Ground state properties of charge and magnetically frustrated two–dimensional quantum Josephson–junction arrays

T. K. Kopeć and T. P. Polak
Institute for Low Temperature and Structure Research, Polish Academy of Sciences, POB 1410, 50-950 Wroclaw 2, Poland
(March 22, 2022)

Abstract

We study a quantum Hamiltonian that models a two–dimensional array of Josephson junctions with short range Josephson couplings, (given by the Josephson energy $E_J$) and charging energy $E_C$ due to the small capacitance of the junctions. We include the effects from both the self-$C_0$ and the junction-$C_1$ capacitances in the presence of external magnetic flux $f = \Phi/\Phi_0$ as well as uniform background of charges $q_x$. We derive an effective quantum nonlinear $\sigma$-model for the array Hamiltonian which enables us a non mean–field treatment of the zero–temperature phase transition scenario. We calculate the ground–state phase diagram, analytically deriving $E_J^{\text{crit}}(E_C, q_x, f)$ for several rational fluxes $f = 0, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ and $\frac{1}{6}$ that improves upon previous theoretical treatments based on mean–field approximations.
I. INTRODUCTION

Advances in the photolithographic micro–fabrication techniques have experimentally allowed to manufacture Josephson–junction arrays (JJA) with tailor specific properties. Because the junction parameters can be accurately controlled JJA offer a unique opportunity to test different quantum mechanical models. In JJA’s the two main energy scales are set by the Josephson coupling, $E_J$, between superconducting islands due to Cooper pair tunneling, and to the electrostatic energy $E_C$ (proportional to the inverse of capacitance matrix setup by island self- $C_0$ and junction- $C_1$ capacitances) due to local deviations from charge neutrality. When $E_J$ is much larger then $E_C$ the phases of the superconducting order parameters on individual islands are well defined. In this regime the semi-classical fluctuations determine the properties of the JJA. In the opposite limit, ie. for $E_C \gg E_J$, the superconducting phases are dominated by strong quantum fluctuations since the Coulomb blockade pins the charge carriers to the islands. Several theoretical and experimental studies have considered the competition between the $E_J$ dominated phase and the $E_C$ dominated charging energy regions in periodic JJA. It has been established that for sufficiently large charging energy the quantum phase fluctuations lead a complete suppression of long–range phase coherence even at zero temperature. This type of quantum phase transition has attracted significant interest in recent years (for a review see Ref. 6).

Because the junction parameters can be controlled accurately JJA offer a unique system where one can test the nature of quantum phase transitions and critical phenomena, in particular the superconductor–insulator (SI) phase transition induced by quantum fluctuations. The experimental systems can be modeled by a quantum generalization of the classical XY model with quantum phase of the superconducting order parameter on each island canonically conjugated to the excess of Cooper pair number. The quantum parameter $\alpha = E_C/E_J$ determines the relevance of the quantum fluctuations. Bulk of theoretical studies have been carried out within the self–capacitance model ($C_0 \neq 0, C_1 = 0$), usually using different kinds of mean–field–theory or self–consistent harmonic approximations (for a comprehensive account see, Ref. 1). In the mutual–capacitance dominated limit ($C_1 \neq 0, C_0 = 0$) the lattice model is equivalent to a quantum Coulomb gas model, with critical properties that are not fully understood at present. Further complication arise when both $C_0$ and $C_1$ are non–zero. The charging energy can also be tuned by an applied gate voltage $V_g$ which control the energy required to change the number of Cooper pairs on the islands. A uniform $V_g$ can be applied by means of gate capacitance $C_g$. Assuming $C_g \ll C_0$ the applied voltage induces a charge $C_g V_g$ on each grain which can be conveniently account for when one defines the a dimensionless charge frustration parameter $q_s = C_g V_g / 2e$. The effects of charge frustration is closely related to the so–called Bose–Hubbard model which describes the strongly interacting bosons under the competing kinetic energy (related to Josephson energy) and the potential energy (i.e charging energy in the JJA) effects. The on–site (chemical) potential corresponds in this analogy to the charge frustration parameter $q_s$ in JJA. Frustration in quantum JJA can be also introduced by applying magnetic field $B$. The presence of $B$ induces vortices in the system described by the magnetic frustration parameter $f$ (≡ $\Phi / \Phi_0$, where $\Phi$ is the magnetic flux piercing a 2D lattice plaquette and $\Phi = h/2e$ stands for the elementary flux quantum). Of special interest are cases when $f = p/q$ with $p$ and $q$ being the rational numbers. Particularly prominent is the case of $f = 1/2$ because of the interplay
between continuous $U(1)$ symmetry of the superconducting parameter and discrete Ising $Z_2$ symmetry associated with antiferromagnetic arrangements of the plaquette chiralities describing directions of the circulating currents in each plaquette.\footnote{11}

