_m(H)$, as determined by the discontinuity in $M(T)$. Estimated errors in $M(T)$ are much smaller than the symbol sizes. $N_\phi \times N_z = 10^2 \times 10$. Right inset: locus of the liquid-solid phase boundary in the $H$-$T$ plane, as determined by our calculations and as measured by Farrell et al. and Safar et al.. Left inset: specific heat $C_H$ as a function of magnetic field, taken at two temperatures, $T = 83$ K and 87 K. The dashed line represents the mean-field value $C_H^{MF}/T$. Arrows indicate the approximate location of the fields at melting $H_m(T)$. Straight lines have slopes $-0.0038$ emu cm$^{-3}$ K$^{-2}$ at 87 K and $-0.0030$ emu cm$^{-3}$ K$^{-2}$ at 83 K (see text). $N_\phi \times N_z = 6^2 \times 6$. 
for $H = 20$ kOe, and $(\partial^2 M/\partial T^2)_H = (-0.0030 \pm 0.002)$ emu cm$^{-3}$K$^{-2}$ for $H = 50$ kOe. Experiment [13] also gives a negative $(\partial^2 M/\partial T^2)_H$ for fields in the range 10-20 kOe, and of the same order of magnitude. In the solid phase, we find our calculated $(\partial^2 M/\partial T^2)_H > 0$.

Another striking feature of our results is the crossing of the magnetization curves as a function of temperature. This crossing is also observed in experiment at a similar temperature [12]. In Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, the same phenomenon has attracted much theoretical attention [14, 15], because it is believed to occur at a unique temperature $T^*$ independent of field. In YBa$_2$Cu$_3$O$_{7-\delta}$, experimental data of Welp et al. [12] reveal that magnetization curves do not cross at a single point, presumably because, although layered, YBa$_2$Cu$_3$O$_{7-\delta}$ is only moderately anisotropic. As may be seen in the Figure, our calculated magnetization curves also fail to cross at a single point. Furthermore, the order of the calculated crossings as a function of field is the same as observed in YBa$_2$Cu$_3$O$_{7-\delta}$ [12].

The second derivative of the magnetization can also be calculated using a Maxwell relation

$$\left(\frac{\partial^2 M}{\partial T^2}\right)_H = \left(\frac{\partial(C_H/T)}{\partial H}\right)_T,$$

where $C_H \equiv -T(\partial^2 G/\partial T^2)_H$ is the specific heat of the sample at constant $H$ [16]. Since eq. 6.7 equates the second derivative of one macroscopic quantity to the first derivative of another, it provides a potentially more precise way of determining $(\partial^2 M/\partial T^2)_H$ than a direct calculation of $M(T)$. We have done an MC calculation of $C_H(H,T)$, using the fluctuation-dissipation theorem [17]. Our results are presented in
Fig. 6.2 (inset). Clearly, \( \frac{d(C_H/T)}{dH} < 0 \) in the vortex liquid phase, which implies, in agreement with experiment [13], that \( M(T) \) has negative curvature throughout the liquid phase, not just in the vicinity of the mean-field critical temperature \( T_{c2}(H) \). The straight lines in the Figure are constructed using slopes determined from independent calculations of the magnetization. To an excellent approximation, they are tangent to the specific heat curves, as expected from eq. 6.7, thus confirming the self-consistency of our approach. Experimental specific heat data [18] confirm that \( \frac{d(C_H/T)}{dH} < 0 \) in the vortex liquid phase. In the solid phase, our work predicts that \( \frac{d(C_H/T)}{dH} > 0 \). This is in agreement with recent, high-accuracy specific heat measurements by Schilling and Jeandupeux [19] on large twinned \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \) crystals.

