Critical properties of two–dimensional Josephson junction arrays with zero-point quantum fluctuations

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Abstract

We present results from an extensive analytic and numerical study of a two-dimensional model of a square array of ultrasmall Josephson junctions. We include the ultrasmall self and mutual capacitances of the junctions, for the same parameter ranges as those produced in the experiments. The model Hamiltonian studied includes the Josephson, $E_J$, as well as the charging, $E_C$, energies between superconducting islands. The corresponding quantum partition function is expressed in different calculationally convenient ways within its path-integral representation. The phase diagram is analytically studied using a WKB renormalization group (WKB-RG) plus a self-consistent harmonic approximation (SCHA) analysis, together with non-perturbative quantum Monte Carlo simulations. Most of the results presented here pertain to the superconductor to normal (S-N) region, although some results for the insulating to normal (I-N) region are also included. We find very good agreement between the WKB-RG and QMC results when compared to the experimental data. To fit the data, we only used the experimentally determined capacitances as fitting parameters. The WKB-RG analysis in the S-N region predicts a low temperature instability i.e. a Quantum Induced Transition (QUIT). We carefully analyze the possible existence of the QUIT via the QMC simulations and carry out a finite size analysis of $T_{QUIT}$ as a function of the magnitude of imaginary time axis $L\tau$. We find that for some relatively large values of $\alpha = \frac{E_C}{E_J}$ ($1 \leq \alpha \leq 2.25$), the $L\tau \to \infty$ limit does appear to give a non-zero $T_{QUIT}$, while for $\alpha \geq 2.5$, $T_{QUIT} = 0$. We use the SCHA to analytically understand the $L\tau$ dependence of the QMC results with good agreement between them. Finally, we also carried out a WKB-RG analysis in the I-N region and found no evidence of a low temperature QUIT, up to lowest order in $\alpha^{-1}$.

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I. INTRODUCTION

The physics of Josephson junctions arrays (JJA) has been a subject of significant interest in the last ten years [1]. A large number of studies, both experimental [2–7] and theoretical [8–23], have been devoted to them. Initially, part of the interest in JJA came from their close relation to one of the most extensively studied theoretical spin models, i.e. the classical 2-D XY model for which JJA give a concrete experimental realization.

In non-dissipative JJA the two main contributions to the energy are the Josephson coupling between superconducting islands due to Cooper pair tunneling, and the electrostatic energy arising from local deviations from charge neutrality. In the initial experimental studies, the size of the islands was large enough so that the charging energy contributions were very small, thus making the arrays’ behavior effectively semi-classical. Recent advances in submicron technology have made it possible to fabricate relatively large arrays of ultrasmall superconducting islands separated by insulating barriers. These islands can have areas of the order of a few µm², with self capacitances \( C_s \approx 3 \times 10^{-2} \) fF, and nearest neighbors’ mutual capacitance \( C_m \approx 1 \) fF [3]. Note that the mutual capacitance can be at least two orders of magnitude larger than the self capacitance. Therefore, these arrays have charging energy contributions, \( E_c \), large enough so that quantum fluctuation effects are of paramount importance.

In the Delft [3] and Harvard [4] experiments, the island sizes were kept constant, while varying the normal state junction resistance, which in turn changes the Josephson coupling energy, \( E_J \). This allows one to obtain arrays with values of the quantum parameter

\[
\alpha_m = \frac{E_{C_m}}{E_J}
\]  

in the range [0.13–4.55] [3], or values as high as 33 [3]. In this equation we have used the definition of charging energy,

\[
E_{C_m} = \frac{e^2}{2C_m}.
\]

The experimental systems can be modeled by a quantum generalization of the classical XY model, because the phase of the order parameter associated with each one of the islands is canonically conjugate to its excess Cooper pair number. The magnitude of \( \alpha_m \) determines the relevance of the quantum fluctuations. For small \( \alpha_m \) the quantum fluctuations of the phases are small and the system is well modeled by a renormalized classical 2-D XY model.

The nature of the phase transition in the classical 2-D XY model is well understood, whereas in its quantum mechanical generalization there still are unsettled issues. One of the most notorious of these is the possibility of having a low temperature instability of the superconducting state. A possible reentrant transition was originally found within a mean field theory treatment of the self-capacitive XY model [16,20–22]. An explicit two-dimensional study of the self-capacitave XY model, within a WKB renormalization group (WKB-RG) analysis also found evidence of a low temperature reentrant instability, triggered by a quantum fluctuation induced proliferation of vortices [13].

Recently, Kim and Choi have studied the quantum induced fluctuations in these arrays, using a variational method [23]. They found that there is a range of values of the ratio
of charging to Josephson energy, for which there is a low temperature reentrance from a superconducting to a normal state. Similar results had been obtained by Simanek, also using a variational calculation, see for example Ref. [22].

A non-perturbative quantum Monte Carlo study of the self-capacitive model found a low temperature transition, but between two superconducting states [14]. The fully frustrated version of this model was also studied by quantum QMC and it yielded a larger jump discontinuity in the superfluid density as compared to the one in zero field as well as the critical temperature one order of magnitude higher [14]. A more recent analysis of the WKB-RG analysis has shown that, to lowest order in the quantum fluctuations, it must have the same critical temperature for a quantum induced phase transition (QUIT) [24]. A recent QMC study of the fully frustrated self-capacitive model by Mikalopas et al. [25] has suggested that the unusually large jump in the superfluid density is dominated by metastability effects due to the particular nature of the excitations in the frustrated model. This result is in agreement then with the reanalysis of the RG equations. However, this study was carried out at relatively high temperatures and the question about the existence of a QUIT, both in the frustrated and unfrustrated cases remains open. We deal extensively with the later question here. Other studies find within MFT that to have reentrance it is necessary to include off-diagonal capacitances [12], while others do not agree with this finding [3,17–19]. The search for a reentrant type transition is encouraged by some evidence of low temperature instabilities found experimentally in arrays of Josephson junctions [2], ultrathin amorphous films [26], a multiphase high-$T_c$ system [27], and in granular superconductors [28].

Most theoretical studies have been carried out using the self-capacitive model and different kinds of MFT or self consistent harmonic approximations (SCHA) [19]. As already mentioned, these studies do not agree among each other on some of the properties of the phase diagram, in particular about the possible existence of a low temperature instability of the superconducting state. No study has been carried out that closely represents the experimental systems where both the self and mutual capacitances are explicitly included. The goal of this paper is to consider a model that is expected to represent the characteristics of the Delft experiments. In particular, we concentrate on calculating the phase diagram using different theoretical tools.

One of the main results of this paper is presented in Fig. 1 which shows the $\alpha_m$ vs. $T$ phase diagram for an array with $C_m > C_s$ both for the unfrustrated ($f = 0$) and fully frustrated ($f = 1/2$) cases. The left hand side of this diagram shows the superconducting to normal phase boundary (S–N) as data points with error bars joined by a continuous line. These data points were calculated using a QMC method, to be described later in the paper. We also show (as squares) the experimental results taken from Refs. [3,4]. For $f = 0$ at small values of $\alpha_m$, the theoretical and experimental results agree quantitatively quite well with each other and with the semiclassical WKB-RG approximation. On the other hand, they only qualitatively agree for the $f = 1/2$ case and on the superconducting to insulating phase boundary. The normal to insulating transition line is shown to the right of the phase diagram. The latter is just a tentative boundary since our numerical calculations were not reliable enough to give the definitive location of this line, as also happens in experiments. The error bars in the calculated points used to draw the N-I line represent a crude estimation of the region where the inverse dielectric constant is different from zero. However, the issue of convergence of the calculation to the path integral limit is not resolved by these error
bars. As we will explain in the main body of the paper we found further evidence for a low temperature instability of the superconducting state in our numerical calculations. We found that this instability depends strongly on the magnitude of $\alpha_m$ and the finite size of the imaginary time axis in the QMC calculations. The latter finding sets strict constraints on some of the reentrant type behavior found in previous theoretical studies. Other studies have found reentrance very close to the superconducting to insulating transition [22]. This possibility is harder to study from our Monte Carlo calculations.

The physical content of the phase diagram is generally understood in terms of the interplay between the Josephson and charging energies. For small $\alpha_m$ and high temperature the spectrum of excitations is dominated by thermally excited vortices, which drive the superconducting to normal transition as the temperature increases, while the charging energy contributes with weak quantum fluctuations of the phases. The latter produces, after averaging over the quantum fluctuations, an effective classical action with a renormalized Josephson coupling that lowers the critical temperature [13].

For large $\alpha_m$ and low temperatures the charging energy dominates. The excitations in this limit are due to the thermally assisted Cooper pair tunneling that produces charged polarized islands. At low temperatures, there is not enough thermal energy to overcome the electrostatic coulomb blockade so that the Cooper pairs are localized and the array is insulating. As the temperature increases, the electric dipole excitations can unbind, driving an insulating to conducting transition (I-C). In the limit $C_m \gg C_s$, it was suggested that the I-C transition could be of the Berezinskii-Kosterlitz-Thouless (BKT) type, for in this case the interaction between charges is essentially logarithmic [29,30,2]. However, for the experimental samples it has been shown that rather than a true phase transition what is measured appears to be a crossover between an insulating to conducting phase, characterized by thermally activated processes [1,4]. It is likely that the reason for the crossover is the short screening length present in the samples ($\Lambda \approx 20$ lattice sites). Both experimental groups [1,4] find that a simple energetic argument gives an explanation for the activation energy found in the experiments. Furthermore, the nature of this crossover may be linked to thermal as well as to dynamical effects. As we shall see, theoretically the I-N phase is hard to study in detail.

For large values of $\alpha_m$ the model can be approximated by a 2-D lattice Coulomb gas, where a perturbative expansion can be carried out using $E_J$ as a small parameter. This type of calculation was performed in Ref. [8] in the limit $C_s \ll C_m$. The analysis lead to a 2-D Coulomb gas with a renormalized coupling constant. Here we will extend this calculation to obtain a more accurate estimation of the renormalized coupling constant. We do this because we are interested in seeing if it is possible to have a QUIT instability in the low temperature insulating phase. This possibility is suggested by the dual symmetry of the effective action between charges and vortices found in Ref. [8], and the fact that the $\alpha_m$ perturbative expansion shows a low temperature QUIT instability in the superconducting phase. We find that the results of a first order expansion in $\alpha_m^{-1}$ does not present this type of low temperature instability.

Among the most interesting regions of the phase diagram is when the Josephson and charging energies are comparable. For this nonperturbative case, using a path integral formulation and the Villain approximation [34], an effective action for logarithmically interacting charges and vortices was derived in Ref. [8] in the case where $C_s \ll C_m$. The action
of the two Coulomb gases shows an almost dual symmetry, so that at an intermediate value of $\alpha_m$, both the S–N and the I–C transitions converge to a single point as $T \to 0$. A similar picture was derived in Ref. [17] using a short range electrostatic interaction and a mean field renormalization group calculation. A nonperturbative calculation is needed to determine the actual shape of the phase diagram in this region. We further discuss this point in the main body of the paper.

It has been argued that at $T = 0$ the self-capacitive model is in the same universality class as the 3-D XY model [9,11], where the ratio $\alpha_s = (q^2/2C_s)/E_J$ would play the role of temperature. This analogy would result in a transition at some finite value of $\alpha_s$ from a superconducting to an insulating phase. Moreover, there should be a marked signature in the nature of the correlation functions when crossing over from a 2-D XY model at high temperatures to a 3-D XY model as $T \to 0$. When $\alpha_s = 0$, the correlation functions decay algebraically in the critical region, with a temperature dependent exponent. At $T=0$ and $\alpha_s \neq 0$ there is a single critical point at $\alpha_s = \alpha_c$, so that the correlations decay exponentially above and below $\alpha_c$, and algebraically at $\alpha_s = \alpha_c$. The question is then, how do we go from algebraic to exponential correlations as $T$ changes? This can only happen by having a change of analyticity in the correlations, thus the possibility of having a QUIT in the self-capacitive model.

The situation is different in the mutual-capacitance dominated limit, of experimental interest. When $C_s = 0$ the model is equivalent to having two interacting lattice Coulomb lattice gas models. The general critical properties of this case are not fully understood at present. A further complication arises when $C_s$ is small but non-zero. The map to a higher dimensional known model does not work in this case, and the problem has to be studied on its own right. Because of the essential differences between the self-capacitive and the mutual-capacitance dominated models one can not just take results from one case and apply them to the other. It is the goal of this paper to explicitly study the mutual capacitance dominated model, but with nonzero $C_s$. A brief report on some of the results of this paper has appeared elsewhere [24].

The outline of the rest of the paper is the following: In Section II we define the model studied and derive the path integral formulation of the partition function used in our calculations. In Section III A we present a derivation of the path integral used in the semiclassical analysis, in the limit where the Josephson energy dominates. We carry out a WKB expansion up to first order in $\alpha_m$, finding an effective classical action where the charging energy contributions are taken into account as a renormalization of the Josephson coupling. In section III B we find general renormalization group (RG) equations from which we obtain the phase diagram for small $\alpha_m$. In Section IV we study the large $\alpha_m$ limit, in which the charging energy is dominant over the Josephson energy. There we obtain an effective 2-D Coulomb gas model with a quantum fluctuations renormalized coupling constant. In Section V A we discuss our QMC calculations and define the physical quantities calculated. In Section V B we present some technical details of the implementation of the QMC simulations. In Section V C we give the QMC results for $f = 0$ mainly, but also for $f = 1/2$. There we make a direct comparison between the semiclassical approximation results, the QMC calculations and experiment which lead to the phase diagram discussed above. In that section we also present an $L_r$ dependent analysis of the apparent $T_{QUIT}$ for three relatively large values of $\alpha_m = 2.0, 2.25$ and 2.5. The $L_r \to \infty$ extrapolation of the results leads to a finite
\( T_{\text{QUIT}} \) for \( \alpha_m = 2.0 \) and 2.25, while for \( \alpha_m = 2.5 \) we get a \( T_{\text{QUIT}}(L_r = \infty) = 0 \). In section \( \text{VI} \) we discuss a self-consistent harmonic approximation (SCHA) analysis, that we use to analytically study the phase diagram, and that helps us understand the finite size effects of the imaginary-time lattices studied in the QMC calculations. At the end of the paper there are two appendices where we give more technical details of the analysis. In Section \( \text{VII} \) we restate the main results of this paper.

II. THE MODEL AND THE PATH INTEGRAL FORMALISM

In this section we define the Josephson junction array model considered in this paper together with the path integral formulation of its corresponding partition function.