Usually, mean–field calculations or semiclassical approaches are not expected to be reliable at $T = 0$ and be capable to handle spatial and quantum fluctuation effects properly especially in two–dimensions. Notably, there are virtually no works beyond mean-field level on 2D JJA in the where the physics is dominated by the by the combination of charge $q_x$, magnetic frustration $f$ and the charging energy related to the self-$C_0$ and junction-$C_1$ capacitances. Recent studies based on perturbative expansions combine either JJA with charge frustration and and charging energy effects\footnote{12} or magnetic frustration and effects of array capacitances.\footnote{13} Therefore, the problem we would like to address is then: What is the effect of having a competition between the magnetic, charge frustration and quantum effects on the ground state ordering in the Josephson–junction network on a square two–dimensional lattice? The purpose of this work is therefore to study these quantum fluctuation effects in an analytical way to understand the ground state phase diagram of the system as a function of various control parameters like $q_x$ and $f$ as well as the ratio of the junction to the self–capacitances $C_1/C_0$. To analyze the 2D JJA beyond the mean–field theory we employ the path–integral formulation explicitly tailored for the macroscopic JJA Hamiltonian. The effective action formalism allows then for an explicit implementation of the magnetic field and offset charges effects with the nearest–neighbor mutual and self–capacitances included. Furthermore, we adopt an approach based on the quantum phase fluctuation algebra, to map the microscopic JJA model Hamiltonian onto an effectively constrained system – a solvable quantum spherical model in two-dimensions that captures both quantum and spatial fluctuation effects beyond the mean field level.

There are four sections in this paper: Section II is devoted for the introduction of the microscopic Hamiltonian of the 2D JJA with a set of parameters describing with interactions and set of control parameters. In Sec. III the system is transformed into quantum action of the XY model under the magnetic field using the “imaginary–time” Matsubara approach. Furthermore, Sec. IV presents the resulting phase diagrams and finally, Sec. V summarizes the results and presents some discussions. In Appendix we gave a derivation of closed–form analytical formulae for the density of states of a two-dimensional square lattice with magnetic flux for a number of rational values $p/q$ which might be also of general interest.

\section*{II. QUANTUM PHASE HAMILTONIAN}

A Josephson junction array can be modeled by a periodic lattice of superconducting islands separated by insulating barriers. Each island becomes independently superconducting about the bulk transition temperature $T_{c0}$ and it is characterized by an order parameter $\psi(\mathbf{r}_i) = |\psi_0(\mathbf{r}_i)|e^{i\phi(\mathbf{r}_i)}$, where $\mathbf{r}_i$ is a two–dimensional vector denoting the position of each island. The magnitude of the order parameter, $|\psi_0(\mathbf{r}_i)|$, is non–fluctuating when the temperature is lowered further and the onset of long range phase coherence due to the tunneling of Cooper pairs between the islands is responsible for the zero resistance drop in the arrays. The competition between the Josephson tunneling and the charging (Coulomb) energy, without dissipation, can be modeled by the Hamiltonian

\begin{equation}
\end{equation}
\[ \mathcal{H} = \mathcal{H}_C + \mathcal{H}_J, \]
\[ \mathcal{H}_C = -\frac{1}{2} \sum_r [C^{-1}]_{rr} \hat{Q}_r \hat{Q}_{r'}, \]
\[ \mathcal{H}_J = \sum_{\langle r_1, r_2 \rangle} J(|r_1 - r_2|) \left[ 1 - \cos(\phi_{r_1} - \phi_{r_2}) \right]. \tag{1} \]