Fig. 6.3 shows the in-plane structure factor \( S(q_{\perp}, 0) \) defined as the thermal average

\[
S(q_{\perp}, 0) = \left\langle \int d^2r \, d^2r' \, |\psi(r)|^2 |\psi(r')|^2 e^{i\mathbf{q}_{\perp} \cdot (r-r')} \right\rangle, \tag{6.8}
\]

for a field \( H = 50 \text{ kOe} \) at two temperatures \( T = 82.8 \text{ K} \) and \( T = 83.0 \text{ K} \), corresponding to the vortex solid and vortex liquid phases. This dramatic change occurs at the temperature of the magnetization discontinuity, thus confirming that this discontinuity signals a melting transition. The regular periodic structure of the maxima in Fig. 6.3 (a) corresponds to an ordered crystalline phase, while the concentric rings of Fig. 6.3 (b) characterize an isotropic fluid. In both cases, the deviations from perfect isotropy can be attributed to the finite size of the sample, as well as to its rectangular shape.

Finally, we address the issue of the order of the melting transition. As indicated
Figure 6.4: (a) In-plane structure factor $S(q_\perp,0)$, divided by the "atomic" structure factor $\exp(-q_\perp^2/4)$, taken in the solid phase at $T = 82.8$ K and $H = 50$ kOe, and averaged over 100 configurations. The central maximum at $q_\perp = 0$ has been removed for clarity. (b) Same as (a), but in the liquid phase at $T = 83.0$ K.
by Fig. 6.3, upon melting, the vortex ensemble undergoes a discontinuous symmetry change. By the well-known argument of Landau [20], the vortex melting transition has to be first-order, with a finite jump in entropy per unit volume $\Delta S$. A critical point (defined by $\Delta S = 0$) cannot exist, and the liquid-solid phase boundary must terminate by intersecting either the coordinate axes or other phase boundaries.

To calculate $\Delta S$, we use a variant of the histogram method of Lee and Kosterlitz [21]. In principle, one should resolve the energy distribution $P(G)$ into two Gaussian peaks at $T_m$, then confirm that the dip between the peaks scales like a surface energy with increasing sample size [22]. In the present case, this would be a formidable computational effort, because $\Delta S$ is small and the two peaks are not resolved at any accessible system sizes. Instead, we perform a long MC run ($\sim 10^6$ passes through the entire lattice) near $T_m$, starting from the system ground state. During the simulation, the system flips $\sim 2-4$ times between the two states in equilibrium. In our standard diffusive sampling algorithm, we can identify continuous (in MC "time") sequences of representatives belonging to the same homogeneous phase. The two phases can be clearly distinguished by their structure factors and mean internal energy.

In Fig. 6.3 we plot the probability distribution of internal energy, $P(G)$, for these two phases in equilibrium at $T_m \sim 83$ K and $H = 50$ kOe, at three system sizes. The low-energy peak always corresponds to the ordered vortex solid phase. Since the entropy change $\Delta S_\phi$ decreases with system size, the value $\Delta S_\phi \sim 0.034 k_B$ should be considered an upper bound to $\Delta S_\phi$ in the thermodynamic limit. $\Delta S_\phi(H = 20$ kOe) has a similar size dependence and is $\sim 30\%$ smaller than $\Delta S_\phi(H = 50$ kOe).
Figure 6.5: Probability distribution $P(G)$ of internal energy at the finite-size melting point $T_m \sim 83$ K, $H = 50$ kOe, and three different system sizes. For each system size, the two separate peaks represent the distributions of energy within the solid and the liquid at the same $T$ and $H$. Because of the weak dependence of $T_m$ on system size, we have used for the zero of $G_\phi$ a size-dependent energy. Horizontal bars denote the calculated latent heats per flux line per layer.
From our calculated $\Delta S$ at melting and the computed slope $(dH/dT)_m$ of the melting curve from Fig. 6.2, we can estimate the magnetization jump $\Delta M$ at melting via the Clausius-Clapeyron relation 6.3. Inserting the calculated values of this slope and of $\Delta S$, we obtain $\Delta M \sim 0.0014 \text{ emu cm}^{-3}$ at $H = 50 \text{ kOe}$, and $\Delta M \sim 0.0005 \text{ emu cm}^{-3}$ at $H = 20 \text{ kOe}$. These values are consistent with the directly calculated $\Delta M$ seen in Fig. 6.2. In experiment, no finite magnetization jump has yet been observed [13, 23], although transport measurements on untwinned YBa$_2$Cu$_3$O$_{7-\delta}$ crystals are widely interpreted as evidence for a first-order melting transition [11, 24].

