Quantum Monte Carlo Studies of 2D Anisotropic Superconductor-Insulator Transitions

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Submitted in partial fulfillment

of the requirements for the degree of

Bachelor of Science in Physics

Department of Physics

Brown University

April 2021

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Abstract

The Superconductor-Insulator Transition (SIT) is one of the most fundamental quantum phase transitions. It refers to the quantum phase transition of the ground state of electrons from a quantum phase coherent state to a quantum phase incoherent state at absolute zero temperature. Anisotropy is a phenomena observed in many natural materials. It refers to the property of a physical property having a different value when measured in different directions. The SIT has been studied in many isotropic 2D structures but systematic studies involving anisotropic materials have yet to be done. Here, we are studying Superconductor-Insulator transitions in 2D anisotropic materials using quantum Monte Carlo simulations. We find that anisotropy affects the superfluid density and the critical coupling constant K_c for the SIT. Further studies will involve more Monte Carlo steps and a more comprehensive adjustment of the formalism.

Acknowledgements

First and foremost, I would like to thank my thesis advisor Professor James Valles. I was inspired to pursue physics after taking PHYS 0070 with Professor Valles. Professor Valles's passion, knowledge, and encouragement constantly inspire me to be a better scientist. Working as a TA for Professor Valles, I was constantly touched and amazed by his care for students and his resourcefulness. He provided much guidance and insights throughout the thesis writing process.

I would like to thank Dr. Hung Q. Nguyen for laying the foundation for my research. His research on Superconductor-Insulator transitions using quantum Monte Carlo simulations inspired this study. His thesis and code base helped me understand the physics and optimize my code.

I would like to thank Ellen Royal, who graduated from Brown last year, for her great experimental work in dimensional crossover and anisotropy. Ellen is a good friend and mentor.

I would like to thank Professor Jay Tang from Brown University, Professor Jonathan Home from ETH Zurich, and Professor Oskar Painter from Caltech for being great research advisors and providing me the amazing opportunities to work on various physics projects alongside physicists from all over the world. I became more passionate about experimental condensed matter physics research after working with these professors.

I would like to thank all the professors from the Department of Physics and the Department of Computer Science for the rigorous training. I feel much more confident working on the intersection of both fields.

I would like to thank my friends for their support and encouragement throughout college. They make my Brown experience much better.

Most importantly, I would like to thank my parents for their unconditional support and love for the last 22 years.

Contents

List of Figures

Chapter 1

Introduction

1.1 Motivation

The Superconductor-Insulator Transition (SIT) is one of the most fundamental quantum phase transitions. The SIT in 2D thin films has been studied extensively both theoretically and experimentally [1][2][3][4][5][6]. The present work is motivated primarily by previous studies where SIT is observed in a 2D material as a function of disorder, induced an applied magnetic field or random chemical potentials [7]. Most previous research focused on 2D isotropic materials and changed the amount of disorder as a parameter. Very little work has been done to study the SIT in 2D anisotropic materials. This paper intends to provide more insights into the superconductor-insulator transitions in 2D anisotropic materials. The paper will first lay out the physics behind the SIT in 2D anisotropic systems, introduce the formalism, expand on the quantum Monte Carlo simulations method, propose two hypotheses, and present the simulation results.

1.2 Superconductor-Insulator Transition

1.2.1 Electronic Properties

The electronic properties refer to a set of parameters and representations that fully describe the state and behavior of electrons in the material. It is a very rich field with a long history of development. For example, the electronic band structure is an electronic property and describes the state of the electrons in terms of the energy E and momentum k [8][9].

In solid state physics, a periodic arrangement of atoms is called a lattice [8]. Electrons in a lattice are then categorized by their movements. According to the band theory, mobile electrons, or conduction electrons, can move freely between atoms and therefore form a conductor. Immobile electrons, or valence electrons, are bound with the atoms and therefore form an insulator.

Under certain conditions, electrons can change their ground state from one arrangement to another, a process called a phase transition. Landau came up with a theory that describes phase transitions and suggested that the free energy of any system should be analytic and obey the symmetry of the Hamiltonian. Given these two conditions, the Landau free energy can be written as a Taylor expansion in the order parameter [8].

$$F = \alpha(T)\psi^2 + \beta(T)\psi^4 + H\psi, \tag{1.1}$$

where $\alpha = \alpha_0(T - T_c)$ and T_c is the transition temperature. To minimize the free energy with respect to the order parameter requires

$$\frac{\partial F}{\partial \psi} = 2\alpha(T)\psi + 2\beta(T)\psi^3 - H = 0. \tag{1.2}$$

The solution of the order parameter is either $\psi = 0$ or

$$\psi^2 = -\frac{\alpha}{\beta}(T - T_c), \tag{1.3}$$

where the nontrivial solution only exists when $T < T_c$. ψ approaches zero as T approaches T_c from below and such a behaviour is typical for a second order phase transition [10].

Landau theory then inspired the Ginzburg-Landau theory of superconductivity.

1.2.2 Superconductivity

Superconductivity is a phenomenon discovered more than one hundred years ago. It refers to the phenomenon that when temperature drops below a transition temperature, the material enters a phase that has zero electrical resistance and zero internal magnetic field.

It is a quantum phase with long quantum phase coherence. Phase coherence refers to the phenomenon where two wave sources have identical frequencies and wave forms and their phase difference is constant [11][12]. In quantum mechanics, all objects have wave-like properties. Quantum phenomena are prevalent at the atomic scale but research has shown that quantum phenomena can be observed on a macroscopic scale too. Superconductivity is a prominent quantum effect at the macroscopic scale [13].

Inspired by the Landau theory of phase transitions, Ginzburg and Landau came up with the theory that describes superconductivity using a macroscopic order parameter ψ [10]. They argued that the free energy of a superconductor near the superconducting transition can be expressed in terms this order parameter

$$F = F_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m}|(-i\hbar\nabla - 2e\mathbf{A})\psi|^2 + \frac{|\mathbf{B}|^2}{2\mu_0}. \tag{1.4}$$

Here F_n is the free energy in the normal phase, α and β are the phenomenological

parameters, m is an effective mass, e is the charge of an electron, $\mathbf{A}$ is the magnetic vector potential, and $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic field [10].

Minimizing the free energy with respect to the variations of the order parameter and the vector potential, the Ginzburg-Landau equations can be written as

$$\alpha\psi + \beta|\psi|^2\psi + \frac{1}{2m}(-i\hbar\nabla - 2e\mathbf{A})^2\psi = 0, \tag{1.5}$$

$$\nabla \times \mathbf{B} = \mu_0\mathbf{j}, \tag{1.6}$$

$$\mathbf{j} = \frac{2e}{m}Re\{\psi^*(-i\hbar\nabla - 2e\mathbf{A})\psi\}, \tag{1.7}$$

$\mathbf{j}$ is the supercurrent, e and m are the electric charge and mass of the carriers.

The equations introduce two new characteristic lengths of a superconductor. The first is the coherence length, ξ:

$$\xi = \sqrt{\frac{\hbar^2}{2m|\alpha|}}, (T > T_c), \tag{1.8}$$

$$\xi = \sqrt{\frac{\hbar^2}{4m|\alpha|}}, (T < T_c). \tag{1.9}$$

The second is penetration depth λ.

$$\lambda = \sqrt{\frac{m}{4\mu_0 e^2\psi_0^2}} = \sqrt{\frac{m\beta}{4\mu_0 e^2|\alpha|}}, \tag{1.10}$$

where ψ_0 is the equilibrium value of the order parameter with no electromagnetic field present.

The coherence length dictates the exponential spatial decay of the small perturbations of the density of superconducting electrons from their equilibrium value. The

penetration depth dictates the exponential law of an external magnetic field decaying with distances inside the superconductor [8].

The ratio between the two lengths $\kappa = \frac{\lambda}{\xi}$ is known as the Ginzburg-Landau parameter [10]. Superconductors that have $0 < \kappa < \frac{1}{\sqrt{2}}$ are Type I superconductors and those have $\kappa > \frac{1}{\sqrt{2}}$ are Type II superconductors [10].

1.2.3 Localization

When disorder is introduced to a lattice system, it can lead to quantum interference of wave functions at low temperatures or low dimensions. When the amount of disorder is significant, electrons will scatter off of the impurities in the materials and follow a more complex path than a straight path. Electrons can travel in a closed loop in two directions. If the phase shift of the electron wave function of the closed loop path is coherent, the probability of finding an electron at its initial location is higher. This phenomenon is known as weak localization [8][14].