Here, \( \hat{Q}_r = (2e/i) \partial/\partial \phi_r \) is the charge operator while \( \phi_r \) represents the superconducting phase operator of the grain at the site \( r \); \( J(|r_1 - r_2|) \) is the site-dependent Josephson coupling and \( [C^{-1}]_{rr'} \) is the inverse capacitance matrix. The first part of the action (8) than defines the electrostatic energy with \( C_{rr'} \) being a geometrical property of the array. This matrix is normally approximated (both theoretically and in experimental interpretation) as a diagonal (so-called self-capacitance \( C_0 \)) and mutual one \( C_1 \) between nearest neighbors. In the case of an square 2D JJA of interest here we write the capacitance matrix as:
\[ C_{rr'} = (C_0 + 4C_1) \delta_{rr'} - C_1 \sum_d \delta_{r,r'+d} \tag{2} \]

with the vector \( d \) running over the nearest neighboring (n.n) islands.

### A. Effect of applied magnetic field

A perpendicular magnetic field \( B \) given by the vector potential \( \mathbf{A} \) enters the Hamiltonian (1) through Peierls phase factor according to
\[ J(|r_i - r_j|) \rightarrow J_B(|r_i - r_j|) = J(|r_i - r_j|) \exp \left( \frac{2\pi i}{\Phi_0} \int_{r_i}^{r_j} \mathbf{A} \cdot d\mathbf{l} \right). \tag{3} \]

Thus, the phase shift on each junction is determined by the vector potential \( \mathbf{A} \) and in a typical experimental situation it can be entirely ascribed to the external field \( B \). We assume throughout this paper that the model (1) is defined on a square lattice with lattice spacing \( a \). From Eq.(3) it follows that the properties if the array will be periodic with a period corresponding to the one flux quantum \( \Phi_0 = hc/2e \) per plaquette. Of special interest are the values of the magnetic field which corresponds to the rational values of \( f = \Phi/\Phi_0 \), e.g. \( f = 1/2, 1/4, 1/4, \ldots \) where \( \Phi = Ba^2 \). Since all properties of the Hamiltonian (1) are invariant under \( f \rightarrow f + 1 \) and also under \( f \rightarrow -f \) it is sufficient to consider \( f \) in the range \( 0 \leq f \leq 1/2 \).

### B. Offset charges

Offset charges are an important ingredient in the experimental array samples made of ultrasmall junctions. Several authors have shown that static background charges can have a pronounced effect on the SI transition at zero temperature.\(^{14,15}\) Including the offset charges, \( q_x \), in the charging energy of Eq. (8) gives
\[ \mathcal{H}_C \rightarrow -\frac{1}{2} \sum_r [C^{-1}]_{rr'} \left( \hat{Q}_r - q_x \right) \left( \hat{Q}_{r'} - q_x \right). \tag{4} \]

Thus, offset charges, or an external gate voltage applied between the array and the substrate, behave like a chemical potential for injection of Cooper pairs into the array.
III. JJA “PHASE–ONLY” ACTION

It is useful to derive a field-theoretic representation of the partition function for Eq (1). A convenient procedure is to introduce a path–integral representation in a basis diagonal in $\phi_j$. Given the Hamiltonian $H$, one can simply perform a Legendre transformation to obtain the corresponding Euclidean Lagrangian in the Matsubara “imaginary time” $\tau$ formulation ($0 \leq \tau \leq 1/k_BT \equiv \beta$):

$$\mathcal{L}[Q,\phi] = i \sum_r Q_r(\tau) \cdot \frac{d}{d\tau} \phi_r(\tau) + \mathcal{H}[Q,\phi]. \quad (5)$$

The partition function $Z = Tr e^{-\mathcal{H}/k_BT}$ of the system is then given by

$$Z = \int \prod_i [D\phi_r] \int \prod_r \left[ \frac{DQ_r}{2\pi} \right] e^{-\int_0^\beta d\tau \mathcal{L}[Q,\phi]}. \quad (6)$$