The null result of Farrell et al. [13] for $\Delta M$ puts an upper bound $\Delta S < 0.003 k_B$ at $H = 20 \text{ kOe}$, a value almost ten times smaller than predicted in the present work. However, as suggested by these authors themselves, the presence of defects may have suppressed the measured $\Delta M$ to some extent. This discrepancy remains to be settled by an experiment which attains perfect reversibility in both temperature and field.

6.4 Line liquid or not?

In the previous section we identified vortex lattice melting by its macroscopic manifestations: discontinuous magnetization and entropy content. Microscopically, there is a discontinuous change of the vortex lattice symmetry as demonstrated by fig. 6.3. This figure, however, does not offer complete information about the structural properties of the two phases. While there is no doubt that the order-parameter density $\langle |\psi(r)|^2 \rangle$ in the solid is periodic in all directions, there are in principle two qualitatively distinct possibilities for the vortex liquid: i) normal liquid in which all correlation lengths are
finite, and ii) line liquid, in which phase coherence along the c-axis is long range. While the normal liquid is non-superconducting, the line liquid would be a superconducting phase with vanishing linear DC resistivity along the c-axis. If the phase which is in equilibrium with the solid were a line liquid (rather than a normal liquid), there would have to be another—possibly continuous—phase transition at a higher temperature from line liquid to normal liquid. We note that it is impossible to just "cross over" from the line liquid to normal liquid, for these two phases are qualitatively different (see below). Also of importance is the fact that should the line-to-normal liquid phase transition turn out to be first order, the phase boundary cannot terminate in a critical point, but must end on the coordinate axes or by intersecting other first-order lines. For unlike water and vapor, which are but quantitatively different phases, line liquid and normal liquid are qualitatively different.

The property which determines whether or not a vortex liquid is normal is whether its helicity modulus is zero or finite. The helicity modulus is a macroscopic quantity defined as

\[ \Upsilon_c = \left( \frac{\partial^2 G}{\partial A'_z^2} \right)_{A'_z=0}, \]  

(6.9)

where \( A' \) is a constant vector potential added to the existing vector potential. This addition does not change the magnetic field, so the free energy \( G \) cannot change either. It would seem therefore that definition 6.9 is trivial. However, the change of \( G \) corresponding to the addition of \( A' \) is to be evaluated in a reference frame where \( A' \) has not been added.

A useful way to think about it is to note that the addition \( A \rightarrow A + A'_z \hat{z} \) induces a
phase twist along the c axis: the Josephson interlayer coupling term of eq. 5.1 becomes

\[ 2\Re\{\psi_{n+1}^*(r)\psi_n(r)\} \rightarrow 2\Re\{\psi_{n+1}^*(r)\psi_n(r)\exp(i2\pi A'_s/\phi_0)\}. \]

In the ground state of the system all layers are in phase, \( \psi_{n+1}(r) = \psi_n(r) \). When \( A' \) is turned on, it will be absorbed in the phases so that \( \psi_{n+1}(r) = \psi_n(r)\exp(i2\pi A'_s/\phi_0) \) for all \( n \). In this new ground state the phase winds along the c-axis. When viewed from the “untwisted” reference frame (without \( A' \) added), this state is an excited state whose energy enters definition 6.9. We note that \( \Gamma_c \) is non-zero only if there is extended phase coherence along the c-axis; in a normal liquid \( \Gamma_c = 0 \), whereas in the solid and line liquid phases \( \Gamma_c > 0 \).
The helicity modulus is also a measurable quantity. Using the definition of the current density $J_z = c(\partial G/\partial A_z)$ and the second London equation $\mathbf{J} = (c/4\pi)\mathbf{A}/\lambda^2$, where $\lambda$ is the magnetic penetration depth, we find