We assume that each superconducting island in a junction can be characterized by a Ginzburg-Landau order parameter \( \Psi(\vec{r}) = |\Psi_0(\vec{r})|e^{i\phi(\vec{r})} \), where \( \vec{r} \) is a two-dimensional vector denoting the position of each island. If the coherence length of the Cooper pairs is larger than the size of the islands, we can assume that the phase of the order parameter is constant in each island. Moreover, the amplitude of the order parameter is expected to have small fluctuations about an electrically neutral island and can then be taken as constant through the array. We will assume that the charge fluctuations have an effect on the electrostatic energy but not on the Josephson contribution to the Hamiltonian. The gauge invariant Hamiltonian studied here is

\[
\hat{H} = \hat{H}_C + \hat{H}_J = \frac{q^2}{2} \sum_{<\vec{r}_1, \vec{r}_2>} \hat{n}(\vec{r}_1)C^{-1}(\vec{r}_1, \vec{r}_2)\hat{n}(\vec{r}_2) + E_J \sum_{<\vec{r}_1, \vec{r}_2>} \left[ 1 - \cos \left( \phi(\vec{r}_1) - \phi(\vec{r}_2) - A_{\vec{r}_1, \vec{r}_2} \right) \right],
\]

(3)

where \( q = 2e \); \( \hat{\phi}(\vec{r}) \) is the quantum phase operator and \( \hat{n}(\vec{r}) \) is its canonically conjugate number operator, which measures the excess number of Cooper pairs in the \( \vec{r} \) island. These operators satisfy the commutation relations \([\hat{n}(\vec{r}_1), \hat{\phi}(\vec{r}_2)] = -i\delta_{\vec{r}_1, \vec{r}_2} \) \([3] \). Here \( A_{\vec{r}_1, \vec{r}_2} \) is defined by the line integral that joins the sites located at \( \vec{r}_1 \) and \( \vec{r}_2 \), \( A_{\vec{r}_1, \vec{r}_2} = \frac{2\pi}{\Phi_0} \int_{\vec{r}_1}^{\vec{r}_2} \vec{A} \cdot d\vec{l} \), where \( \vec{A} \) is the vector potential and \( \Phi_0 \) is the flux quantum. In Eq. (3) \( \hat{H}_C \) is the charging energy due to the electrostatic interaction between the excess Cooper pairs in the islands. The \( C^{-1}(\vec{r}_1, \vec{r}_2) \) matrix is the electric field propagator and its inverse, \( C(\vec{r}_1, \vec{r}_2) \), is the geometric capacitance matrix, which must be calculated by solving Poisson’s equation subject to the appropriate boundary conditions. This is not easy to do in general and typically this matrix is approximated, both theoretically and in the experimental analysis of the data, by diagonal plus nearest neighbor contributions \([3] \):

\[
C(\vec{r}_1, \vec{r}_2) = (C_s + zC_m)\delta_{\vec{r}_1, \vec{r}_2} - C_m \sum_{\vec{d}} \delta_{\vec{r}_1, \vec{r}_2 + \vec{d}}.
\]

(4)

Here the vector \( \vec{d} \) runs over nearest neighboring islands, \( z \) is the coordination number, \( C_s \) is the self-capacitance of each island, and \( C_m \) is the mutual capacitance between nearest neighbor islands. In the experimental arrays, typically \( C_m \sim 10^2 C_s \sim 1 \text{F} \) \([3] \).

The second term in Eq.(3) is the Josephson energy, which represents the probability of Cooper pair tunneling between nearest neighboring islands. The Josephson coupling energy
\[ E_J = \Phi_0 i_c / (2\pi) \] is assumed to be temperature independent, where \( i_c \) is the junction critical current and \( \Phi_0 \) the flux quantum. Here we are interested in calculating the thermodynamic properties of the model defined by \( \hat{\mathcal{H}} \). The quantity of interest is the partition function

\[ Z \equiv \text{Tr} \{ e^{-\beta \hat{\mathcal{H}}} \}. \]  

(5)

The trace is taken either over the phase variables, \( \hat{\phi} \), or the numbers operator, \( \hat{n} \). To evaluate the partition function we will use its path integral representation \([3, 33]\). To derive the path integral we use the states

\[ < n(\vec{r}_1) | \phi(\vec{r}_2) > = \delta_{\vec{r}_1, \vec{r}_2} \exp\{in(\vec{r}_1)\phi(\vec{r}_1)\} / \sqrt{2\pi}. \]  

(6)

We will also use the fact that both \( \{|n(\vec{r})\rangle\} \) and \( \{\{\phi(\vec{r})\rangle\} \) form complete sets. To start we write the partition function as a trace in the phase representation

\[ Z = \prod_{\vec{r}} \int_0^{2\pi} d\phi(0, \vec{r}) < \{\phi(0, \vec{r})\} | \exp \left\{ -\beta \hat{\mathcal{H}} \right\} | \{\phi(0, \vec{r})\} >. \]  

(7)

As usual we use the Trotter formula

\[ \exp \left\{ -\beta (\hat{\mathcal{H}}_C(\hat{n}) + \hat{\mathcal{H}}_J(\hat{\phi})) \right\} = \left[ \exp\{-\beta(\mathcal{L}_\tau)\hat{\mathcal{H}}_C(\hat{n})\} \exp\{-\beta(\mathcal{L}_\tau)\hat{\mathcal{H}}_J(\hat{\phi})\} \right]^{L_\tau} \]  

\[ + O \left( 1/L_\tau^2 \right). \]  

(8)

Next we introduce \( L_\tau - 1 \) complete sets \( \{\{\phi(\tau, \vec{r})\rangle\} \), \( \tau = 1, 2, \ldots, L_\tau - 1 \) in Eq. (7) so that

\[ Z = \prod_{\vec{r}} \prod_{\tau=0}^{L_\tau-1} \int_0^{2\pi} d\phi(\tau, \vec{r}) < \{\phi(0, \vec{r})\} | \exp \left\{ -\beta \hat{\mathcal{H}} \right\} | \{\phi(1, \vec{r})\} > \times \]  

\[ \times < \{\phi(1, \vec{r})\} | \exp \left\{ -\beta \hat{\mathcal{H}} \right\} | \{\phi(2, \vec{r})\} > \times \]  

\[ \times \cdots \times < \{\phi(L_\tau - 1, \vec{r})\} | \exp \left\{ -\beta \hat{\mathcal{H}} \right\} | \{\phi(0, \vec{r})\} > \]  

\[ + O \left( 1/L_\tau^2 \right). \]  

(9)

At this point we need to calculate the short time propagator,

\[ < \{\phi(\tau, \vec{r})\} | e^{-(\beta/(L\tau))\hat{\mathcal{H}}} | \{\phi(\tau + 1, \vec{r})\} > = \sum_{n(\tau, \vec{r})=-\infty}^{\infty} < \{\phi(\tau, \vec{r})\} | e^{-(\beta/L\tau)\hat{\mathcal{H}}} | \{n(\tau, \vec{r})\} > \times \]  

\[ \times < \{n(\tau, \vec{r})\} | \{\phi(\tau + 1, \vec{r})\} >, \]  

(10)

where we used a summation over the complete set \( \{|n(\tau, \vec{r})\rangle\} \). From Eqs. (3) and (8) this propagator can be written as

\[ < \{\phi(\tau, \vec{r})\} | e^{-(\beta/(L\tau))\hat{\mathcal{H}}} | \{\phi(\tau + 1, \vec{r})\} > = \prod_{\vec{r}} \frac{1}{2\pi} \sum_{n(\tau, \vec{r})=-\infty}^{\infty} e^{i n(\tau, \vec{r})[\phi(\tau + 1, \vec{r}) - \phi(\tau, \vec{r})]} \times \]  

\[ e^{-(\beta/L\tau)\mathcal{H}(\{n(\tau, \vec{r})\}, \{\phi(\tau, \vec{r})\})} + \]  

\[ + O(1/L^2_\tau). \]  

(11)
Inserting this equation in Eq. (3) we obtain the following path integral representation of the partition function

\[
Z = \prod_{\tau=0}^{L_\tau} \prod_{\vec{r}} \int_0^{2\pi} \frac{d\phi(\tau, \vec{r})}{2\pi} \sum_{\{n(\tau, \vec{r})\}=-\infty}^{\infty} \exp \left[ i \sum_{\tau=0}^{L_\tau-1} n(\tau, \vec{r}) [\phi(\tau+1, \vec{r}) - \phi(\tau, \vec{r})] \right] \times \\
\times \exp \left[ -\frac{\beta}{L_\tau} \sum_{\tau=0}^{L_\tau-1} \left[ H_J(\{\phi(\tau, \vec{r})\}) + \sum_{\vec{r}_1, \vec{r}_2} \frac{q^2}{2} n(\tau, \vec{r}_1) C^{-1}(\vec{r}_1, \vec{r}_2) n(\tau, \vec{r}_2) \right] \right] + \\
+ O(1/L_\tau^2).
\]  
(12)

together with the important boundary condition \(\phi(L_\tau, \vec{r}) = \phi(0, \vec{r})\). These equations are our starting point for the semiclassical approximation analysis discussed in the next section.

### III. WKB AND RENORMALIZATION GROUP EQUATIONS

#### A. Semiclassical limit

The semiclassical limit corresponds to taking \(q^2 \to 0\), or \(\alpha_m \to 0\). The summations over \(\{n(\tau, \vec{r})\}\) in Eq. (12) can be carried out and the result leads to \(\phi(\tau+1, \vec{r}) = \phi(\tau, \vec{r})\), for \(\tau = 0, 1, \ldots, L_\tau - 1\). In other words, in this limit all the phase variables are constant along the imaginary time axis, and we recover the classical 2-D XY model [34,35]. As the charging energy increases the value of \(\phi(\tau, \vec{r})\) fluctuates along the \(\tau\)-axis; these fluctuations suppress the XY phase coherence in the model lowering its critical temperature. For the self-capacitive model \((C_m = 0)\), at \(T = 0\), one can map the model to an anisotropic three-dimensional XY model [3]. This model should have a transition between ordered and disorder phases at a critical coupling \((E_{C_s}/E_J)_{c}\). Here \(E_{C_s} = e^2/2C_s\), so we would expect the phase boundary to go all the way down to \(T = 0\) for large enough charging energy.

In this section we study the change of the critical temperature as \(E_{C_m}\) increases, for small values of the ratio \(\alpha_m = E_{C_m}/E_J\). We start by eliminating the \(\{n's\}\) from Eq.(12) using the Poisson summation formula

\[
\sum_{n=-\infty}^{\infty} f(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{2\pi i m x} dx, 
\]  
(13)

obtaining

\[
Z = \prod_{\tau=0}^{L_\tau-1} \sqrt{\det[C]} \prod_{\vec{r}} \int_0^{2\pi} \sqrt{\frac{L_\tau}{2\pi \beta q^2}} d\phi(\vec{r}, \tau) \sum_{\{m(\tau, \vec{r})\}=-\infty}^{\infty} \exp \left[ -\frac{1}{\hbar} S[\{\phi\}, \{m\}] \right].
\]  
(14)

Here we defined the action

\[
\frac{1}{\hbar} S[\{\phi\}, \{m\}] = \sum_{\tau=0}^{L_\tau-1} \left[ \beta \frac{L_\tau}{q^2} H_J(\{\phi(\tau, \vec{r})\}) + \frac{L_\tau}{2\beta q^2} \sum_{\vec{r}_1, \vec{r}_2} [\phi(\tau+1, \vec{r}_1) - \phi(\tau, \vec{r}_1) + 2\pi m(\tau, \vec{r}_1)] \times \\
\times C(\vec{r}_1, \vec{r}_2) [\phi(\tau+1, \vec{r}_2) - \phi(\tau, \vec{r}_2) + 2\pi m(\tau, \vec{r}_2)] \right] + \\
+ O(1/L_\tau^2).
\]  
(15)
It is convenient to write the paths in the partition function separated into a constant part, that corresponds to the classical model, plus a quantum fluctuating contribution, over which we will perform the integrations to find an effective classical action. First we eliminate the summations over the \( \{m'\} \). This is done at the same time that the integrals over the \( \{\phi'\} \) are extended from \([0, 2\pi)\) to \((-\infty, \infty)\). After a couple of standard variable changes \([32,33]\) we get an action where the phases and the charges are separated,

\[
\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau L_E = \frac{1}{2} \frac{(2\pi)^2}{\beta q^2} \sum_{\vec{r}_1, \vec{r}_2} m(\vec{r}_1) C(\vec{r}_1, \vec{r}_2) m(\vec{r}_2) + \frac{1}{\hbar} \int_0^{\beta \hbar} d\tau \times \left[ \frac{\hbar^2}{2q^2} \sum_{\vec{r}_1, \vec{r}_2} \frac{d\psi}{d\tau}(\tau, \vec{r}_1) C(\vec{r}_1, \vec{r}_2) \frac{d\psi}{d\tau}(\tau, \vec{r}_2) + H_J(\{\psi(\tau, \vec{r}) + (2\pi/\beta \hbar)m(\vec{r})\} \right].
\]

Here the variables \( \psi(\beta \hbar, \vec{r}) = \psi(0, \vec{r}) \), and the integers \( m(\vec{r}) \) are called the winding numbers.

This equation shows that the winding numbers are the charge degrees of freedom and that the coupling between phases and charges appears only in the Josephson term. We can also see from this equation that in the semi-classical limit (small charging energy) the charge fluctuations are exponentially suppressed. This is more so for the \( m' \)s because they have a discrete excitation spectrum. Therefore, to lowest order in the semiclassical analysis we will set \( m(\vec{r}) = 0 \), leaving integrals only over the phases. Next we separate the \( \psi' \)s into a constant plus a fluctuating part

\[
\psi(\tau, \vec{r}) = \bar{\phi}(\vec{r}) + \phi_f(\tau, \vec{r}).
\]

At this point we use the following argument \([35,36]\). First that the Lagrangian is invariant under the transformation \( \psi(0, \vec{r}) \to \psi(0, \vec{r}) + 2\pi l(\vec{r}) \) for all integers \( l(\vec{r}) \), so that we can extend the limits of integration over \( \psi(0, \vec{r}) \) to \((-\infty, \infty)\), safe for an extra overall multiplicative constant. Now, the limits of integration for \( \phi_f(\tau, \vec{r}) \in (-\infty, \infty) \), and because of the periodicity of \( \phi_f \), we can Fourier series expand it as

\[
\phi_f(\tau, \vec{r}) = (\beta \hbar)^{-1/2} \sum_{k=1}^{\infty} [\phi_k(\vec{r}) e^{i\omega_k \tau} + C.C.],
\]

where the \( \omega_k = 2\pi k/\beta \hbar \) are the Bose-Matsubara frequencies. We have then the partition function \([33]\)

\[
Z = \prod_{\vec{r}} \sqrt{\det[C]} \int_{-\infty}^{\infty} \frac{d\bar{\phi}(\vec{r})}{(2\pi \beta q^2)^{1/2}} \prod_{k=1}^{\infty} \left[ \frac{\omega_k^2 \hbar^2}{\pi q^2} \det[C] \int_{-\infty}^{\infty} d\text{Re}\phi_k(\vec{r}) \int_{-\infty}^{\infty} d\text{Im}\phi_k(\vec{r}) \right] \times \exp \left\{ -\frac{1}{\hbar} S[\{\bar{\phi}\}, \{\phi_f\}] \right\}.
\]

Next, we expand the Josephson term in the action up to second order in \( \phi_f \), for higher order terms are suppressed in the integrations. After performing the integrations over the Euclidean time \( \tau \), and the Gaussian integrations, the effective partition function reads
Here we want to expand this partition function in powers of the charging energy. This is equivalent to expanding in powers of $q^2$, so our next step is to expand the determinant. We use the following identities

$$\det[I + D] = \exp\{\text{Tr}[\ln(I + D)]\},$$

$$\ln(I + D) = -\sum_{n=1}^{\infty} \frac{(-1)^n}{n} D^n,$$

where $I$ is the identity matrix. To lowest order in $q^2$ and using the result $\sum_{k=1}^{\infty} [q^2/(\hbar \omega_k)^2] = (q\beta)^2/24$, the effective partition function for $\bar{\phi}$ is then

$$Z_{\text{eff}} = \prod_{\bar{r}} \sqrt{\det[C]} \int_{-\infty}^{\infty} \frac{d\bar{\phi}(\bar{r})}{(2\pi \beta q^2)^{1/2}} \exp\left\{-\beta H_J(\{\bar{\phi}\}) \right\} \times$$

$$\times \prod_{k=1}^{\infty} \left[ \det\left\{ \delta_{\bar{r}_1,\bar{r}_2} + \frac{q^2}{\hbar^2 \omega_k^2} \sum_{\bar{r}} C^{-1}(\bar{r}_1, \bar{r}) \frac{\partial^2 H_J}{\partial \phi(\bar{r}) \partial \phi(\bar{r}_2)} |_{\bar{r}} \right\} \right]^{-1}.$$

(20)

To further advance the calculation we now use the properties of the Josephson energy. We start by using the fact that it is a local nearest neighbor interaction, so from Eq. (3)

$$H_J(\{\phi\}) = \sum_{\bar{r}} \sum_d f(\phi(\bar{r} + \bar{d}) - \phi(\bar{r})),$$

(24)

with the $\bar{d}$ running over the nearest neighbors to $\bar{r}$ in the lattice. From this equation we can see that the second derivative of $H_J(\{\phi\})$ is given by

$$\frac{\partial^2 H_J}{\partial \phi(\bar{r}_1) \partial \phi(\bar{r}_2)} = \sum_d \left[ f''(\phi(\bar{r}_1) - \phi(\bar{r}_1 - \bar{d})) \left( \delta_{\bar{r}_1,\bar{r}_2} - \delta_{\bar{r}_1,\bar{r}_2 + \bar{d}} \right) + 
+f''(\phi(\bar{r}_1 + \bar{d}) - \phi(\bar{r}_1)) \left( \delta_{\bar{r}_1,\bar{r}_2} - \delta_{\bar{r}_1 + \bar{d},\bar{r}_2} \right) \right],$$

(25)

where $f''(x) = d^2 f(x)/dx^2$.