Performing the integration over the charge variables the partition function is expressed as

$$Z = \int \left[ \prod_r D\phi_r \right] e^{-S[\phi]}. \quad (7)$$

Here the functional integral is evaluated over the phases restricted to the compact interval $[0, 2\pi]$ and with an effective “phase–only” action ($\hbar = 1$)

$$S[\phi] = S_C[\phi] + S_J[\phi];$$
$$S_C[\phi] = \frac{1}{8e^2} \int_0^\beta d\tau \sum_{r,r'} C_{rr'} \left( \frac{\partial \phi_r}{\partial \tau} \right) \left( \frac{\partial \phi_{r'}}{\partial \tau} \right) - \frac{iq_x}{2e} \int_0^\beta d\tau \sum_r \left( \frac{\partial \phi_r}{\partial \tau} \right),$$
$$S_J[\phi] = \int_0^\beta d\tau \sum_{(r_1,r_2)} J_B(|r_1 - r_2|) \left\{ 1 - \cos[\phi_{r_1}(\tau) - \phi_{r_2}(\tau)] \right\}. \quad (8)$$

Since the values of the phases $\phi_i$ in Eq.(8) which differ by $2\pi$ are equivalent, the path integral in Eq.(7) can be written in terms of non–compact phase variables $\theta_r(\tau)$, defined on the unrestricted interval $[-\infty, +\infty]$, and by a set of winding numbers $\{n_r\} = 0, \pm 1, \pm 2, \ldots$, which are integers running from $-\infty$ to $+\infty$ (and physically reflects the discreteness of the charge$^{14}$), so that $\phi_r(\tau) = \theta_r(0) + 2\pi n_r \tau / \beta + \theta_r(\tau)$.

A. Effective non–linear $\sigma$ model

Bulk of existing analytical works on quantum JJA have employed variety of mean–field–like approximations$^{1,16–18}$ which, unfortunately, are not reliable for treatment spatial and temporal quantum phase fluctuations in a low dimensional systems. To study the JJA model it appears at first natural to use a description in terms of an effective Ginsburg–Landau functional derived from the microscopic model of Eq. (8). Several studies of JJA have followed this route, also known as the coarse grained approach first developed by Doniach.$^{19}$ The essence of this method is to introduce a complex field order parameter $\psi_r$ (or equivalently a two component real field) whose expectation value is proportional to
\[ \langle \exp(i\phi_r) \rangle. \] The non-zero value of this quantity describes the “phase-locking” or long–range phase ordering in the model. Unfortunately, the system is governed by the Ginzburg-Landau functional only as long as the order parameter is small. This is a serious shortcoming of the coarse grained approach since the method is restricted to the region of parameters in the vicinity of the critical point. It is therefore desirable to extend the coarse–grained method in a way which enables one a self–consistent description of the phase transitions in JJA in an extended parameter range. Following Ref. 20 we note that the model (8) encodes phase fluctuation algebra given by the Euclidean group \( E_2 \) in an extended parameter range. Following Ref. 20 we note that the model (8) encodes phase ordering in the vicinity of the critical point. It is therefore desirable to extend the coarse–grained method since the method is restricted to the region of parameters in the functional only as long as the order parameter is small. This is a serious shortcoming of the phase ordering in the model. Unfortunately, the system is governed by the Ginzburg-Landau evaluation of the effective action in terms of the \( \psi \).

To proceed we write the partition function

\[ Z = \int [\prod_r D\phi_r] e^{S[\phi]} \] for the model (8) in terms path integral representation\(^{21}\) by introducing the auxiliary complex fields \( \psi_r(\tau) \) which replace the original ladder operators \( P_r \). Furthermore, relaxing the original “rigid” constraint (9) and imposing the weaker (spherical) condition \( \sum_r P_r P_r^\dagger = N \) allows us to formulate the problem in terms of the (exactly) soluble quantum spherical (QS) model (see, Ref. 22). This can be conveniently done using the Fadeev–Popov method with Dirac delta-functional which facilitate both the change of integration variables and superimposition of the spherical constraint:

\[ Z = \int [\prod_r D\psi_r D\psi_r^\dagger] \left( \sum_r |\psi_r(\tau)|^2 - N \right) e^{-S[\psi]} \times \]

\[ \times \int [\prod_r D\phi_r] e^{-S_C[\psi]} \prod_r \delta [\Re \psi_r(\tau) - S^r(\phi(\tau))] \]

\[ \times \delta [\Im \psi_r(\tau) - S^v(\phi(\tau))]. \] (10)