If the wave functions interfere constructively, the probability of finding the electron at its initial location is

$$|A_1 + A_2|^2 = |A_1|^2 + |A_2|^2 + 2|A_1 A_2| = 4A^2, \tag{1.11}$$

where A_1 and A_2 are the amplitudes of the two loops. The probability is higher in this quantum case compared to the classical case where the probability is $|A_1|^2 + |A_2|^2 = 2A^2$.

In the strong disorder limit, even wave diffusion will be absent, a phenomenon called strong localization or Anderson localization. In low dimensional systems ($d = 1, 2$), even tiny disorder can lead to localization. In 3D systems, localization only occurs with large disorder. By tuning the amount of disorder, the ground state of electrons can change from a localized state to an extended state, a phenomenon known

as the Metal-Insulator Transition [15].

When strong localization is applied to a superconductor, it will go through a superconductor-insulator quantum phase transition. It is a quantum phase transition of the ground state of electrons from a quantum phase coherent state to a quantum phase incoherent state. The superconductor-insulator transition has been observed and measured experimentally [4][5][6].

1.2.4 Josephson Junction Array

The SIT model can be described using Josephson Junction Arrays. A Josephson junction is a structure formed by two superconductors linked by a non-conducting material.

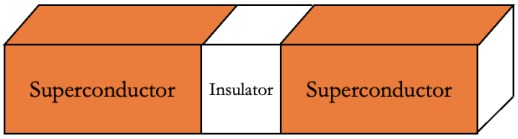

Figure 1.1: Josephson Junction

The current through a Josephson Junction is written as

$$J = J_c \sin(\phi_1 - \phi_2), \tag{1.12}$$

where the J_c is the critical current of the Josephson junction and it depends on the properties of the superconductors. ϕ_1 and ϕ_2 refer to the phases of the two superconducting islands.

Josephson junctions can be capacitively coupled into 2D arrays as shown in Figure 1.2, where each cross represents a junction and the square represents an island with a charging energy E_c, where $E_c = \frac{e^2}{2C}$ and C is the junction capacitance [16][17].

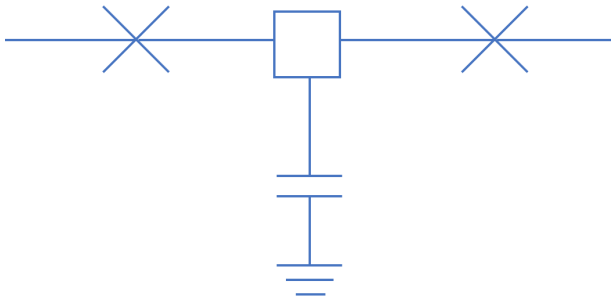

Figure 1.2: Josephson Junction Array

The superconducting island has a charging energy E_C and the two islands have the Josephson coupling energy E_J. Josephson Junctions only allow current to pass through when $E_J > E_C$. Therefore, $E_J > E_C$ can be used to describe the delocalized state and $E_J < E_C$ can be used to describe the localized state.

Josephson Junction Arrays can model granular thin films well. Superconductivity in granular thin films is defined within each grain island and transport is allowed by tunneling between the islands. E_c and E_j could be tuned by changing the thickness of the film. Experimentally SIT has been observed in In, Ga, Pb, Al films [18] and has been realized using Josephon Junction Arrays [19]. These models all showed direct superconductor-insulator transitions but did not agree on an universal value [19].

1.3 2D Anisotropy

Anisotropy refers to the property of a material that allows it to have different properties along different directions, as opposed to isotropy [20]. Anisotropy is observed in many natural materials [21]. Josephson Junction Arrays can be used to model anisotropic thin films. The Josephson coupling energy J will be different along X and Y directions in the anisotropic case. The amount of anisotropy a material has is defined as the ratio between the two Josephson energies

$$\epsilon = \frac{J_y}{J_x}. \tag{1.13}$$

Figure 1.3 and 1.4 illustrate the isotropic and anisotropic structures formed in Josephson Junction Arrays. Each cross represents a junction and each square represents an island.

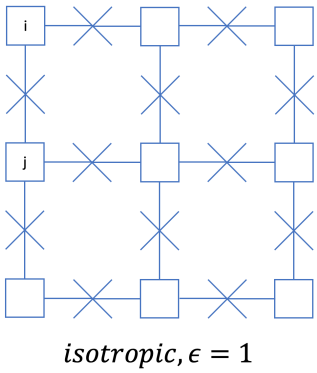

Figure 1.3: 2D isotropic structure, $\epsilon = 1$

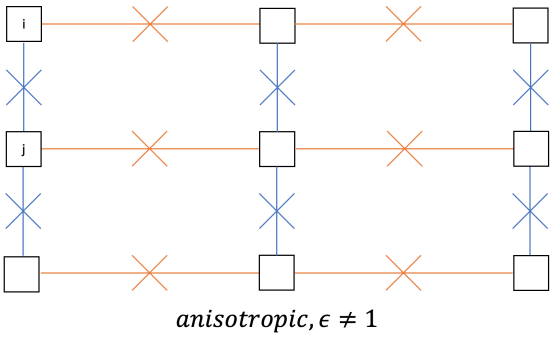

Figure 1.4: 2D anisotropic structure, $\epsilon \neq 1$

1.4 Formalism

1.4.1 Model Hamiltonian

The Hamiltonian of SIT in 2D anisotropic materials can be written as

$$H = U\sum_j n_j^2 - \sum_{<ij>} J_{ij} cos(\theta_i - \theta_j), \tag{1.14}$$

where U is the charging energy of an island which is identical for all islands, n_j is the operator of the number of Cooper pairs on island j, J_{ij} is the Josephson coupling energy between island i and j, $< i, j >$ identifies summation over the nearest neighbor i and j, θ_i and θ_j are the phases of the two islands [7].

From the Hamiltonian (Eq.1.14), SIT can be thought of a competition between the charging energy U and the coupling energy J. When the ratio between the two energies is tuned to a certain, the system will undergo the superconductor-insulator transition. The ratio at which the system go through the phase transition is the critical ratio and the theory implies that there exists an universal value for the critical resistance [22]. θ_j is canonically conjugate to n_j so the Bose-Hubbard model can be expressed in the quantum rotor model form [2].

When the phase θ_j is well defined, we have

$$n_j = \frac{1}{i}\frac{\partial}{\partial\theta_j}. \tag{1.15}$$

Using the Josephson relation

$$V_j = \frac{\hbar}{2e}\dot{\theta_j}^2, \tag{1.16}$$

$$E_{Cj} = \frac{1}{2}CV_j^2 = \frac{C\hbar^2}{2(2e)^2}\dot{\theta_j}^2 = \frac{\hbar^2}{4U}\dot{\theta_j}^2. \tag{1.17}$$

The Hamiltonian can be rewritten as

$$H' = \frac{\hbar}{4U}\sum_j \dot{\theta_j}^2 - \sum_{<ij>} J_{ij}\cos(\theta_i - \theta_j). \tag{1.18}$$

Even though the model is artificial, it resembles a real, physically achievable system. Specifically, the model resembles a 2D Josephson junction array on a square lattice in a uniform magnetic field [7].

1.4.2 Path Integral Formalism

With the Hamiltonian, the action can be obtained in the form of a standard path integral over imaginary time as follows:

$$\frac{S}{\hbar} = \frac{1}{\hbar} \int \mathcal{L} d\tau, \tag{1.19}$$

where $\mathcal{L}$ is the Lagrangian written as

$$\mathcal{L} = \frac{\hbar}{4U} \sum_j \left(\frac{\partial \theta_j}{\partial \tau} \right)^2 - \sum_{<ij>} J_{ij} \cos[\theta_i(\tau) - \theta_j(\tau)]. \tag{1.20}$$

The partition function is given by a path integral of $e^{-S/\hbar}$ over all possible paths described by the variables $\theta_i(\tau)$ in imaginary time τ [kim], integrated from $\tau = 0$ to $\tau = \beta\hbar$ where $\beta = \frac{1}{k_B T}$ [7] [8].