In this paper we consider a periodic array, which implies that the inverse capacitance matrix is invariant under translations and rotations, that is $C^{-1}(\bar{r}_1, \bar{r}_2) = C^{-1}(|\bar{r}_1 - \bar{r}_2|)$. In particular, this makes $C^{-1}(\bar{r}, \bar{r} \pm \bar{d}) = C^{-1}(|\bar{d}|)$, independent of the direction of $\bar{d}$. Notice that here we are using $\bar{d}$ to denote the vectors that connect nearest neighboring islands, therefore in a periodic and symmetric array all of them have the same magnitude, allowing us to take the terms $C^{-1}(|\bar{d}|)$ out of the summations. From these considerations the trace gives
\[
\sum_{\vec{r}_1, \vec{r}_2} C^{-1}(\vec{r}_1, \vec{r}_2) \frac{\partial^2 H_J}{\partial \phi(\vec{r}_1) \partial \phi(\vec{r}_2)} \bigg|_{\phi} = 2 \left[ C^{-1}(|\vec{0}|) - C^{-1}(|\vec{d}|) \right] \sum_{\vec{r}} \sum_{\vec{d}} f''(\vec{\phi}(\vec{r} + \vec{d}) - \vec{\phi}(\vec{r})) \right). \quad (26)
\]

Next notice that since \( f''(x) = -f(x) \) (up to a constant), both terms in the argument of the exponential in Eq. (23) are the same cosine function of the classical phase variables, with only different coupling constants. Finally, the effective semi-classical partition function can be written as

\[
Z_{\text{eff}} = \prod_{\vec{r}} \sqrt{\text{det}[C]} \int_{-\infty}^{\infty} \frac{d\vec{\phi}(\vec{r})}{(2\pi \beta q^2)^{1/2}} \exp \left\{ -\beta_{\text{eff}} H_J(\{\vec{\phi}\}) \right\}, \quad (27)
\]

where the effective temperature is explicitly given by

\[
\beta_{\text{eff}} = \beta - q^2 \frac{\beta^2}{12} \left[ C^{-1}(|\vec{0}|) - C^{-1}(|\vec{d}|) \right]. \quad (28)
\]

Notice that to obtain this result we have used an argument that could be questionable, namely the extension of the \( \phi(0, \vec{r}) \) to the \((-\infty, \infty)\) range in the path integrals. All the other approximations are consistent with the semiclassical approximation and the symmetries used are exact. However, to continue we will now restore the \([0, 2\pi]\) range of the phases to use the results known from the BKT theory. As we will show later in the paper, the nonperturbative QMC results do agree quantitatively with the WKB results and experimental results to be discussed later. A similar effective result was first obtained but for the self-capacitive model in [13].

One of the important properties of Eqs. (27) and (28) is that up to this point we have made no assumptions about the structure of the capacitance matrix that go beyond translational invariance. Later on we will make specific choices of this matrix when we make direct contact with experimental findings [3].

**B. Renormalization group analysis**

Now that we have expressed the quantum mechanical problem as a modified 2-D classical XY model we can directly apply the well known results for this model [34,35]. The standard physical picture of the excitation spectrum in this model is of spin-waves plus vortex pair excitations. At low temperatures the energy to create an isolated vortex grows logarithmically with the size of the system, therefore excitations are created as bounded vortex-antivortex pairs. As the temperature increases, the vortex pair density increases until they unbind at a critical dimensionless temperature \( T_{\text{BKT}} = 0.894(5) \) [37,40]. The BKT scenario is best understood in terms of a renormalization group (RG) analysis [34,35]. The RG flow diagram is obtained from a perturbative expansion in powers of the vortex pair fugacity \( y \). To lowest order in \( y \), the RG equations corresponding to our problem are

\[
\frac{dK_{\text{eff}}}{dl} = -4\pi^3 K_{\text{eff}}^2 y^2, \quad (29)
\]

\[
\frac{dy}{dl} = [2 - \pi K_{\text{eff}}] y. \quad (30)
\]
Here we have used the following definitions:

\[ K_{\text{eff}} = K - xK^2, \]

\[ x = \frac{q^2}{12E_J} \left[ C^{-1}(|0\rangle) - C^{-1}(|d\rangle) \right], \]

\[ K = \beta E_J. \]

Then the equations for the coupling constants \( K \) and \( y \) are

\[ \frac{dK}{dl} = 4\pi^3 K^2 y^2 \frac{(1 - xK)^2}{(2Kx - 1)}, \]

\[ \frac{dy}{dl} = [2 - \pi K(1 - xK)]y. \]

To find the critical temperature, we use the initial conditions from the temperature and the bare vortex pair fugacity

\[ K_{\text{eff}}(l = 0) = \beta_{\text{eff}} E_J \left[ 1 + \frac{1}{2\beta_{\text{eff}} E_J} + O \left( \frac{1}{(\beta_{\text{eff}} E_J)^2} \right) \right]^{-1}, \]

\[ y(l = 0) = \exp \left\{ -\frac{\pi^2}{2} K_{\text{eff}}(l = 0) \right\}. \]

The RG equations have two nontrivial fixed points (for \( x < \pi/8 \)). One corresponds to the effective BKT thermal fluctuations driven transition, and the other to a quantum fluctuations induced transition (QUIT) [13–15].

One way to analyze the structure of the RG flow in the \((y, K)\) phase space is to use a conserved quantity associated with Eqs. (29) and (30)

\[ A = -\pi \ln K_{\text{eff}} - \frac{2}{2K} + 2\pi^3 y^2. \]

Using Eq. (32) and expanding up to first order in \( x \) we find

\[ A = \pi xK - \pi \ln K - \frac{2}{K} + 2\pi^3 y^2. \]

Figure 2 shows the RG flows obtained from numerically solving the RG equations for different values of \( A \), where the arrows indicate the direction of increasing \( l \). We have also plotted the set of initial conditions from Eqs. (36) and (37) as a discontinuous line. One important flow line is the separatrix between the lines for which \( y(l \to \infty) \to \infty \) and those for \( y(l \to \infty) \to 0 \). This line has \( A_c = -\pi [1 + \ln(2/\pi)] \), which is determined by the condition that it must pass through the point \( (y = 0, K_{\text{eff}} = 2/\pi) \). The critical temperature is obtained from the intersection of the separatrix with the initial conditions given in Eqs. (36) and (37). This intersection exists only if \( x \) is less than the critical value \( x_c < \pi/8 \), to be estimated below. Fortunately, we do not need to find this intersection explicitly since we already know the critical value of the effective coupling \( K_{\text{eff}} \), which is the usual critical coupling of the classical XY model, \( K_{\text{eff}} = K_{\text{XY}}^{(c)} \approx 1.1186 \) [37]. Therefore, the values of the two critical couplings are
\[ K(1 - xK) = K_{c}^{XY}, \quad (40) \]

\[ K_{\pm} = \frac{1}{2x} \left[ 1 \pm \sqrt{1 - 4xK_{c}^{XY}} \right], \quad (41) \]

which leads to \( x_{c} = 1/(4K_{c}^{XY}) \approx 0.2235 \).

We note from Fig. 2 that the \( K^{-1} \) axis can be divided into three different regions. If we set \( K_{+} = K_{QUIT} \), and \( K_{-} = K_{BKT} \), then in the region \([K_{QUIT}^{-1}, K_{BKT}^{-1}]\), as \( l \) increases, the fugacity of the vortex-antivortex pairs decreases. In the limit \( l \to \infty \) the energy to create a macroscopic vortex pair becomes infinite. Therefore, the system is superconducting for temperatures in this interval. For temperatures \( T > E_{J}K_{BKT}^{-1} \) the renormalized fugacity \( y(l) \) increases and the low \( y \) approximation breaks down. For these temperatures, the array is normal. For \( T < E_{J}K_{QUIT}^{-1} \), the vortex pair density increases due to the quantum fluctuations, leading us to think that there may be a low temperature transition driven by the quantum fluctuations (QUIT).

To obtain the results described above we used a high temperature perturbative calculation. Therefore the QUIT results are in principle outside the regimen of validity of the WKB-RG calculation. We need, then, other calculations and approaches valid at low temperatures to prove or disprove the existence of the QUIT. Expanding Eq. (41), up to first order in \( x \) and using Eq. (33) we find the critical temperatures,

\[ T_{BKT} \approx T_{BKT}^{(0)} - \frac{E_{J}}{k_{B}}x + O(x^{2}), \quad (42) \]

\[ T_{QUIT} \approx \frac{E_{J}}{k_{B}}x + O(x^{2}). \quad (43) \]

Note that these equations are applicable not only in 2-D, for if the system described by Eq. (27) has a transition point at some \( K_{c}^{eff} \) then the equation \( K_{c}^{eff} = K - xK^{2} \) has two solutions for \( K \). In this argument we should notice that the existence of the second solution for \( K \) depends on the higher order terms in the \( x \) expansion. Note that the change of \( T_{BKT} \) for small \( x \) is correctly given by the small \( x \) result. The existence of a low temperature quantum phase is of a nonperturbative nature, however. That is one of the reasons why we resort to using the nonperturbative quantum QMC approach latter in the paper.

Another interesting property of Eqs. (42) and (43) is that the first order correction does not depend on the specific value of \( T_{BKT}^{(0)} \). In particular, if we add a magnetic field to the Hamiltonian in Eq. (3), all the calculations leading to Eqs. (27) and (28) would be unchanged. Therefore, if \( T_{c}^{(0)}(B) \) is the superconducting to normal transition temperature for the array in a finite magnetic field \( B \) at \( x = 0 \), then to first order in \( x \) we must have

\[ T_{c}(B) \approx T_{c}^{(0)}(B) - (E_{J}/k_{B})x + O(x^{2}). \quad (44) \]

This equation is in agreement with the results obtained in Ref. [14]. Furthermore, we notice that to lowest order in \( x \), the \( T_{QUIT} \) must be the same with then without a magnetic field. This result was not noted before and it can be used as a test of the QMC calculations, in particular those of Mikalopas et al. [25].

To make comparisons with experiment, we need to specify the capacitance matrix. In particular, if we use Eq. (4) and the specific geometry of the array, we find that \( x \) is given by
The function \( g(w) \) can be written as an elliptic integral for a two-dimensional square lattice [38]. For a general lattice geometry, we find the following limiting behavior

\[
g(w) \approx \begin{cases} 
  z - z(1 + z)w, & \text{if } w \ll 1, \\
  w^{-1} \{1 - (4\pi w)^{-1} \ln w\}, & \text{if } w \gg 1.
\end{cases}
\] (46)

Using Eqs. (42) and (46) we get

\[
\frac{k_B T_{BKT}}{E_J} \approx \frac{k_B T_{BKT}^{(0)}}{E_J} - \begin{cases} 
  (2/3)\alpha_s + O(\alpha_s^2), & \text{if } C_s \gg C_m, \\
  (2/3)\alpha_m + O(\alpha_m^2), & \text{if } C_s \ll C_m.
\end{cases}
\] (47)

This result is in agreement with the Monte Carlo calculation of the superconducting to normal transition temperature carried out in Ref. [14] for the self-capacitive model. As we will show later in this paper, it is also in good agreement with our QMC calculations for the model dominated by the mutual capacitances.

IV. INSULATING TO NORMAL CROSS OVER.

So far we have studied the normal to superconducting transition in the limit where the Josephson energy dominates over the charging energy. In the opposite limit, when the relevant excitations are charge fluctuations, the transition is expected to be from a normal conducting state, where the charges are free to move, to an insulating state where the charges are bound into neutral dipole pairs (see Fig. [1]). It has been suggested that in the limit \((C_s/C_m) \to 0\) this I-N transition would be of a BKT type [29,50,2,8]. Experimental results have shown, however, that the behavior of the fabricated samples is better explained by a crossover from a normal to an insulating phase [34,4]. In finite systems, like the experimental ones, we would expect a rounding of the transition. Furthermore, in the experiments, the screening length is shorter than the sample size \(\Lambda \sim \sqrt{C_m/C_s} \approx 18\) lattice spacings [3]. Minnhagen et al. have argued that for any finite screening length, the transition is washed out even for an infinite array [42]. This is not difficult to understand since in the BKT scenario the superconducting to normal transition depends on the unscreened nature of the vortex logarithmic interaction [34,35].

In this section we present results from a perturbative calculation of the effect of the Josephson energy on the expected I-N crossover temperature. We start with Eqs. (16) and (17) leading to

\[
Z = \sqrt{\det[C]} \int_0^{2\pi} \prod_\tau \sqrt{\frac{L_\tau}{2\pi \beta q^2}} d\phi(\vec{r}) \sum_{m(\vec{r})=-\infty}^{\infty} \int_{-\infty}^{\infty} \prod_{\tau=1}^{L_\tau-1} \sqrt{\det[C]} \prod_\tau \sqrt{\frac{L_\tau}{2\pi \beta q^2}} d\phi_f(\tau, \vec{r}) \times \exp \left[ -\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau L_E \right],
\] (48)
where the action is now given by

\[
\frac{1}{\hbar} \int_0^{\beta h} d\tau L_E = \frac{1}{2} \frac{(2\pi)^2}{\beta q^2} \sum_{\vec{r}_1, \vec{r}_2} m(\vec{r}_1) C(\vec{r}_1, \vec{r}_2)m(\vec{r}_2) + \frac{1}{\hbar} \int_0^{\beta h} d\tau \times \\
\times \left[ \frac{\hbar^2}{2q^2} \sum_{\vec{r}_1, \vec{r}_2} \frac{d\phi_f}{d\tau}(\tau, \vec{r}_1) C(\vec{r}_1, \vec{r}_2) \frac{d\phi_f}{d\tau}(\tau, \vec{r}_2) + \\
+ H_J(\{\phi(\vec{r}) + \phi_f(\tau, \vec{r}) + (2\pi/\beta h)m(\vec{r})\}) \right],
\]

(49)

with the boundary condition

\[
\phi_f(0, \vec{r}) = \phi_f(\beta h, \vec{r}) = 0.
\]

(50)

Since we are interested in the charge degrees of freedom, our task here is to integrate out the phases. This limit has been studied before, in particular in Ref. [8]. Here we are not only interested in the crossover temperature, but we mostly want to ascertain if there is an equivalent QUIT in the insulating phase at low temperatures.