A convenient way to enforce the spherical constraint is the functional analog of the \( \delta \)–function representation \( \delta(x) = \int_{-\infty}^{\infty} (d\lambda/2\pi) e^{i\lambda x} \) which introduces the Lagrange multiplier \( \lambda(\tau) \) thus adding an additional quadratic term (in \( \psi \)–fields) to the action (8). The evaluation of the effective action in terms of the \( \psi \) to the second order in \( \psi_r(\tau) \) gives the partition function of the quantum–spherical model \( Z \equiv Z_{QS} \):

\[ Z_{QS} = \int [\prod_r D\psi_r D\psi_r^\dagger] \int \left[ \frac{d\lambda}{2\pi i} \right] e^{-S_{QS}[\psi,\lambda]}, \] (11)

where the action of the effective non-linear \( \sigma \)-model reads

\[ S_{QS}[\psi, \lambda] = \int_0^\beta d\tau d\tau' \left\{ \sum_{(r_1, r_2)} [(\mathbf{J}(r_1 - r_2) + \lambda(\tau)\delta_{r_1, r_2}) \delta(\tau - \tau') \]

\[ + \Gamma_{02}^+(r_1; r_2) \psi_{r_1}^+(\tau) \psi_{r_2}(\tau') - N\lambda(\tau)\delta(\tau - \tau')] \right\}, \] (12)

Furthermore, \( \Gamma_{02}^+(r_1; r_2) = [W_{02}^{-1}]^+(r_1; r_2; r_2') \) is the two–point phase vertex correlator and
\[ W_{02}^{\pm}(\mathbf{r}_1, \mathbf{r}_2, \tau; \mathbf{r}_2', \tau') = \frac{1}{Z_0} \sum_{\{n_r\}} \prod_r \int_0^{2\pi} d\theta(0) \int_{\theta(0)}^{\theta(0)+2\pi n_r} D\theta_r(\tau) e^{i[\theta_{\mathbf{r}_1}(\tau) - \theta_{\mathbf{r}_2}(\tau)']} e^{-S_C[\theta]}, \]  

with

\[ Z_0 = \sum_{\{n_r\}} \prod_r \int_0^{2\pi} d\theta(0) \int_{\theta(0)}^{\theta(0)+2\pi n_r} D\theta_r(\tau) e^{-S_C[\theta]}, \]  

where \( Z_0 \) is the statistical sum of the “non–interacting” system described by the action \( S_C[\theta] \). The phase–phase correlation function becomes:

\[ W_{02}(\omega_\ell) = \frac{8E_C}{Z_0} \sum_q \exp \left[ -4\beta E_C(q - q_x)^2 \right] \frac{\exp \left[ -4\beta E_C(q - q_x)^2 \right]}{(4E_C)^2 - [8E_C(q - q_x) - i\omega_\ell]^2}, \]  

where \( Z_0 = \sum_q \exp \left[ -4\beta E_C(q - q_x)^2 \right] \), and the summation is performed over all integer–valued charge states \( q = 0, \pm 1, \pm 2, \ldots \), which makes the function \( W_{02}(\omega_\ell) \) periodic. At low temperatures the sum over \( q \) in Eq.(15) is dominated by the charge \( q \) which makes the exponent in the numerator of Eq.(15) smallest (for \( T = 0 \) this value is \( q = 0 \)).