1.4.3 Coupling Constant K

The coupling constant can be viewed as the ratio between the charging energy U and the Josephson coupling energy J. Since SIT is essentially driven by the competition between U and J, the coupling constant $K = \sqrt{\frac{J}{2U}}$ could be used and tuned as a parameter dictating SIT [7][22].

Since the model is quantum in nature but has to be simulated on a classical machine, the imaginary time τ is thus treated as a third dimension. The path integral can be viewed as the partition function of an anisotropic classical XY model in three dimensions. In this case, the anisotropy refers to the coupling constants K and K_τ in the xy plane and the τ direction are different [7].

To map the third dimension, we can use the expansion of $\cos\Delta\theta$ to second order in the small quantity of $\Delta\theta$,

$$\left(\frac{\partial\theta_i}{\partial\tau}\right)^2 \sim \left(\frac{\Delta\theta_i}{\Delta\tau}\right)^2 \sim \frac{2-2\cos\Delta\theta_i}{(\Delta\tau)^2}, \tag{1.21}$$

where $\Delta\tau$ is the width of the imaginary time slice, $\Delta\theta_i = \theta_i(\tau+\Delta\tau) - \theta_i(\tau)$.

Then the action can be rewritten as

$$\frac{S}{\hbar} = -K_\tau \sum \cos[\theta_i(\tau) - \theta_i(\tau+\Delta\tau)] - \sum_{ij} K_{ij}\cos[\theta_i(\tau) - \theta_j(\tau)]. \tag{1.22}$$

The values of the coupling constants K and K_τ can be obtained assuming that the time integral is broken into M slices, each of width $\frac{\beta\hbar}{M}$. The coupling constant in the x direction is

$$K_x = \frac{\beta J_x}{M}, \tag{1.23}$$

and that of the y direction is

$$K_y = \frac{\beta J_y}{M}. \tag{1.24}$$

The coupling constant in the τ direction is then

$$K_\tau = \frac{\hbar}{4U}\frac{1}{\hbar}(\Delta\tau)\frac{2}{(\Delta\tau)^2} = \frac{1}{2U}\frac{\hbar}{\Delta\tau} = \frac{M}{2\beta U}. \tag{1.25}$$

With K_i and K_τ, the partition function is obtained from the anisotropic 3D XY classical Hamiltonian with coupling constants K and K_τ [7][23]. Therefore, the equilibrium quantities can be obtained by averaging over all configurations using Monte Carlo techniques.

1.4.4 Helicity Modulus

With the time-slice formulation of the partition function, we can use Monte Carlo techniques to evaluate various properties.

For a classical XY system in d dimensions, the helicity modulus tensor is a measure of phase stiffness [24]. Phase stiffness can be seen as a measure of the response of a system in an ordered phase to a slow in-plane phase twist of the order parameter [7]. It is a measure of the superconductivity of the system. It is a $d \times d$ matrix defined as the second derivative of the free energy with respect to an infinitesimal phase twist as follows:

$$\gamma_{\alpha\beta} = \frac{1}{N} \frac{\partial^2 F}{\partial A'_\alpha \partial A'_\beta}, \tag{1.26}$$

where N is the number of sites in the system.

For the diagonal elements, the derivative takes the following explicit form:

$$\begin{aligned} \gamma_{\alpha\alpha} =& \frac{1}{N} \left\langle \sum_{<ij>} J_{ij} \cos(\theta_i - \theta_j)(\hat{e}_{ij} \cdot \hat{e}_\alpha)^2 \right\rangle \\ & - \frac{1}{N} \left\langle \left[\sum_{<ij>} J_{ij} \sin(\theta_i - \theta_j)(\hat{e}_{ij} \cdot \hat{e}_\alpha) \right]^2 \right\rangle \\ & + \frac{1}{N} \left\langle \sum_{<ij>} J_{ij} \sin(\theta_i - \theta_j)(\hat{e}_{ij} \cdot \hat{e}_\alpha) \right\rangle^2, \end{aligned} \tag{1.27}$$

where the triangular brackets denote an average in the canonical ensemble, $\hat{e}_{ij}$ is a unit vector from the ith to the jth site, and $\hat{e}_\alpha$ is a unit vector in the α direction.

When applied to a time-slice representation of the quantum mechanical Hamiltonian, the coupling constants J_{ij} will be different in the xy plane and in the τ direction:

$$\begin{aligned}\gamma_{xx} =& \frac{1}{N_x N_y}\left\langle \frac{1}{M}\sum_{<ij>||\hat{x}} J_{ij||\hat{x}}\cos(\theta_i-\theta_j)\right\rangle \\ &- \frac{1}{N_x N_y k_B T}\left\langle \frac{1}{M}\left[\sum_{<ij>||\hat{x}} J_{ij||\hat{x}}\sin(\theta_i-\theta_j)\right]^2\right\rangle \\ &+ \frac{1}{N_x N_y k_B T}\left\langle \frac{1}{M}\sum_{<ij>||\hat{x}} J_{ij||\hat{x}}\sin(\theta_i-\theta_j)\right\rangle^2,\end{aligned} \tag{1.28}$$

where $N_x N_y$ represent the total number of sites. The sums run over all bonds in the $\hat{x}$ direction and there are $N_x N_y M$ bonds. The expression is similar for γ_{yy}.

To incorporate the coupling constant K, we can multiply Equation 1.25 by $\frac{\beta}{M}$:

$$\begin{aligned}\frac{\beta\gamma_{xx}}{M} =& \frac{1}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} K_{ij||\hat{x}}\cos(\theta_i-\theta_j)\right\rangle \\ &- \frac{1}{N_x N_y M}\left\langle \left[\sum_{<ij>||\hat{x}} K_{ij||\hat{x}}\sin(\theta_i-\theta_j)\right]^2\right\rangle \\ &+ \frac{1}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} K_{ij||\hat{x}}\sin(\theta_i-\theta_j)\right\rangle^2,\end{aligned} \tag{1.29}$$

where $K = \frac{\beta J}{M}$ and $K_\tau = \frac{M}{2\beta U}$. We can choose M so that $K = K_\tau$ in the limit $\beta \gg 1$, which is equivalent to

$$\frac{\beta}{M} = \frac{1}{\sqrt{2JU}}. \tag{1.30}$$

$$\begin{aligned}\frac{\gamma_{xx}}{\sqrt{2J_xU}} =& \frac{1}{N_xN_yM}\left\langle \sum_{<ij>||\hat{x}} K_x\cos(\theta_i-\theta_j)\right\rangle \\ &- \frac{1}{N_xN_yM}\left\langle \left[\sum_{<ij>||\hat{x}} K_x\sin(\theta_i-\theta_j)\right]^2\right\rangle \\ &+ \frac{1}{N_xN_yM}\left\langle \sum_{<ij>||\hat{x}} K_x\sin(\theta_i-\theta_j)\right\rangle^2,\end{aligned} \tag{1.31}$$

$$\begin{aligned}\frac{\gamma_{yy}}{\sqrt{2J_yU}} =& \frac{1}{N_xN_yM}\left\langle \sum_{<ij>||\hat{y}} K_y\cos(\theta_i-\theta_j)\right\rangle \\ &- \frac{1}{N_xN_yM}\left\langle \left[\sum_{<ij>||\hat{y}} K_y\sin(\theta_i-\theta_j)\right]^2\right\rangle \\ &+ \frac{1}{N_xN_yM}\left\langle \sum_{<ij>||\hat{y}} K_y\sin(\theta_i-\theta_j)\right\rangle^2,\end{aligned} \tag{1.32}$$

1.4.5 Superfluid Density

A similar measure of the superconductivity is called superfluid density ρ_s[25]. We can calculate the quantity $\rho(0)$ from the helicity modulus and the coupling constant [7]:

$$\rho(0) = K\gamma \equiv \frac{K(\gamma_{xx}+\gamma_{yy})}{2}. \tag{1.33}$$

Since we are dealing with a 2D anisotropic model, $\gamma_{xx} \neq \gamma_{yy}$, so $\rho(0)$ is given by

$$\begin{aligned}\rho(0) =& \frac{J_x K_x}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} \cos(\theta_i - \theta_j)\right\rangle + \frac{J_y K_y}{N_x N_y M}\left\langle \sum_{<ij>||\hat{y}} \cos(\theta_i - \theta_j)\right\rangle \\ & - \frac{J_x K_x^2}{N_x N_y M}\left\langle \left[\sum_{<ij>||\hat{x}} \sin(\theta_i - \theta_j)\right]^2\right\rangle - \frac{J_y K_y^2}{N_x N_y M}\left\langle \left[\sum_{<ij>||\hat{y}} \sin(\theta_i - \theta_j)\right]^2\right\rangle \\ & + \frac{J_x K_x^2}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} \sin(\theta_i - \theta_j)\right\rangle^2 + \frac{J_y K_y^2}{N_x N_y M}\left\langle \sum_{<ij>||\hat{y}} \sin(\theta_i - \theta_j)\right\rangle^2 .\end{aligned} \tag{1.34}$$