Since we are at the limit \(E_J \ll E_C\), the Josephson energy can be treated as perturbation. We expand the exponential

\[
\exp \left[ -\frac{1}{\hbar} \int_0^{\beta h} d\tau H_J(\tau) \right] \approx 1 - \frac{1}{\hbar} \int_0^{\beta h} d\tau H_J(\tau) + \frac{1}{2\hbar^2} \int_0^{\beta h} d\tau \int_0^{\beta h} d\tau' H_J(\tau) H_J(\tau') + \ldots
\]

(51)

We note that Eq. (48) can be written as

\[
Z = Z_\phi \prod_{\vec{r}} \sum_{m(\vec{r})=-\infty}^{\infty} \exp \left[ -\frac{(2\pi)^2}{2\beta q^2} \sum_{\vec{r}_1, \vec{r}_2} m(\vec{r}_1) C(\vec{r}_1, \vec{r}_2)m(\vec{r}_2) \right] Z_{\text{eff}}(\{m\}),
\]

(52)

where \(Z_\phi\) contains only phase degrees of freedom and can formally be written as

\[
Z_\phi = \prod_{\vec{r}} \int_{-\infty}^{\infty} D\phi_f(\vec{r}) \exp \left[ -\frac{1}{\hbar} S_f[\phi_f] \right],
\]

(53)

\[
S_f[\phi_f] = -\frac{\hbar^2}{2q^2} \int_0^{\beta h} d\tau \sum_{\vec{r}_1, \vec{r}_2} \frac{d\phi_f}{d\tau}(\tau, \vec{r}_1) C(\vec{r}_1, \vec{r}_2) \frac{d\phi_f}{d\tau}(\tau, \vec{r}_2).
\]

(54)

Here we have used the following short hand notation for the measure

\[
D\phi_f(\vec{r}) = \lim_{L_r \to \infty} \prod_{\tau=1}^{L_r-1} \sqrt{\det[C]} \prod_{\vec{r}} \sqrt{\frac{L_r}{2\pi \beta q^2}} d\phi_f(\tau, \vec{r}),
\]

(55)

noting that strictly speaking the integrals over a finite number of \(L_r\)’s have to be calculated before the limit \(L_r \to \infty\) is taken [39].

All the interactions between phases and charges are contained in \(Z_{\text{eff}}(\{m\})\), the effective partition function for the charges. The details of the explicit evaluations of \(Z_{\text{eff}}\) are given in Appendix A. The result for Eq. (52) can then be written, up to second order in \(E_J\), as
The effective coupling constant is given by

\[
Z = Z_{\phi} \prod_{\vec{r}} \sum_{m(\vec{r})=-\infty}^{\infty} \exp \left[ -\frac{1}{2K} \sum_{<\vec{r}_1,\vec{r}_2>} (m(\vec{r}_1) - m(\vec{r}_2))^2 - \frac{1}{2K} \left( \frac{C_s}{C_m} \right) \sum_{\vec{r}} m(\vec{r})^2 + \frac{K^2}{2} \left( \frac{(2\pi)^2 E_f C_m}{q^2} \right)^2 \sum_{<\vec{r}_1,\vec{r}_2>} \mathcal{I}(m(\vec{r}_1) - m(\vec{r}_2), \tilde{K}[1 - C_s C^{-1}(|\tilde{0}|)]) \right] + O(E_f^4). \tag{56}
\]

Here we have defined

\[
\tilde{K} = \frac{\beta q^2}{(2\pi)^2 C_m},
\]

\[
\mathcal{I}(m, \tilde{K}) = \int_{0}^{1/2} dx_1 \cos(2\pi mx_1) \exp \left[ -\{2(2\pi)^2/z\} \tilde{K} x_1(1-x_1) \right]. \tag{58}
\]

The function \( \mathcal{I}(m, \tilde{K}) \) is an even function of \( m \), so it can be expanded in a Taylor series in \( m^2 \). One way to do it is to take \( \cos(x_1) \approx 1 + (1/2)x_1^2 - (1/24)x_1^4 + \ldots \), This is a good approximation if the coefficient in the exponential is large. Since we are interested in discrete values of \( m \), and considering that values of \( m \) greater than one are suppressed even near the transition point, we can use the following approximation

\[
\mathcal{I}(m, \tilde{K}) = \mathcal{I}(0, \tilde{K}) - \mathcal{I}(0, \tilde{K}) - \mathcal{I}(1, \tilde{K}) = m^2. \tag{59}
\]

With this approximation we can write Eq. \( \text{(56)} \) as

\[
Z = Z_{\phi} \prod_{\vec{r}} \sum_{m(\vec{r})=-\infty}^{\infty} \exp \left[ -\frac{1}{2\tilde{K}_{\text{eff}}} \sum_{<\vec{r}_1,\vec{r}_2>} (m(\vec{r}_1) - m(\vec{r}_2))^2 - \frac{1}{2K} \left( \frac{C_s}{C_m} \right) \sum_{\vec{r}} m(\vec{r})^2 \right] + O(E_f^4). \tag{60}
\]

The effective coupling constant is given by

\[
\tilde{K}_{\text{eff}} = \tilde{K} \left[ 1 + \left( \frac{(2\pi)^2 E_f C_m}{q^2} \right)^2 h\left( \tilde{K}[1 - C_s C^{-1}(|\tilde{0}|)] \right) \right]^{-1}, \tag{61}
\]

\[
h(w) = w^3 \int_{0}^{1/2} dx \left[ 1 - \cos(2\pi x) \right] \exp \left[ -\{2(2\pi)^2/z\} w x(1-x) \right]. \tag{62}
\]

The function \( h(w) \) has the following limiting asymptotic behavior

\[
h(w) = \begin{cases} 
(1/2)w^3 \left[ 1 - w (1/z)(12 + (2\pi)^2/3) \right] + O(w^5), & \text{if } w \ll 1, \\
\frac{(z/2)^3}{(2\pi)^3} \left[ 1 + \frac{12}{(2\pi)^2}(z/2)w^{-1} - \frac{1}{(2\pi)^2}(z/2)^2 w^{-2} \right] + O(w^{-3}), & \text{if } w \gg 1.
\end{cases} \tag{63}
\]

We now use the fact that for the experimental systems \( C_s \ll C_m \), so that in the limit \( (C_s/C_m) \to 0 \) we can use

\[
\lim_{(C_s/C_m) \to 0} \left[ 1 - C_s C^{-1}(|\tilde{0}|) \right] = \lim_{(C_s/C_m) \to 0} \left[ 1 + \frac{1}{4\pi} \left( \frac{C_s}{C_m} \right) \ln \left( \frac{C_s}{C_m} \right) \right] = 1. \tag{64}
\]
The end result is a discrete Gaussian model with an effective coupling constant given by Eq. (61). This effective model can be transformed into a Villain model [40,43]. The critical points of this model are given by the equation \( \tilde{K}_{\text{eff}} = \tilde{K}_c \), where \( \tilde{K}_c \) is the critical coupling for the Villain model, \( \tilde{K}_c \approx 0.752(5) \) for a square array [40]. In other words we have to solve the equations,

\[
\tilde{K}_c = \tilde{K}_c + \Omega h(\tilde{K}_c), \quad \Omega = \tilde{K}_c (\pi^4/4) (E_J/E_{Cm})^2. \tag{65}
\]

From these equations we find the first order correction to the crossover temperature for a square array

\[
\frac{T_c}{T_c^{(0)}} \approx 1 - 0.259 \left( \frac{E_J}{E_{Cm}} \right)^2 + O\left( \left( \frac{E_J}{E_{Cm}} \right)^4 \right). \tag{67}
\]

Here we have used \( h(\tilde{K}_c) \approx 0.0106 \).

An important property of Eq. (65) is that we can show that it has only one solution, since the function \( h(\tilde{K}) \) is concave for small \( \tilde{K} \) and it has an inflection point at \( \tilde{K}_{\text{infl}} \),

\[
\tilde{K}_{\text{infl}} \approx \frac{6.2}{2(2\pi)^2}. \tag{68}
\]

A sufficient condition for Eq. (65) to have only one solution is \( \tilde{K}_c > \tilde{K}_{\text{infl}} \). This condition is satisfied for square as well as triangular arrays. This result shows that there is no insulating QUIT phase and it is in clear contrast to the existence of the QUIT found using the WKB-RG approximation in the superconducting phase.

V. QUANTUM MONTE CARLO RESULTS

A. Definition of Physical Quantities Calculated

The two important physical parameters in our analysis are the temperature and \( \alpha = \frac{E_{Cm}}{E_J} \). Since in the experiments the self-capacitance is much smaller than the mutual capacitance, the relevant quantum parameter here is

\[
\alpha_m = \frac{E_{Cm}}{E_J} = \frac{e^2}{2C_mE_J}. \tag{69}
\]

In the region where \( \alpha_m \) is small, the phases dominate and we expect a superconducting to normal transition. The quantity we will use to characterize the coherent superconducting phase is the helicity modulus [45,41] defined as

\[
\Upsilon = \frac{\partial^2 F}{\partial A^2_{\hat{x},\hat{y}+\hat{z}}} \bigg|_{A=0}. \tag{70}
\]

Here \( \hat{x} \) is the unitary vector in the \( x \) direction. The superfluid density per unit mass, \( \rho_s \), is proportional \( \Upsilon \), with \( \rho_s(T) = \frac{1}{V} \left( \frac{ma}{\hbar} \right)^2 \Upsilon(T) \), where \( a \) is the distance between superconducting islands, \( m \) is the mass of the Cooper pairs, and \( V \) is the volume. From Eqs. (12) and (70) we get
\[
\frac{1}{E_J L_x L_y} \gamma(T) = \frac{1}{L_x L_y L_T} \left[ \left( \sum_{\tau=0}^{L_T-1} \sum_{\vec{r}} \cos \left( \phi(\tau, \vec{r}) - \phi(\tau, \vec{r} + \hat{x}) - A_{\vec{r}, \vec{r} + \hat{x}} \right) \right) - \right. \\
\left. - \frac{E_J \beta}{L_T} \left\{ \left[ \sum_{\tau=0}^{L_T-1} \sum_{\vec{r}} \sin \left( \phi(\tau, \vec{r}) - \phi(\tau, \vec{r} + \hat{x}) - A_{\vec{r}, \vec{r} + \hat{x}} \right) \right]^2 \right\} \right].
\]

(71)

The quantity we shall use to probe the possible charge coherence in the array is the inverse dielectric constant of the gas of Cooper pairs, defined as [47,48],

\[
\frac{1}{\varepsilon} = \lim_{k \to 0} \left[ 1 - \frac{q^2}{k_B T} \frac{1}{C(k)} n(k) n(-k) \right].
\]

(72)

We can obtain the Fourier transform \( C(\vec{k}) \) from Eq. (4) for the capacitance matrix to get,

\[
C(\vec{k}) = C_s + 2C_m \left[ 1 - \cos(k_x) \right] + 2C_m \left[ 1 - \cos(k_y) \right].
\]

(73)

The Fourier transform of the charge number is defined by

\[
n(\vec{k}) = \frac{1}{\sqrt{L_x L_y}} \sum_{\vec{r}} n(\vec{r}) \exp \left[ i\vec{k} \cdot \vec{r} \right].
\]

(74)

Using this equation we can obtain a path integral representation for this correlation function, given by

\[
\langle n(\vec{r}_1) n(\vec{r}_2) \rangle = -\frac{1}{Z} \prod_{\tau=0}^{L_T-1} \sqrt{\text{det}[C]} \prod_{\vec{r}} \int_0^{2\pi} \frac{L_T}{2\pi \beta q^2} d\phi(\tau, \vec{r}) \sum_{\{m(\tau, \vec{r})\} = -\infty}^\infty \times \\
\times \frac{\partial^2}{\partial \phi(L_\tau, \vec{r}_1) \partial \phi(L_\tau, \vec{r}_2)} \left\{ \exp \left[ -\frac{1}{\hbar} S[\{\phi\}, \{m\}] \right] \right\}_{\phi(L_\tau, \vec{r}) = \phi(0, \vec{r})}.
\]

(75)

The action is given in Eq. (13). This equation becomes

\[
\langle n(\vec{r}_1) n(\vec{r}_2) \rangle = \lim_{L_T \to \infty} \left\{ \frac{L_T}{\beta q^2} C(\vec{r}_1, \vec{r}_2) - \frac{1}{Z} \prod_{\tau=0}^{L_T-1} \sqrt{\text{det}[C]} \prod_{\vec{r}} \int_0^{2\pi} \sqrt{\frac{L_T}{2\pi \beta q^2}} d\phi(\vec{r}, \tau) \times \\
\times \sum_{\{m(\tau, \vec{r})\} = -\infty}^\infty \left( \frac{1}{\hbar} \frac{\partial S}{\partial \phi(L_\tau, \vec{r}_1)} \frac{1}{\hbar} \frac{\partial S}{\partial \phi(L_\tau, \vec{r}_2)} \right) \exp \left[ -\frac{1}{\hbar} S[\{\phi\}, \{m\}] \right] \right\},
\]

(76)

with

\[
\frac{1}{\hbar} \frac{\partial S}{\partial \phi(L_\tau, \vec{r}_1)} = \frac{L_x}{\beta q^2} \sum_{\vec{r}} C(\vec{r}_1, \vec{r}) \left[ \phi(L_\tau, \vec{r}) - \phi(L_\tau - 1, \vec{r}) + 2\pi m(L_\tau - 1, \vec{r}) \right].
\]

(77)
Notice, that this is not a well behaved operator since in the limit $L \tau \to \infty$ we would have to subtract two large numbers and the path integral in the second term in Eq. (76) would diverge. This divergence is canceled out by the first term in Eq. (76). This can be seen explicitly by doing the calculation of $\epsilon^{-1}$ setting $E_J = 0$, which leads to

$$< n(\vec{r}_1)n(\vec{r}_2) > = \frac{1}{\beta q^2} C(\vec{r}_1, \vec{r}_2) + \left( \frac{2\pi}{\beta L \tau} \right)^2 \sum_{\vec{r}_3, \vec{r}_4} C(\vec{r}_1, \vec{r}_3) C(\vec{r}_2, \vec{r}_4) < m(\vec{r}_3)m(\vec{r}_4) >. \quad (78)$$

This result can be put into Eq. (72) to obtain a finite inverse dielectric constant,

$$\frac{1}{\varepsilon} = \lim_{\vec{k} \to 0} \left[ \frac{(2\pi)^2}{\beta q^2} C(\vec{k}) < |m(\vec{k})|^2 > \right]. \quad (79)$$

Here we have used the Fourier transform defined in Eq. (74) and the $m(\vec{r})$ defined as $m(\vec{r}) = \sum_{\tau = 0}^{L \tau - 1} m(\tau, \vec{r})$. Note that in general this operator will not exactly be the inverse dielectric constant of a gas of Cooper pairs, since it will depend on $L \tau$. But we expect that it does contain most of the relevant information of the inverse dielectric constant of our charged system. In our Monte Carlo calculations we have used the general result Eq. (76) valid for $E_J \neq 0$ and finite $L \tau$.

