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THEORY OF SUPERCONDUCTING ARRAYS IN A MAGNETIC FIELD

The Ohio State University

Ph.D. 1984

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THEORY OF SUPERCONDUCTING ARRAYS IN A MAGNETIC FIELD

DISSERTATION

Presented in Partial Fulfillment of the Requirements

for the Degree Doctor of Philosophy in the

Graduate School of the Ohio State University

by

Wan Y. Shih, B.S.

* * * * *

The Ohio State University

1984

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"Molecular-field Approximation for Josephson-Coupled Superconducting Arrays in a Magnetic Field," W. Y. Shih and D. Stroud, Phys. Rev. B28, 6575 (1983).

"Frustration and Disorder in Granular Superconductors," W. Y. Shih, C. Ebner, and D. Stroud, Phys. Rev. B30, 134 (1984)

"Superconducting Arrays in a Magnetic Field: Evidence of a New Double Transition," W. Y. Shih and D. Stroud, to be published.

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CHAPTER 1: INTRODUCTION

One of the most novel superconducting materials is composed of small grains of superconductor embedded in a non-superconducting host.¹ The latter can be insulator, normal metal or superconductor with a lower transition temperature. The grains can vary in size from 100 Å to microns and can be spherical, square or irregular in shape. A striking feature of such materials is the two-step resistivity transition^{2,3} as is shown schematically in Fig. 1.1. The transition is characterized by two temperatures: T_{co} , the bulk transition temperature of the superconducting grains, and T_c , at which the composite becomes superconducting as a whole. At a temperature near T_{co} , the grains become superconducting but the host remains normal, causing the resistivity of the system to drop dramatically but remain finite. Finally, at a lower temperature T_c , the system as a whole becomes non-resistive at a sufficiently small current density. The lower transition is often due to the onset of weak coupling between grains via the host -- Josephson coupling, if the matrix is an insulator; proximity coupling, for a normal metal host.

While this type of behavior is believed to occur in a number of materials, an even more interesting phenomenon is revealed by

Fig.1.1.1 A schematic of the resistivity vs. temperature of a granular array. T_{C0} is the superconducting transition temperature of the grains and T_C is the temperature at which the system acquires infinite conductivity.

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 specially prepared 2d arrays. The magnetoresistance above T_c is oscillatory in field with a period one flux quantum per lattice cell. This serves as an evidence to support that the lower resistivity transition is due to the phase coherence between grains. The oscillation is due to the modulation of coupling by the field.

The purpose of this thesis is to describe the behavior of such composites in a magnetic field, especially the phase coherence transition at T_c . We will deal with 2d and 3d, ordered arrays as well as disordered ones. By 3d is meant that all of the three dimensions are many times the grain lattice constant, and by 2d that one of the dimensions is only approximately one grain in width.

The model we use to describe these behaviors is a pseudospin one, which has been used by several authors⁷⁻¹³ to describe other properties of the granular superconductors. The grains acquire a gap or superconducting order parameter below the single-grain transition temperature T_{co} . The gap is a two-component order parameter and both its magnitude and phase can vary. The pseudospin model treats the magnitude as if it is fixed at a given temperature but allows the phase to vary freely in the absence of coupling. Moreover, the gap amplitude is absorbed into the intergrain coupling constant. Thus a granular array looks exactly like a collection of "XY" spins with temperature-dependent couplings. The weak intergrain coupling (Josephson or proximity) causes the phases to be coherent below T_c .

The purpose of the introduction of a magnetic field is to affect the coupling. The field produces "frustration"¹⁴ in the coupling so that some of the couplings are ferromagnetic while others tend to orient at an angle other than zero degrees. The existence of frustration means that an ordered state cannot be obtained by minimizing the energies of all weak bonds. Increasing the field serves to vary the frustration continuously.

We consider N superconducting grains in volume V . The i th grain is at $\vec{x}_i$ and has a gap $\Delta_i = |\Delta_i(T)|e^{i\phi_i}$. The coupling energy between grain i and grain j in the absence of a magnetic field is

$$E_{ij} = -J_{ij} \cos(\phi_i - \phi_j) , \quad (1.1)$$

where J_{ij} is the weak coupling between grains. Its form depends on the medium through which the coupling occurs. If the host is an insulator, the coupling is via the Josephson effect and

$$J_{ij} = \frac{\hbar}{2e} I_{ij} \quad (1.2)$$

with¹⁵

$$I_{ij} = \frac{\pi}{2} \frac{|\Delta(T)|}{eR_{ij}} \tanh \frac{|\Delta(T)|}{2k_B T} , \quad (1.3)$$

where I_{ij} is the critical current of a junction between two identical grains each having the same $|\Delta(T)|$. In Eq.(1.3), R_{ij} is the resistance between grains i and j in their normal state and

T is the absolute temperature. If the coupling is through a normal metal via the proximity effect, J_{ij} takes the following form¹⁶

$$J_{ij} = C(1 - T/T_{cs})^2 e^{-r_{ij}/\xi(T)}, \quad (1.4)$$

where C is a constant, T_{cs} is the transition temperature of the superconducting grains, $r_{ij} = |\vec{x}_j - \vec{x}_i|$ is the separation between grains and $\xi(T)$ is the coherence length of the normal metal.

The Hamiltonian describing the entire array in the absence of a magnetic field thus takes the form

$$H = - \sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j), \quad (1.5)$$

where $\langle ij \rangle$ denotes all distinct pairs. The thermodynamics of the model are obtained from the classical partition function

$$Z = \int \prod_i \pi d\phi_i e^{-H/k_B T}, \quad (1.6)$$

which shows the behaviors of the system can be described by a classical XY model with temperature-dependent coupling constants. Thus, in the absence of a magnetic field, the behaviors of an array can be deduced from the known properties of the XY-spin systems. In two dimensions, the arrays would undergo a Kosterlitz-Thouless^{2-5,17-20} transition to become phase coherent at low temperatures while in three dimensions, the phase coherence transition would be a second order

21
one.

With the presence of an external magnetic field the behaviors of the array change dramatically. The Hamiltonian becomes²²

$$H = - \sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \quad , \quad (1.7)$$

where

$$A_{ij} = \frac{2\pi}{\Phi_0} \int_{\vec{x}_i}^{\vec{x}_j} \vec{A} \cdot d\vec{l} \quad . \quad (1.8)$$

In Eq.(1.8), $\Phi_0 = hc/2e$ is an elementary flux quantum and the integral is taken along the path joining the centers of grain i and grain j . There are several approximations involved here. First, the possibility that J_{ij} might depend on the field as well as the temperature is excluded. Secondly, the grain penetration depth is assumed to be much larger than the grain size and so is the host penetration depth than the separation between grains in order that the local field can be approximated by the applied one. Finally, we assume the junctions are not too wide, otherwise A_{ij} should be replaced by an average over the junction width. The model presents a considerable idealization of the composite systems; nonetheless, its behavior is still interesting enough to consider it in detail.

For convenience, throughout the text, we assume that the magnetic field is in z direction, $\vec{B} = B\hat{z}$ and use the gauge $\vec{A} = Bx\hat{y}$. Of

course, the partition function is gauge invariant and so are the properties deduced from it; with this choice, the magnetic phase factor then takes the form

$$A_{ij} = \frac{2\pi}{\Phi_0} B x_{ij} (y_j - y_i) , \quad (1.9)$$

where $x_{ij} = 1/2(x_i + x_j)$ and x_i and y_i are the coordinates of grain i in x and y directions respectively.

It is shown in Appendix B that for an ordered array, the Hamiltonian is periodic in field. Consequently, the thermodynamic properties should also be periodic in field; for example, we find below that for an ordered array, the ground state energy E_g , the phase coherence transition temperature T_c , the helicity modulus Y and the critical current I_c are all periodic in field. The variations of these quantities with field within one period are all extremely non-monotonic, having cusps at all rational values of f , where f is the number of flux quanta per lattice cell. The relative heights of these cusps depend very much on the underlying lattice structure. For example, in the variation of the mean-field transition temperature $T_c^{MF}(f)$ with f , the most conspicuous cusps occur at $f = 1/2$ for a square lattice, at $f = 1/3$ for honeycomb and at $f = 1/2$ and $f = 1/4$ for triangular. It is shown below, that $T_c^{MF}(f)$ as a function of f can be mapped onto the highest energy eigenvalue of a tight-binding electron in a similar lattice in the

presence of a magnetic field.²³⁻²⁴

Furthermore, from careful Monte Carlo simulations, it is found that the presence of a magnetic field may change the nature of the phase coherence transition at T_c . For example, in the case of $f = 1/2$ for both square and triangular lattices, the ground state forms an "antiferromagnetic-Ising-like" vortex configuration and the specific heat diverges at T_c , suggesting that the transition may be of an "Ising-like" variety, as discussed below. Moreover, evidence is found to support the hypothesis that in a triangular lattice at $f = 1/4$, the phase coherence is achieved via a double transition, with the intermediate state being partially ordered.

For a disordered array, at a sufficiently large field, the magnetic phase factors A_{ij} all become larger than 2π . Thus the couplings are essentially randomized so that the array looks very much like a spin glass. After the couplings are randomized, further increase in field will not change the thermodynamics of the array. One therefore expects T_c to drop from its zero-field value at small fields and to saturate at a "spin-glass" value at high fields. Thus, increasing the field allows a disordered array to transform from a disordered ferromagnet to a spin glass.

Recently, Pannetier, Chaussy and Rammal²⁵ have solved the linearized Landau-Ginzburg equations for a honeycomb superconducting wire network to explain the periodic variation of the resistivity

above T_c with magnetic field. The network problem proves to be closely related to the solution of the Schrödinger equation of a tight-binding electron on a similar network in the presence of a magnetic field. This same equation also plays a role in the present problem. Thus the two problems are closely related although not identical.

The rest of this thesis is organized as follows. Chapter 2 deals with small clusters of grains, especially closed loops in various geometries. In Chapter 3, Section 3.1 and Section 3.2 give a brief description of the mean-field approximation and the Monte Carlo method respectively. The rest of Chapter 3 shows the results of 2d arrays: Section 3.3 is for square lattice, Section 3.4 for honeycomb and Section 3.5 for triangular lattice. Chapter 4 discusses various situations in a simple cubic lattice. Finally, we study the effect of disorder in Chapter 5.

CHAPTER 2: LOOPS

In a dilute disordered Josephson or proximity-coupled junction array, the diamagnetism is due to the tunneling currents flowing in a closed loop.²⁶ de Gennes²⁷ has already pointed out that for a disordered superconducting wire network, the topology of the network will affect its diamagnetism. Analyzing the linearized Ginzburg-Landau equations, he noted that a small loop has a critical field beyond which the loop will be driven normal and that the dead-end parts of the network do have a role even though they can not carry currents. A dead-end branch tends to prevent the closed loop from being driven normal. These predictions were later confirmed by Straley and Visscher²⁸ by solving the full Ginzburg-Landau equations although the effects are not as dramatic as predicted by the linearized equations. Therefore, it is of interest to examine the topological effects of a disordered superconducting array, since a superconducting array is a discrete version of a wire network but with more adjustable parameters. We find that a granular loop will behave similarly to a wire loop in the strong-coupling limit while in the weak-coupling regime, it will not be driven normal by an external

field and is unaffected by its dead-end branches.

2.1 Fixed-Amplitude Approximation

A. Single Loop

(i) Derivation

Consider a loop of N weak links in the presence of a transverse magnetic field. For simplicity, we assume the magnitude of the superconducting order parameter in each grain is temperature-independent.

The Hamiltonian is then

$$H = - \sum_{i=1}^N J_{i,i+1} \cos(\phi_i - \phi_{i+1} - A_{i,i+1}) \quad (2.1)$$

where ϕ_i is the phase of the superconducting order parameter of grain i . $J_{i,i+1}$ is the nearest-neighbor coupling energy and $A_{i,i+1}$ is the magnetic phase factor due to the presence of a flux through the loop.

$$A_{i,i+1} = \frac{2\pi}{\Phi_0} \int_{\vec{x}_i}^{\vec{x}_{i+1}} \vec{A} \cdot d\vec{\ell} \quad , \quad (2.2)$$

where $\Phi = \frac{hc}{2e}$ is an elementary flux quantum and $\vec{A}$ is the vector potential. For convenience, we assume a constant nearest-neighbor coupling energy and a constant magnetic phase factor across all junctions. Thus the Hamiltonian simply becomes

$$H = -J \sum_{i=1}^N \cos(\phi_i - \phi_{i+1} - \Delta) \quad , \quad (2.3)$$

where $\Delta = A_{i,i+1}$ is the constant magnetic phase factor across a junction.

The partition function can then be obtained by integrating over all phases ϕ_i ,

$$Z = \int \prod_{i=1}^N \pi d\phi_i \prod_{i=1}^N e^{-\beta H(\phi_i, \phi_{i+1})}, \quad (2.4)$$

where $H(\phi_i, \phi_{i+1}) = -J \cos(\phi_i - \phi_{i+1} - \Delta)$. Let λ_n and $f_n(\phi)$ be the eigenvalue and eigenfunction of

$$\int d\phi' e^{-\beta H(\phi, \phi')}$$

such that λ_n and $f_n(\phi)$ satisfy

$$\lambda_n f_n(\phi) = \int d\phi' e^{-\beta H(\phi, \phi')} f_n(\phi'). \quad (2.5)$$

Let $f_n(\phi) = \frac{1}{\sqrt{2\pi}} e^{in\phi}$ and n be an integer. The integral in Eq.(2.5) thus gives

$$\lambda_n = 2\pi e^{in\Delta} I_n(x), \quad (2.6)$$

where $x = \beta J$ and I_n is the modified Bessel function of order n .

Combining the identity

$$e^{-\beta H(\phi, \phi')} = \int d\phi'' e^{-\beta H(\phi, \phi'')} \delta(\phi' - \phi'') \quad (2.7)$$

and the completeness of the eigenfunctions

$$\sum_n f_n(\phi'') f_n^*(\phi') = \delta(\phi' - \phi''), \quad (2.8)$$

we get

$$e^{-\beta H(\phi, \phi')} = \sum_n \int d\phi'' e^{-\beta H(\phi, \phi'')} f_n(\phi'') f_n^*(\phi') \quad (2.9)$$

The integral over ϕ'' gives $\lambda_n f_n(\phi)$ and $e^{-\beta H(\phi, \phi')}$ is hence completely expressed in terms of λ_n , $f_n(\phi)$ and $f_n^*(\phi')$.

$$e^{-\beta H(\phi, \phi')} = \sum_n \lambda_n f_n(\phi) f_n^*(\phi') \quad (2.10)$$

Plugging Eq.(2.10) back into the expression for the partition function

and integrating over all phases ϕ_1 with the boundary condition

$f_n(\phi_1) = f_n(\phi_{1+N})$, we get

$$Z = \sum_n \lambda_n^N \quad (2.11)$$

$$= (2\pi)^N [I_0^N(x) + 2 \sum_{n=1}^{\infty} \cos(2\pi n f) I_n^N(x)] ,$$

where $f = \frac{N\Delta}{\Phi_0}$ is the number of flux quanta through the loop. Note that this expression for the partition function is exact and so are the thermodynamic quantities derived from it.