Introducing the parameter for anisotropy $\epsilon = \frac{J_y}{J_x}$ to the equation, the superfluid density can be written as

$$\begin{aligned}\rho(0) =& \frac{J_x K_x}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} \cos(\theta_i - \theta_j)\right\rangle + \frac{\epsilon J_x \sqrt{\epsilon} K_x}{N_x N_y M}\left\langle \sum_{<ij>||\hat{y}} \cos(\theta_i - \theta_j)\right\rangle \\ & - \frac{J_x K_x^2}{N_x N_y M}\left\langle \left[\sum_{<ij>||\hat{x}} \sin(\theta_i - \theta_j)\right]^2\right\rangle - \frac{\epsilon J_x \epsilon K_x^2}{N_x N_y M}\left\langle \left[\sum_{<ij>||\hat{y}} \sin(\theta_i - \theta_j)\right]^2\right\rangle \\ & + \frac{J_x K_x^2}{N_x N_y M}\left\langle \sum_{<ij>||\hat{x}} \sin(\theta_i - \theta_j)\right\rangle^2 + \frac{\epsilon J_x \epsilon K_x^2}{N_x N_y M}\left\langle \sum_{<ij>||\hat{y}} \sin(\theta_i - \theta_j)\right\rangle^2 ,\end{aligned} \tag{1.35}$$

1.4.6 Finite-size Scaling

If the phase transition is continuous as a function of some parameter, such as the coupling constant K, the critical behavior near the transition can be analyzed through a finite-size scaling analysis. The basic finite-size scaling hypothesis is that, given the correlation length ξ, the size of the system only appears in the ratio of N/ξ and the corresponding ratio in the time direction is N_τ/ξ_τ [2].

The quantity we are interested in, helicity modulus at zero frequency $\gamma(0)$, can be

written as

$$\gamma(0) = \frac{1}{L^{d+z-2}}\tilde{\gamma}\left(\frac{L_\tau}{L^z}\right), \tag{1.36}$$

where d is the spatial dimensionality, z is the dynamic exponent, $\tilde{\gamma}$ is a scaling function, v is the critical exponent of the correlation length ξ, $\delta = \frac{K-K_c}{K_c}$ and K_c is the critical value of the coupling constant, L_τ is the thickness in the imaginary time direction [7].

For the 2D model, $d = 2$ and let $\tilde{\gamma}(L^{1/v}\delta, L_\tau/L^z) = (L^z/L_\tau)\tilde{G}(L^{1/v}\delta, L_\tau/L^z)$, the scaling relation is then

$$L_\tau\gamma(0) = \tilde{G}\left(L^{1/v}\delta, \frac{L_\tau}{L^z}\right). \tag{1.37}$$

The simulation has a total of $N_x \times N_y \times M$ sites, the scaling relation can then be written as

$$KM\gamma(0) = \tilde{G}\left(N_x^{1/v}\delta, \frac{M}{N_x^z}\right). \tag{1.38}$$

Therefore, K_c can be found by plotting $KM\gamma(0)$ as a function of δ for different lattice sizes as long as the $M = cN_x^z$ is satisfied. The point where all the lines cross, which correspond to $\delta = 0$, is the critical point. We used $z = 1$, which is known to be correct when there is no magnetic field in the system. The scaling function is thus

$$KM\gamma(0) = \tilde{G}(M^{1/v}\delta, 1). \tag{1.39}$$

Chapter 2

Method

2.1 Quantum Monte Carlo Simulation

2.1.1 Metropolis Algorithm

To evaluate the superfluid density as a function of the coupling constant K, we can use quantum Monte Carlo techniques. In this case, we use the Metropolis algorithm with periodic boundary conditions satisfied both in the spatial directions and the imaginary time direction [7][26].

In most applications, we want to estimate the mean of some function f because the quantity gives us a first-principles estimate of certain physical quantities. In the 2D anisotropic model, the mean is taken over all configurations

$$\mathcal{F} = \frac{1}{Z(T)} \sum_{x} f(x) exp(-E(x)/k_B T). \tag{2.1}$$

The weights come from the expression of the configuration's energy. A natural approach would be to select some configurations from the distribution but it is challenging to determine what samples to choose. Nick Metropolis and others came up with the observation that if we only change one site, it is easy to evaluate the change

in energy ΔE because only a few terms change [26]. The transition probability $p_{\xi,\sigma}$ is such that for each configuration σ,

$$\mu(\sigma) = \sum_{\xi} \mu(\xi) p_{\xi,\sigma}. \tag{2.2}$$

The sum includes all configurations ξ that differ from σ by one site, and

$$p_{\xi,\sigma} = \frac{\mu(\sigma)}{\mu(\xi)} = \exp(-\Delta E(\sigma)/k_B T). \tag{2.3}$$

This transition probability indicates that if the change of one site lowers the energy, we should proceed, otherwise, we proceed with a probability p and reject the change with the probability $p - 1$.

In order to choose the site to flip, we can use a probability distribution

$$cv(\sigma) = \frac{min(1, exp(\Delta E(\sigma)/k_B T))}{n}, \tag{2.4}$$

where n is the number of sites and this too follows the Metropolis rejection algorithm.

2.1.2 Procedure

The quantum Monte Carlo calculation with Metropolis algorithm is carried out in Python [27]. The overall procedure is as follows [8]:

1. Choose a specific lattice size, n = 6, 8, 10.

2. Generate a random initial configuration for the lattice. The phase θ_i of each site is randomly chosen from [1, 360].

3. Checks for periodic boundary conditions, $\theta_1 = \theta_{n+1}$.

4. Randomly pick a site i and consider whether to change the phase θ_i to an arbitrary integer value in [1, 360].

5. Compute the energy change δS associated with the change. Since the new

energy only differs from the old energy at the chosen site i, δS can be calculated as

$$\begin{aligned}\delta S = &- K_\tau \cos[\theta_i^{new}(\tau) - \theta_i^{new}(\tau + \Delta\tau)] - K \cos[\theta_i^{new}(\tau) - \theta_j^{new}(\tau)] \\ &+ K_\tau \cos[\theta_i^{old}(\tau) - \theta_i^{old}(\tau + \Delta\tau)] + K \cos[\theta_i^{old}(\tau) - \theta_j^{old}(\tau)].\end{aligned} \tag{2.5}$$

6. Calculate the transition probability p associated with the energy change

$$p = e^{\frac{-\delta S}{k_B T}} \tag{2.6}$$

7. Randomly choose a number Z between [0, 1]
8. If $Z < p$, change the phase on site i, reject the change otherwise.
9. Calculate γ_i associated with the new configuration.

2.1.3 Python Implementation

For 2D isotropic materials with no disorder in a uniform magnetic field, the theoretical critical coupling constant K_c is calculated to be around 0.452 using both analytical and numerical approaches. Therefore, we used K ranging from 0.42 - 0.46, with 0.01 as the step size.

$N_x = N_y = m$ takes values of 6, 8, and 10. To stabilize the initial configuration, we used $N = 40000 \times N_x \times N_y \times M$ Monte Carlo steps. Once the configuration is stabilized, we used $N_1 = 50000 \times N_x \times N_y \times m$ steps to calculate the helicity modulus of the configuration.

The ***nearest_neighbor*** function takes in the lattice size N_x and N_y and generates the initial random configuration.

The ***sample_generation*** function takes in a randomly generated site indices idi, idj and generate a new phase θ_i for the chosen site.

The ***deltaH*** function takes in the old phase and the new phase of chosen site and calculate the energy change associated with the change.

The ***HelicityModulus*** function takes in the old configuration and calculates its helicity modulus.

The ***newGamma*** function takes in the new configuration and calculates its helicity modulus.