**B. The Simulation Approach**

Up to now we have seen that the partition function defined by the Hamiltonian in Eq. (3) can be expressed in different convenient representations for analytic analyses. To carry out our QMC calculations, we have used what is, in principle, the most straightforward representation of $Z$ given by Eqs. (14) and (15); it involves the phases and the charge integer as statistical variables. This representation is general enough to be used over all the whole parameter range covered in the phase diagram.

In this case we have a set of angles $\phi(\tau, \vec{r}) \in [0, 2\pi)$, located at the nodes of a three-dimensional lattice, with two space dimensions, $L_x$ and $L_y$, and one imaginary time dimension, $L \tau$. The periodic boundary condition, comes from the trace condition in Eq. (5), and we also have chosen to use periodic boundary conditions in both space directions. The link variables $m(\tau, \vec{r})$ are defined in the bonds between two nodes in the $\tau$ direction and they can take any integer value.

We have basically used the standard Metropolis algorithm to move about in phase space [44]. As the phases are updated we restrict their values to the interval $[0, 2\pi)$. Moreover, the shifts along a $\tau$-column and the individual phase moves are adjusted to keep the acceptance rates in the range $[0.2, 0.3]$. If $\alpha_m$ is small, the system is in the semiclassical limit. In this case the fluctuations of the phases along the imaginary time axis as well as the fluctuations in the $m$’s are suppressed by the second term in Eq. (13). Attempts to change a phase variable will have a very small success rate. Therefore we implemented two kinds of Monte Carlo moves in the phase degrees of freedom. In one sweep of the array we update the $L_x \times L_y$ imaginary time columns, by shifting all the phases along a given column by the same angle. This move does not change the second term in Eq. (13), and thus it probes only the Josephson energy [14]. To account
for phase fluctuations along the imaginary time axis, which become more likely as \((\alpha_m/T)\) increases, we also make local updates of the phases along the planes.

Another aspect of the implementation of the QMC algorithm is the order in which we visit the array. This is relevant for the optimization of the computer code in different computer architectures. In a scalar machine we have used an algorithm that updates column by column in the array. For a vector machine we have used the fact that for local updates, like the ones we use, the lattice can be separated into four sublattices in a checkerboard-like pattern. This separation is done in such a way that each of the sublattices can be updated using a long vector loop without problems of data dependency. Using this last visiting scheme, the cpu time grows sublinearly with the size of the array. One of the problems that this type of visiting scheme has in a vector machine, like the Cray C90, is that the array’s dimensions have to be even, and this produces memory conflicts. We have not made attempts to optimize this part of the code. We have not used parallel machines in our calculations but the same type of checkerboard visiting scheme would lead to a fast algorithm.

We followed Ref. [14] and replaced the U(1) symmetry of the problem by a discrete \(Z_N\) subgroup. We took \(N = 5000\). This allows us to use integer arithmetic for the values of the phase variables, and to store lookup tables for the Josephson cosine part of the Boltzmann factors. This simplification can not be used for the charging energy part of the Boltzmann factors, except in the \(C_m = 0\) case, where the \(m\)’s can be summed up in a virtually exact form. In the latter case we can also store lookup tables using the following definition of an effective potential \(V_{\text{eff}}\),

\[
\exp \left[ -\left( \frac{L_s C_s}{q^2 \beta} \right) V_{\text{eff}}(\phi) \right] = \sum_{m=-\infty}^{\infty} \exp \left[ -\frac{1}{2} \left( \frac{L_s C_s}{q^2 \beta} \right) (\phi + 2\pi m)^2 \right].
\] (80)

We notice that this summation can be evaluated numerically to any desired accuracy.

We calculated the thermodynamic averages after we had made \(N\) visits to the array updating the phases and \(M\) visits updating the \(m\)’s. Typically, if \(\alpha_m\) is small we used \(N = 4\) and \(M = 1\). In the opposite limit we used \(N = 1\) and \(M = 8, 10, \ldots\) This is so because our local updating algorithms for the \(m\)’s have serious decorrelation time problems, due to the long range interaction among the charges. We typically found that in order to get reasonably small statistical errors, we needed to perform, in most cases, about \(N_{\text{meas}} = 2^{12} = 4096\) measurements of the thermodynamical quantities, other times we took up to \(N_{\text{meas}} = 2^{13} = 8192\) measurements.

Once we have a long stationary string of values for the measured operators we calculated their mean values and uncertainties. We also have used the algorithm proposed in Ref. [43] for the efficient calculation of the helicity modulus. This method has a bias problem due to the last term in Eq. (71). However, in the zero magnetic field case this problem is not present, since this term is identically zero.

### C. Results for f=0

In this subsection we present the bulk of our Monte Carlo results. We have mostly calculated the helicity modulus in the small \(\alpha_m\) region and the inverse dielectric constant in the large \(\alpha_m\) regime, and both quantities in the intermediate region.
Most of the calculations we performed were for parameter values close to or at the experimental ones. In particular, the ratio between the self and mutual capacitances was kept fixed between the values $C_s/C_m \approx 0.01$ and 0.03, with the bulk of the calculations carried out for 0.01. We found that for the helicity modulus both values gave essentially the same results. Almost all of the calculations were done by lowering the temperature, in order to reduce the possibility for the system to be trapped in metastable states.

We have a clear physical understanding of the behavior of the system in the very small $\alpha_m$ limit, since this limit is close to the classical 2-D XY model. Moreover, we have the semiclassical calculation results, mentioned before, up to first order in $\alpha_m$, which, as we shall see, agree very well with the Monte Carlo results. In this limit the results are solid because the discrete imaginary time path integral calculations converge very rapidly to the infinite $L_\tau$ limit. Therefore in this section we will discuss our numerical results for increasing values of $\alpha_m$. This will allow us to go from a well understood physical and calculational picture to the nonperturbative region of parameter space which is less understood. Here is where we will explore the limits of our numerical calculational schemes. The end result will be that a significant portion of the phase diagram can be understood. However, some of the most interesting intermediate regimes of the phase diagram are still very difficult to fully understand with our present calculational techniques.

In Fig. 3 we show a typical curve for the helicity modulus as a function of temperature, in the small $\alpha_m$ limit. As $\alpha_m$ increases $\Upsilon$ flattens in the superconducting region. In order to calculate the transition temperature we used the fact that the critical temperature and the helicity modulus still satisfy the universal relation,

$$\Upsilon(T_c) = \frac{2}{\pi} T_c.$$  \hspace{1cm} (81)

Based on the first order results from the semiclassical approximation analysis we know that this universal result is independent of $\alpha_m$. In other words, we can determine the critical temperature by the intercept of $\Upsilon(T)$ with the line $(2/\pi)T$, as shown in Fig. 3.

As can be seen from Fig. 3, at high temperatures and small $\alpha_m$ the asymptotic limit $L_\tau \to \infty$ is already reached for small $L_\tau$. From Eq. (15), we can see that the parameter that determines this rate of convergence is

$$P = \frac{L_\tau}{(\beta E_J)\alpha_m}.$$  \hspace{1cm} (82)

The deep quantum limit is reached for a relatively large $P \gg 1$. This progression is shown in Fig. 4 where we plot the helicity modulus as a function of temperature for a relatively large $\alpha_m = 1.25$, $L_x = L_y = 20$, and three values of $L_\tau$. It can be seen that convergence is reached for $P > 5$, as found before in the self capacitive model in Ref. [14].

As shown in Fig. 5 for a larger $\alpha_m$ the behavior changes and the departure from the $L_\tau \to \infty$ limit is manifested as a small dip in $\Upsilon$ at low temperature [15]. As the temperature is lowered $\Upsilon$ shows an upward behavior. This is also seen in Fig. 6 from more extensive calculation for a still larger $\alpha_m$'s. This finite $L_\tau$ behavior can be understood in terms of a plane decoupling along the imaginary time direction. A way to see this is to notice that if we take both contributions to the action given in Eq. (13) as independent, both of them would yield a low temperature transition. If all the $L_\tau$ planes are considered decoupled, then the
Josephson coupling would be $\beta/L$. Therefore in this case the N–S transition would happen at $T_{N-S} \approx 1/L\tau$. On the other hand, if we only consider the second term in Eq. (15) we see that plane decoupling would take place at $T_{\text{decl}} \approx (\alpha_m/L\tau)$. Now, if $T_{N-S} > T_{\text{decl}}$ which implies $\alpha_m < 1$, then only the first transition would take place. If however $\alpha_m$ is large enough, we could have $T_{N-S} < T_{\text{decl}}$, producing the observed dip in the helicity modulus. This is seen in Fig. 7 where the helicity modulus is shown together with the inverse dielectric constant. There it can be seen that the dip starts at about the same temperature where $\epsilon^{-1}$ becomes finite, signaling that the nonzero winding numbers have become relevant. In this region the fluctuations between planes have a small energy cost in the action given by Eq. (15).

As we increase $\alpha_m$ further we arrive at a point where at low temperatures, and fixed $L\tau$, $\Upsilon$ goes to zero as shown in Fig. 8. To understand the nature of the low temperature imaginary time phase we have computed the equal space imaginary time correlation function

$$C_{\tau}(\tau) = \langle \cos (\phi(\vec{r},\tau) - \phi(\vec{r},0)) \rangle.$$

(83)

We evaluated this function at three different temperatures, for $\alpha_m = 1.75$ and $L\tau = 32$. The results are shown in Fig. 9 where we see that the appropriate value for $L\tau$ needs to be increased as $T$ is lowered. More extreme are the two temperature results for $\alpha_m = 2.5$ and $L\tau = 64$, shown in Fig. 10. The upper curve corresponds to $k_BT/E_J = 0.36$. As seen in Fig. 8 at this temperature a value of $L\tau = 64$ is enough to reliably calculate the helicity modulus, for in this case the planes are correlated with a short decorrelation time. The lower curve has $k_BT/E_J = 0.1$. At this temperature the helicity modulus is zero and the correlation function has a very short decorrelation time. These results show that the low temperature discontinuity is related to a decoupling of the planes along the imaginary time axis.

This plane decoupling does not show any dependence on $(L_x, L_y)$ for the cases considered, and the curves shown in Fig. 8 are reproducible within the statistical errors for other values of $L_x$ and $L_y$. Again we point out that upon increasing $L\tau$ the decoupling temperature moves closer to zero temperature. We should note that from the WKB analysis there is a critical value for $\alpha$ above which the superconducting state is no longer stable. So as we consider larger values of $\alpha_m$, the superconducting state will become less and less stable. As we mentioned the simulations were performed while lowering the temperature. In contrast, in Fig. 11 we show results from lowering the temperature for $\alpha_m = 2.75$. In this case $\Upsilon$ reaches a zero for $T \leq 0.2$. We reversed the process increasing the temperature. Up to the last temperature calculated the results are consistent with having zero $\Upsilon$ for $\alpha_m = 2.75$. The low temperature state arises from a decoupling transition between the imaginary time planes which leads to an ensemble of decorrelated planes. Maybe the planes could get recoupled at higher temperatures but, as already mentioned, our local algorithm would take too long to realign these planes so as to produce a coherent state.

As shown in Fig. 8 the temperature where $\Upsilon$ has a sharp drop changes with the size of the system. To see if in the limit $L\tau \to \infty$ we still have a finite low temperature transition, we tried to extract it from the data for three different $\alpha_m$ values by plotting them against $1/L\tau$ as shown in Figs. 12, 13 and 14. From these figures it appears that for $\alpha_m = 2.0$ and 2.25 there is a nonzero transition temperature in the $L\tau \to \infty$ limit. We used a jackknife calculation to estimate the infinite $L\tau$ temperature and we found

$$T_{\text{decl}}(\alpha_m = 2, L\tau \to \infty) = (0.0183 \pm 0.009)(E_J/k_B),$$
and
\[ T_{\text{decl}}(\alpha_m = 2.25, L_\tau \to \infty) = (0.0067 \pm 0.0025)(E_J/k_B). \]
The same type of calculation was done for \( \alpha_m = 2.5 \). The results are shown in Fig. \[ ] . Here we found that
\[ T_{\text{decl}}(\alpha_m = 2.5, L_\tau \to \infty) = (-0.013 \pm 0.005)(E_J/k_B). \]
Therefore from these estimates we surmise that the critical value for \( \alpha_m \sim 2.5 \), which is larger than the one estimated from the WKB-RG analysis. However, our QMC calculations, in particular at low temperatures, are not precise enough to make a definitive determination of the critical \( \alpha_m \).

The calculations of the S–N transition line seem to indicate that the superconductor to insulator zero temperature transition occurs at \( \alpha_m \approx 3 \), which is quantitatively different from the \( T=0 \) estimate \[ ] .

The evaluation of the inverse dielectric constant is considerably more complicated since the insulating region we have \( \alpha_m > 3 \), needing larger values of \( L_\tau \) at low temperatures. Moreover there are serious critical slowing down problems due to the long range charge interactions which worsen as the size of the system increases.

We should point out that, in comparing with the purely classical case \[ ] , the quantum 2-D Coulomb gas studied here has the extra complication of the \( n - \phi \) coupling, as seen in Eq. (12). This introduces an imaginary component to the action. Therefore we are forced to integrate the \( n \)’s introducing the new variables \( \{m\} \) leading to the action given in Eq. (15). This is the action that we used to perform the Monte Carlo calculations.

We use the expression given in Eq. (79), which for finite \( \vec{k} \) and \( L_x = L_y \) gives \( |\vec{k}| = 2\pi/L_x \), as an upper bound for the inverse dielectric constant \[ ] . The technical problems mentioned above made the calculation of the dielectric constant less reliable than that of \( \Upsilon \). The results obtained from the Monte Carlo runs were too noisy to give us a quantitative estimate of the conductor to insulator transition temperature if there was one. Our quoted results give only tentative values for the transition line.

The results are shown in Fig. [], where we also plotted the results of the Monte Carlo calculation of the normal to superconductor transition temperature as well as the experimental results from the Delft group []. We have fitted a straight line to the first seven points in this line and used a jackknife calculation of \( T_c(\alpha_m) \) for small \( \alpha_m \). We obtained
\[ \frac{k_B T_c}{E_J} = (0.9430 \pm 0.0042) - (0.1800 \pm 0.0040)\alpha_m + O(\alpha_m^2). \] (84)

The value of the slope is in good agreement with the semiclassical approximation result given in Eq. (47). The dashed line gives \( \alpha_m = 2.8 \) at \( T=0 \) and joins the last QMC point to \( T = 0 \). The line is only a guide to the eye. We have not performed detailed calculations around \( \alpha_m = 3 \) since the required values of \( L_\tau \) makes reliable calculations too computationally intensive to be carried out with current algorithms and computer capabilities.