(ii) Properties

We first examine the correlation function between the phases of the superconducting grains in a loop.

$$\begin{aligned}
\langle \cos(\phi_1 - \phi_{1+l}) \rangle &= \frac{1}{Z} \int \prod_{i=1}^N d\phi_i \cos(\phi_1 - \phi_{1+l}) \prod_{i=1}^N e^{-\beta H(\phi_i, \phi_{i+1})} \\
&= \frac{1}{2Z} \sum_{n=-\infty}^{\infty} \lambda_n^l \lambda_{n+1}^{N-l} + \lambda_n^l \lambda_{n-1}^{N-l} ,
\end{aligned} \tag{2.12}$$

where $1 \leq l \leq N-1$, an integer. Equation (2.12) describes the correlation between two grains with separation l . Note the symmetry of l and $N-l$ in Eq.(2.12), which is simply a result of the loop geometry. In a loop, separation l specifies the same pair of grains as separation $N-l$ does, i.e.,

$$\langle \cos(\phi_1 - \phi_{1+l}) \rangle = \langle \cos(\phi_1 - \phi_{1+N-l}) \rangle . \tag{2.13}$$

We plot in Fig. 2.1 $\langle \cos(\phi_1 - \phi_{1+l}) \rangle$ as a function of l at various temperatures for a loop of 40 junctions at $f = 0$. The correlation function decreases with increasing separation and increases with decreasing temperature as is expected.

We also examine the tunneling current resulting from the presence of a magnetic flux through the loop

$$\begin{aligned}
I_{1,i+1} &= \frac{2e}{h} J \langle \sin(\phi_1 - \phi_{i+1} - \Delta) \rangle \\
&= \frac{-4eJ}{h} \frac{1}{xz} \sum_{n=1}^{\infty} n \sin(n2\pi f) I_n^N(x) .
\end{aligned} \tag{2.14}$$

In Fig. 2.2, $-\langle \sin(\phi_1 - \phi_{i+1} - \Delta) \rangle$ as a function of temperature is

Fig.2.1 $\langle \cos(\phi_i - \phi_{i+l}) \rangle$ vs. l in a 40-junction loop in the absence of a magnetic field at various temperatures.

Fig.2.2 $-\langle \sin(\phi_i - \phi_{i+1} - \Delta) \rangle$ vs. T for a 4-junction loop at $f=.025$.

plotted for a loop of 4 junctions at $f = .025$. The currents are clearly diamagnetic. $-\langle \sin(\phi_i - \phi_{i+1} - \Delta) \rangle$ increases with decreasing temperature, approaching $-\sin(.05 \pi)$ at $T = 0$, as is consistent with the variation of the correlation function with temperature.

In Fig. 2.3, we plot $-\langle \sin(\phi_i - \phi_{i+1} - \Delta) \rangle$ for a 4-junction loop as a function of f at various temperatures. At all temperatures we have considered, the tunneling currents are periodic in f and are diamagnetic at small fields. Note that the variation of the tunneling currents with f becomes more sinusoidal at high temperatures. This implies that there is no critical flux even for a small loop of 4 junctions.

B. Other Geometry

(i) Two Loops

Consider the geometry as shown schematically in Fig. 2.4a. A loop of N_1 junctions is attached to another loop of N_2 junctions at a common grain. We write down the Hamiltonian H_1 and H_2 for each loop.

$$\begin{aligned}
 H_1 &= -J \sum_{i=1}^{N_1} \cos(\phi_i - \phi_{i+1} - \Delta) \\
 H_2 &= -J \sum_{j=1}^{N_2} \cos(\psi_j - \psi_{j+1} - \Delta) ,
 \end{aligned}
 \tag{2.15}$$

Fig.2.3 $-\langle \sin(\phi_i - \phi_{i+1} - \Delta) \rangle$ vs. f for a 4-junction loop at various temperatures.

(a)

(b)

Fig.2.4 A schematic of (a) two attached loops with one common grain and (b) a loop with a dead-end branch..

where ϕ_1 and ψ_j are the phases of the superconducting order parameter of the grains in loop 1 and loop 2, respectively.

For convenience, we assume the same parameter J and Δ . The partition function is thus

$$A = \int \prod_i \pi d\phi_i \prod_j \pi d\psi_j e^{-\beta H_1} e^{-\beta H_2} \delta(\psi_1 - \phi_1) , \quad (2.16)$$

where $\delta(\phi_1 - \psi_1)$ means loop 1 touches loop 2 at $\phi_1 = \psi_1$.

Integrating over all phases, we are left with

$$Z = \frac{1}{2\pi} \sum_n \lambda_n^{N_1} \sum_m \lambda_m^{N_2} = \frac{1}{2\pi} Z_1 Z_2 , \quad (2.17)$$

where Z_1 and Z_2 are the partition function of a single loop of N_1 and N_2 junctions respectively. It is clear that the thermodynamics of such two loops are just the same as those of two separate loops. We therefore conclude that the tunneling current in a closed loop is unaffected by an attached loop as long as the two loops have only one common grain.

(ii) A Loop With Attached Arms

Shown schematically in Fig. 2.4b is a loop of N_1 grains attached with an arm of N_2 grains. We use H_1 and H_2 to denote the Hamiltonian for the loop and for the arm respectively.

$$H_1 = -J \sum_{i=1}^{N_1} \cos(\phi_i - \phi_{i+1} - \Delta_1) \quad (2.18)$$

$$H_2 = -J \sum_{j=1}^{N_2} \cos(\psi_j - \psi_{j+1} - \Delta_2) ,$$

where we assume the same coupling energy for both the loop and the arm but allow the magnetic phase factors to be different. The partition function is then the following integral

$$Z = \int \prod_{i=1}^{N_1} \pi d\phi_i \prod_{j=1}^{N_2} \pi d\psi_j e^{-\beta H_1} e^{-\beta H_2} \delta(\phi_1 - \psi_1) . \quad (2.19)$$

Again, $\delta(\phi_1 - \psi_1)$ means that the arm is connected with the loop at $\phi_1 = \psi_1$. Integrating over all phases except ϕ_1 and ψ_{N_2} , we are left with

$$Z = \sum_{n,m} \lambda_n^{N_1} \lambda_m^{N_2-1} \int d\phi_1 f_n(\phi_1) f_n^*(\phi_1) f_m(\phi_1) \int d\psi_{N_2} f_m^*(\psi_{N_2}) . \quad (2.20)$$

It is clear that the integral over ψ_{N_2} is non-zero only when $m = 0$.

Thus the partition function becomes

$$Z = I_0^{N_2-1}(x) \sum_n \lambda_n^{N_1} . \quad (2.21)$$

Equation (2.21) clearly states the following. First, only closed loops carry supercurrents in response to a field. Secondly, the tunneling currents in a closed loop are unaffected by a dead-end

branch.

2.2 Amplitude Correction

A. Derivation

We now consider the full Landau-Ginzburg free energy functional for a cluster of N superconducting grains in the presence of a magnetic field.

$$F[\psi_i] = \sum_{i=1}^N a_i |\psi_i|^2 + \frac{b}{2} |\psi_i|^4 + \sum_{\langle i,j \rangle} C_{ij} |\psi_i e^{i\Delta_i} - \psi_j e^{i\Delta_j}|^2, \quad (2.22)$$

where ψ_i is the superconducting order parameter of grain i ,

$a_i = N(0)v_i T_{co}$. $N(0)$ is the density of states at Fermi level of the superconducting grains and v_i is the volume of grain i . T_{co} is

the bulk superconducting transition temperature of the grains and

$t = \frac{T-T_{co}}{T_{co}}$ is the reduced temperature. $C_{ij} = \frac{\pi}{8} \frac{R_o}{R_{ij}}$ where $R_o = \frac{\hbar}{e^2}$

is approximately 4000Ω and R_{ij} is the resistance of the normal

region between grain i and grain j . Δ_i is the magnetic phase

factor at site i due to the presence of a flux through the cluster.

The partition function and the thermal average of an operator

$\mathcal{O}(\psi_1, \dots, \psi_N)$ are then calculated as follows.

$$Z = \int \prod_{i=1}^N \pi |\psi_i| d|\psi_i| d\phi_i e^{-\beta F[\psi_i]} \quad (2.23)$$

$$\langle \vartheta(\psi_1, \dots, \psi_N) \rangle = \frac{1}{Z} \int \prod_{i=1}^N \pi |\psi_i| d|\psi_i| d\phi_i \vartheta(\psi_1, \dots, \psi_N) e^{-\beta F[\psi_i]} \quad (2.24)$$

For simplicity, we assume all grains to be identical. That is, all the volumes v_i and all the magnitudes $|\psi_i|$ of the grains are equal. We further assume that all the normal resistances between neighboring grains are also identical. Therefore, the free energy functional [Eq.(2.22)] becomes

$$F[\psi] = \sum_{i=1}^N [(a+2c)|\psi|^2 + \frac{b}{2} |\psi|^4] - 2c \sum_{i=1}^N |\psi|^2 \cos(\phi_i - \phi_{i+1} - A_{i,i+1}) \quad (2.25)$$

where ϕ_i is the phase of grain i and $|\psi|$ is the constant amplitude of all grains. $c = \frac{\pi}{8} \frac{R_0}{R}$ where R is a the constant normal resistance between neighboring grains and $A_{i,i+1}$ is the magnetic phase factor between neighbors as defined in Eq.(2.2).

The second term of the free energy functional Eq.(2.25) looks exactly the same as the XY-like Hamiltonian Eq.(2.1) except that $J_{i,i+1}$ in Eq.(2.1) is replaced by $2c|\psi|^2$ in Eq.(2.25). Therefore, the integral over the phase part of Eq.(2.23) can be done analytically. Integrating over all phases ϕ_i , the partition function now becomes

$$Z = \int \prod_{i=1}^N \pi |\psi| d|\psi| e^{-\beta F[|\psi|]} \quad (2.26)$$

where

$$F[|\psi|] = -\frac{1}{\beta} \ln Z_\phi + \sum_{i=1}^N [(a + 2c)|\psi|^2 + \frac{b}{2} |\psi|^4] \quad (2.27)$$

and

$$Z_\phi = \int \prod_{i=1}^N \pi d\phi_i e^{+2\beta c |\psi|^2 \sum_i \cos(\phi_i - \phi_{i+1} - A_{i,i+1})} \quad (2.28)$$

Z_ϕ is the integral over all phases and can be done analytically. The expressions for Z_ϕ for various situations have been written down in Section 2.1 and those expressions are exact.

To simplify the calculation, instead of doing the integral in Eq.(2.26), we make the steepest descent approximation. That is, we approximate the total free energy to be the minimum of $F[|\psi|]$. The minimization of $F[|\psi|]$ with respect to $|\psi|$

$$\frac{\delta F[|\psi|]}{\delta |\psi|} = 0 \quad (2.29)$$

gives a self-consistent equation for $|\psi|^2$:

$$|\psi|^2 = \frac{|a|}{b} - \frac{2c}{b} (1 - f_\phi) \quad , \quad (2.30)$$

where

$$f_\phi = \frac{1}{N} \frac{1}{Z_\phi} \frac{dZ_\phi}{dx} \quad , \quad (2.31)$$

where $x = 2\beta c |\psi|^2$ and N is the total number of grains of the

cluster. At low temperatures, i.e., $c/kT \gg 1$, f_{ϕ} is converging to zero, and f_{ϕ} increases with increasing temperature, approaching unity at higher temperatures. Consequently, the reduction of $|\psi|^2$ due to phase fluctuations is nearly zero at low temperatures and is at most $2c/b$ at a higher temperature. The ratio c/a_0 is thus crucial to the magnetic behavior of a cluster where, $a_0 = a/t$ and $-a_0^2/b$ is the energy gained by a single grain at $T = 0$ for being superconducting.

If $c/a_0 \ll 1$, the reduction of $|\psi|^2$ is small compared to $|a|/b$, one expects that the fix-amplitude XY-like model in Section 2.1 should work well. On the other hand, if $c/a_0 \lesssim 1$, the reduction of $|\psi|^2$ due to phase fluctuations is comparable to $|a|/b$. Thus the XY-like model becomes insufficient.

After solving Eq.(2.30) for $|\psi|^2$, we then use the obtained $|\psi|^2$ to calculate other quantities. For example, the tunneling currents $I_{i,i+1}$ between grains are

$$I_{i,i+1} = |\psi|^2 \langle \sin(\phi_i - \phi_{i+1} - A_{i,i+1}) \rangle_{\phi}, \quad (2.32)$$

where $I_{i,i+1}$ is in unit of $\frac{4ec}{h}$. $\langle \rangle_{\phi}$ denotes the thermal average over the phases.

B. Results

Since in Section 2.1 we have studied the weak-coupling limit, i.e., $c/a_o \ll 1$, in great detail, we will now concentrate on cases of stronger coupling. In the calculation, we let b be 1 since b is only a multiplying constant in Eq.(2.30). Also, for convenience, we choose $c = k T_{Bco}$. Therefore, increasing the ratio c/a_o from 0, we then are able to show how the diamagnetic behavior of a cluster changes from that of the weak-coupling limit to that in the stronger-coupling regime. We find that for $c = k T_{Bco}$, the crossover c/a_o is about .4. For small c/a_o , $|\psi|^2$ remains non-zero at all fields even for a small loop when the temperature is lower than $T_c \approx T_{co} (1 - 2c/a_o)$. The behavior of a single loop is very similar to what is described in Section 2.1. For $c/a_o \geq .4$, $|\psi|^2$ begins to vanish at larger fields in a small loop. By large fields is meant that the number of flux quanta through a loop is close to a half integer since the physical properties of a loop are periodic with the flux through the loop. To illustrate this point, we let $c/a_o = 1$ and calculate the tunneling currents in a small loop of 4 grains with a dead-end branch and without one.

The resulting negative tunneling currents $-I_{i,i+1}$ for a single 4-grain loop as a function of f are plotted in Fig. 2.5 for several temperatures where f is the number of flux quanta through the loop and the currents are in unit of $4ec/h$. It is clear that for a

Fig.2.5 $-I_{i,i+1}$ vs. f for a 4-junction loop with $c/a_s = 1$ at various temperatures. $I_{i,i+1}$ is in unit of $4ec/h$.

Fig.2.6 $-I_{i, i+1}$ vs. f for a 4-junction loop with a N_2 -grain dead-end branch where $c/a_0=1$ and $T=.1 T_{C0}$. $I_{i, i+1}$ is in unit of $4ec/h$.

4-grain loop, there indeed exists a critical flux which decreases as the temperature is increased. Note that only a small loop has a critical flux, as is similar to the behavior of a wire network.²⁸ For a larger loop, say, of 20 grains, $|\psi|^2$ remains non-zero at all fields. Thus a large loop does not have a critical flux.