The ***configuration*** function acts as the main function that takes in the lattice size, K, and the anisotropy ϵ. The pseudocode for the algorithm is shown below:

```
Result: Helicity modulus of the configuration
θ_j = nearest_neighbor(lattice size) ;
idi, idj = random indices of site i;
newTheta, idi, idj = sample_generator(idi, idj);
for each step in N1 steps do
    energy change of a flip = deltaH();
    prob = random number;
    if f the transition probability ¿ prob then
        set the configuration to the new configuration;
    end
    generate a new configuration;
end
old helicity modulus = HelicityModulux();
for each step in N steps do
    energy change = deltaH();
    prob = random number;
    if f transition probability ¿ prob then
        new helicity modulus = newGamma();
        gx += new helicity modulus;
        sets the configuration to the new configuration;
    end
    generates new samples;
end
calculates the helicity modulus for the ;
```

Algorithm 1: Metropolis Algorithm

The complete Python implementation can be found in Appendix A.

2.2 Google Cloud Platform

Since the Monte Carlo simulation involves as many as 50 million steps of calculations, to speed up the process, we can use a Virtual Machine instance from the Compute Engines on Google Cloud Platform. With the VM instance, it takes around 8 hours to finish the calculations for lattice size $n = 10$.

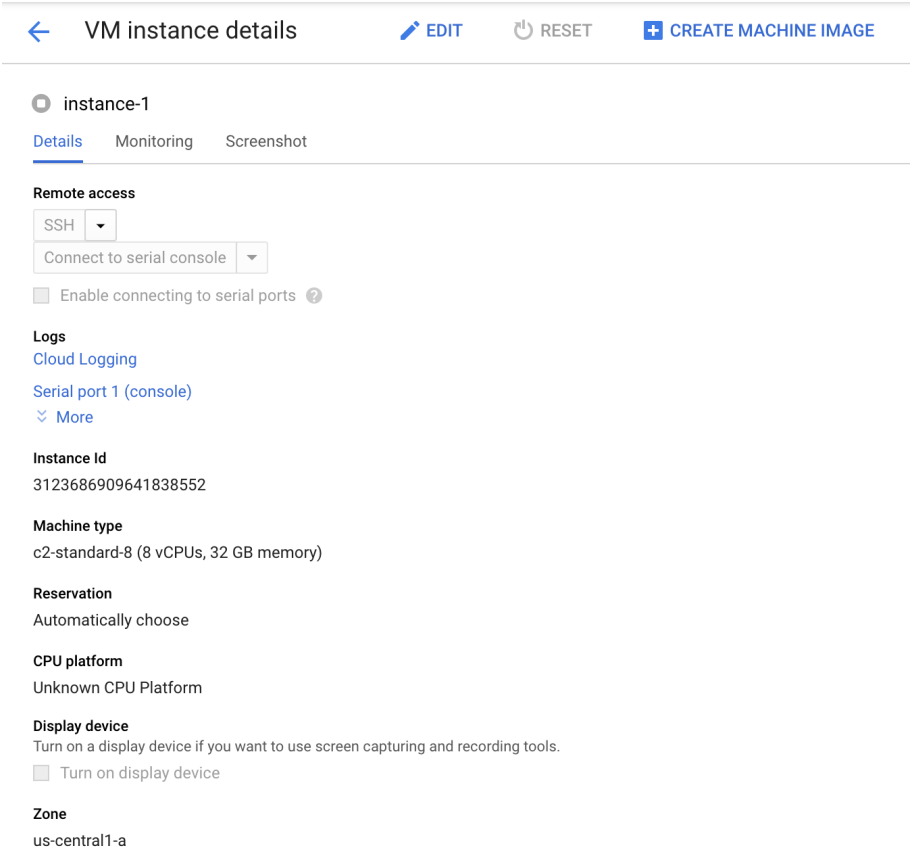

Figure 2.1: Virtual Machine Instance Setup

Chapter 3

Results

3.1 Baseline Model

Before introducing anisotropy to the model, the 2D isotropic model was tested to ensure the baseline model is working. We calculated K_c for the square lattice case with no magnetic field involved. Based on the finite-size scaling method, we plotted the superfluid density, $\gamma \times K \times M$ as a function of K.

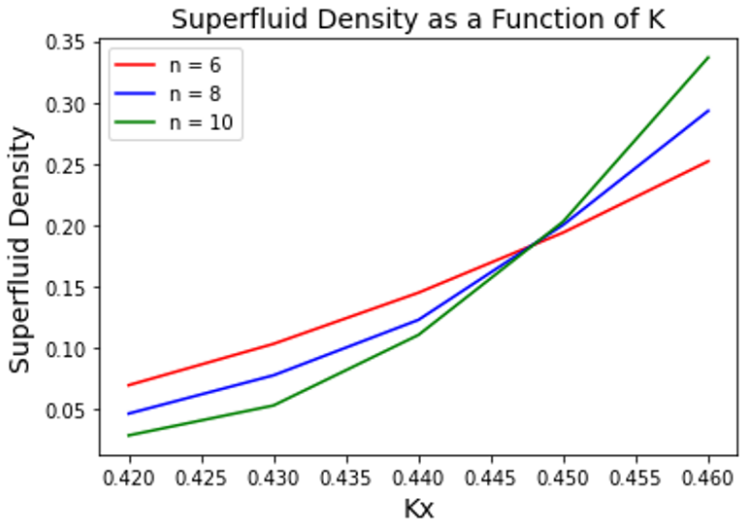

Figure 3.1: Baseline Model for 2D Isotropic Lattice

The three lines correspond to three different lattice sizes and the lines cross at the

critical coupling constant $K_c \approx 0.448 \pm 0.001$. The figure agrees with the baseline model done by Nguyen. The similar crossing point indicates the baseline model without anisotropy is correct.

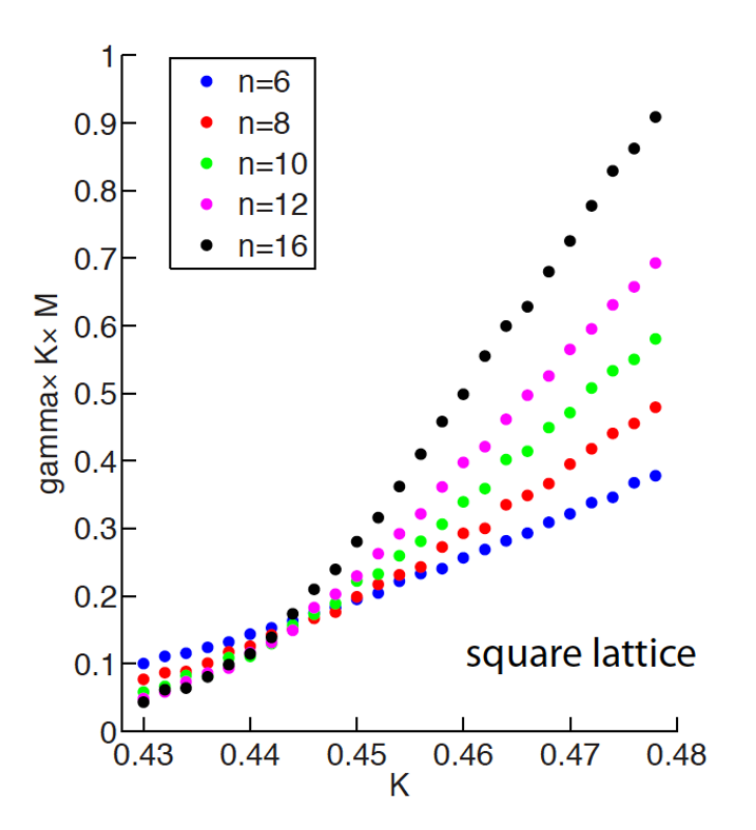

Figure 3.2: Baseline Model for 2D Isotropic Lattice, Hung Q. Nguyen

3.2 Anisotropic Model

We then introduced anisotropy to the model. The measure of anisotropy is defined in Eq.1.13 as the ratio between two Josephson coupling energies. We used $\epsilon = \frac{J_y}{J_x}$ with values 0.5, 0.6, 0.7, 0.8, 0.9, 1, which represented rectangular lattice all the way to isotropic square lattice. We then plotted the $\gamma \times K \times M$ as a function of K_x.