D. Results for \( f=1/2 \).

We also have performed a few calculations of the helicity modulus for the fully frustrated case \( f=1/2 \). The results of these calculations are shown in Fig. []. The experimental results
of the Delft group show a transition temperature for $\alpha_m = 0$ at $(k_B T/E_J) \approx 0.3$, while the classical fully frustrated case has a critical temperature close to $(k_B T/E_J) \approx 0.5$. Taking this into account we have rescaled the Monte Carlo results so that the calculated value for the transition temperature for $\alpha_m = 0$, $f=1/2$ coincides with the experimental result.

Taking the experimental value of the critical temperature for the $f = 0$ case, we performed a least square fit for the five smallest $\alpha_m$’s considered and found, using a jackknife calculation,

$$\left(\frac{k_B T}{E_J}\right)_{f=0} \approx (0.9787 \pm 0.0070) - (0.256 \pm 0.017)\alpha_m + O(\alpha_m^2). \tag{85}$$

In the same way, but now for the $f = 1/2$ case, we found

$$\left(\frac{k_B T}{E_J}\right)_{f=1/2} \approx (0.3188 \pm 0.0015) - (0.2929 \pm 0.0066)\alpha_m + O(\alpha_m^2). \tag{86}$$

These rough calculations show that the slopes of both curves are very close. This result can be compared with Eq. (14), which confirms that the first order correction in $\alpha_m$ to the critical temperature should not depend on the value of the magnetic field. A similar result for the equality of slopes was obtained in Ref. [14], using a Monte Carlo calculation for the self-capacitive model.

VI. SELF-CONSISTENT HARMONIC APPROXIMATION

We need an alternative analytic approach, in principle exact for fixed and finite $L_\tau$, to further understand the QMC results at low temperatures. This is important because of the strong $L_\tau$ dependence in the study of the QUIT temperature, and the analytic WKB results are only strictly valid at high temperatures and $L_\tau = \infty$. In this section we use a variational principle to evaluate the free energy for the JJA within a self-consistent harmonic approximation (SCHA). This approximation gives increasingly better results as the temperature is lowered. Previous SCHA calculations [3,10,19] did not explicitly include the charge degrees of freedom, which are of significant importance in the analysis presented here. As a bonus, we note that the SCHA developed here could be used as the basis for developing an alternative QMC algorithm to study the model at low temperatures and intermediate $\alpha$ values, were both the WKB and the standard QMC analyses have problems.

We start with the following decomposition of the Hamiltonian given in Eq. (3)

$$H = H_0 + \{H_J - H_H\}. \tag{87}$$

where $H_0 = \{H + (H_H - H_J)\}$, and

$$H_J = \sum_{\tau=1}^{L_\tau - 1} \sum_{\langle \vec{r}_1, \vec{r}_2 \rangle} \left[1 - \cos (\phi(\tau, \vec{r}_1) - \phi(\tau, \vec{r}_2))\right], \tag{88}$$

$$H_H = \frac{E_J}{2L_\tau} \sum_{\tau=1}^{L_\tau - 1} \sum_{\langle \vec{r}_1, \vec{r}_2 \rangle} \left[\phi(\tau, \vec{r}_1) - \phi(\tau, \vec{r}_2)\right]^2. \tag{89}$$
In other words, we replace the Josephson Hamiltonian by a spin wave term and introduce its stiffness $\Gamma$ as the variational parameter. $\Gamma$ is of course the helicity modulus, but to emphasize that it is evaluated within the SCHA we use the $\Gamma$ notation instead of $\Upsilon$. The spin wave approximation does not have a phase transition at any temperature so the variational calculation is going to give a vanishing $\Gamma$ as the signature of the JJA transition. The variational free energy is given by $F_V = F_H + \langle H_J - H_H \rangle_H$, where $\beta F_H = -\ln Z_H$, and $Z_H = \text{Tr} \{ \exp \{ -\beta H_0 \} \}$, with the average $<A>_H = \text{Tr} \{ A \exp \{ -\beta H_0 \} \} / Z_H$. We use the change of variables

$$\psi(\tau, \vec{r}) = \psi(0, \vec{r}) + \sqrt{\frac{2}{L_\tau}} \sum_{n=1}^{L_\tau-1} \chi_n(\vec{r}) \sin \left( \frac{\pi n}{L_\tau} \tau \right),$$

$$\tau = 1, 2, \ldots, L_\tau - 1,$$

and perform the integrals over the variables $\chi_n(\vec{r})$. The result is

$$Z_H = \sqrt{\text{det}[C]} \prod_{\vec{r}} \sum_{m(\vec{r}) = -\infty}^{\infty} \exp \left\{ -\frac{1}{\hbar} \tilde{S}_m \right\} \left[ \prod_{n=1}^{L_\tau-1} \left[ 1 + \frac{(\beta q^2 E_J \Gamma / C_m)^n}{2L_\tau^2 [1 - \cos \left( \frac{\pi n}{L_\tau} \right)]} \right] \right]^{-L_\tau L_y/2} \times \prod_{\vec{r}} \int_0^{2\pi} \frac{\phi(0, \vec{r})}{\sqrt{2\pi}}} \exp \left\{ -\frac{1}{2} \sum_{\vec{r}_1, \vec{r}_2} \phi(0, \vec{r}_1) \mathbf{N}(\vec{r}_1, \vec{r}_2) \phi(0, \vec{r}_2) + \sum_{\vec{r}} j(\vec{r}) \phi(0, \vec{r}) \right\}.$$ (92)

where

$$\frac{1}{\hbar} \tilde{S}_m = \frac{(2\pi)^2}{2} \left[ \frac{C_m}{\beta q^2} + \frac{\beta E_J \Gamma}{6} \left( 1 - \frac{1}{L_\tau} \right) \left( 2 - \frac{1}{L_\tau} \right) - (\beta E_J \Gamma) g(\beta q \sqrt{E_J \Gamma / C_m}) \right] \times \sum_{\vec{r}_1, \vec{r}_2} m(\vec{r}_1) \mathbf{O}(\vec{r}_1, \vec{r}_2) m(\vec{r}_2).$$ (93)

To obtain this equation we have taken $C_s = 0$, while the general case can also be treated as well, but since $C_s \ll C_m$ in the experiment this assumption simplifies the calculations. We also have used the following definitions to write the previous equations,

$$\sum_{\langle \vec{r}_1, \vec{r}_2 \rangle} [\phi(\vec{r}_1) - \phi(\vec{r}_2)]^2 = \sum_{\vec{r}_1, \vec{r}_2} \phi(\vec{r}_1) \mathbf{O}(\vec{r}_1, \vec{r}_2) \phi(\vec{r}_2),$$

$$\mathbf{C} = C_m \mathbf{O},$$

$$\mathbf{N} = (\beta E_J \Gamma) \left[ 1 - \hbar \left( \beta q \sqrt{E_J \Gamma / C_m} \right) \right] \mathbf{O},$$

with $\mathbf{O}$ the lattice Laplacian operator, and $g(*)$ and $f(*)$ are functions defined in terms of a Matsubara sum and given in Appendix B.

The details of the variational calculation of the free energy are presented in Appendix B. Here we discuss the main conclusions from the calculation. The results for $\alpha_m = 0$, and 1 are shown in Fig. [13]. There we see that the $\alpha_m = 0$ case has the right low temperature linear $T$ dependence. The result for $\alpha_m = 1.0$ has an essentially flat low temperature behavior for $\Gamma$, which is due to quantum phase slips tunneling processes. In Appendix B it is shown that the helicity modulus can be expressed as
\[ \Gamma = \exp \left\{ -\frac{1}{2} \left\langle (\Delta \phi)^2 \right\rangle \right\}. \]  

(97)

with the fluctuations in the phase given by,

\[ < (\Delta \phi)^2 > _H = \frac{1}{2} \sqrt{\frac{2\alpha_m}{\Gamma}} \left\{ \frac{\sinh (\beta E_J \sqrt{8\alpha_m \Gamma})}{\cosh (\beta E_J \sqrt{8\alpha_m \Gamma}) - 1} \right\}. \]  

(98)

The classical limit corresponds to setting \( \alpha_m \to 0 \), which gives \( < (\Delta \phi)^2 > _{H(d)} = \frac{1}{2\beta E_J} \). Using this result and Eq. (97), at low temperatures \( \Gamma \) is given by \( \Gamma \approx 1 - k_B T / 4E_J + O(T^2) \). This is precisely the same low temperature behavior obtained from a spin wave analysis in two dimensions [11]. From \( < (\Delta \phi)^2 > _{H(d)} \) we find the transition temperature within this approximation, \( \Gamma_c = \frac{1}{4} \left( \frac{k_B T_c}{E_J} \right) \), \( \Gamma_c = 1/e \), and \( k_B T_c^{(0)}/E_J = 4/e \approx 1.472 \), which is an overestimate, (since the dimensionless 2-D critical temperature is \( T_c^{XY} \approx 0.9 \)). The problem with this approximation is extending the integration intervals from \([ -\pi, \pi ]\) to \([ -\infty, \infty ]\). As we have discussed this is a good approximation at low temperatures but it breaks down near the transition point. Our conclusions from this analysis are that for \( \alpha_m = 0 \) the classical SCHA gives good results for low temperatures while it overestimates the critical temperature at higher ones.

In the \( \alpha_m \not= 0 \) case the quantization of the spin wave excitations leads to a non-vanishing result for \( < (\Delta \phi)^2 > _H \), given in Eq. (98). For \( (k_B T/E_J) \ll 1 \) we get

\[ < (\Delta \phi)^2 > _H \approx \frac{1}{2} \sqrt{\frac{2\alpha_m}{\Gamma}} \left( 1 + 2 \exp \left\{ -\beta E_J \sqrt{8\alpha_m \Gamma} \right\} \right), \]  

(99)

\[ \Gamma \approx \Gamma_0 \left( 1 - \frac{1}{2} \sqrt{\frac{2\alpha_m}{\Gamma_0}} \exp \left\{ -\beta E_J \sqrt{8\alpha_m \Gamma_0} \right\} \right), \]  

(100)

where \( \Gamma_0 \) is the helicity modulus at zero temperature and it is the self-consistent solution to the equation \( \Gamma_0 = \exp \left\{ -\frac{\alpha_m}{\sqrt{8 z}} \right\} \), with \( \Gamma_0 \approx 1 - \sqrt{\frac{\alpha_m}{8}} \) for \( \alpha_m \ll 1 \). The solution to this equation is shown as a function of \( \alpha_m \) in Fig. [3], where we also show some Monte Carlo simulation results. The \( \Gamma_0 \) result also presents a transition to a zero \( \Gamma \) state at \( \alpha_m(T = 0) = 32/e^2 \approx 4.33 \), with a jump from \( \Gamma_0 = 1/e^2 \) to zero. Again the result of the SCHA overestimates the stability of the superconducting state. Both the extension of the integration intervals and ignoring the \( m \)'s in these calculations are probably responsible for the deviations at large \( \alpha_m \). An interesting observation is that the result for \( \Gamma_c \) is exact up to first order in \( \alpha_m \). This is equal to the result we obtained from the WKB-RG analysis. Also surprising is that the first order correction to the critical temperature agrees with Eq. (17)

\[ \left( \frac{k_B T_c}{E_J} \right) = \left( \frac{k_B T_c^{(0)}}{E_J} \right) - \left( \frac{2}{3z} \right) \alpha_m + O(\alpha_m^2), \]  

(101)

where \( z \) is the coordination number of the lattice. In Fig. [7] we show \( \Gamma \) for \( \alpha_m = 1.0 \) as a function of the temperature for increasing values of \( L_\tau \), which should be compared with Fig. [4]. This result strongly suggests that the upward tendency of the helicity modulus at low temperatures seen in the QMC results may be an artifact of the finite \( L_\tau \) nature of the
calculations. The origin of this increase is in the low temperature result for the finite $L_\tau$ calculation of Eq. (B16)

$$< (\Delta \phi)^2 >_H \approx \frac{L_\tau}{\beta E_J \Gamma} \left( 1 - \frac{(L_\tau + 2) L_\tau}{16(\beta E_J)^2 \alpha_m \Gamma} + O(T^3) \right),$$

(102)

so that for finite $L_\tau$ and at low temperatures the helicity modulus is given by

$$\Gamma \approx 1 - \frac{L_\tau}{2} \left( \frac{k_B T}{E_J} \right) + O(T^2).$$

(103)

We have been able to explain the shape of the helicity modulus curves for low temperatures, but Figs. 4 and 5 show that if $\alpha_m > \alpha_m^*$, where $\alpha_m^* \in (1.25, 1.75)$, then the helicity modulus has a dip before it may go to one at low temperatures. So far we have ignored the contribution of the Discrete Gaussian Model (DGM) to the variational free energy which is a good approximation only for small $\alpha_m$. We calculated the helicity modulus for the model ignoring the DGM and then including it as a continuous Gaussian model for finite $L_\tau$, which is a good approximation for the effective coupling $J_{\text{eff}} \ll 1$. For large $\alpha_m$ the crossover point, which is when $J_{\text{eff}}$ becomes soft, is seen as a finite dip in the helicity modulus. Unfortunately, the $T^*$ found in the Monte Carlo calculations is much larger than the one given by Eq. (B7). It is apparent that the effective coupling $J_{\text{eff}}$ does not contain all the contributions to the renormalization of the DGM due to the integration over the phases. To illustrate the nature of this crossover we performed several calculations of the helicity modulus for $L_\tau = 10, 20$, and $40$ with $\alpha_m = 1$. The results are shown in Fig. 18. There we took $\frac{L_\tau}{E_J \alpha_m} = 6$ for the crossover temperature. These results can be compared with those of Fig. 18.

The Monte Carlo calculations show that this dip occurs simultaneously with the rise in the inverse dielectric constant. This is a signal that the non-zero effective constant for the winding numbers becomes soft, making their contribution to the helicity modulus non-vanishing. We note that the effect of a finite lattice, necessary for the Monte Carlo calculation, increases the softening temperature of $J_{\text{eff}}$. On the other hand, the variational calculation for $C_s = 0$ does not depend on the size of the lattice, therefore it can not capture these finite space size effects.

VII. CONCLUSIONS

We have presented a thorough study of the $\alpha_m$ vs. $T$ phase diagram for an array of ultrasmall Josephson junctions using a series of theoretical tools. One of our main goals was to perform these calculations for these arrays using experimentally realistic parameters. The model we used for the JJA is defined by a Hamiltonian that has two contributions, a Josephson coupling and an electrostatic interaction between the superconducting islands. The ratio of these two contributions was defined as $\alpha_m = \frac{\text{charging energy}}{\text{Josephson energy}}$. This was the important quantum parameter in our analysis.

For convenience of calculation we derived different path integral formulations of the quantum partition function of the JJA. In the small $\alpha_m$ limit we used a WKB-RG approximation to find the first order correction in $\alpha_m$ to the classical partition function. The result of this
calculation was an effective classical partition function of a 2-D XY model type, where the coupling constant is modified by the quantum fluctuations. We used the modified renormalization group equations for the 2-D model to find the superconducting to normal phase boundary. We also found that up to first order in $\alpha_m$, the correction to the transition temperature was independent of magnetic field. One interesting finding from this calculation was the possible existence of a low temperature instability QUIT of the superconducting state. We found evidence for the QUIT, but the evidence is at the border of validity of the calculational approaches used. To have a definite theoretical proof of the existence of the QUIT one needs to have better algorithms and/or improvements in computer power. The results presented here are, however, rather encouraging. Of course the ultimate test will be furnished by experiment, and there too incipient indications of a low temperature instability have also been reported in [3].