Shown in Fig. 2.6 are the tunneling currents in a 4-grain loop at $T = .1 T_c$ as a function of f while the loop has a dead-end branch. N_2 denotes the number of the grains of the branch and the different curves in Fig. 2.6 correspond to various N_2 's. Clearly, the critical flux shrinks as N_2 decreases. A dead-end part of a loop does have a role in the diamagnetism of a cluster. It tends to stabilize the loop even though it does not carry any supercurrents, as is also similar to that of a wire network.²⁸

2.3 Discussion

The diamagnetism of a granular cluster depends very much on the ratio c/a_o . For $c/a_o \ll 1$, the XY-like model is expected to be proper for describing the system. The expression for the partition function is exact within this model and so are those for other quantities. In this regime, the diamagnetism of a loop is unaffected by its dangling branches and no field can ever drive a loop normal even if the loop is small, in contrast to a wire network.

For $c/a_o \simeq 1$, a granular cluster begins to behave similar to a

dilute wire network. A small loop can be driven normal by a large field, that is, a small loop has a critical flux, and a dead-end branch tends to stabilize the loop even though it does not carry any supercurrents.

Experimentally, how does one vary the ratio c/a_o to see these effects?. By definition $c = \pi/8 R_o/R$ and $a_o = N(0) v_{F1} k T_{co}$. $N(0)$ and T_{co} do not vary much among superconducting materials.

Therefore, it is most likely either to reduce the resistance between grains or to reduce the grain volume in order to increase the ratio of c/a_o . A rough estimate is as follows. Say, $c = k T_{Bco}$. For a cluster of grains $10^3 \text{ \AA}$ in diameter, c/a_o is about .001. The system is therefore well described by the XY-like model of

Section 2.1. To achieve the high c/a_o limit, i.e., $c/a_o \approx 1$, the size of the grains must be reduced to about $10^2 \text{ \AA}$ in diameter. A cluster of such grains will then behave similarly to a wire network.

CHAPTER 3: TWO-DIMENSIONAL ORDERED ARRAYS

3-1 Mean-Field Approximation

A. Self-Consistent Equations

In this section, we will derive a set of self-consistent equations for the order parameters with a mean-field approximation. The advantage of making a mean-field approximation is that we have a one-body effective Hamiltonian and hence an analytic expression for the partition function, from which we can calculate thermodynamic quantities easily. On the other hand, the mean-field solutions leave out fluctuation effects which are known to be especially important in two dimensions. Also, mean-field approximations provide no information about the universality class of the transitions, and they generally overestimate transition temperatures substantially, especially in 2d. Despite these disadvantages, mean-field theory is still a powerful and quick way to investigate qualitatively the behaviors of a complicated system such as the one under consideration.

We will start by rewriting the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \quad (3.1)$$

in a vector form to avoid tediously complicated expressions in the course of our derivation.

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} (\psi_i \psi_j^* e^{-iA_{ij}} + \psi_i^* \psi_j e^{+iA_{ij}}) , \quad (3.2)$$

where J_{ij} is the coupling energy, in which the magnitude of the superconducting order parameter has been absorbed, between two grains and $\langle ij \rangle$ denotes all relevant neighbors. $\psi_i = e^{i\phi_i}$ and ϕ_i is the phase of the superconducting order parameter of grain i . A_{ij} is the path integral

$$A_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \vec{A} \cdot d\vec{l} \quad (3.3)$$

where $\Phi_0 = \frac{hc}{2e}$ is the flux quantum and $\vec{A}$ is the vector potential due to the presence of the transverse magnetic field. $\vec{A}$ is chosen to be

$$\vec{A} = Bx\hat{y} . \quad (3.4)$$

where $\vec{B} = B\hat{z}$ is the applied magnetic field. The integral in (3.3) runs from the center of grain i to that of grain j .

Now ψ_i can be expressed as the sum of its thermal average and a fluctuation as:

$$\psi_i = \langle \psi_i \rangle + \delta\psi_i , \quad (3.5)$$

where $\langle \rangle$ denotes the thermal averages. The Hamiltonian is thus

$$\begin{aligned}
H = & -\sum_{\langle ij \rangle} \frac{1}{2} J_{ij} (\langle \psi_i \rangle \langle \psi_j^* \rangle e^{-iA_{ij}} + \langle \psi_i \rangle \delta \psi_j^* e^{-iA_{ij}} \\
& + \delta \psi_i^* \langle \psi_j \rangle e^{-iA_{ij}} + \delta \psi_i^* \delta \psi_j^* e^{-iA_{ij}} + \langle \psi_i^* \rangle \langle \psi_j \rangle e^{iA_{ij}} \\
& + \langle \psi_i^* \rangle \delta \psi_j e^{iA_{ij}} + \delta \psi_i^* \langle \psi_j \rangle e^{iA_{ij}} + \delta \psi_i^* \delta \psi_j e^{iA_{ij}}) .
\end{aligned} \tag{3.6}$$

If we neglect the quadratic terms in $\delta\psi$'s, we get

$$H \sim H_{\text{eff}} + \frac{1}{4} \sum_i (\langle \psi_i \rangle h_i^* + \langle \psi_i^* \rangle h_i) \tag{3.7}$$

where

$$H_{\text{eff}} = \frac{-1}{2} \sum_i (\psi_i h_i^* + \psi_i^* h_i) \tag{3.8}$$

and

$$h_i = \sum_j J_{ij} \langle \psi_j \rangle e^{iA_{ij}} , \tag{3.9}$$

where j denotes all nearest neighbors of i . Thus we see that ψ_i couples to an average field due to its neighboring grains. Note that the second term of Eq.(3.7) is just a constant which does not affect any thermal average. We will henceforth use H_{eff} as the effective Hamiltonian for thermal averaging.

In the canonical ensemble, the partition function and the thermal average of an operator $\mathcal{O}(\phi_1, \dots, \phi_N)$ are given by

$$Z = \int \prod_{i=1}^N \pi d\phi_i e^{-\beta H_{\text{eff}}} \quad (3.10)$$

and

$$\langle g(\phi_1, \dots, \phi_N) \rangle = \frac{1}{Z} \int \prod_{i=1}^N \pi d\phi_i g(\phi_1, \dots, \phi_N) e^{-\beta H_{\text{eff}}} \quad (3.11)$$

where N is the total number of grains. The constant term in Eq.(3.7) does not affect these averages. However, we must keep in mind that when calculating free energy, we have to include the second term of Eq.(3.7).

For convenience in carrying out the required integrals, we again express the effective Hamiltonian in terms of the cosines of the phases:

$$H_{\text{eff}} = - \sum_i |h_i| \cos(\phi_i - \phi_{h_i}) , \quad (3.12)$$

where ϕ_{h_i} is the phase angle of h_i , defined by

$$h_i = |h_i| e^{i\phi_{h_i}} . \quad (3.13)$$

With the change of variables, $\phi_i' = \phi_i - \phi_{h_i}$, Z takes the form

$$Z = \prod_{i=1}^N \int_0^{2\pi} \pi d\phi_i' e^{-\beta |h_i| \cos \phi_i'} . \quad (3.14)$$

The integrations in Eq.(3.14) give modified Bessel function of zeroth

order.

$$Z = \prod_{i=1}^N \int_0^{2\pi} d\phi_i I_0(\beta|h_i|) \quad (3.15)$$

and the free energy is thus

$$F = -T \sum_i \ln[2\pi I_0(\beta|h_i|)] + \frac{1}{4} \sum_i [\langle \psi_i \rangle h_i^* + \langle \psi_i^* \rangle h_i] \quad (3.16)$$

The second term of Eq.(3.16) is the part of Eq.(3.7) that was previously omitted.

Our aim is to find an approximate expression for $\eta_i \equiv \langle e^{i\phi_i} \rangle$ as the order parameter to indicate phase coherence. Writing

$$\eta_i \equiv \langle e^{i\phi_i} \rangle \equiv \langle \cos \phi_i \rangle + i \langle \sin \phi_i \rangle \quad (3.17)$$

and integrating over all phases except ϕ_i , for $\langle \cos \phi_i \rangle$, we are left with

$$\langle \cos \phi_i \rangle = \frac{1}{2\pi I_0(\beta|h_i|)} \int_0^{2\pi} d\phi_i e^{-\beta|h_i|\cos(\phi_i - \phi_{h_i})} \quad (3.18)$$

With change of variables, $\phi_i' = \phi_i - \phi_{h_i}$, Eq.(3.18) becomes

$$\langle \cos \phi_i \rangle = \frac{1}{2\pi I_0(\beta|h_i|)} \int_0^{2\pi} d\phi_i' (\cos \phi_i' \cos \phi_{h_i} - \sin \phi_i' \sin \phi_{h_i}) e^{-\beta|h_i|\cos \phi_i'} \quad (3.19)$$

The second term of the integrand is odd and hence does not contribute to the integral. The first term gives I_1 , the modified Bessel

function of order 1.

$$\langle \cos \phi_i \rangle = \frac{I_1(\beta |h_i|)}{I_0(\beta |h_i|)} \cos \phi_{h_i} \quad (3.20)$$

Similarly, $\langle \sin \phi_i \rangle$ can be expressed in terms of modified Bessel functions. We thus finally obtain

$$\eta_i \equiv \langle e^{i\phi_i} \rangle = \frac{I_1(\beta |h_i|)}{I_0(\beta |h_i|)} \frac{h_i}{|h_i|} \quad (3.21)$$

$$h_i \equiv \sum_j J_{ij} \eta_j e^{iA_{ij}}$$

where j denotes all nearest neighbors of i .

Equation (3.21) represents a set of N coupled complex equations in the N unknown phase order parameters η_i 's, and must be solved numerically. Note that the derivation so far is quite general. These equations can be applied to both ordered and disordered arrays and to two-dimensional systems as well as three-dimensional ones. In practice, Eq.(3.21) will be solved by iteration in a lattice of $10 \sim 1600$ sites with periodic boundary conditions. The transition temperature is thus identified as that above which Eq.(3.21) no longer has a non-trivial solution.

B. Ground State Configurations

One characteristic feature of the solution to the self-consistent

equations [Eq.(3.21)] at finite temperatures is that the relative phase angles between the complex order parameters η_i remain almost unchanged as the temperature is varied while the magnitudes $|\eta_i|$, which may vary from site to site, decrease with increasing temperature and finally go to zero at the transition temperature. We therefore extrapolate the ground state configurations by means of "annealing". That is, we take the finite-temperature configurations with all $|\eta_i|$'s taken to be unity as the input. We obtain the ground state configurations by further iterating

$$\psi_i = \frac{\sum_j J_{ij} \psi_j e^{iA_{ij}}}{|\sum_j J_{ij} \psi_j e^{iA_{ij}}|} \quad (3.22)$$

to convergence with periodic boundary conditions, where $\psi_i = e^{i\phi_i}$. Equation (3.22) is just another way of writing the minimization condition for the ground states, namely,

$$\sum_j J_{ij} \sin(\phi_i - \phi_j - A_{ij}) = 0, \quad (3.23)$$

where j denotes all nearest neighbors of i in both Eq.(3.22) and Eq.(3.23). Equation (3.23) is the equivalent of Kirchhoff's law in these superconducting arrays, which states that the net tunneling current into one grain must be equal to that coming out of the grain. The ground states obtained by this annealing procedure are exact since

mean-field theory is exact at $T = 0$. Compared to other methods, for example, the Monte Carlo annealing, this mean-field annealing proves to be a better way of obtaining the ground states because of its much faster convergence.

C. Ground State Energy $E_g(f)$

Once the ground state configuration is obtained, the ground state energy per site is calculated according to the following formula:

$$E_g(f) = \frac{-1}{N} \sum_{\langle ij \rangle} J_{ij} \cos(\phi_i^0 - \phi_j^0 - A_{ij}) , \quad (3.24)$$

with periodic boundary condition, where ϕ_i^0 stands for the ground state configuration and N is the total number of grains.

D. Critical Current I_c at $T = 0$

We compute the critical currents at $T = 0$ by considering the following. If one twists the sample at the boundaries, there will be a net current resulting from the twist. For convenience, rather than applying the twist externally and using twisted boundary conditions, we will use periodic boundary conditions and put the twist explicitly in the expression for the currents. Thus at $T = 0$ a net current, due to the twist $\vec{\delta}$, flowing in a bond lying in a lattice direction ℓ is

$$I_{\ell}(f, \vec{\delta}) = \frac{2e}{\hbar N_{\ell}} \sum_{\langle i,j \rangle_{\ell}} J_{ij} \sin(\phi_i - \phi_j - A_{ij} - \vec{\delta} \cdot \vec{e}_{ij})$$

or

(3.25)

$$I_{\ell}(f, \vec{\delta}) = \frac{2e}{\hbar N_{\ell}} \sum_{\langle i,j \rangle_{\ell}} J_{ij} \operatorname{Im}(\psi_i \psi_j^* e^{-iA_{ij}} e^{-\vec{\delta} \cdot \vec{e}_{ij}}),$$

where $\psi_i = e^{i\phi_i}$ and $\vec{\delta}$ is the applied twist. N_{ℓ} denotes the number of bonds and $\langle i,j \rangle_{\ell}$ all nearest neighbors in ℓ direction. ψ_i 's are the solution to the following $T = 0$ mean-field coupled equations with periodic boundary conditions.

$$\psi_i = \frac{\sum_j J_{ij} \psi_j e^{iA_{ij}} e^{i\vec{\delta} \cdot \vec{e}_{ij}}}{\left| \sum_j J_{ij} \psi_j e^{iA_{ij}} e^{i\vec{\delta} \cdot \vec{e}_{ij}} \right|}. \quad (3.26)$$

These mean-field equations [Eq.(3.26)] are exact at $T = 0$. Note that Eq.(3.26) with periodic boundary conditions is equivalent to a change of variables from Eq.(3.22) with twisted boundary conditions and hence is also an equivalent statement of Kirchhoff's law. In practice, to solve for ψ_i at a given $\vec{\delta}$, we let the configuration evolve continuously from the ground state as $\vec{\delta}$ is increased. That is, we first iterate Eq.(3.26) to convergence with periodic boundary conditions, using the ground state configuration as an input, at a small $\vec{\delta}$. Then we increase $\vec{\delta}$ by a small amount each time and use

the preceding configuration as an initial state to iterate Eq.(3.26) to convergence with periodic boundary conditions. Doing so, we then are able to put the system into a current-carrying state.

The $T = 0$ critical current density is then just the maximum current density that the system can carry

$$I_c^{\hat{\delta}} = \max_{\delta} F(I_l(\hat{\delta}, f)) , \quad (3.27)$$

where $I_c^{\hat{\delta}}$ denotes the critical current density in $\hat{\delta}$, the direction of the twist, and F denotes some combination of I_l , which depends on the lattice structure. In general, the critical current can be anisotropic, namely, it depends very much on the symmetry of the ground state configuration.