$$\Gamma_c = \frac{1}{4\pi} \frac{1}{\lambda_c^2}. \quad (6.10)$$

Here $\lambda_c$ is the penetration depth in the $c$-direction for external infinitesimal fields applied in the $ab$ plane. When $\Gamma_c > 0$, $\lambda_c$ is finite and the sample exhibits transverse Meissner effect. When $\Gamma_c = 0$, $\lambda_c$ diverges and the sample becomes transparent to external magnetic fields, i.e., normal.

Figure 6.4 shows the helicity modulus of YBa$_2$Cu$_3$O$_{7-\delta}$ as a function of temperature. The most remarkable feature is the discontinuous drop of $\Gamma_c$. Comparison with fig. 6.2 shows that the drop coincides with the melting temperature $T_m$. We conclude that vortex lattice melting for this range of fields is a single-step process in which vortex solid melts directly into a normal liquid, without the intervening line liquid phase. This was experimentally confirmed very recently by López et al. [25].

### 6.5 Magnetic field fluctuations; susceptibility $\chi$

We have seen that the present model gives results for magnetization and specific heat that are consistent with the appropriate Maxwell relation. Another important test of the model, and the assumption of a uniformly fluctuating flux density in particular,
Figure 6.7: Finite-size scaling of fluctuation magnetization.

is the finite-size scaling of fluctuations\(^1\). Magnetic permeability \(\mu\) can be written as

\[
\mu \equiv \left( \frac{\partial B}{\partial H} \right)_T = \frac{4\pi V}{k_B T} \left[ \langle M^2 \rangle - \langle M \rangle^2 \right],
\]

(6.11)

therefore

\[
\langle M^2 \rangle - \langle M \rangle^2 = \mu \frac{k_B T}{4\pi (\phi_0 s / H) N N_z} \frac{1}{N N_z}
\]

(6.12)

In fig. 6.5 we plot the calculated values of \(\langle M^2 \rangle - \langle M \rangle^2\) for two representative points in the \(H-T\) plane; one in the vortex solid and one in the vortex liquid phase. The data points follow approximately straight lines, as expected from eq. 6.11, with a slope close to unity. This is expected, since \(B \sim H\) in the extreme type-II limit at high fields.

\(^1\)I am indebted to Prof. Steven Teitel for bringing this point to my attention.
As straightforward as it is to determine magnetization by the present method, it is very difficult to determine magnetic susceptibility $\chi$ with any accuracy. This is because magnetic field fluctuations lead directly to permeability, not susceptibility (see eq. 6.11). Since $\mu \sim 1$ and $\chi = (1 - \mu)/(4\pi)$, evaluation of $\chi$ would be made unreliable by large statistical errors.

6.6 Conclusions

To summarize, we have presented the first non-mean-field calculation of magnetization in YBa$_2$Cu$_3$O$_{7-\delta}$, using a constant-$H$ Monte Carlo technique in conjunction with a lowest Landau level approximation. Our results yield a magnetization in very good agreement with experiment in both the flux liquid and flux lattice state, as well as a melting curve very close to experiment. Our results provide perhaps the most detailed evidence to date that a Ginzburg-Landau free energy functional, based on a complex scalar order parameter, adequately describes the thermodynamic properties of YBa$_2$Cu$_3$O$_{7-\delta}$ near the flux lattice melting curve.
CHAPTER VI REFERENCES


[16] In actuality $C_H$ is just the superconducting part of the specific heat of a crystal.

[17] Care must be taken here, for $G[\psi, A]$ is explicitly temperature dependent.


[23] A reversible magnetization jump in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ has been recently reported by E. Zeldov et al. Nature 375, 373 (1995).