In the large $\alpha_m$ limit we used a perturbative expansion in $1/\alpha_m$ to find an effective partition function for a quantum a 2-D Coulomb gas. This model shows a renormalized conducting to insulating transition as the temperature is lowered. We did not find a low temperature QUIT instability in the large $\alpha_m$ insulating phase.

We also performed extensive nonperturbative quantum Monte Carlo calculations of the JJA model. We concentrated our analysis on the helicity modulus $\Upsilon$. This quantity is directly related to the superfluid density in the array. Using $\Upsilon$ we determined the superconducting to normal transition boundary. We found good agreement between the critical temperatures obtained by QMC calculation and the semiclassical approximation. We also carried out a low temperature $1/L_\tau$ extrapolation analysis of the $T_{\text{QUIT}}$ and found evidence for $T_{\text{QUIT}} \neq 0$ for relatively large values of $\alpha_m = 2.0$ and 2.25 but $T_{\text{QUIT}} = 0$ for $\alpha_m = 2.5$. These calculations have, however, a strong $L_\tau$ dependence and our QMC algorithm is not precise enough to completely ascertain the nature of the low temperature phase. Nonetheless, the results found here together with the scant emerging experimental evidence for a low temperature instability yields further support for the possible existence of a QUIT.

We also presented some QMC calculations of the inverse dielectric constant of the 2-D quantum Coulomb gas, in order to find the conducting to insulating phase boundary. We found that the present Monte Carlo path integral implementation of our model, that includes phase and charge degrees of freedom, does not allow us to make reliable calculations of this quantity. Our results for this transition are only qualitative. Further technical improvements are needed in order to make solid quantitative statements about the $N-I$ phase boundary.

To use a QMC calculation to prove or disprove the presence of a low temperature instability in the superconducting state is not an easy task. However, these type of calculations give us upper temperature limits for the instability region. As far as our calculations could determine, the results for the superfluid density as a function of temperature are in rather good agreement with experimental findings in JJA [4], except for the incipient data on the reentrant transition in the nonperturbative region of $\alpha_m$.

To further understand the QMC results at low temperatures and as a function of $L_\tau$, we have also implemented a self-consistent harmonic approximation analysis of the model, that includes phases and charge freedoms. We were able to make successful qualitative, and in some instances even quantitative comparisons between both calculational approaches. One of the conclusions from these calculations is that the general trend of the QMC results for $\Upsilon$ can be traced to the discretization of the imaginary time axis. For small $\alpha_m$, the decrease
of the helicity modulus at low temperature is clearly due to this effect.

Among the most significant aspects of the results presented in this paper is the quantitative agreement between our different calculational approaches and the corresponding experimental results in the superconducting-normal phase boundary with essentially only the measured capacitances as adjustable parameters. The existence of the QUIT is also a significant result of this paper, for it had not been studied in a model including realistic capacitances in the model.

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APPENDIX: A

In this appendix we present the derivation of the renormalization group equations in the insulating to normal region of the phase diagram up to first order in $\alpha m^{-1}$. We begin by writing the effective partition function from Eqs. (52), (53), and (54)

$$Z_{\text{eff}}(\{m\}) = \left\langle \exp \left[ -\frac{1}{\hbar} \int_0^{\beta \hbar} d\tau \mathcal{H}_J(\{\overline{\phi} (\vec{r}) + \phi_f(\tau, \vec{r}) + (2\pi / \beta \hbar) m(\vec{r}) \tau \}) \right] \right\rangle_\phi.$$  

(A1)

The phase average $\langle \rangle_\phi$ is defined by

$$\langle A \rangle_\phi = \frac{1}{Z_\phi} \prod_{\vec{r}} \int_0^{2\pi} d\phi(\vec{r}) \int_{-\infty}^{\infty} D\phi_f(\vec{r}) \ A(\{\overline{\phi} (\vec{r}) + \phi_f(\tau, \vec{r}) \}) \exp \left[ -\frac{1}{\hbar} S_f[\phi_f] \right].$$  

(A2)

From Eq.(3) the Josephson energy is

$$H_J(\{\phi\}) = -E_J \sum_{\langle \vec{r}_1, \vec{r}_2 \rangle} \cos \left( \phi(\vec{r}_1) - \phi(\vec{r}_2) \right).$$  

(A3)

Inserting this equation into Eq. (A2), and using the expansion given in Eq. (51), we first see that the integrations over the $\{\phi\}$’s eliminate all the odd powers in $E_J$. Moreover up to the third term in Eq. (51) we have integrals of the form

$$\prod_{\vec{r}} \int_0^{2\pi} \frac{d\phi(\vec{r})}{2\pi} \exp \left[ \overline{\phi}(\vec{r}_1) - \overline{\phi}(\vec{r}_2) + \overline{\phi}(\vec{r}_3) - \overline{\phi}(\vec{r}_4) \right] = \delta_{\vec{r}_1, \vec{r}_4} \delta_{\vec{r}_2, \vec{r}_3},$$  

(A4)

where $\vec{r}_1 \neq \vec{r}_2$ and $\vec{r}_3 \neq \vec{r}_4$, because they are pairs of nearest neighbors.

Using this equation and the fact that Eq. (54) is an even function of the $\phi_f$’s we end up with
\[ Z_{\text{eff}}(\{m\}) \approx 1 + \left( \frac{E_f}{2\hbar} \right)^2 \int_0^{\beta \hbar} d\tau \int_0^{\beta \hbar} d\tau' \sum_{\langle \vec{r}_1, \vec{r}_2 \rangle} \exp \left[ -G(\vec{r}_1, \vec{r}_2; \tau, \tau') \right] \times \cos \left( (2\pi/\beta \hbar)[m(\vec{r}_1) - m(\vec{r}_2)](\tau - \tau') \right) + O(E_f^4). \] (A5)

Here we have defined the correlation function

\[ G(\vec{r}_1, \vec{r}_2; \tau, \tau_2) = -\ln \left\{ \frac{1}{Z_{\phi}} \prod_{\vec{r}} \int_{-\infty}^{\infty} D\phi_f(\vec{r}) e^{-\frac{1}{2}S_f[\phi_f]} \exp \left[ \int_0^{\beta \hbar} \sum_{\vec{r}} j(\tau, \vec{r}) \phi_f(\tau, \vec{r}) \right] \right\}, \] (A6)

\[ j(\tau, \vec{r}) = i \left[ \delta(\tau - \tau_1) - \delta(\tau - \tau_2) \right] \left[ \bar{\delta}_{\vec{r}, \vec{r}_1} - \delta_{\vec{r}, \vec{r}_2} \right]. \] (A7)

The easiest way to perform this integral is to go to Fourier space, and using Eq. (A6) we can write

\[ \phi_f(\tau, \vec{r}) = \sqrt{\frac{2}{\beta \hbar}} \sum_{n=1}^{\infty} \psi_n(\vec{r}) \sin(\nu_n \tau), \] (A8)

\[ \nu_n = \left( \frac{\pi}{\beta \hbar} \right) n. \] (A9)

From this equation, Eq. (A4) can be written as

\[ G(\vec{r}_1, \vec{r}_2; \tau_1, \tau_2) = -\ln \left\{ \frac{1}{Z_{\phi}} \prod_{\vec{r}} \int_{-\infty}^{\infty} d\psi_n(\vec{r}) e^{-\frac{1}{2}S_f[\psi_n]} \exp \left[ \sum_{n=1}^{\infty} \sum_{\vec{r}} j_n(\vec{r}) \psi_n(\vec{r}) \right] \right\}, \] (A10)

\[ S_f[\psi_n] = \frac{1}{2} \sum_{n=1}^{\infty} \sum_{\vec{r}_3, \vec{r}_4} \psi_n(\vec{r}_3) \left\{ (\hbar \nu_n/q)^2 C(\vec{r}_3, \vec{r}_4) \right\} \psi_n(\vec{r}_4), \] (A11)

\[ j_n(\vec{r}) = \sqrt{\frac{2}{\beta \hbar}} \int_0^{\beta \hbar} d\tau \sin(\nu_n \tau) j(\tau, \vec{r}). \] (A12)

Therefore the correlation function is

\[ G(\vec{r}_1, \vec{r}_2; \tau_1, \tau_2) = -q^2 \beta \sum_{n=1}^{\infty} \sum_{\vec{r}_3, \vec{r}_4} \frac{1}{\nu_n^2} j_n(\vec{r}_3) C^{-1}(\vec{r}_3, \vec{r}_4) j_n(\vec{r}_4), \] (A13)

\[ = -q^2 \beta \sum_{\vec{r}_3, \vec{r}_4} \int_0^{\beta \hbar} d\tau \int_0^{\beta \hbar} d\tau' j(\tau, \vec{r}_3) \{ g(\tau, \tau') C^{-1}(\vec{r}_3, \vec{r}_4) \} j(\tau', \vec{r}_4), \] (A14)

where we have used the result \((\tau < \tau')\)

\[ g(\tau, \tau') = \frac{1}{(\beta \hbar)^2} \sum_{n=1}^{\infty} \frac{\sin(\nu_n \tau) \sin(\nu_n \tau')}{\nu_n^2} = \left( 1 - \frac{\tau'}{\beta \hbar} \right) \frac{\tau}{\beta \hbar}. \] (A15)

Using Eq. (A7) we finally find

\[ G(\vec{r}_1, \vec{r}_2; \tau_1, \tau_2) = 2q^2 \beta \frac{|\tau_1 - \tau_2|}{\beta \hbar} \left( 1 - \frac{|\tau_1 - \tau_2|}{\beta \hbar} \right) \left[ C^{-1}(|\vec{0}|) - C^{-1}(|\vec{r}_1 - \vec{r}_2|) \right]. \] (A16)
Inserting this equation in Eq. (A3), and noting that here $|\vec{r}_1 - \vec{r}_2| = |d|$ we have

$$Z_{\text{eff}}\{m\} \approx 1 + \left(\frac{E_J}{2\hbar}\right)^2 \int_0^{\hbar} d\tau \int_0^{\hbar} d\tau' \times$$

$$\times \sum_{<\vec{r}_1,\vec{r}_2>} \exp\left\{-\frac{2q^2\beta}{\beta\hbar}\left[1 - \frac{|\tau - \tau'|}{\beta\hbar}\right]\left[1 - C_sC^{-1}(|\vec{0}|)\right]\right\} \times$$

$$\times \cos\left(2\pi/\beta h)[m(\vec{r}_1) - m(\vec{r}_2)](\tau - \tau')\right) + O(E_J^4).$$

(A17)

At this point we can perform the following symmetrical change of variables

$$x_1 = \frac{1}{\sqrt{2}} \frac{(\tau - \tau')}{\beta\hbar},$$

(A18)

$$x_2 = \frac{1}{\sqrt{2}} \frac{(\tau + \tau')}{\beta\hbar}.$$  

(A19)

Now we see that the integral over $x_2$ can be calculated explicitly leaving only $x_1$ to be integrated. We find then

$$Z_{\text{eff}}\{m\} \approx 1 + \frac{(\beta E_J)^2}{2} \sum_{<\vec{r}_1,\vec{r}_2>} \int_0^{1/2} dx_1 \exp\left\{-\frac{2q^2\beta}{\beta\hbar}\left[1 - C_sC^{-1}(|\vec{0}|)\right] x_1 (1 - x_1)\right\} \times$$

$$\times \cos\left(2\pi|\vec{m}(\vec{r}_1) - \vec{m}(\vec{r}_2)|x_1\right) + O(E_J^4).$$

(A20)

Which is the result used in Eq. (50).

**APPENDIX: B**

Here we give the details of the derivation of the effective free energy in the variational calculation, from which we obtain the expressions for $<\Delta \phi^2>_H$ which was used to obtain the helicity modulus in Section VI.

We start by defining the following effective quantities for the $m$’s and the $\phi(0, \vec{r})$ interaction terms

$$j(\vec{r}) = -\pi \beta E_J \Gamma \left[1 - \frac{1}{L_T}\right] - \hbar \left(\beta q \sqrt{E_J \Gamma / C_m}\right) \sum_{\vec{r}_1} m(\vec{r}_1) O(\vec{r}_1, \vec{r}),$$

(B1)

$$\frac{1}{\hbar} \tilde{S}_m = \frac{(2\pi)^2}{2} \frac{C_m}{\beta q^2} + \frac{\beta E_J \Gamma}{6} \left[1 - \frac{1}{L_T}\right] \left[2 - \frac{1}{L_T}\right] - (\beta E_J \Gamma) g \left(\beta q \sqrt{E_J \Gamma / C_m}\right) \times$$

$$\times \sum_{\vec{r}_1, \vec{r}_2} m(\vec{r}_1) O(\vec{r}_1, \vec{r}_2) m(\vec{r}_2).$$

(B2)

The functions $h(\Lambda)$ and $g(\Lambda)$ are given in terms of Matsubara frequency summations

$$h(\Lambda) = \frac{1}{2} \left(\frac{\Lambda}{L_T}\right)^2 \sum_{n=1}^{L_T-1} \frac{\sin^2(\pi n / L_T)}{\Lambda^2 + 2L_T^2(1 - \cos(\pi n / L_T))} \left[1 - \cos(\pi n)\right]^2$$

$$= 1 - \frac{1}{L_T} + \frac{2}{L_T} \left(\frac{L_T}{\Lambda}\right)^2 \left[\frac{\sin((L_T - 1)\Lambda + \sin(\Lambda))}{\sin(L_T \Lambda)} - 1\right],$$

(B3)
therefore

and find that Eq. 92 becomes overestimation of the transition temperature. After extending the limits of integration we extend the limits of integration to the entire real axis. We expect that this approximation integral can not be explicitly calculated due to the finite limits of integration. Therefore we find that Eq. (B4) becomes

\[
g(\Lambda) = \frac{1}{2} \left( \frac{\Lambda}{L_\tau} \right)^2 \sum_{n=1}^{L_\tau-1} \frac{\sin^2(\pi n/L_\tau)}{\left[ \Lambda^2 + 2L_\tau^2 (1 - \cos(\pi n/L_\tau)) \right] \left[ 1 - \cos(\pi n/L_\tau) \right]^2} \int \frac{1}{L_\tau} \left( \frac{L_\tau}{\Lambda} \right)^2 \left[ \frac{\sinh((L_\tau - 1)\Lambda)}{\sinh(L_\tau \Lambda)} - \frac{(L_\tau - 1)}{L_\tau} \right] \left\{ 1 - \frac{1}{6} \left( \frac{\Lambda}{L_\tau} \right)^2 (2L_\tau - 1) \right\},
\]

(B4)

\[
\lambda = \ln \left\{ 1 + \frac{1}{2} \left( \frac{\Lambda}{L_\tau} \right) \left[ \frac{(\Lambda)}{L_\tau} + \sqrt{4 + \left( \frac{(\Lambda)}{L_\tau} \right)^2} \right] \right\}.
\]

(B5)