E. Helicity Modulus γ at $T = 0$

The helicity modulus which will be described in more detail in Section 3.2 is defined as the second derivative of the free energy with respect to an infinitesimal twist. The diagonal component of the helicity modulus tensor can be approximated at a small twist as

$$\gamma_{\alpha\alpha} \approx \frac{1}{N} \frac{\sum_l N_l I_l \vec{e}_l \cdot \vec{e}_\alpha}{\vec{\delta} \cdot \vec{e}_\alpha} , \quad (3.28)$$

where α denotes x , y , and z , and l the lattice direction. In two dimensions, the helicity modulus is always isotropic while in

three dimensions, it may not be so.

3.2 Monte Carlo Simulations

A. Metropolis Algorithm

As noted in the previous section, given the Hamiltonian [Eq.(3.1)], any observable is given by an average of the form

$$\langle A(\phi_1, \dots, \phi_N) \rangle = \frac{\int \prod_{i=1}^N d\phi_i e^{-\beta H} A(\phi_1, \dots, \phi_N)}{\int \prod_{i=1}^N d\phi_i e^{-\beta H}}, \quad (3.29)$$

where N is the total number of grains. Numerically, one has to turn the integration into a sum over a set of points. The Monte Carlo method introduced by Metropolis et al.²⁹ is a sampling algorithm based on the idea of "importance sampling"³⁰ which we now describe.

Let Φ_n denote a phase space point which represents a certain configuration of $(\phi_1, \dots, \phi_N)$. M phase space points which are chosen according to a probability $p(\Phi_n)$ are used to calculate thermal averages. Equation (3.29) is then approximated by

$$\langle A \rangle \approx \bar{A} = \frac{\sum_{n=1}^M A(\Phi_n) p^{-1}(\Phi_n) e^{-\beta H(\Phi_n)}}{\sum_{n=1}^M p^{-1}(\Phi_n) e^{-\beta H(\Phi_n)}}, \quad (3.30)$$

where $p^{-1}(\Phi_n)$ appears in both sums to cancel the artificial weight

$p(\Phi_n)$ which one creates in the selection process. The simplest way of choosing $p(\Phi_n)$ is to $p(\Phi_n) = p_{eq}(\Phi_n) \propto e^{-\beta H(\Phi_n)}$, in this case,

Eq.(3.30) reduces to a simple arithmetic average,

$$\bar{A} = \frac{1}{M} \sum_{n=1}^M A(\Phi_n) . \quad (3.31)$$

In order that our process of generating configurations has the desired property that $p(\Phi_n)$ converges to $p_{eq}(\Phi_n)$, it is sufficient to impose the detailed balance condition

$$p_{eq}(\Phi_n) w(\Phi_n \rightarrow \Phi_{n'}) = p_{eq}(\Phi_{n'}) w(\Phi_{n'} \rightarrow \Phi_n) , \quad (3.32)$$

where $w(\Phi_n \rightarrow \Phi_{n'})$ is the transition rate from configuration Φ_n to $\Phi_{n'}$. Equation (3.32) can be rewritten as

$$\frac{w(\Phi_n \rightarrow \Phi_{n'})}{w(\Phi_{n'} \rightarrow \Phi_n)} = e^{-\beta \delta H} , \quad (3.33)$$

where $\delta H = H(\Phi_{n'}) - H(\Phi_n)$. The ratio of the transition rates only depends upon the change in energy.

Equation (3.33) clearly does not uniquely specify $w(\Phi_n \rightarrow \Phi_{n'})$. There are many possible choices of w . In the calculations described here, we have used

$$\begin{aligned} w(\Phi_n \rightarrow \Phi_{n'}) &= e^{-\beta \delta H} & \text{if } \delta H > 0 \\ &= 1 & \text{otherwise} \end{aligned} \quad (3.34)$$

Equation (3.34) means that a change of configuration towards a lower energy state is always favorable.

B. Simulation

Simulations are carried out in a sample of 100-3000 sites with periodic boundary conditions. The way we generate a new configuration $\Phi_{n'}$ from the preceding one Φ_n is to rotate one of the phases $(\phi_1, \dots, \phi_N)$ by an arbitrary angle between 0 and 2π and then to compute $e^{-\beta\delta H}$ where δH is the change in energy. $e^{-\beta\delta H}$ is then compared to a random number R between 0 and 1 and selected from a uniform distribution. $\Phi_{n'}$ is thus determined according to the selection criterion.

$$\begin{aligned} \Phi_{n'} &= \text{new configuration} & \text{if } e^{-\beta\delta H} \geq R \\ \Phi_{n'} &= \Phi_n & \text{otherwise} \end{aligned} \quad (3.35)$$

By repeating this process at every site in succession we thus generate a set of configurations over which a thermal average of interesting quantities can be calculated according to Eq.(3.31).

Typically 15,000 ~ 25,000 passes through the entire lattice are made in each run, with approximately 5,000 passes discarded to make sure that the averages are taken at equilibrium. Moreover, we always initiate the Monte Carlo procedure using as a start configuration one

of the equilibrium configurations of a neighboring temperature so as to avoid becoming trapped in the metastable states which are characteristic of the system. In order to better describe the behavior near the transition temperatures where fluctuations are large, the reported results are the average over 4-6 independent runs.

C. Order Parameters

Although we have used $\eta_i \equiv \langle e^{i\phi_i} \rangle$ as the order parameter in the mean-field approximation, it turns out the $\langle e^{i\phi_i} \rangle$ is not really a good order parameter in Monte Carlo simulations. First of all, it is well known¹⁷ that in two dimensional XY systems (the zero-field case in our problem), there is no conventional long range order at low temperatures. That is, the correlation function $\langle e^{i(\phi_i - \phi_j)} \rangle$ between spin i and spin j varies as $\frac{1}{|\vec{r}_i - \vec{r}_j|^\eta}$ at large separations rather than as a constant independent of position i and j . Thus the quantity $\langle e^{i\phi_i} \rangle$ is actually zero at all temperatures. Secondly, in spite of its validity in 3d, $\langle e^{i\phi_i} \rangle$ is numerically unstable because the simulated sample of "spins" can rotate as a whole.

For these reasons we use a different quantity known as the helicity modulus^{9-11,31} as the order parameter in our simulations. The helicity modulus measures the "stiffness" of the spins (the phases of the superconducting order parameter of the grains) and is analogous

to the superfluid density. Ohta and Jasnow³¹ have studied it in great detail within the framework of the two dimensional XY model. They showed that helicity modulus first decreases linearly with increasing temperature with a slope $1/4$ at low temperature where only spin wave excitations are important; as the temperature is increased further, the vortex contribution becomes significant and helicity modulus drops more dramatically. It finally jumps discontinuously from the value $2/\pi$ to zero at the Kosterlitz-Thouless transition temperature at which the first vortex pair unbinds and the system can no longer maintain its ordered state. More recently Teitel and Jayaprakash⁹ have extensively used the helicity modulus as the order parameter in their Monte Carlo simulation of Josephson junction arrays in a square lattice at several values of magnetic field. It turns out that helicity modulus is a good order parameter because of its general numerical stability as well as its capacity to describe the characteristics of two dimensional arrays.

To define the helicity modulus precisely, imagine that a long-wavelength "twist" of wave vector $\vec{k}$ is imposed in the system. The free energy of the system will then increase by an amount proportional to k^2 relative to the untwisted state. We therefore define helicity modulus to be the second derivative of the free energy with respect to an infinitesimal "twist":

$$\gamma_{\alpha\beta} \equiv \lim_{k \rightarrow 0} \frac{\partial^2 F(T, \vec{k})}{\partial k_\alpha \partial k_\beta}, \quad (3.36)$$

where α and β are x , y or z . Rather than imposing the twist externally it is more convenient to include the "twist" explicitly in the Hamiltonian and use periodic boundary conditions. Thus one considers

$$H(k) = -\sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij} - \vec{k} \cdot \vec{e}_{ij}) , \quad (3.37)$$

and carries out the second derivative indicated in Eq.(3.36), obtaining explicit expressions for the components of the helicity modulus tensor. The diagonal terms, for example, are written as

$$\begin{aligned} \gamma_{\alpha\alpha} = & \frac{1}{N} \left[\left\langle \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j - A_{ij}) (\vec{e}_{ij} \cdot \vec{e}_\alpha)^2 \right\rangle \right. \\ & - \frac{1}{T} \left(\left\langle \sum_{\langle ij \rangle} \sin(\phi_i - \phi_j - A_{ij}) \vec{e}_{ij} \cdot \vec{e}_\alpha \right\rangle^2 \right. \\ & \left. \left. - \left\langle \sum_{\langle ij \rangle} \sin(\phi_i - \phi_j - A_{ij}) \vec{e}_{ij} \cdot \vec{e}_\alpha \right\rangle^2 \right) \right] , \end{aligned} \quad (3.38)$$

where N is the total number of grains and $\vec{e}_{ij}$ a unit vector directed from i to j . The experimental interpretation of the helicity modulus will be given in Appendix C.

Besides this order parameter, we also calculate specific heat C according to the following formula:

$$C = \frac{1}{NT} [\langle H^2 \rangle - \langle H \rangle^2] . \quad (3.39)$$

The behavior of the specific heat is of great help in identifying a second order transition at which the specific heat usually has an anomaly.

3.3 Square Lattice

A. Explicit Form of the Hamiltonian

Figure 3.1 shows the coordinates (I,J) of a square lattice. I represents the index along x direction and J in y . Both I and J are measured in units of the lattice constant a . The magnetic field is applied perpendicularly in the z direction. The magnetic phase factor between grain (I,J) and $(I,J+1)$ is

$$A((I,J),(I,J+1)) = \frac{2\pi}{\Phi_0} \int_{(I,J)}^{(I,J+1)} Bx dy = \frac{2\pi a^2 B}{\Phi_0} I , \quad (3.40)$$

where a is the lattice constant. It is convenient to use a new parameter f to describe the strength of the magnetic field,

$$f \equiv \frac{Ba^2}{\Phi_0} , \quad (3.41)$$

which measures the numbers of flux quanta through each unit square.

In terms of f , Eq.(3.41) becomes

Fig.3.1 The coordinates of a square lattice.

$$A((I,J),(I,J+1)) = 2\pi f I \quad (3.42)$$

Similarly,

$$A((I,J),(I,J-1)) = -2\pi f I \quad (3.43)$$

$$A((I,J),(I+1,J)) = A((I,J),(I-1,J)) = 0$$

The Hamiltonian for square lattice is thus

$$H = -J \sum_{\langle I,J \rangle} \cos(\phi(I,J) - \phi(I+1,J)) + \cos(\phi(I,J) - \phi(I,J+1) - 2\pi f I) \quad (3.44)$$

where J is the nearest-neighbor coupling and (I,J) the coordinates.

B. Mean-Field Transition temperature, T_c^{MF}

Numerical Results

The self-consistent equations for the order parameters $\eta(I,J)$ in a square lattice take the explicit form:

$$h(I,J) = J[\eta(I+1,J) + \eta(I-1,J) + \eta(I,J+1)e^{12\pi f I} + \eta(I,J-1)e^{-12\pi f I}]$$

and (3.45)

$$\eta(I,J) = \frac{I_1(\beta |h(I,J)|)}{I_0(\beta |h(I,J)|)} \frac{h(I,J)}{|h(I,J)|}.$$

We solve the coupled equations [Eq.(3.45)] self-consistently for

$f = p/q$, $q \leq 15$. For each f , we assume the system to be periodic

in $m \times m$ cell with $m \geq 1$, an integer, and solve the resulting $(mq)^2$ equations by iteration. Transition temperatures are identified as those above which Eq.(3.45) no longer has non-trivial solutions. For all the values of f we have considered, the system proves to be periodic with a $q \times q$ cell.

The mean-field transition temperature $T_c^{MF}(f)$ for several values of f are plotted in Fig. 3.2. $T_c^{MF}(f)$ is a periodic function of f with period 1 and is symmetric about $f = \frac{1}{2}$ as implied by the periodic dependence of the model Hamiltonian [Eq.(3.44)] on f .²² The most striking feature of $T_c^{MF}(f)$ is that it is extremely non-monotonic, with cusps at rational values of f and hence have complicated structures on a small scale. The line connecting the data points is merely to guide the eye. Note especially, the cusp at $f = \frac{1}{2}$, a feature that has been seen in the measurements of the resistivity above T_c of Josephson or proximity-coupled junction arrays⁵⁻⁷ as well as superconducting wire networks.³²

Linearization near $T_c^{MF}(f)$

Near $T_c^{MF}(f)$, presumably, all $|\eta_1|$'s are small, hence $I_0(\beta|h(I,J)|)$ and $I_1(\beta|h(I,J)|)$ can be expanded in power series in $\beta|h(I,J)|$. To the lowest order of $\beta|h(I,J)|$, Eq.(3.45) becomes

$$\eta(I,J) = \frac{1}{2T}(\eta(I+1,J) + \eta(I-1,J) + \eta(I,J+1)e^{i2\pi fI} + \eta(I,J-1)e^{-i2\pi fI}) \quad (3.46)$$

Fig.3.2 T_c^{MF} and $-E_g$ vs. f of a square lattice. The lines connecting the data points are merely to guide the eye.

Equation (3.46) is identical to the Schrödinger equation for a tight-binding electron in a magnetic field, which was treated in detail by Holfstadter²³. The temperature $2T$ in Eq.(3.46) plays the same role as the energy eigenvalue in the electronic problem. Hence the variation of $T_c^{MF}(f)$ with f can be mapped onto the highest band edge of the magnetic spectrum of a tight-binding electron as a function of field. Scaled properly, our numerical values of $T_c^{MF}(f)$ do indeed fall on Halfstadter's band edge.

We can also handle Eq.(3.46) analytically by means of transfer matrix technique (Appendix A). We show in Appendix A that for $f = 0$, $1/2$ and $1/3$, $T_c^{MF}(f)$ is 2 , $\sqrt{2}$ and $\frac{1+\sqrt{3}}{2}$ respectively, and that for f near 0 and $1/2$, T_c^{MF} is

$$\begin{aligned} T_c^{MF} &= 2 - \pi|f| & |f| \ll 1 \\ &= \sqrt{2} - \frac{\pi}{\sqrt{2}} \left| f - \frac{1}{2} \right| & \left| f - \frac{1}{2} \right| \ll 1 \end{aligned} \quad (3.47)$$

All these linearized results are correctly reflected in the numerical curve of $T_c^{MF}(f)$ vs. f within numerical accuracy.

C. Ground State Properties

We show as examples in Fig. 3.3a the ground state phase configuration within a unit cell and in Fig. 3.3b the vortex configuration at $f = 1/2$, $1/3$ and $1/4$. A shaded square denotes a

Fig.3.3a Phase configurations at $f = 1/2, 1/3$ and $1/4$ within a unit cell of a square lattice.

$$f = 1/2$$

$$f = 1/3$$

$$f = 1/4$$

Fig.3.3b Ground-state vortex configurations at $f = 1/2, 1/3$ and $1/4$ within a unit cell of a square lattice. A shaded area denotes a positive vortex of charge $1-f$ and a white square of negative charge $-f$. The arrows indicate the directions of the supercurrents.

positive vortex of charge $1 - f$ and a white one has charge $-f$. The vortex charge of a square is defined as $1/2\pi \sum \Delta\phi - f$ where $\sum \Delta\phi$ denotes the sum of the differences of the phases between neighboring grains along the edges of a square. In practice we may identify the vortex charge by the current loops around the squares in the ground state as illustrated in Fig. 3.3b.