CHAPTER VII

Dynamics

7.1 Introduction

In the previous chapters we considered type-II superconductors in thermal equilibrium and calculated their macroscopic static properties. Nevertheless, there are situations when one is more interested in dynamical properties. An example of such a property is DC conductivity, the most important transport property of superconductors. Although the process of measurement itself may be perfectly stationary, the transport current results in the time dependence of the phase of the order parameter $\psi(r)$, even at zero temperature. Any transport measurement therefore drives the superconductor out of equilibrium. As a result, DC conductivity is a dynamical quantity.

In the next section we outline the formalism necessary to calculate the c-axis conductivity and $I-V$ characteristics of a layered superconductor in a high magnetic field.
7.2 Ginzburg-Landau dynamics

We construct equations of motion for the order parameter \( \psi(r) \) based on the following assumptions: i) the system is always sufficiently near equilibrium, so that GL functional can be used, and ii) equations of motions are first-order, i.e., dynamics is \textit{overdamped} and the vortex mass is zero:

\[
\frac{\partial \psi(r,t)}{\partial t} = \frac{i e^*}{\hbar} V(r) \psi(r,t) - \Gamma \frac{\delta F[\psi]}{\delta \psi^*(r)} + \eta(r,t) \tag{7.1}
\]

The first term on the right-hand side is the Josephson term; \( V(r) \) is the scalar potential (voltage) at point \( r \) which, in the absence of the remaining terms, rotates the phase of the order parameter according to the Josephson equation \( \dot{\theta}(r) = (e^*/\hbar) V(r) \). The second term is the restoring force, \( \Gamma \) is an (unknown) rate constant. The perturbing influence of the thermal reservoir on the system is included via a random Gaussian force term (Langevin noise) \( \eta(r,t) \), of the following characteristics:

\[
\langle \eta(r,t) \rangle = 0 \tag{7.2}
\]

\[
\langle \eta(r,t) \eta^*(r',t') \rangle = 2 \Gamma k_B T \delta(r-r') \delta(t-t'). \tag{7.3}
\]

A layered high-\( T_c \) system may be well represented by an energy functional of the form 5.1. We will assume this form in the following. Electric current is defined as a functional derivative

\[
j(r) = e \frac{\delta F[\psi]}{\delta A(r)}. \tag{7.4}
\]

In particular, for a layered superconductor, the net current in the \( z \)-direction, \( J_z \equiv \)
\((L_z)^{-1}\langle f d^3r j_z(r) \rangle\), is
\[
J_z = \frac{2\cos}{N_z} \left( \frac{2\pi}{\phi_0} \right) \sum_n \int d^3r \Im(\psi_{n+1}^* \psi_n(r)). \tag{7.5}
\]

Here \(\langle \cdots \rangle\) represents a time average. For completeness we note that \(\psi_n(r)\) is the order parameter in the \(n\)-th layer, and \(r\) is a two-dimensional coordinate. By solving eq. 7.1 for a given \(V(r)\) and by evaluating eq. 7.5, one obtains \(c\)-axis \(I-V\) characteristics of the superconductor.

### 7.3 \(c\)-axis transport at high fields

We will now project eq. 7.1 into the LLL manifold, which, as we noted earlier, represents the high field approximation. It is necessary to expand both order parameter \(\psi_n(r, t)\) and the noise \(\eta_n(r, t)\) in the Landau level basis as follows:
\[
\psi_n(r, t) = \sum_k c_{k,n}(t) \psi_k(r) + \cdots \tag{7.6}
\]
\[
\eta_n(r, t) = \sum_k \eta_{k,n}(t) \psi_k(r) + \cdots \tag{7.7}
\]