As seen in Figures 3.3-3.7, the crossing point and the superfluid density at the critical point change as the amount of anisotropy changes. To quantitatively view the

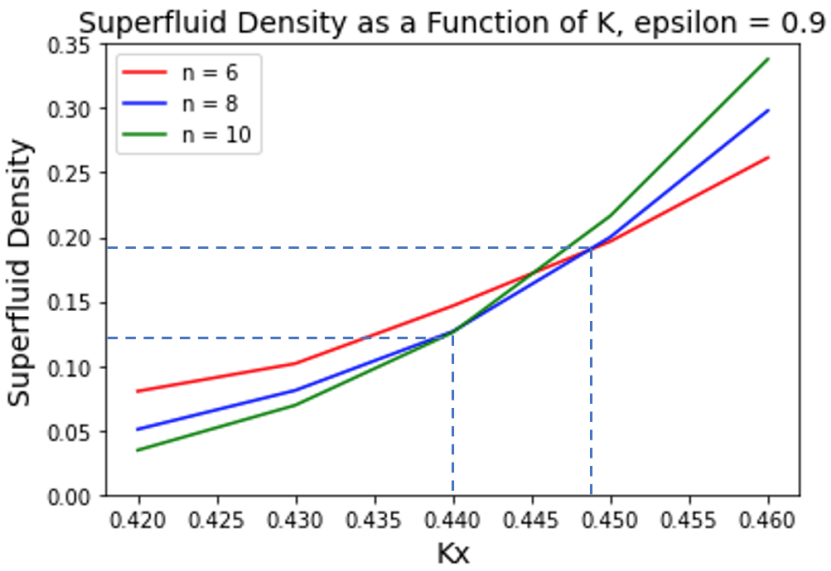

Figure 3.3: Superfluid density as a function of K_x, $\epsilon = 0.9$

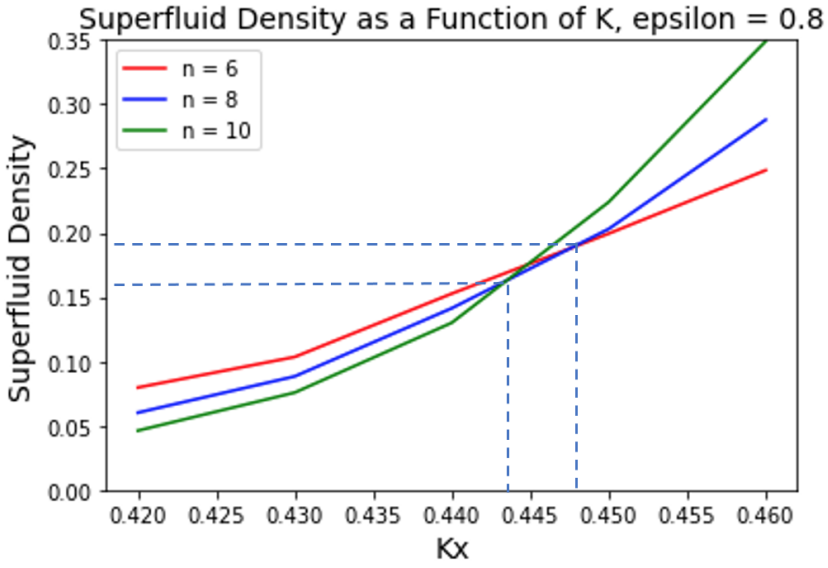

Figure 3.4: Superfluid density as a function of K_x, $\epsilon = 0.8$

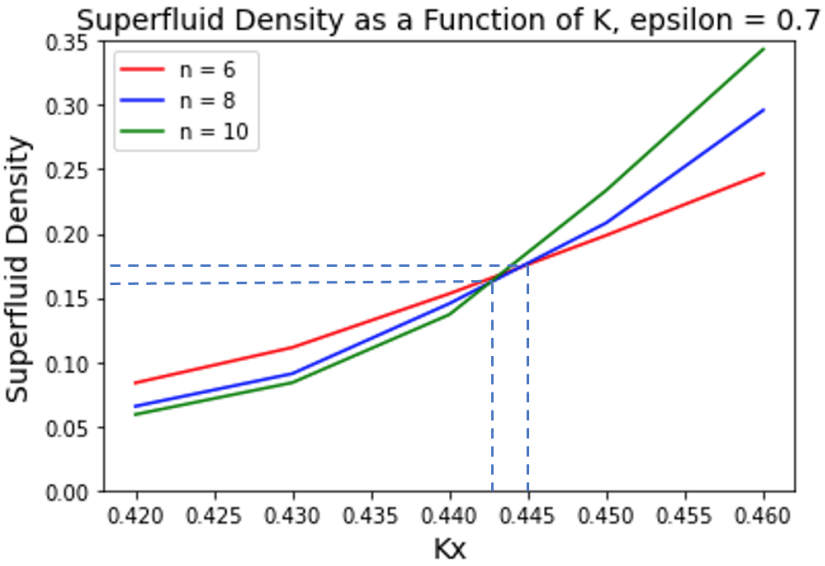

Figure 3.5: Superfluid density as a function of K_x, $\epsilon = 0.7$

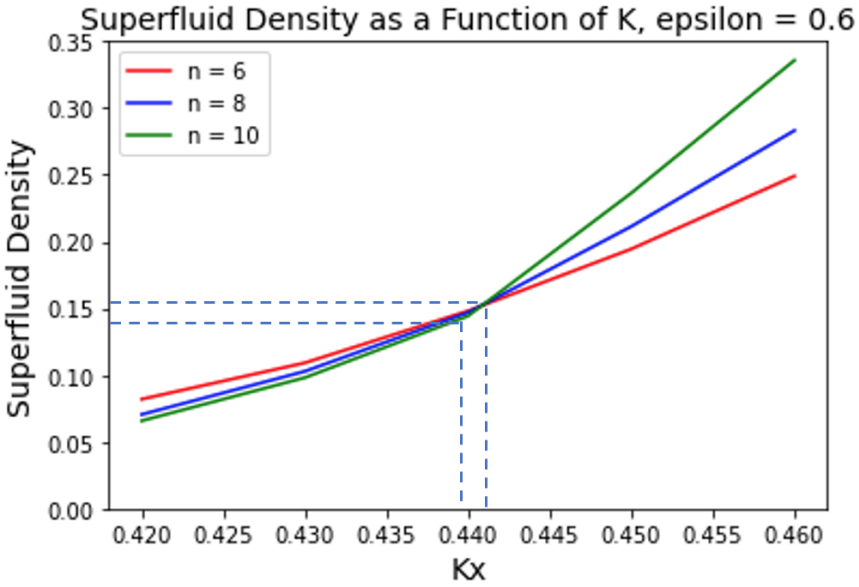

Figure 3.6: Superfluid density as a function of K_x, $\epsilon = 0.6$

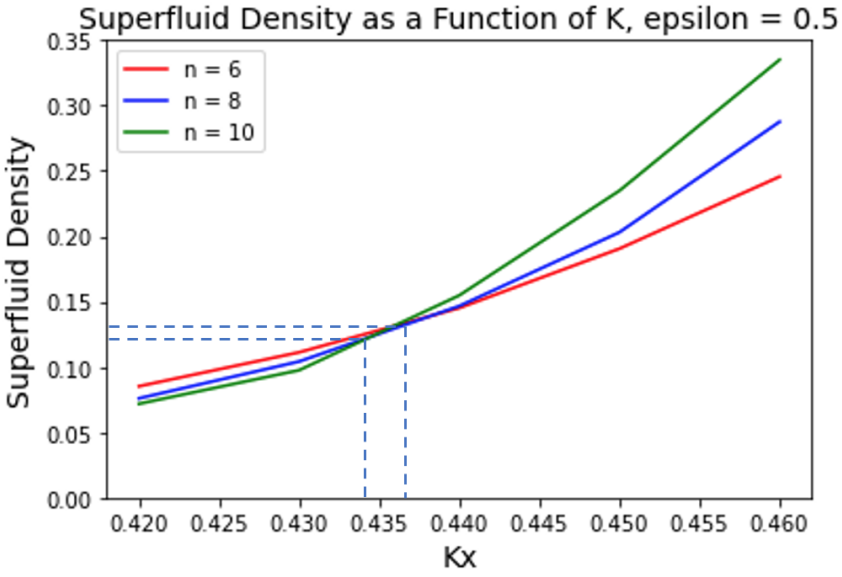

Figure 3.7: Superfluid density as a function of K_x, $\epsilon = 0.5$

relationships, we plotted the superfluid density at the critical points as a function of ϵ, shown in Figure 3.8, and the critical coupling constant K_c as a function of ϵ, shown in Figure 3.9.