$-E_g(f)$ vs. f is also plotted in Fig. 3.2. Again, $-E_g(f)$ is non-monotonic with f and the line connecting the data points are just to guide the eye. Note that $-E_g(f)$ always lies below $T_c^{MF}(f)$. This may be explained as follows. At $T = 0$, the equation which $\psi(I,J)$'s obey becomes

$$\begin{aligned} E\psi(I,J) = & -\frac{J}{2} [\psi(I+1,J) + \psi(I-1,J) + \psi(I,J+1)e^{i2\pi fI} \\ & + \psi(I,J-1)e^{-i2\pi fI}] , \end{aligned} \quad (3.48)$$

where $\psi(I,J) = e^{i\phi(I,J)}$. Equation (3.48) is identical to the linearized equation [Eq.(3.46)] near T_c , except that the factor $2T$ in Eq.(3.46) is replaced by $-2E$ in Eq.(3.48). $-2E_g(f)$ is thus the highest eigenvalue of Eq.(3.48). $-E_g(f)$ will always be smaller than or equal to $T_c^{MF}(f)$ because Eq.(3.48) has the additional constraint that all the magnitudes $|\psi(I,J)|$ be the same.

D. Critical Current I_c at $T = 0$

We calculate the critical currents at $T = 0$ by imposing twist

in both x and y directions. The expression for critical current density [Eq.(3.27)] now takes the following form in a square lattice,

$$I_c(f)_\alpha = \frac{1}{a} \max_\delta I_\alpha(f, \delta \hat{e}_\alpha) , \quad (3.49)$$

where α is x and y and a is the lattice constant. The critical current density is measured by the critical current of a single junction per lattice constant. It turns out the critical currents are identical in x and y direction. We plot $I_c(f)$ as a function of f in Fig. 3.4 for $f = 1/q$, $q \leq 13$. Teitel and Jayaprakash[3.12] have also calculated critical currents for $q \leq 7$, using the same prescription [Eq.(3.25)] but with Monte Carlo method. Our $I_c(f)$ for $q \leq 7$ agree very well with theirs.

E. Helicity Modulus Y at $T = 0$

In square lattice, Eq.(3.28) is simply

$$Y_{\alpha\alpha} \approx \frac{I_\alpha(f, \delta \hat{e}_\alpha)}{\delta} \quad \text{at small } \delta , \quad (3.50)$$

where α is x and y . Our calculations show that Y_{xx} and Y_{yy} are always equal within numerical accuracy. This isotropy of the helicity modulus is later confirmed by Monte Carlo simulation. The resulting values of Y are also plotted in Fig. 3.4.

Fig.3.4 $I_C(T=0)$ and $Y(T=0)$ vs. f of a square lattice for $f = 1/q$, $q \leq 13$. The lines connecting the data points are merely to guide the eye.

F. Comparison of T_c^{MC} to T_c^{MF}

Monte Carlo simulations of superconducting arrays in a square lattice was first done by Teitel and Jayaprakash⁹ at $f = 0, 1/2, 1/3$ and $1/4$. The most interesting finding in their simulations is probably that the presence of the magnetic field may change the nature of the transition. This was demonstrated in the case $f = 1/2$. The divergence of the specific heat at T_c plus the anti-ferromagnetic-Ising-like arrangement of the ground state vortices (shown in Fig. 3.3b) suggests that the system may become disordered via a transition of Ising-like variety instead of simply via a Kosterlitz-Thouless transition.

The Monte Carlo transition temperatures $T_c^{MC}(f)$, although much smaller than those of mean-field theory, display a cusp at $f = 1/2$, in agreement with mean-field theory, while $T_c^{MC}(f=1/4)$ is smaller than $T_c^{MC}(f=1/3)$, suggesting that $T_c(f)$ approaches c/q at small f , where c is a field-independent constant, in disagreement with mean-field theory.

3.4 Honeycomb Lattice

A. Explicit Expression for the Hamiltonian

Figure 3.5 shows the coordinate (I, J) we use for honeycomb lattice. Both I and J are indices in x and y directions and

Fig.3.5 The coordinates of a honeycomb lattice. I and J are in unit of $\frac{3}{2}a$ and $\frac{\sqrt{3}}{2}a$ respectively. 1 and 2 are denoting lattice directions.

are measured in units of $3/2a$ and $\frac{\sqrt{3}}{2}a$ respectively. The Hamiltonian is thus given explicitly

$$H = -\frac{J}{2} \sum_{I,J} \cos(\phi(I,J) - \phi(I,J+1) - \pi f I) + \cos(\phi(I,J) - \phi(I,J-1) + \pi f I) + \cos(\phi(I,J) - \phi(I+(-1)^{I+J}, J)) \quad (3.51)$$

where $f = \frac{3\sqrt{3}}{2} B a^2 / \Phi_0$ is the number of flux quanta through each hexagon.

B. Mean-field transition temperature $T_c^{MF}(f)$:

We solve the following self-consistent equations

$$\eta(I,J) = \frac{I_1(\beta |h(I,J)|)}{I_0(\beta |h(I,J)|)} \frac{h(I,J)}{|h(I,J)|} \quad (3.52)$$

$$h(I,J) = J[\eta(I,J+1)e^{i\pi f I} + \eta(I,J-1)e^{-i\pi f I} + \eta(I+(-1)^{I+J}, J)]$$

with periodic boundary conditions on a $m \times n$ cell where m and

n are integers. The obtained $T_c^{MF}(f)$ are plotted in Fig. 3.6.

Again, $T_c^{MF}(f)$ varies periodically with f with period 1 and is symmetric about $f = 1/2$. Note that the most conspicuous cusp occurs at $f = 1/3$. This has been seen experimentally in the measurements of the resistivity above T_c of a honeycomb network.²⁵

C. Ground State Properties

We also plot $-E_q(f)$ in Fig. 3.6. In the variation of $-E_g(f)$ with f , the cusp at $f = 1/3$ is strengthened. This can be understood by looking at the ground state configurations. In a honeycomb lattice, the phase configurations are rather complicated even for small q 's. However, the current distributions still preserve simple patterns. We show the ground state vortex configurations for $f = 1/2$, $1/3$ and $1/4$ in Fig. 3.7 as examples. The shaded hexagons represent positive vortices with charge $1 - f$ and the white are of charge $-f$.

At $f = 1/2$, the currents just flow in a zig-zag pattern and hence the system does not form a specific vortex configuration. There are in fact many degenerate states and Fig. 3.7a shows just one of these. The high degeneracy makes the system rather unstable at finite temperatures.

At $f = 1/3$, the vortices fit nicely into the dual lattice and form a rather symmetric pattern. The stability of this configuration helps the system to lower its energy at $T = 0$ as well as to maintain its ordered state at finite temperatures. The contrast between the curves of $T_c^{MF}(f)$ and $-E_g(f)$ for square and for honeycomb lattices demonstrates that the system not only reacts sensitively to the external field strength but also to its underlying lattice structure.

Fig.3.6 T_C^{MF} and $-E_g$ vs. f for a honeycomb lattice. The lines connecting the data points are merely to guide the eye. The insert shows the Monte Carlo transition temperatures T_C^{MC} for $f=0, 1/2, 1/3$, and $1/4$. Note that all curves show a cusp at $f=1/3$.

$$f = 1/2$$

$$f = 1/3$$

$$f = 1/4$$

Fig.3.7 Ground-state vortex configuration for $f=1/2, 1/3$ and $1/4$ of a honeycomb lattice. The shaded hexagons represent positive vortices with charge $1-f$ and a white one of charge $-f$. At $f=1/2$, the currents do not form a specific vortex configuration while at $f=1/3$, the vortices fit nicely into the dual lattice and form a symmetric pattern.

D. Critical Current I_c at $T = 0$

For the hexagonal lattice, the critical current densities in x (parallel to one of the lattice directions) and y (perpendicular to one of the lattice directions) take the form,

$$\begin{aligned} I_c(f)_x &= \frac{1}{\sqrt{3}a} \max_{\delta} I_1(f, \delta \hat{e}_x) \\ I_c(f)_y &= \frac{1}{\frac{3}{2}a} \max_{\delta} I_2(f, \delta \hat{e}_y) \end{aligned} \quad (3.53)$$

where 1 and 2 denote the lattice directions as indicated in Fig. 3.5. The obtained critical current densities are plotted in Fig. 3.8 for $q \leq 6$. Once again, the critical current densities are measured in unit of the critical current of a single junction per lattice constant. The larger critical current densities are perpendicular to the lattice direction. Both critical current densities show a conspicuous cusp at $f = 1/3$.

E. Helicity Modulus Y at $T = 0$

The $T = 0$ helicity modulus in honeycomb lattice is now expressed as

$$Y_{\alpha\alpha} = \frac{1}{2} \frac{\sum_{l=1}^3 I_l(f, \delta \hat{e}_{\alpha}) \hat{e}_l \cdot \hat{e}_{\alpha}}{\delta} \quad (3.54)$$

Fig.3.8 $I_c(T=0)$ and $\gamma(T=0)$ vs. f in a honeycomb lattice for $f = p/q$, $q \leq 6$. The lines are merely connecting the data points. The critical current densities are in unit of the critical current of a single junction per lattice constant and are anisotropic. The symbols $\perp$ and $\parallel$ denote perpendicular and parallel to the lattice direction respectively. All curves show a cusp at $f = 1/3$.

where $\alpha = x$ and y and z denotes the lattice directions. Again, we find that at any field Y is symmetric within numerical accuracy. The calculated $T = 0$ helicity moduli are also plotted in Fig. 3.8. Y also shows the cusp at $f = 1/3$.

F. Monte Carlo Simulation

In order to determine finite temperature properties in a honeycomb lattice, we have done MC simulations at $f = 0, 1/2, 1/3$ and $1/4$. The diagonal components Y_{xx} and Y_{yy} of the helicity modulus tensor are used as the order parameters. It turns out that the helicity modulus is symmetric also at finite temperatures, as is consistent with the $T = 0$ result.

We plot the helicity modulus for $f = 0, 1/2, 1/3$ and $1/4$ in Fig. 3.9. At $f = 0$, the helicity modulus is linear in T with a slope $-1/4$ at low temperatures, in agreement with Ohta and Jasnow's³¹ analytic result. The transition temperatures are estimated as those above which the helicity modulus falls below $2/\pi$. The tails of the helicity moduli above T_c are due to the finite size of the Monte Carlo samples. They can in principle be eliminated by increasing the sample size.

In all of the four cases, we find that the specific heat shows at most a smooth maximum at the transition temperature. To illustrate this point, we plot the specific heat as a function of temperature

Fig.3.9 Monte Carlo helicity modulus vs. T for $f=0, 1/2, 1/3$, and $1/4$ of a honeycomb lattice. The transition temperatures are estimated as those at which the helicity modulus falls below $2/\pi$.

Fig.3.10 Specific heat vs. T for $f=1/2$ of a honeycomb lattice, as an illustration of the lack of a specific heat anomaly of a KT-like transition.

for $f = 1/2$ in Fig. 3.10 as a demonstration. We therefore classify these as KT-like transitions to indicate the absence of the specific heat anomaly at the transition temperature. This classification does not necessarily mean that we are actually able to determine the universality class of these transitions, but only that they are not conventional second-order transitions with divergent specific heat peaks.

The estimated transition temperatures are also plotted in Fig. 3.6, where they are compared to the mean-field values. The Monte Carlo transition temperatures, although much reduced in value relative to mean-field, clearly demonstrate the minimum at $f = 1/2$ and the cusp at $f = 1/3$ in agreement with the mean-field theory.

3.5 Triangular Lattice

A. Explicit Expression for the Hamiltonian

Figure 3.11 shows how we label the lattice sites: 1 , 2 and 3 denote lattice directions and I and J are indices along directions 1 and 2 respectively.

The Hamiltonian is given explicitly as

$$\begin{aligned}
 H = -J \sum_{I,J} & \cos(\phi(I,J) - \phi(I+1,J)) + \cos(\phi(I,J) - \phi(I,J+1) - 2\pi f(2I+J+\frac{1}{2})) \\
 & + \cos(\phi(I,J) - \phi(I-1,J+1) - 2\pi f(2I+J-\frac{1}{2})) \quad ,
 \end{aligned}
 \tag{3.55}$$

Fig.3.11 The coordinates of a triangular lattice. I and J are the indices in the lattice direction 1 and 2 respectively.

where $f = \frac{\sqrt{3}}{4} B a^2 / \Phi_0$ is the number of flux quanta through each triangle.

B. $\underline{T_c^{MF}(f) \text{ and } -E_g(f)}$

To obtain the transition temperatures, we solve the following self-consistent equations,

$$\eta(I, J) = \frac{I_1(\beta |h(I, J)|)}{I_0(\beta |h(I, J)|)} \frac{h(I, J)}{|h(I, J)|} \quad (3.55)$$

$$\begin{aligned} h(I, J) = & J[\eta(I+1, J) + \eta(I-1, J) + \eta(I, J+1)e^{i2\pi f(2I+J+\frac{1}{2})} \\ & + \eta(I+1, J-1)e^{-i2\pi f(2I+J+\frac{1}{2})} + \eta(I, J-1)e^{-i2\pi f(2I+J-\frac{1}{2})} \\ & + \eta(I-1, J+1)e^{+i2\pi f(2I+J-\frac{1}{2})}] , \end{aligned}$$

with periodic boundary conditions for $q \leq 11$. The obtained $T_c^{MF}(f)$ are plotted in Fig. 3.12 as a function of f . Again, $T_c^{MF}(f)$ is non-monotonic and can be mapped onto the highest edge of the energy bands as a function of the magnetic field of a tight-binding electron in a triangular lattice, which was treated by Claro and Wannier.²⁴ Also shown in Fig. 3.12 are the negative ground state energy $-E_g(f)$ for $q \leq 11$ and the Monte Carlo transition temperatures for $f = 0, 1/2, 1/3$ and $1/4$. Note the especially outstanding cusp at $f = 1/4$ besides that at $f = 1/2$ in all three of these curves. This

Fig.3.12 T_C and $-E_g$ vs. f of a triangular lattice. The lines connecting the data points are merely to guide the eye. Note that in the curve of T_C^{MF} , the cusp at $f=1/4$ is also very conspicuous (unlike square and honeycomb lattices). The insert shows the Monte Carlo T_C^{MC} for $f=0, 1/2, 1/3$, and $1/4$ in comparison with mean-field results.

$$f=1/2$$

$$f=1/3$$

Fig.3.13 Ground-state vortex configurations for $f=1/2$ and $1/3$ of a triangular lattice. The arrows indicate the current directions. A shaded triangle denotes a positive vortex of charge $1-f$ and a white one of charge $-f$.

is a feature which is only seen in triangular lattice and is confirmed experimentally.⁴

C. Ground State Configurations, $I_c(T = 0)$ and $\gamma(T = 0)$

We show the ground state configurations of $f = 1/2$ and $f = 1/3$ in Fig. 3.13. The shaded triangles, again, denote positive vortices of charge $1 - f$, while the white triangles denote charge $-f$. Note that the vortex configuration of $f = 1/2$ looks very much like an antiferromagnetic-Ising arrangement: the two sublattices of "up spins" (shaded triangles) and "down spins" (white triangles) are interpenetrating. Later we will demonstrate from our Monte Carlo simulation that this Ising-like vortex configuration results in a specific heat divergence at the transition temperature just as for $f = 1/2$ in a square lattice.