Here \(\psi_k(r)\) is the LLL basis 2.6, \(c_{k,n}(t)\) and \(\eta_{k,n}(t)\) are time-dependent complex amplitudes, and the ellipses suggest higher Landau levels. The LLL approximation consists of erasing the ellipses in equations 7.6, 7.7. Particular care must be taken in order to meet the requirements on noise correlations. When we set
\[
\langle \eta_{k,n}(t) \eta_{k',n'}^*(t') \rangle = \frac{1}{2} \Gamma k_B T \delta_{n,n'} \delta_{k,k'} \delta(t' - t), \tag{7.8}
\]
the real-space correlations are
\[
\langle \eta_n(r, t) \eta_{n'}^*(r', t') \rangle = \Gamma k_B T \frac{e^{-|r-r'|^2/4\ell^2}}{4\pi \ell^2} \delta_{n,n'} \delta(t - t'). \tag{7.9}
\]
Note that in the LLL representation the noise no longer looks “white” in space; instead, the coherence length equals the magnetic length $\ell$. The Gaussian term on the right-hand side of eq. 7.9 integrates to unity and can be considered as the “best” approximation to the delta function within the LLL manifold. This is a result of the incompleteness of the LLL set. Furthermore, the pre-factor $\Gamma k_B T$ is only a half of that in eq. 7.3. The other half is carried by the higher LL’s which do not perturb the system by assumption. It is also noteworthy that the perturbing force $\eta_n(r,t)$ at any given time $t$ has the same properties as the vortex liquid at infinite temperature (compare with eq. 4.3).

The energy functional 5.1 becomes

$$F[\{c_{k,n}\}] = s \sum_{k,n} \left\{ \frac{(8\pi)^{1/2} \kappa^2}{\ell L_y} \sum_{q,q'} c_{k,n}^* c_{k+q,n} c_{k+q',n} c_{k+q+q',n} e^{-\kappa^2/2} \right\}, \quad (7.10)$$

and eq. 7.5 becomes

$$J_z = \frac{2c}{N_z \gamma^2} \sum_{k,n} \Im \langle c_{k,n+1}^* c_{k,n} \rangle. \quad (7.11)$$

Equation 7.1 can now be written

$$\dot{c}_{k,n}(t) = -\frac{\epsilon^*}{\hbar} E_0 n s c_{k,n} - \Gamma \frac{\partial F}{\partial c_{k,n}^*} + \eta_{k,n}(t) \quad (7.12)$$

Here we chose $V(r) = -E_0 z \hat{z}$.

Equations 7.10–7.12 form the basis for a future calculation of the c-axis transport properties of high-$T_c$ superconductors.
CHAPTER VIII

Conclusions

In the spirit of the mean-field theory of Abrikosov of 1957, we have applied the lowest Landau level approximation to describe thermodynamics of vortices, vortex lattice melting, and magnetic properties of high-$T_c$ superconductors. We also outlined an extension of this formalism to describe dynamical transport properties of layered superconductors.

The good overall agreement of the theory with experiment is encouraging; however, there are several aspects of the LLL method which deserve further study. We will briefly state two that are most immediate:

- What is the region of validity of the LLL approximation? Common sense suggests a criterion $B > H_{c2}(T)/3$, but our personal conviction is that the LLL method is qualitatively valid to much lower fields. A detailed, quantitative, numerical study of this problem is lacking at present.

- The LLL and the London pictures, often termed respectively the “high-field” and the “low-field” approximations, describe two qualitatively different and mutually exclusive fluctuation regimes. In the former all fluctuations are vortex
fluctuation, while in the latter there are only phase fluctuations. One has to ask whether the intermediate regime has been understood at all. Presently there is no formalism—other than the full Ginzburg-Landau theory—that covers the intermediate fluctuation regime.

These are but two open issues that await solution. Another broad area of topical interest, which we touched upon only tangentially in this thesis, is the thermodynamics and dynamics of superconductivity in disordered media. In this area few things are known for certain and even the experimental situation is far from being clear. To any research worker in the field of high-temperature superconductivity, this is an area of great challenge and opportunity. We hope to address some of the problems related to disorder in a future work.
BIBLIOGRAPHY


[36] H. Kamerlingh Onnes, Leiden Comm. 120b, 122b, 124c (1911).