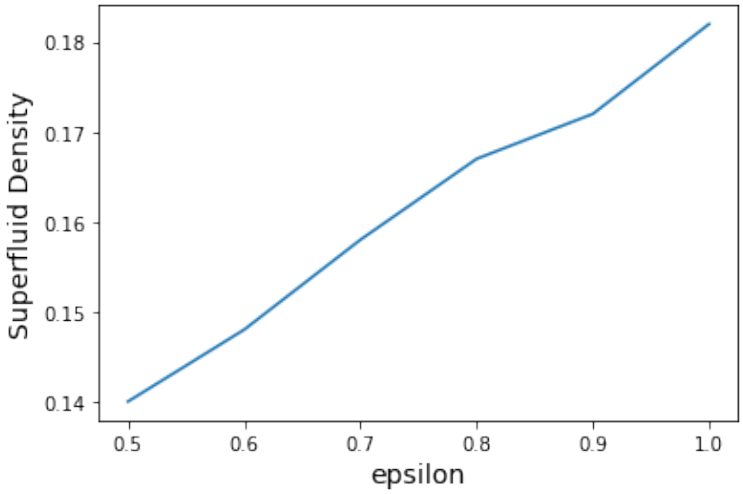

Figure 3.8: Superfluid density as a function of anisotropy ϵ

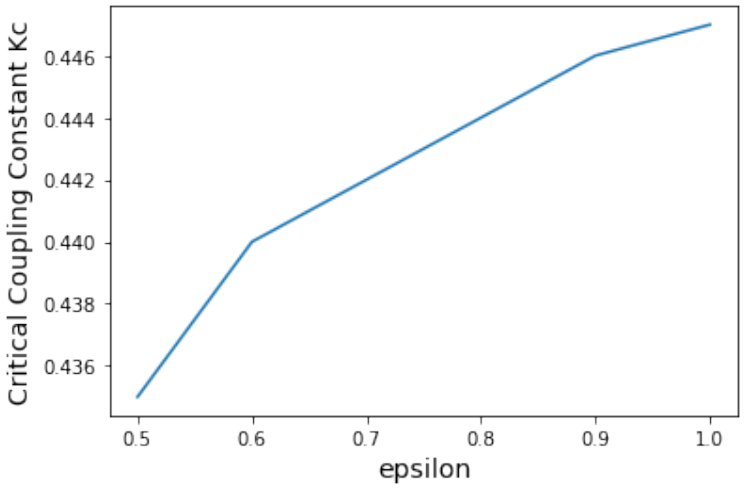

Figure 3.9: Critical coupling constant K_c as a function of anisotropy ϵ

3.3 Discussion

Previous research using the quantum U(1) rotor approach to study 2D anisotropic optical lattice suggests that the $K_c \propto \frac{J}{U}$ increases as the amount of anisotropy increases [28]. Similarly, we predicted that the critical coupling constant would increase as the amount of anisotropy increases. We also predicted that as we increase the amount of anisotropy, the phase stiffness or helicity modulus would decrease since the interaction along one direction overpowers that of the other direction.

Our results suggest that anisotropy does affect the superfluid density and the critical coupling constant. Figure 3.8 also suggests the superfluid density decreases as we introduce more anisotropy. However, for the critical coupling constant, our result indicates the opposite of the hypothesis, such that as the critical coupling constant decreases as the amount of anisotropy increases.

There are multiple explanations for the discrepancy. First, Monte Carlo simulations will be more precise and close to the true distribution with more steps. The amount of Monte Carlo step significantly affects the precision and the accuracy of our model. When using only $4000 \times N_x \times N_y \times M$ steps, we did observe a similar crossing behavior but the crossing point was around $K_c \approx 0.440$, which differed

from the true model. Due to the computational time and power limits, we used $40000 \times N_x \times N_y \times M$ steps, which gave us relatively stable results but could still lead to imprecision. Therefore, if we perform more Monte Carlo steps, the crossing points may shift and we will obtain more precise results. Second, when introducing anisotropy to the model, we adjusted the Josephson energy and the coupling constant K along x and y directions. However, more parameters may be affected by the anisotropy and some forms of normalization should be involved to reflect the new property. Lastly, we made our predictions from the intuition that the phase stiffness is lowered when two directions have different coupling energies. If we take the model to be the accurate model, it suggests that new physics intuition is needed to explain the results.

Chapter 4

Conclusion

In this study, we investigated the Superconductor-Insulator Transition (SIT) in 2D anisotropic materials using quantum Monte Carlo simulation. SIT is a quantum phase transition that is driven by the competition between the Josephson coupling energy and the charging energy of each island. In 2D isotropic materials with no magnetic field, SIT happens at a universal critical coupling constant $K_c = 0.4538$, which is confirmed through both analytical and numerical calculations. When anisotropy is introduced to the 2D structure, we predicted that the helicity modulus would decrease as anisotropy increases and the critical coupling constant would increase as the anisotropy increases.

Through quantum Monte Carlo simulation using the Metropolis algorithm, we were able to simulate both the isotropic and anisotropic systems numerically. Using finite-size scaling, we were able to find the critical coupling constant at which point the superfluid density lines of different lattice sizes cross. We found that the superfluid density did decrease as anisotropy increases but the critical coupling constant also decreased as more anisotropy was introduced.

Both hypotheses were driven by the same intuition and mechanism, which is that it is easier to twist the phase of each site along one direction when the coupling energies

are different along different directions and thus it requires more Josephson coupling energy along one direction for the system to enter the superconducting phase. The discrepancy in our results suggest that future revision is required.

Future investigation should revisit the formalism of the helicity modulus and the superfluid density derivations and check if more parameters should be revised to incorporate anisotropy. Once the formalism is confirmed, subsequent studies can use more Monte Carlo steps to generate a more stablized configuration and calculate a more precise superfluid density value. That being said, one should always consider the trade-off between computational time and model accuracy. If further investigation indicates similar trends as the current results, it means we should introduce new insights to the physical system and the quantum phase transition.

Appendix A

Python Implementation

```
import numpy as np
from random import *
from scipy import *
import time
from matplotlib import pyplot as plt
N_x = 10
N_y = N_x
m = N_x
N = 50000 * N_x **3
N_1 = 40000 * N_x **3
epsilon = 0.6
K = np.arange(0.4, 0.5, 0.01)
Aij = 0
theta_j = np.zeros((N_x * N_y, 4))
cos_list = []
sin_list = []
for i in range(360):
    cos_list.append(np.cos(2 * np.pi * i/360))
    sin_list.append(np.sin(2 * np.pi * i/360))

"""
```

```
returns the theta_j matrix
"""
def nearest_neighbor(N_x, N_y):
    temp = np.zeros((N_x * N_y, 4))
    for i in range(N_x * N_y):
        ii = np.mod(i, N_x) + 1
        ij = np.ceil((i + 1) / N_y)
        temp[i][0] = int((ij - 1) * N_y + np.mod(ii, N_x))
        temp[i][1] = int(np.mod(ij, N_y) * N_y + ii) - 1
        temp[i][2] = int((ij - 1) * N_y + np.mod(ii + N_x - 2, N_x))
        temp[i][3] = int((np.mod(ij + N_y - 2, N_y)) * N_y + ii) - 1
    theta_j = temp
    return theta_j
```

Listing A.1: Initial Configuration Generation

```
"""
returns new theta
"""
def sample_generator(idi, idj, oldTheta, N_x, N_y, m):
    newTheta = np.copy(oldTheta)
    #get the new i, j for the next flip site
    idj_r = np.random.random()
    index = np.round(idj_r * (N_x * N_y * m - 1) + 1)
    idi = int(np.mod(index - 1, N_x * N_y))
    idj = int((index - idi) / (N_x * N_y))
    rr = np.random.rand()
    newTheta[idi][idj] = np.round(rr * 359) + 1
    return newTheta, idi, idj
```