The critical current densities at $T = 0$ are now calculated according to the following formula:

$$I_{c_x} = \frac{1}{\sqrt{3}a} \max_{\delta} (2I_1(f, \delta \hat{e}_x) + I_2(f, \delta \hat{e}_x) + I_3(f, \delta \hat{e}_x))$$

$$I_{c_y} = \frac{1}{a} \max_{\delta} (I_2(f, \delta \hat{e}_y) - I_3(f, \delta \hat{e}_y)) ,$$
(3.57)

where 1, 2 and 3 are the lattice directions and I_{c_x} and I_{c_y} denote the critical current densities parallel and perpendicular to the lattice direction 1 respectively. The resulting critical

Table 3.1. T_c , $-E_g$, I_c , γ and type of transition for $f=0, 1/4, 1/3$ and $1/2$ of a triangular lattice. Transition temperatures, $-E_g$ and γ are measured by the coupling constant J . Critical current densities I_c are in unit of the critical current of a single junction per lattice constant and the symbols $\perp$ and $\parallel$ denote perpendicular and parallel to a lattice direction. In the last column, KT and Ising merely indicate the absence or presence of a specific heat anomaly at the transition.

f	MC T_c	MF T_c	$-E_g$	$I_{c\parallel}(T=0)$	$I_{c\perp}(T=0)$	$\gamma(T=0)$	transition
0	1.45	3	3	2	2	1.5	KT
1/4	~.13, 0.3	1.27, 1.73	1.5	0.43	0.43	.75	KT
1/3	0.16	1.5	1½				KT
1/2	0.53	1.5	1.5	0.43	0.83	.75	Ising

current densities for $f=0, 1/4$ and $1/2$ are shown in table 3.1 along with T_c and $-E_q$ and types of transition. The critical current densities are generally anisotropic and the larger ones in table 3.1 are perpendicular to the lattice direction. Again, the critical current densities at $T = 0$ are in units of the critical current of a single junction per lattice constant. Also shown in table 3.1 are the $T = 0$ helicity moduli which are now approximated at small δ by:

$$\gamma_{\alpha\alpha} = \frac{\sum_{\ell=1} I_{\ell}(f, \delta \hat{e}_{\alpha}) \hat{e}_{\alpha} \cdot \hat{e}_{\ell}}{\delta}, \quad (3.58)$$

where α denotes x and y and ℓ denotes the lattice direction.

Again, the helicity modulus tensor proves to be isotropic.

D. Monte Carlo Simulation

We have carried out simulations for the cases $f = 0, 1/2, 1/3$ and $1/4$. In all cases, the helicity modulus proves to be symmetric at all temperatures. We plot the helicity modulus for $f = 0$, $f = 1/2$ and $f = 1/3$ as a function of temperature in Fig. 3.14. The $f = 0$ helicity modulus is indeed linear in T with a slope $-1/4$ at low temperatures, in agreement with Ohta and Jasnow.³¹ In the cases $f = 0$ and $f = 1/3$ the specific heat only shows a size-independent maximum as illustrated in Fig. 3.10 by the case at $f = 1/2$ in honeycomb lattice. The transition temperature is thus estimated as that above which the helicity modulus is less than $2/\pi$.

Fig3.14 Monte Carlo helicity modulus vs. T for $f=0, 1/2$ and $1/3$ of a triangular lattice. For $f=0$ and $1/3$, the transition temperatures are estimated as those above which the helicity modulus falls below $2/\pi$ while at $f=1/2$, T_C is estimated as that at which the specific heat diverges.

Fig.3.15 Specific heat vs. T for $f=1/2$ of a triangular lattice to illustrate the specific heat anomaly of a Ising-like transition.

At $f = 1/2$, as we have mentioned earlier, the specific heat diverges, i.e., the peak of the specific heat grows with increasing sample size and moves from higher temperatures towards T_c , as is commonly seen in a second order transition in two-dimensional systems.³³ We plot the specific heat as a function of temperature at $f = 1/2$ in Fig. 3.15. The transition temperature for $f = 1/2$ is approximated to be that at which the largest Monte Carlo sample has a peak in the specific heat. This estimated transition temperature is very close to that above which the helicity modulus falls below $2/\pi$. We call this transition "Ising-like" merely to indicate the presence of a specific heat anomaly. Our simulations can not, in fact, truly determine the universality class of the transition.

E. Evidence of a double transition at $f = 1/4$

As indicated earlier, a plot of mean-field transition temperatures versus field f shows an unusually high cusp at $f = 1/4$. We now focus on this case. First note that the ground state at $f = 1/4$ is periodic with a unit cell of eight elementary triangles, shown in the insert A of Fig. 3.16, two of which have charge $3/4$, denoted by shaded triangles and six have charge $-1/4$. As shown in Fig. 3.16, we have traced the mean-field order parameters $|\langle e^{i\phi_1} \rangle|$ closely as the temperature is increased and we find that within this approximation the system becomes disordered via two

Fig.3.16 Mean-field local order parameter $|\eta_i|$ vs. T for $f = 1/4$ of a triangular lattice. The abrupt drop of the $|\eta_i|$ at the center of a hexagon at $T_{c1} = 1.27J$ suggests that the lower transition be first order. Insert (a) shows the configuration of the ground state and insert (b) that of the intermediate state. All $|\eta_i|$ vanish at $T_{c2} = 1.73J$.

transitions. As the temperature approaches T_{c1} from below, the phase order parameters at the center of a hexagon drops discontinuously to zero while those on the perimeter of a hexagon take the opportunity to strengthen themselves by slightly adjusting their phase angles (insert B of Fig. 3.16). These phase order parameters then gradually decrease with increasing temperature. Finally the whole system becomes disordered at a higher temperature T_{c2} .

Strictly speaking, the phase order parameters $|\langle e^{i\phi_1} \rangle|$ are zero in two dimensions and hence can not be used as order parameters to indicate a true thermodynamic phase transition. Nonetheless, within a finite number of MC steps, $|\langle e^{i\phi_1} \rangle|$ are non-zero. The comparison of $|\langle e^{i\phi_1} \rangle|$ at different sites can tell us the stability of one grain relative to the others. We therefore plot $|\langle e^{i\phi_1} \rangle|$ obtained from MC method in Fig. 3.17a as a supporting evidence of the double transition. The abrupt drop in $|\langle e^{i\phi_1} \rangle|$ at the center of a hexagon indeed supports the mean-field suggestion that the lower transition is first order. Also shown in Fig. 3.17b and Fig. 3.17c are the helicity modulus Y and the specific heat as obtained from MC. The helicity modulus appears at least to have a change in slope at T_{c1} , at which the phase order parameter $|\langle e^{i\phi_1} \rangle|$ at the center of a hexagon drops abruptly. We estimate the upper transition temperature as that above which the helicity modulus falls below $2/\pi$. The tail of Y above T_{c2} is probably due to the finite size effect. There is also

Fig.3.17 Monte Carlo (a) $|\langle e^{i\phi_c} \rangle|$ (b) specific heat (c) helicity modulus vs. T . Around $T \approx 0.13J$, $|\langle e^{i\phi_c} \rangle|$ at the center of the a hexagon drops abruptly and the specific heat shows an unusual peak while the helicity modulus persists, falling below $2/\pi$ near $T \approx 0.25J$ where the specific heat shows a weaker maximum, supporting the double transition suggested by the mean-field approximation.

a distinct peak in the specific heat at T_{c1} , while T_{c2} is at most related to a weaker maximum in the specific heat. The two mean-field transitions occur at temperatures about a factor of 10 above the Monte Carlo transition temperatures, indicating that the fluctuations are important here.

The experimental realization of this seeming double transition would be as follows. The higher transition at T_{c2} is the point at which the system becomes non-resistive with respect to an infinitesimal external current. The most significant evidence of the other transition at T_{c1} would most likely be a jump in critical current. The phase between T_{c1} and T_{c2} could have some strange properties arising from the inhomogeneous distributions of normal and superconducting weak links. For example, the a.c. properties would probably be those of an impedance network composed of pure inductive elements (the Josephson or proximity-coupled junctions) and resistors (normal links) distributed regularly in a two-dimensional lattice. Such a network would be likely to show substantial absorption below the superconducting energy gap. Further similar transitions seem likely to occur in other lattices and in other magnetic fields.

3.6 Summary

1. If we compare our calculations with experiments in all three lattices, we find, surprisingly, that $T_c^{MF}(f)$ or $-E_g(f)$, plotted as

a function of field, correctly reflects the resistivity measurements above T_c in all these arrays. This is especially so in superconducting wire networks^{25,32} where fluctuations are not as large as in the granular arrays.

2. The extensive mean-field calculations and the Monte Carlo simulations at several values of f in each lattice prove that it is characteristic of the system that all quantities such as T_c , E_g , I_c and Y as a function of field are non-monotonic, while the underlying lattice may change the height of a cusp at rational values of f .

3. Careful Monte Carlo simulations bring the message: the presence of the magnetic field not only reduces the transition temperature periodically with field but also adds much complexity to the system. Among the greatest complexities are the Ising-like transitions at $f = 1/2$ in both square and triangular lattices, and the double transition at $f = 1/4$ in triangular lattice.

CHAPTER 4: THREE-DIMENSIONAL ORDERED ARRAYS: SIMPLE CUBIC

In three dimensions, the direction of the magnetic field can be varied as well as the magnitude and both can cause T_c and E_g to change. We will use $\vec{f} = (f_1, f_2, f_3)$ to describe the magnetic field where f_1 , f_2 and f_3 are the number of flux quanta through a unit square in x , y and z direction respectively.

In a three dimensional ordered array, the physical properties are in general anisotropic with respect to the direction of the applied field. The reason for this lies in the nature of the Hamiltonian: the coupling between phases in the field direction is unchanged by the applied field, while the field will produce frustration between phases in a plane perpendicular to the field. In Section 4.1, we will focus on the case $\vec{f} = (0,0,f)$ to demonstrate this anisotropy as well as to examine the physical properties of the system at different field strengths.

Varying the field direction will change the ground state configuration of the system and hence all of its physical quantities. In Section 4.2, we will compare the ground state energies in two different field directions as a function of field strength to

illustrate the sensitivity of the system to field direction.

$$4.1 \quad \vec{f} = (0,0,f)$$

$$A. \quad \underline{T_c^{MF}(f) \text{ and } -Eg(f)}$$

At $\vec{f} = (0,0,f)$ the Hamiltonian is given as

$$H = -J \sum_{I,J,K} \cos(\phi(I,J,K) - \phi(I+1,J,K)) + \cos(\phi(I,J,K) - \phi(I,J+1,K)) + 2\pi f I \quad (4.1)$$

$$+ \cos(\phi(I,J,K) - \phi(I,J,K+1)) \quad ,$$

where I , J and K are the indices in x , y and z directions.

From Eq.(4.1) it is already clear that the coupling along the field direction is unaffected by application of the field. Indeed, it turns out that the ground state phase configurations for a simple cubic lattice at $\vec{f} = (0,0,f)$ are just obtained by stacking those for a square lattice (Fig. 3.3a). That is, the phases of the superconducting grains are parallel in the field direction. Consequently, $T_c^{MF}(f)$ and $-Eg(f)$ at $\vec{f} = (0,0,f)$ in a simple cubic lattice are just those in a square lattice (shown in Fig. 3.2) plus J at each f .

$$(T_c^{MF})_{sc}(f) = (T_c^{MF})_{sq}(f) + J \quad (4.2)$$

$$(-Eg)_{sc}(f) = (-Eg)_{sq}(f) + J \quad ,$$

where sc stands for simple cubic and sq square.

B. Anisotropy of γ

As noted, the presence of a magnetic field in one of the axes produces frustration only in the planes perpendicular to the field. The helicity modulus, which is analogous to the superfluid density, clearly reflects this anisotropy. At $T = 0$, γ_{zz} , the helicity modulus in the field direction, equals J at all field strengths, while γ_{xx} and γ_{yy} are identical to those of a square lattice (Fig. 3.4) at $T = 0$. Both are less than γ_{zz} because the phases are parallel in field direction and it costs more energy to twist phases that are parallel.

C. I_c at $T = 0$

This critical current densities at $T = 0$ also show this anisotropy. If we express the critical current density in units of the critical current of a single junction per unit square, then I_{cz} , the critical current density in the field direction, equals unity at any field strength, while I_{cx} and I_{cy} just have the values of a square lattice (Fig. 3.4).

D. Monte Carlo Simulations

In order to gain further information, we have done extensive simulations for a simple cubic lattice at $\vec{f} = (0,0,f)$ in the cases $f = 1/q$ and $1 \leq q \leq 6$. As examples, we plot the helicity moduli parallel and perpendicular to the field in Fig. 4.1a and Fig. 4.1b respectively for $f = 0, 1/2$ and $1/3$. The transition temperatures are estimated as those at which the helicity moduli have an inflection point. The tails above T_c are due to the well known Monte Carlo finite-size effect.³⁴ This can in principle be eliminated by increasing the sample size, as illustrated by the case $f = 0$ in Fig. 4.1a. The two arrows indicate $T_c(0)$, the estimated transition temperature for $f = 0$ from our simulation and $T_{c\infty}$, the transition temperature obtained by the method of high-temperature series expansion.²¹ $T_c(0)$ is slightly lower than $T_{c\infty}$, as is commonly seen in estimates of the Monte Carlo transition temperatures in three dimensions.³⁴

We also plot the specific heat for $\vec{f} = (0,0,1/3)$ as a function of temperature in Fig. 4.2. The peak in specific heat not only grows but also moves from lower temperatures towards T_c as the size of the Monte Carlo sample is increased, indicating a real specific heat anomaly.

The anomaly in the specific heat will be more difficult to observe at large q 's. The reasons are the following. First, the

Fig.4.1(a) Monte Carlo helicity modulus parallel to the field vs. T for $\vec{f}=(0,0,0)$, $(0,0,1/3)$, and $(0,0,1/2)$ of a simple cubic lattice. The transition temperatures are estimated as those at which the helicity modulus has an inflection point. $T_{c\infty}$ denotes the transition temperature of $\vec{f}=(0,0,0)$ obtained by the high temperature series expansion.

Fig.4.1(b) Monte Carlo helicity modulus perpendicular to the field vs. T for $\vec{F}=(0,0,0)$, $(0,0,1/3)$ and $(0,0,1/2)$ of a simple cubic lattice. The determination of T_c is described in the caption of Fig.4.1(a).