To complete the calculation of \( Z_H \) we need to make one more approximation because the integral can not be explicitly calculated due to the finite limits of integration. Therefore we extend the limits of integration to the entire real axis. We expect that this approximation is good for large \( \Gamma \) or small \( T \), which is our region of interest. For small \( \Gamma \) it would give an overestimation of the transition temperature. After extending the limits of integration we find that Eq. (B2) becomes

\[
Z_H = \left( \frac{C_m}{\beta^2 q^2 E_J \Gamma} \right)^{L_x L_y/2} \left[ 1 - h \left( \beta q \sqrt{E_J \Gamma / C_m} \right) \right]^{-L_x L_y/2} \times \prod_{\tilde{r}} \sum_{m(\tilde{r})=\infty} \exp \left\{ -\frac{1}{h} S_m \right\},
\]

(B6)

where the effective action for the \( m \)'s is given by

\[
\frac{1}{h} S_m = \frac{J_{\text{eff}}}{2} \sum_{\tilde{r}_1,\tilde{r}_2} m(\tilde{r}_1) O(\tilde{r}_1,\tilde{r}_2) m(\tilde{r}_2),
\]

\[
J_{\text{eff}} = (2\pi)^2 \left[ \frac{C_m}{\beta q^2} + \frac{\beta E_J \Gamma}{6} \left( 1 - \frac{1}{L_\tau} \right) \left( 2 - \frac{1}{L_\tau} \right) - (\beta E_J \Gamma) g \left( \beta q \sqrt{E_J \Gamma / C_m} \right) - \frac{\beta E_J \Gamma \left( 1 - 1/L_\tau \right) - h \left( \beta q \sqrt{E_J \Gamma / C_m} \right)^2}{4 \left( 1 - h \left( \beta q \sqrt{E_J \Gamma / C_m} \right) \right)} \right].
\]

(B7)

and \( O \) is the lattice Laplacian operator. The free energy in the harmonic approximation is therefore

\[
\frac{\beta F_H}{L_x L_y} = \frac{\beta F_{DG}(J_{\text{eff}})}{L_x L_y} + \frac{1}{2} \left\{ \ln \left( \frac{\beta^2 q^2 E_J \Gamma}{C_m} \right) \right\} + \ln \left[ 1 - h \left( \beta q \sqrt{E_J \Gamma / C_m} \right) \right] + \sum_{n=1}^{L_\tau-1} \ln \left[ 1 + \frac{(\beta^2 q^2 E_J \Gamma / C_m)}{2L_\tau^2 (1 - \cos(\pi n/L_\tau))} \right].
\]

(B8)

The function \( F_{DG} \) is related to the partition function of the Discrete Gaussian Model (DGM) defined by

\[
\frac{\beta F_{DG}(J)}{L_x L_y} = -\ln \left[ \prod_{\tilde{r}} \sum_{m(\tilde{r})=\infty} \exp \left\{ -\frac{J}{2} \sum_{\tilde{r}_1,\tilde{r}_2} \left[ m(\tilde{r}_1) - m(\tilde{r}_2) \right]^2 \right\} \right].
\]

(B9)
We will ignore this term for the moment, since the discrete nature of its excitations makes it very small. We need to calculate the average of the harmonic part of the Hamiltonian, i.e.

\[
<H_H> = E_J \Gamma L_x L_y \left\langle \left[ \phi(\tau, \vec{r} + \vec{d}) - \phi(\tau, \vec{r}) \right]^2 \right\rangle_H = -\frac{\Gamma}{\beta} \frac{\partial \ln Z_H}{\partial \Gamma} = \Gamma \frac{\partial F_H}{\partial \Gamma} = L_x L_y \frac{1}{2\beta} \left\{ 1 - \frac{\beta q}{2} \sqrt{\frac{E_J \Gamma}{C_m}} \frac{h' \left( \beta q \sqrt{E_J \Gamma / C_m} \right)}{1 - h \left( \beta q \sqrt{E_J \Gamma / C_m} \right)} + f \left( \beta q \sqrt{E_J \Gamma / C_m} \right) \right\},
\]

(B10)

where \( \vec{d} \) joins nearest neighbors, and \( f(\Lambda) \) is given by a summation over Matsubara frequencies resulting in,

\[
f(\Lambda) = \frac{1}{2} \left\{ (L_{\tau} - 1) - \frac{L_{\tau}}{1 + (\Lambda / L_{\tau})^2 / 2} \frac{\sinh \left( (L_{\tau} - 1)\Lambda \right)}{\sinh \left( L_{\tau} \Lambda \right)} \right\}.
\]

(B11)

On the other hand we know that if the Hamiltonian is Gaussian, then the calculation of the average over the Josephson Hamiltonian is

\[
<H_J> = 2E_J L_x L_y \left[ 1 - \exp \left\{ -\frac{1}{2} \left\langle \left[ \phi(\tau, \vec{r} + \vec{d}) - \phi(\tau, \vec{r}) \right]^2 \right\rangle \right\} \right].
\]

(B12)

Therefore, the relevant term in the variational free energy is given by the average of the square of the lattice derivative over the harmonic Hamiltonian. Finally, we can write the variational free energy

\[
\frac{\beta F_V}{L_x L_y} = \frac{\beta F_H}{L_x L_y} + 2\beta E_J \left[ 1 - \exp \left\{ -\frac{1}{2} \left\langle (\Delta \phi)^2 \right\rangle \right\} \right] - \beta E_J \Gamma \left\langle (\Delta \phi)^2 \right\rangle,
\]

(B13)

\[
< (\Delta \phi)^2 >_H = < \left[ \phi(\tau, \vec{r} + \vec{d}) - \phi(\tau, \vec{r}) \right]^2 >_H.
\]

(B14)

with \( < (\Delta \phi)^2 >_H \) given in Eq. (B10).

The variational condition requires minimizing this function with respect to \( \Gamma \). Taking the derivative of this equation, and using Eq. (B10), we find that

\[
\Gamma = \exp \left\{ -\frac{1}{2} \left\langle (\Delta \phi)^2 \right\rangle \right\}.
\]

(B15)

\( \Gamma \) is then the normalized coupling constant of the spin wave Hamiltonian, i.e. the normalized helicity modulus. Eq. (B7) gives the condition to identify the phase transition as the point at which \( \Gamma \neq 0 \) becomes a solution to the variational equations. The complete problem is to solve the combination of Eqs. (B14) and (B17). We can write Eqs. (B14) as a function of \( \Gamma \)

\[
< (\Delta \phi)^2 >_H = \frac{1}{2\beta E_J \Gamma} \left\{ 1 - \beta E_J \sqrt{2\alpha_m \Gamma} \frac{h' \left( \beta E_J \sqrt{8\alpha_m \Gamma} \right)}{1 - h \left( \beta E_J \sqrt{8\alpha_m \Gamma} \right)} + f \left( \beta E_J \sqrt{8\alpha_m \Gamma} \right) \right\}.
\]

(B16)
We now study the behavior of the helicity modulus as a function of $\alpha_m$ in the continuum limit, that is in the $L_r \rightarrow \infty$ limit. In this limit we get

\begin{align}
    h(\Lambda) &= 1 - \frac{2}{\Lambda} \left( \frac{\cosh(\Lambda) - 1}{\sinh(\Lambda)} \right), \\
g(\Lambda) &= \frac{1}{\Lambda^2} \left[ 1 + \frac{2^3}{3} - \Lambda \frac{\cosh(\Lambda)}{\sinh(\Lambda)} \right], \\
f(\Lambda) &= \frac{\Lambda \cosh(\Lambda)}{2 \sinh(\Lambda)} - \frac{1}{2}, \\
< (\Delta \phi)^2 >_H &= \frac{1}{2} \sqrt{\frac{2 \alpha_m}{\Gamma}} \left( \frac{\sinh \left( \beta E_J \sqrt{8 \alpha_m \Gamma} \right)}{\cosh \left( \beta E_J \sqrt{8 \alpha_m \Gamma} \right) - 1} \right).
\end{align}

We used Eqs. (B15) and (B20) to find the helicity modulus for $\alpha_m = 0$ and 1. The results of these calculations are shown in Fig. 15. This figure shows several interesting features. First the helicity modulus for $\alpha_m = 0$ has the right shape, i.e., a linear $T$ behavior near $T = 0$, and a jump at the transition temperature. The transition temperature is, however, overestimated. Note that the $\alpha_m = 1$ helicity modulus has a flat behavior at low temperatures, which must be contrasted with the $\alpha_m = 0$ result.
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FIGURES

FIG. 1. The phase diagram for unfrustrated (f=0) and fully frustrated (f=1/2) arrays. Squares denote the experimental results from Ref. [5]. The other symbols give the QMC results including their statistical errors. The dotted lines for f=0 is a naive extrapolation of the QMC results to zero temperature, while the dot-dashed curve is the result of the WKB-RG calculation. In the f=1/2 case we have rescaled the MC results so that the MC curve would coincide with the experimental result at $\alpha_m(f = 1/2) = 0.1$.

FIG. 2. Renormalization group flow diagram. The discontinuous line indicates the vortex pair density as a function of temperature. See text for a discussion of the analysis of this RG flow diagram.

FIG. 3. The helicity modulus $\Upsilon$ vs. temperature $T$ for $\alpha_m = 0.5$, $L_x = L_y = 32$, and two different values of $L_\tau = 6$, and 8. This figure shows that for this value of $\alpha_m$ the results have converged to the infinite $L_\tau$ limit already for $L_\tau = 6$. The line is $(2k_BT/EJ\pi)$. The intersection of this line with $\Upsilon(T)$ is used to determine the normal to superconducting transition temperature.

FIG. 4. The helicity modulus vs. temperature for $\alpha_m = 1.25$, $L_x = L_y = 20$, and three different values of $L_\tau = 8$, 16, and 32. This figure shows that a convenient convergence criteria for the $L_\tau \to \infty$ limit is $P = L_\tau/(\beta E_J\alpha_m) > 5$.

FIG. 5. The same as Fig. 4 with $\alpha_m = 1.75$, $L_x = L_y = 20$, and $L_\tau = 16, 32$ and 64. Again the criteria for convergence $P > 5$ works in this figure. Note that the departure from the infinite $L_\tau$ limit is in the form of a small reentrant type dip in $\Upsilon$ as the temperature is lowered.

FIG. 6. The helicity modulus vs. temperature for $\alpha_m = 2.25$, $L_x = L_y = 20$, and $L_\tau = 32, 48, 64$, and 96. As in Fig. 5, $\Upsilon$ has a dip as the temperature is lowered and shows a reentrant–like behavior at lower temperatures.

FIG. 7. $\Upsilon$ and inverse dielectric constant $\epsilon^{-1}$ vs temperature for $\alpha_m = 2.25$, $L_x = L_y = 20$, and $L_\tau = 32$. As the temperature is lowered, the drop in the helicity modulus is correlated with the rise in the inverse dielectric constant, signaling the decoupling between imaginary time planes.

FIG. 8. $\Upsilon$ vs temperature for $\alpha_m = 2.5$, $L_x = L_y = 20$, and $L_\tau = 32, 48, 64, 80, 96$, and 128. At this value of $\alpha_m$ the drop in the helicity modulus at low temperatures yields essentially $\Upsilon = 0$. This abrupt drop is probably due to having a finite $L_\tau$. Note that the decrease of the $\Upsilon$ as $T$ is lowered happens even before the plane decoupling temperature.
FIG. 9. The imaginary time correlation function $C(\tau)$ vs. $\tau$, for $\alpha_m = 1.75$, $L_x = L_y = 20$, and $L_\tau = 32$ for $T = 0.35$, 0.30, and 0.18. As the temperature is lowered, the correlation time decreases until at $(k_B T/E_J) \approx 0.3$ the correlation time is shorter than one lattice spacing in the time direction. At this point the value of $L_\tau$ is too small to produce a convergent calculation of the helicity modulus.

FIG. 10. The imaginary time correlation function $C(\tau)$ vs $\tau$ for $\alpha_m = 2.5$, $L_x = L_y = 20$, and $L_\tau = 64$, at $(k_B T/E_J) = 0.36$ and 0.10. As in Fig. 9 this correlation function for temperatures below the decoupling temperature is consistent with having zero decorrelation time.

FIG. 11. The helicity modulus vs. temperature for $\alpha_m = 2.75$, $L_x = L_y = 20$, and $L_\tau = 64$. The upper curve was obtained while lowering the temperature. The lower curve corresponds to increasing it. The disparity in the results is most likely due to the difficulty in establishing phase coherence in the 64 equal time planes as $T$ is increased, above the plane decoupling temperature.

FIG. 12. Estimate of the plane decoupling transition vs $1/L_\tau$ extracted from results similar to those of Fig. 9 for $\alpha_m = 2.0$, $L_x = L_y = 20$ and $L_\tau = 48, 64, 80, 96, 128$. The line from a least squares fit suggests a non zero decoupling temperature in the limit $1/L_\tau = 0$. This figure is also consistent with the condition $P \approx 5$.

FIG. 13. The same as Fig. 12. Data extracted from Fig. 9 for $\alpha_m = 2.25$ and $L_x = L_y = 20$. The line from a least squares fit also seems to suggest a non zero decoupling temperature in the limit $L_\tau \to \infty$. This figure is also consistent with the $P \approx 5$ condition.

FIG. 14. Same as Fig. 12. In this case, extracted from Fig. 8, for $\alpha_m = 2.5$ and $L_x = L_y = 20$. The least squares straight line fit seems to suggest a negative decoupling temperature in the limit $1/L_\tau = 0$.

FIG. 15. The spin wave stiffness vs $T$ (related to the normalized helicity modulus) obtained from the self-consistent-harmonic approximation for $\alpha_m = 0$ and $\alpha_m = 1$.

FIG. 16. The $T = 0$ helicity modulus at as a function of $\alpha_m$, obtained from the SCHA. Extrapolated $T = 0 \ U$ results from the Monte Carlo simulations are shown as diamonds joined by a line. From this figure it is clear that the SCHA gives reasonable results at low temperatures and for small values of $\alpha_m$.

FIG. 17. The normalized helicity modulus $\Gamma$ for $\alpha_m = 1.0$ as a function of $T$ for increasing values of $L_\tau = 5, 10, 20, \text{and } 100$. The extrapolated plot for $L_\tau = \infty$ is shown as a solid line.
FIG. 18. The normalized helicity modulus $\Gamma$ for $\alpha_m = 1.0$ and $L_\tau = 10$, 20, and 40. The crossover temperature $T^*$ is calculated using $(L_\tau/(\beta E_J)\alpha_m) = 6$, so that as $L_\tau$ increases the crossover temperature decreases. Here the solid line correspond to $L_\tau = 10$, the dashed line to $L_\tau = 20$ and the dot-dashed line to $L_\tau = 40$. See text for discussion of these results.
\( \alpha \)

\( m \)

\( k_B \)

\( T / E_j \)

\( \alpha_m \)

\( f=0 \)

\( f=1/2 \)

\( \text{SC} \)

\( \text{N} \)

\( \text{I} \)
\[ \sum \rightarrow L_\tau = 8 \]
\[ \Diamond \rightarrow L_\tau = 6 \]
$Y$ vs. $(k_B T/E_J)$

- $L_\tau = 8$
- $L_\tau = 16$
- $L_\tau = 32$
$Y$, $1/\varepsilon$

$\left( k_B T/E_J \right)$
$C(\tau)$ vs $\tau$

- $T = 0.36$
- $T = 0.10$
\( (k_B T_{\text{decl}}/E_J) \) vs. \( 1/L_\tau \)