Listing A.2: New Sample Generator

```
"""
return delta H
"""
```

```
def deltaH(newTheta, oldTheta, idi, idj, N_x, N_y, m, cos_list,
    theta_j, A_ij):
     iOd = np.zeros(4)
     iNd = np.zeros(4)
     if (idj == m - 1):
         idj2 = 0
         idj1 = idj - 1
     elif (idj == 0):
         idj1 = m - 1
         idj2 = idj + 1
     else:
         idj1 = idj - 1
         idj2 = idj + 1
     id1 = int(np.mod(oldTheta[idi][idj1] - oldTheta[idi][idj], 360))
     id2 = int(np.mod(oldTheta[idi][idj] - oldTheta[idi][idj2], 360))
     id3 = int(np.mod(newTheta[idi][idj1] - newTheta[idi][idj], 360))
     id4 = int(np.mod(newTheta[idi][idj] - newTheta[idi][idj2], 360))
     for ii in range(4):
         iOd[ii] = np.mod(oldTheta[idi][idj] - oldTheta[int(theta_j[
    idi][ii])][idj] - A_ij, 360)
         iNd[ii] = np.mod(newTheta[idi][idj] - newTheta[int(theta_j[
    idi][ii])][idj] - A_ij, 360)
     DH = cos_list[id1] + cos_list[id2] - cos_list[id3] - cos_list[
    id4] + \
              cos_list[int(iOd[0])]+cos_list[int(iOd[1])]+\
                  cos_list[int(iOd[2])]+cos_list[int(iOd[3])] - \
                      cos_list[int(iNd[0])]-cos_list[int(iNd[1])]- \
                          cos_list[int(iNd[2])]-cos_list[int(iNd[3])]
     return -DH
```

Listing A.3: Energy Change Associated with the Flip

```
"""
return helicity modulus as an array
```

```
"""
def HelicityModulux(oldTheta,nx,ny,m,cosx,sinx,theta_j,Aij):
    x1 = 0
    x2 = 0
    x3 = 0
    x4 = 0
    gx = np.zeros(6)
    for i in range(m):
        for j in range(N_x * N_y):
            i1 = np.mod(int(oldTheta[j][i]) - int(oldTheta[int(
theta_j[j][0])][i]) - A_ij, 360)
            i2 = np.mod(int(oldTheta[j][i]) - int(oldTheta[int(
theta_j[j][1])][i]) - A_ij, 360)
            x1 += cos_list[i1]
            x2 += cos_list[i2]
            x3 += sin_list[i1]
            x4 += sin_list[i2]
    gx[0] = x1
    gx[1] = x2
    gx[2] = x3**2
    gx[3] = x4**2
    gx[4] = x3
    gx[5] = x4
    return gx
```

Listing A.4: Helicity Modulus Calculation for the Old Configuration

```
def newGamma(oldG, oldTheta, newTheta, idi, idj, N_x, N_y, m,
cos_list, sin_list, theta_j, A_ij):
    newG = np.zeros(6)
    iO1 = np.mod(int(oldTheta[idi][idj]) - int(oldTheta[int(theta_j[
idi][0])][idj]) - A_ij, 360)
    iO2 = np.mod(int(oldTheta[idi][idj]) - int(oldTheta[int(theta_j[
idi][1])][idj]) - A_ij, 360)
```

```
    iO3 = np.mod(int(oldTheta[int(theta_j[idi][2])][idj]) - int(
    oldTheta[idi][idj]) - A_ij, 360)
    iO4 = np.mod(int(oldTheta[int(theta_j[idi][3])][idj]) - int(
    oldTheta[idi][idj]) - A_ij, 360)

    iN1 = np.mod(int(newTheta[idi][idj]) - int(newTheta[int(theta_j[
    idi][0])][idj]) - A_ij, 360)
    iN2 = np.mod(int(newTheta[idi][idj]) - int(newTheta[int(theta_j[
    idi][1])][idj]) - A_ij, 360)
    iN3 = np.mod(int(newTheta[int(theta_j[idi][2])][idj]) - int(
    newTheta[idi][idj]) - A_ij, 360)
    iN4 = np.mod(int(newTheta[int(theta_j[idi][3])][idj]) - int(
    newTheta[idi][idj]) - A_ij, 360)

    newG[0] = oldG[0] - cos_list[iO1] - cos_list[iO3] + cos_list[iN1
    ] + cos_list[iN3]
    newG[1] = oldG[1] - cos_list[iO2] - cos_list[iO4] + cos_list[iN2
    ] + cos_list[iN4]
    newG[4] = oldG[4] - sin_list[iO1] - sin_list[iO3] + sin_list[iN1
    ] + sin_list[iN3]
    newG[5] = oldG[5] - sin_list[iO2] - sin_list[iO4] + sin_list[iN2
    ] + sin_list[iN4]
    newG[2] = newG[4]**2
    newG[3] = newG[5]**2
    return newG
```

Listing A.5: Helicity Modulus Calculation for the New Configuration

```
"""
Metropolis algorithm
1. find a random theta_i
2. flip the theta_i to a new value [1, 360] degrees from a
   probability density function
3. the new probability dTheta_i is dTheta_i x probability density
```

```
    matrix
4. accept the flip with probability min (1, transition prob)
5. if accepted, then theta -> theta_new, otherwise theta is
    unflipped
"""
def configuration(epsilon, coeff, N_x, N_y, m, N, N_1, A_ij):
    theta_j = nearest_neighbor(N_x, N_y)
    idj_r = np.random.random()
    index = np.round(idj_r * (N_x * N_y * m - 1) + 1)
    idi = int(np.mod(index - 1, N_x * N_y))
    idj = int((index - idi) / (N_x * N_y)) #6 out of bound so
    deleted +1
    g = np.zeros(6)
    r = np.random.rand(N_x * N_y, m)
    oldTheta = np.round(r * 359) + 1
    newTheta, idi, idj = sample_generator(idi, idj, oldTheta, N_x,
    N_y, m)
    start_config = time.time()
    for i in range (N_1):
        DH = deltaH(newTheta, oldTheta, idi, idj, N_x, N_y, m,
    cos_list, theta_j, A_ij)
        prob = np.random.random()
        if (np.exp(coeff * DH) >= prob):
            oldTheta = newTheta
        newTheta, idi, idj = sample_generator(idi, idj, oldTheta,
    N_x, N_y, m)
    # Stabilization step 1-5
    end_config = time.time()
    print("Config Done", end_config - start_config)
    oldG = HelicityModulux(oldTheta, N_x, N_y, m, cos_list, sin_list
    , theta_j, A_ij)
    start_gamma = time.time()
```

```
    count = N
    g = np.zeros(6)
    # calculate gamma
    gx = np.copy(oldG)
    counter = 0
    while count >= 1:
        DH = deltaH(newTheta, oldTheta, idi, idj, N_x, N_y, m,
cos_list, theta_j, A_ij)
        prob = np.random.random()
        if (np.exp(coeff * DH) >= prob):
            newG = newGamma(oldG, oldTheta, newTheta, idi, idj, N_x,
 N_y, m, cos_list, sin_list, theta_j, A_ij)
            gx += newG
            oldTheta = newTheta
            oldG = newG
            count -= 1
        counter += 1
        newTheta, idi, idj = sample_generator(idi, idj, oldTheta,
N_x, N_y, m)
    end_gamma = time.time()
    print("QMC done", end_gamma - start_gamma)
    g[0] = gx[0] / N
    g[1] = gx[1] / N
    g[2] = gx[2] / N
    g[3] = gx[3] / N
    g[4] = (gx[4] / N)**2
    g[5] = (gx[5] / N)**2
    gamma = (1 + epsilon**2) * coeff / (2 * N_x * N_y * m) * (g[0] +
 g[1]) \
        - ((1 + epsilon**3) * coeff**2)/(2*N_x*N_y*m)*(g[2]+g[3]) \
            + ((1 + epsilon**3) * coeff**2)/(2*N_x*N_y*m)*(g[4]+g
[5])
```

```
58      return gamma, gx
```

Listing A.6: Main Function

```
1  def plot(epsilon, N_x, N_y, m, N, N_1, A_ij):
2      gamma_list = []
3      for i in K:
4          gamma, gx = configuration(epsilon, i, N_x, N_y, m, N, N_1,
       A_ij)
5          print(gamma * i * m)
6          gamma_list.append(gamma * i * m)
7      return gamma_list
```

Listing A.7: Saves the Data

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