Fig.4.2 Monte Carlo specific heat vs. T for $\vec{f}=(0,0,1/3)$ of a simple cubic lattice to illustrate the specific heat divergence at T_c .

Fig.4.3 Monte Carlo helicity modulus parallel and perpendicular to the field for $\vec{F}=(0,0,1/3)$ of a simple cubic lattice to illustrate the anisotropy of the helicity modulus of a 3d array.

Monte Carlo convergence becomes slower at large q 's. Secondly, the large unit cell at large q greatly reduces the number of proper sizes of the Monte Carlo sample. Nonetheless, we find that in all of the cases we have considered, the temperatures at which the specific heat anomaly occurs are always coincident with those at which the helicity moduli have an inflection point, indicating that the transitions are second order. However, we do not have enough calculations to determine the precise universality class of the transitions.

Our results should be contrasted to two dimensional systems, in which the helicity modulus seems to jump discontinuously at T_c , either with a specific heat anomaly (Ising-like transitions) or without one (KT-like transition). Note that the transitions in three dimensions are all second order. The helicity moduli go to zero continuously at the same T_c at which the specific heat diverges.

To illustrate the anisotropy of the helicity modulus at finite temperatures, we plot the helicity moduli both parallel and perpendicular to field for $\vec{f} = (0,0,1/3)$ in Fig. 4.3. One can see that the anisotropy is increased with increasing temperature and becomes very large in the vicinity of the transition temperature. For large q 's, the anisotropy near the transition temperature gets even bigger.

The two components of the helicity modulus tensor may vanish with

Fig.4.4 Estimated Monte Carlo transition temperatures T_c^{MC} vs. f of a simple cubic lattice at $\vec{f}=(0,0,f)$ in comparison with mean-field results.

a different power law behavior near T_c . Experimentally, an anisotropic superfluid might be probed by measurements of the kinetic inductance, i.e., the imaginary part of the conductivity, as discussed in Appendix C.

The estimated Monte Carlo transition temperatures are plotted in Fig. 4.4 as a function of field. Also shown in Fig. 4.4 are the mean-field transition temperatures $T_c^{MF}(f)$. In comparison with $T_c^{MF}(f)$, the Monte Carlo transition temperatures are much lower, indicating that fluctuations are important here. Nevertheless, $T_c^{MF}(f)$ generally reflects the variation of $T_c^{MF}(f)$ with f , especially the cusp at $f = 1/2$ and the trend of an increasing T_c as f approaches zero.

4.2 Sensitivity to the Field Direction

To illustrate how sensitive the system is to a change of field direction, we plot the ground state energy for both $\vec{f} = (0,0,f)$ and $\vec{f} = \frac{1}{\sqrt{3}}(f,f,f)$ as a function of f , the field strength, in Fig. 4.5. The ground state energy for $\vec{f} = \frac{1}{\sqrt{3}}(f,f,f)$ is calculated from the following Hamiltonian:

$$H = -J \sum_{I,J,K} [\cos(\phi(I,J,K) - \phi(I+1,J,K) - 2\pi \frac{f}{\sqrt{3}} K) + \cos(\phi(I,J,K) - \phi(I,J+1,K) - 2\pi \frac{f}{\sqrt{3}} I) + \cos(\phi(I,J,K) - \phi(I,J,K+1) - 2\pi \frac{f}{\sqrt{3}} J)] \quad (4.3)$$

Fig.4.5 $-E_g$ vs. f for $\vec{f} = f(0,0,1)$ and $\vec{f} = \frac{f}{\sqrt{3}}(1,1,1)$ in a simple cubic lattice to illustrate the sensitivity of the system to the direction of the field.

We use the same method as before, namely, the "mean-field annealing."

From Fig. 4.4, it is clear that rotating the field from (001) direction to (111) direction causes the ground state energy to change dramatically except for small f . Note that the minimum of $-E_g(f)$ in (111) direction is much deeper than that of $-E_g(f)$ in (001) direction. The reason for this is that the magnetic field in (111) direction frustrates the coupling between phases in all three directions, while the field in (001) direction only affects the coupling in a plane perpendicular to the field.

Conceivably, if one rotates the magnetic field gradually, the ground state energy will vary non-monotonically. That is, the variation of the ground state energy, and hence other quantities with field direction, will have cusps at certain directions, causing the system to undergo numerous commensurate-incommensurate transitions. thus, in three dimensions, the variation of physical quantities with the direction of the field is no less complicated than with the magnitude of the field.

CHAPTER 5: DISORDERED ARRAYS

5.1 Speculation

In previous chapters, we have studied two- and three-dimensional ordered arrays, showing that the transition temperatures and other physical quantities of a perfectly ordered array are periodic with the applied field, even though the variations within a period are complicated and may depend upon the underlying lattice structure.

In reality, there exist no perfectly ordered arrays. A real sample always has some non-uniformity. Moreover, even an approximately ordered three-dimensional array is difficult to prepare in practice. A more realistic three dimensional array would be a composite made of superconducting grains randomly embedded in a normal or insulating host. Therefore, it is of great interest to know how disorder affects the physical properties of the system.

Consider the coupling between two grains of a disordered array in the presence of a magnetic field:

$$E_{ij} = -J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \quad , \quad (5.1)$$

where J_{ij} is the coupling energy between grain i and grain j and is now dependent on the separation of the two grains, and A_{ij} is the phase factor due to the presence of the magnetic field. If we choose the field direction to be $\hat{z}$, i.e.,

$$\vec{B} = B\hat{z} \quad (5.2)$$

and use the gauge

$$A = Bx\hat{y} \quad , \quad (5.3)$$

we can express the magnetic phase factor in the following form:

$$A_{ij} = 2\pi B x_{ij}(y_j - y_i) \quad , \quad (5.4)$$

where $x_{ij} = \frac{1}{2}(x_i + x_j)$, and x_i and y_i are the coordinates of grain i in x and y directions respectively.

At zero field, the system will behave like a disordered ferromagnet since the XY couplings are all ferromagnetic. At sufficiently large field, however, nearly all the phase factors A_{ij} are large compared to 2π (the only exceptions are those in the xz plane). The couplings would tend to orient the phases of the grains at random angles. Thus the system will behave very much like a "spin glass." In fact, it is a physical realization of a "gauge glass" mentioned by several authors.³⁵ After the "spin glass" limit has been reached, further increase in magnetic field will not change the thermodynamic properties, since the couplings have already been

randomized. However, in this regime, a change in field is equivalent to a jump from one "spin-glass replica" to another. Thus the phase-ordering transition temperature should decrease from its zero-field value, as the field is increased, finally saturating at a lower, "spin-glass" value. The crossover field dividing low-field from high-field behavior should be of order one flux quantum per d^2 where d is a typical separation between two grains with non-zero coupling.

A schematic of the behaviors of T_c versus field in various cases is shown in Fig. 5.1. In an ordered array, all the closed loops of non-zero bonds have the same projected area perpendicular to the field. Thus the system has only one natural period with field as shown in Fig. 5.1a. In a strongly disordered array, different closed loops of non-zero bonds have different projected areas perpendicular to the field, corresponding to various periods. Thus, integrating over various periodicities, the system as a whole is not expected to show any oscillations with field. T_c should decrease from its zero field value at small fields and saturate at a high-field value as the field is further increased, as is shown in Fig. 5.1c. In a weakly disordered array, all the closed loops of non-zero bonds have projected areas very close to the fundamental one. Therefore, there are fields at which all the couplings are nearly ferromagnetic, like the zero-field case. One thus expects T_c to vary with field like a

Fig.5.1 A schematic of T_c vs. B of a (a) ordered array (b) weakly disordered array and (c) strongly disordered array.

damped oscillation, as shown in Fig. 5.1b, approaching a "spin-glass" value at high fields.

5.2 Slightly Disordered Array: Mean-Field Theory

To model a weakly disordered two-dimensional array, we put 400 grains in a square lattice and allow the grains to sit a little bit off the lattice sites. Let $|\Delta x_i|$ and $|\Delta y_i|$ denote the deviation of grain i from its ideal position measured in x and y directions respectively. We restrict both $|\Delta x_i|$ and $|\Delta y_i|$ to be within one hundredth of a lattice constant. For simplicity, a nearest-neighbor constant coupling energy is assumed. The following mean-field coupled equations are then solved by iteration with periodic boundary conditions:

$$\eta_i = \frac{I_1(\beta|h_i|)}{I_0(\beta|h_i|)} \frac{h_i}{|h_i|} \quad (5.5)$$

$$h_i = \sum_j J_{ij} \eta_j e^{iA_{ij}},$$

where J_{ij} is the constant nearest-neighbor coupling energy and A_{ij} takes the form of Eq.(5.4).

the resulting transition temperatures are plotted in Fig. 5.2 as a function of f up to $f = 14$, where f is the number of flux quanta per lattice square. Clearly, the oscillation of $T_c^{MF}(f)$ with

Fig.5.2 T_c^{MF} vs. f of a slightly disordered square array of 400 grains.

f becomes damped and distorted as f is increased from zero.

Finally, for $f \geq 10$, $T_c^{MF}(f)$ simply fluctuates about 1.4 J. The fluctuation of $T_c^{MF}(f)$ at large fields in Fig. 5.2 is probably due to the small size of the sample. Nonetheless, Fig. 5.2 confirms our speculation in Section 5.1: Weak disorder will damp the oscillations of T_c at small fields and cause T_c to saturate at a "spin-glass" value at high fields.

Experimentally, the measured variations of the resistivity above T_c as a function of field for a superconducting array³⁻⁷ as well as for a wire network^{25,32} all behave like a damped oscillation. Our simple mean-field calculation clearly demonstrates how this damping effect could result from the non-uniformity of the sample. Of course, there could be other mechanisms, too, such as finite junction width, finite grain size and variation in junction resistance.

5.3 Site-Diluted Three-Dimensional Array

To examine the effect of stronger disorder other than just weak non-uniformity, we first carry out the mean-field calculations on a site-diluted array. The sample is a $12 \times 12 \times 12$ simple cubic lattice with 48.96% of the sites randomly occupied by superconducting grains. Assuming a constant nearest-neighbor coupling energy, we solve the following mean-field coupled equations by iteration with periodic boundary conditions:

$$\begin{aligned}
 n_1 &= \frac{I_1(\beta|h_1|)}{I_0(\beta|h_1|)} \frac{h_1}{|h_1|} && \text{if site 1 is occupied} \\
 &= 0 && \text{otherwise}
 \end{aligned}
 \tag{5.6}$$

$$h_1 = \sum_j J_{1j} n_j e^{iA_{1j}},$$

where A_{ij} is the magnetic phase factor between nearest neighbors in a simple cubic lattice with the field pointing in one of the axial directions and J_{ij} is the nearest-neighbor coupling constant.

The resulting $T_c^{MF}(f)$ as a function of f is plotted in Fig. 5.3b, where f is the number of flux quanta per lattice square. Again, Fig. 5.3b can be mapped onto the highest energy eigenvalue of an electron in a site-diluted tight-binding band in the presence of a magnetic field.

Also shown in Fig. 5.3a are the mean-field transition temperatures of an ordered simple cubic lattice as a comparison. Note the variation of $T_c^{MF}(f)$ as a function of f in a site-diluted array (Fig. 5.3b) no longer has the complicated structures of the ordered array (Fig. 5.3a). The reason for this is that various projected areas perpendicular to the field of different closed loops of non-zero coupling strength are present in a site-diluted array. In Fig. 5.3b, $T_c^{MF}(f)$ decreases monotonically as the field is increased from zero,

Fig.5.3 T_c^{MF} vs. f of a (a) ordered simple cubic (b) site-dilute simple cubic array. $\vec{f}=(0,0,f)$. In (b), the site-diluteness washes out the non-monotonic variation of T_c^{MF} with f of a ordered array shown in (a) and T_c^{MF} flattens when f approaches $1/2$. The periodic dependence of T_c^{MF} on f is merely due to the artifact that all grains are still sitting on lattice sites.

flattening out when f approaches $\frac{1}{2}$, in agreement with the speculation in Section 5.1 for a disordered array. The periodicity of $T_c^{MF}(f)$ with f and the symmetry of $T_c^{MF}(f)$ about $f = \frac{1}{2}$ in a site-diluted array are merely due to the artifact that all the grains are still sitting on lattice sites.

5.4 Three-Dimensional Granular Composite

A. Mean-Field Approximation

To model an amorphous granular composite, we put the superconducting grains randomly in a fine grid at a small dilution so that the system has various separations between two grains. In the actual calculation, we put 158 superconducting grains in a $24 \times 24 \times 24$ grid. The separations between any two grains are all greater than or equal to $\sqrt{3}$ grid lattice constants. We then iterate the mean-field coupled equations [Eq.(5.5)] to convergence with periodic boundary conditions on this sample. In Eq.(5.5), A_{ij} is defined by Eq.(5.4) and J_{ij} now takes the form

$$J_{ij} = J e^{-|\vec{r}_i - \vec{r}_j|/\xi(T)}, \quad (5.7)$$

where $\vec{r}_i$ is the position of grain i and $\xi(T)$ is the coherence length of the normal metal. Here we assume ξ to be 1.6 grid

Fig.5.4 T_C^{MF} vs. f of a positionally disordered 3d array. f denotes the number of flux quanta through a square whose side is the average separation between grains.

lattice constants and to be independent of temperature. The exponentially decaying coupling is cut off at separations larger than 7 grid lattice constants. At this distance, the coupling is approximately one twentieth of that for nearest neighbors. On average, a given grain interacts with 25 neighbors.

The resulting transition temperatures $T_c^{MF}(f)$ as a function of f are plotted in Fig. 5.4, where f is the number of flux quanta per d^2 . d is the average separation between two grains. The transition temperature does drop monotonically at small fields and flattens out at large fields, in agreement with the speculation in Section 5.1. The variation in the projected areas of closed loops of non-zero coupling strength wash out any oscillatory behavior of T_c with field.

B. Monte Carlo Results

Monte Carlo simulation for a disordered array was first done by Shih, Ebner and Stroud.¹⁰ The Monte Carlo sample is intended to model a composite of Pb spheres dilutely embedded in a Zn host. The helicity modulus is used as the order parameter in the simulations. The results revealed several interesting properties of a disordered array, which confirm our speculations in Section 5.1.

First, the convergence of physical quantities is much slower than in an ordered array. Secondly, in contrast to an ordered array the

specific heat peak does not show any size dependence when the size of the Monte Carlo sample is increased. Thirdly, the helicity modulus relaxes on some occasions, that is, a group of 20-30 "spins" rotate together, causing the helicity modulus to have a sudden jump. Also, the anisotropy of the helicity modulus that is the characteristic of a three-dimensional ordered array disappears at high fields. At last, the estimated Monte Carlo transition temperatures as a function of field do behave like what is predicted by mean-field theory: T_c drops monotonically at small fields and is totally insensitive to the change in field at high fields.

The lack of a divergent specific heat at T_c , the slow convergence of physical quantities, the relaxational phenomena, the isotropy of the helicity modulus tensor and the insensitivity of T_c to the change in field at high fields together provide evidence to support our speculation: In the high-field limit, the system behaves like a spin glass.

It is interesting that a disordered array presents the possibility of a system which can be transformed from a disordered ferromagnet to a spin glass by continuous variation of an external parameter -- the magnetic field. In a sufficiently strong field, the disorder of the array and the frustration produced by the field together create many metastable states each of which lies only a small energy above the ground state. At low temperatures, the system can be

easily trapped in the metastable states and the measured quantities are very likely to be the metastable ones. Therefore, the system should show many of the typical characteristics of other glasses, such as time-dependence of supposedly equilibrium quantities and various kinds of hysteresis. The Monte Carlo simulations, for example, show the relaxation of the helicity modulus as mentioned earlier. Thus the existence of a true phase transition is somewhat doubtful, just as it is in other types of spin glass ordering. All these relaxation phenomena can probably be studied experimentally via low frequency conductivity as discussed in Appendix C.

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APPENDIX A

We will use the linearized equation (3.41) to evaluate $T_c^{MF}(f)$ at $f = 0$, $1/2$ and $1/3$ and find an analytical expression for $T_c^{MF}(f)$ near $f = 0$ and near $f = 1/2$. Since we are below $T_c^{MF}(f)$, all $\eta(I,J)$'s should be non-zero and periodic in both x and y directions. We should be able to express $\eta(I,J)$'s as Fourier sums. Let us assume the period to be q in both x and y directions (this will be justified numerically). $\eta(I,J)$ can then be written as

$$\eta(I,J) = \frac{1}{\sqrt{q}} \sum_k \eta(I,k) e^{ikJa}, \quad (A.1)$$

where k is a multiple of $2\pi/qa$, running from 0 to 2π , and a is the lattice constant. The linearized equation (3.41) is thus

$$\sum_k 2T \eta(I,k) e^{ikJa} = \sum_k e^{ikJa} (\eta(I+1,k) + \eta(I-1,k) + 2\eta(I,k) \cos(2\pi fI + ka)). \quad (A.2)$$

To have Eq.(A.2) as an identity, we expect the Fourier coefficients on both sides of Eq.(A.2) should individually be equal

$$2T\eta(I,k) = \eta(I+1,k) + \eta(I-1,k) + 2\eta(I,k) \cos(2\pi fI + ka) \quad (A.3)$$

From the argument of the cosine in (3.33), we observe that the

effect of ka is like a translation of $(k/(2\pi/qa))$ steps in x direction and it will not affect the analysis of $T_c^{MF}(f)$. It is therefore sufficient to deal with the simplest case, namely, $k = 0$.

Let us call $\eta(I, k = 0) = \eta(I)$. Then Eq.(A.3) becomes

$$\frac{2T}{J} \eta(I) = \eta(I+1) + \eta(I-1) + 2\eta(I) \cos(2\pi f I) . \quad (A.4)$$

We then rewrite (A.4) in the form of transfer matrix.

$$\begin{pmatrix} \eta(I+1) \\ \eta(I) \end{pmatrix} = \begin{pmatrix} \frac{2T}{J} - 2 \cos(2\pi f I) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \eta(I) \\ \eta(I-1) \end{pmatrix} . \quad (A.5)$$

The condition for $\eta(I)$'s to be non-vanishing and to have period q is that the eigenvalues of the total transfer matrix M , which is the product of q successive transfer matrices, have absolute value unity. We thus use this condition to find T_c^{MF} for several values of f .

Case 1: $f = 0$

At $f = 0$, the period is 1 and the eigenvalues λ of the total transfer matrix obey the following equation,

$$\lambda^2 - (2 \frac{T}{J} - 2)\lambda + 1 = 0 . \quad (A.6)$$

The condition for $|\lambda| = 1$ is

$$(2 \frac{T}{J} - 2)^2 \leq 4 , \quad (A.7)$$

and hence $T_c^{MF}(f = 0) = 2J$ is the maximum temperature satisfying Eq.(A.7).

Case 2: Near $f = 0$

We follow the analysis of Ref. 36. Since f is small we treat the configuration at small f as a slight variation from that of $f = 0$. Therefore, $\eta(I+1)$ and $\eta(I-1)$ are related to $\eta(I)$ in the following form,

$$\begin{aligned}\eta(I+1) &= e^{ip} \eta(I) \\ \eta(I-1) &= e^{-ip} \eta(I)\end{aligned}\tag{A.8}$$

where p is the momentum operator in unit a^{-1} , and a is the lattice constant. Equation (A.4) becomes

$$2\frac{T}{J} \eta(I) = 2(\cos p + \cos(2\pi f I)) \eta(I) .\tag{A.9}$$

For small f , p must be also small; therefore,

$$\begin{aligned}\cos p &\approx 1 - \frac{1}{2} p^2 \\ \text{and} \\ \cos 2\pi f I &\approx 1 - \frac{1}{2} (2\pi f I)^2 .\end{aligned}\tag{A.10}$$

To the lowest order of p and f , Eq.(A.9) becomes

$$(2 - \frac{T}{J}) \eta(I) = (\frac{1}{2} p^2 + \frac{1}{2} (2\pi f I)^2) \eta(I) .\tag{A.11}$$

Equation (A.11) is just like the Schrödinger equation for a simple harmonic oscillator with unit mass and spring constant $(2\pi f)^2$.

$2 - T_c^{MF}(f)$ corresponds to the lowest energy eigenvalue of the harmonic oscillator.

$$2 - \frac{T_c^{MF}}{J}(f) = \frac{1}{2} \omega^2, \quad (\text{A.12})$$

where $\omega = \sqrt{\frac{(2\pi f)^2}{1}} = 2\pi|f|$ is the frequency of the harmonic oscillator. $T_c^{MF}(f)$ is thus

$$T_c^{MF}(f) = (2 - \pi|f|)J \quad \text{for } |f| \ll 1. \quad (\text{A.13})$$

Case 3: $f = 1/2$

The period of $\eta(I)$'s is 2. The total transfer matrix M is then the product of 2 successive matrices.

$$\begin{aligned} M &= \begin{pmatrix} 2\frac{T}{J} + 2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2\frac{T}{J} - 2 & -1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 4(\frac{T}{J})^2 - 5 & -2\frac{T}{J} - 2 \\ 2\frac{T}{J} - 2 & -1 \end{pmatrix}. \end{aligned} \quad (\text{A.14})$$

The eigenvalues λ of matrix M obey

$$\lambda^2 - (4(\frac{T}{J})^2 - 6)\lambda + 1 = 0. \quad (\text{A.15})$$

requiring $|\lambda| = 1$, we obtain an inequality for T .

$$\left(2\left(\frac{T}{J}\right)^2 - 3\right)^2 - 1 \leq 0. \quad (\text{A.16})$$

Therefore, $T_c^{\text{MF}}(f = 1/2) = \sqrt{2} J$ is the maximum temperature satisfying Eq.(A.16).

Case 4: Near $f = 1/2$

We extend the analysis near $f = 0$. Let $f = 1/2 + \delta$. For small δ , the configuration of $\eta(I)$ can be treated as a deviation from that at $f = 1/2$. Since the system has period 2 at $f = 1/2$, we will treat two adjacent η 's, say, $\eta(I)$ and $\eta(I+1)$ as two independent variables

$$\begin{aligned} \eta(I+2) &= e^{12p} \eta(I) \\ \eta(I-1) &= e^{-12p} \eta(I+1), \end{aligned} \quad (\text{A.17})$$

where p is the momentum operator. Plugging Eq.(A.17) into Eq.(A.4) we get two coupled equations for $\eta(I)$ and $\eta(I+1)$.

$$2 \frac{T}{J} \eta(I) = (1 + e^{-12p}) \eta(I+1) + \eta(I) \cos(2\pi f I) \quad (\text{A.18})$$

$$2 \frac{T}{J} \eta(I+1) = (1 + e^{12p}) \eta(I) + \eta(I+1) \cos(2\pi f (I+1)) \quad (\text{A.19})$$

Substituting Eq.(A.19) into Eq.(A.18), we get

$$\frac{T}{J} \eta(I+1) = \frac{\cos^2 p}{\frac{T}{J} - \cos(2\pi f I)} \eta(I+1) + \cos(2\pi f(I+1)) \eta(I+1) \quad . \quad (A.20)$$

Let $\frac{T}{J} = \sqrt{2} + \varepsilon$ and $f = \frac{1}{2} + \delta$. To the lowest order in ε , δ and p , Eq.(A.20) becomes

$$- \varepsilon \eta(I+1) \approx [(\pi \delta(I+1))^2 + \frac{1}{2} p^2] \eta(I+1) \quad . \quad (A.21)$$

Again, Eq.(A.21) looks like a Schrödinger equation for a harmonic oscillator with mass 1 and spring constant $2(\pi \delta)^2$. $T_c^{MF}(f)$ is given by the lowest energy eigenvalue of the harmonic oscillator,

$$- \varepsilon_c = \frac{1}{2} \omega^2 \quad , \quad (A.22)$$

where $\omega = \sqrt{2(\pi \delta)^2} = \sqrt{2} \pi |\delta|$, the frequency of the harmonic oscillator. $T_c^{MF}(f)$ is thus

$$T_c^{MF}(f) = (\sqrt{2} - \frac{\pi}{\sqrt{2}} |f - \frac{1}{2}|)J \quad \text{near } f = \frac{1}{2} \quad . \quad (A.23)$$

Case 5: $f = 1/3$

The system now has period 3. The total transfer matrix is the product of 3 successive matrices

$$\begin{aligned}
 M &= \begin{pmatrix} 2T+1 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2T+1 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2T-2 & -1 \\ 1 & 0 \end{pmatrix} \\
 &= \begin{pmatrix} (2T+1)(4T^2-4T-1) & -2T(2T+1) \\ (2T+1)(2T-2)-1 & -(2T+1) \end{pmatrix}.
 \end{aligned} \tag{A.24}$$

The eigenvalues λ of M obey

$$\lambda^2 + 2 \frac{T}{J} (2 \frac{T}{J} + 1) (2 \frac{T}{J} - 2) \lambda - 1 = 0. \tag{A.25}$$

Requiring $|\lambda|$ to be 1, we get an inequality for T :

$$\left(\frac{T}{J} (2 \frac{T}{J} + 1) (2 \frac{T}{J} - 2) \right)^2 - 1 \leq 0. \tag{A.26}$$

Thus, $T_c^{MF}(f = \frac{1}{3}) = \frac{1 + \sqrt{3}}{2} J$ is the maximum temperature satisfying Eq.(A.26).

APPENDIX B

In the presence of a magnetic field, the superconducting order parameter Δ_i of grain i is modified as follows

$$\Delta_i = \Delta_i e^{iA_i}$$

or (B.1)

$$\Delta_i = |\Delta_i| e^{i(\phi_i + A_i)},$$

where A_i is the phase factor at site i due to the presence of the magnetic field

$$A_i = \frac{2\pi}{\Phi_0} \int_0^{\vec{x}_i} \vec{A} \cdot d\vec{l}, \quad (B.2)$$

where Φ_0 is the elementary flux quantum and $\vec{A}$ is the vector potential. The coupling energy between grain i and grain j thus becomes

$$E_{ij} = -J_{ij} \cos(\phi_i - \phi_j - A_{ij}), \quad (B.3)$$

where

$$A_{ij} = A_j - A_i = \frac{2\pi}{\Phi_0} \int_{\vec{x}_j}^{\vec{x}_i} \vec{A} \cdot d\vec{l}. \quad (B.4)$$

It is clear from Eq.(B.4) that A_{ij} is independent of the choice of the origin. The Hamiltonian thus takes the form of Eq.(1.7).

$$H = - \sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \quad . \quad (B.5)$$

Next, we would like to demonstrate the periodic dependence of the Hamiltonian of an ordered array on the magnetic field. We examine 2d arrays as examples. For convenience, let us use the gauge $\vec{A} = B\hat{x}\hat{y}$ and assume nearest-neighbor couplings. The Hamiltonian Eq.(B.5) then takes the following forms:

$$H = -J \sum_{I,J} \cos(\phi(I,J) - \phi(I+1,J)) + \cos(\phi(I,J) - \phi(I,J+1)) + 2\pi f I \quad (B.6)$$

for a square lattice,

$$H = -\frac{J}{2} \sum_{I,J} \cos(\phi(I,J) - \phi(I,J+1) - \pi f I) + \cos(\phi(I,J) - \phi(I,J-1) + \pi f I) + \cos(\phi(I,J) - \phi(I+(-1)^{I+J}, J)) \quad (B.7)$$

for a honeycomb lattice and

$$H = -J \sum_{I,J} \cos(\phi(I,J) - \phi(I+1,J)) + \cos(\phi(I,J) - \phi(I,J+1) - 2\pi f(2I+J+\frac{1}{2})) + \cos(\phi(I,J) - \phi(I-1,J+1) - 2\pi f(I+J-\frac{1}{2})) \quad (B.8)$$

for a triangular lattice, where f is the number of flux quanta per

lattice cell and I, J are integers, denoting the coordinates of the lattices as shown in Fig. 3.1 for a square lattice, in Fig. 3.5 for honeycomb and in Fig. 3.11 for triangular.

Equation (B.6) clearly shows that in a square lattice the Hamiltonian is periodic in f with period 1. Equation (B.7) and Eq.(B.8) show that in a honeycomb or a triangular lattice, the Hamiltonian is periodic in f with period 2. Nonetheless, at $f = 1$, spins can lie antiparallel in some of the bonds without frustration. The ground state energy for $f = 1$ is thus the same as that for $f = 0$, even though spins are not all parallel at $f = 1$. As a result, the ground state energy and hence other physical quantities are periodic in f with period 1 despite the fact that the period of the Hamiltonian is 2.

APPENDIX C

The following arguments are basically following the discussion by Shih, Ebner and Stroud¹⁰. The helicity modulus has a somewhat less obvious experimental interpretation. It appears the γ_{ij} may be equivalent to the inductive part of the low-frequency conductivity,³⁷ and thus accessible to a.c. measurement. By definition, γ_{ij} is the second derivative of the Helmholtz free energy with respect to vector potential

$$\gamma_{ij} \equiv \left(\frac{\partial^2 F}{\partial A_i \partial A_j} \right)_{T,V} \quad (C.1)$$

or

$$\gamma_{ij} \propto \left(\frac{\partial I_i}{\partial A_j} \right)_{T,V} , \quad (C.2)$$

where I_i is the i^{th} component of the supercurrent density and A_j is the j^{th} component of the vector potential in addition to that which generates the magnetic field. Such vector potential can be produced by an applied a.c. electric field. In this case,

$A_j = icE_j/\omega$ and it follows that γ_{ij} is related to the imaginary

part of the a.c. conductivity $\sigma_{ij}(\omega)$ by

$$\text{Im } \sigma_{ij}(\omega) \propto \frac{\gamma_{ij}}{\omega} . \quad (\text{C.3})$$

The low-frequency a.c. response of the composite should thus exhibit the features of the helicity modulus described in the text.