In the thermodynamic limit, \( N \rightarrow \infty \), we can calculate the functional integral in Eq.(11) by the steepest–descent method. To proceed, we introduce propagators associated with the order parameter field defined by

\[ G(\mathbf{r}_1, \tau; \mathbf{r}_2, \tau') = \langle \psi^\dagger_{\mathbf{r}_1}(\tau) \psi_{\mathbf{r}_2}(\tau') \rangle_{QS}. \]  

The condition that the integrand in Eq.(11) has a saddle point \( \lambda(\tau) = \lambda_0 \) is that

\[ 1 = \frac{1}{N} \sum_{\mathbf{r}} G(\mathbf{r} \tau; \mathbf{r} \tau + 0^+), \]

which becomes an implicit equation for \( \lambda_0 \). The QS ensemble average is now defined by

\[ \langle \ldots \rangle_{QS} = \frac{\int \left[ \prod_r \mathcal{D} \psi^\dagger_r \mathcal{D} \psi^\dagger_r \right] \ldots e^{-S_{QS}[\psi, \lambda_0]}}{\int \left[ \prod_r \mathcal{D} \psi_r \mathcal{D} \psi_r^\dagger \right] e^{-S_{QS}[\psi, \lambda_0]}}. \]  

To proceed, it is desirable to introduce the density of states for a 2D lattice with the magnetic flux \( f = p/q \) in the form

\[ \rho_{p/q}(E) = \frac{1}{N} \sum_k \delta \left[ E - \frac{J_B(k)}{E_J} \right], \]  

with \( J_B(k) \) the Fourier transform of the Josephson interactions \( \mathbf{J}_B(|\mathbf{r}_1 - \mathbf{r}_2|) \) (cf. Eq.(3)) in a magnetic field. The problem of computing of \( \rho_{p/q}(E) \) reduces effectively to the solution of the Harper’s equation\(^{23}\) relevant e.g. for tight-binding electrons on a two-dimensional lattice with a a uniform magnetic flux per unit plaquette.\(^{24}\) In Appendix we give an analytical derivation of \( \rho_{p/q}(E) \) in a closed form for several rational values of \( p/q \). A Fourier transform of Eq. (12) in momentum and frequency space enables one to write the spherical constraint (17) with the help of the density of states (19) in the form

\[ \langle \ldots \rangle_{QS} = \frac{\int \left[ \prod_r \mathcal{D} \psi^\dagger_r \mathcal{D} \psi^\dagger_r \right] \ldots e^{-S_{QS}[\psi, \lambda_0]}}{\int \left[ \prod_r \mathcal{D} \psi_r \mathcal{D} \psi_r^\dagger \right] e^{-S_{QS}[\psi, \lambda_0]}}. \]  

To proceed, it is desirable to introduce the density of states for a 2D lattice with the magnetic flux \( f = p/q \) in the form

\[ \rho_{p/q}(E) = \frac{1}{N} \sum_k \delta \left[ E - \frac{J_B(k)}{E_J} \right], \]  

with \( J_B(k) \) the Fourier transform of the Josephson interactions \( \mathbf{J}_B(|\mathbf{r}_1 - \mathbf{r}_2|) \) (cf. Eq.(3)) in a magnetic field. The problem of computing of \( \rho_{p/q}(E) \) reduces effectively to the solution of the Harper’s equation\(^{23}\) relevant e.g. for tight-binding electrons on a two-dimensional lattice with a a uniform magnetic flux per unit plaquette.\(^{24}\) In Appendix we give an analytical derivation of \( \rho_{p/q}(E) \) in a closed form for several rational values of \( p/q \). A Fourier transform of Eq. (12) in momentum and frequency space enables one to write the spherical constraint (17) with the help of the density of states (19) in the form
\[
1 = \frac{1}{\beta} \int_{-\infty}^{+\infty} d\xi \sum_{\ell} \frac{\rho_{p/q}(\xi)}{\lambda - \xi E_J + [W_{\ell}(\omega)]^{-1}},
\] (20)

where \( W_{\ell}(\omega) \) is the frequency transformed phase–phase correlator of Eq. (13) and \( \omega = 2\pi \ell/\beta \) (\( \ell = 0, \pm 1, \pm 2, \ldots \)) the (Bose) Matsubara frequencies. As usual in a spherical model the critical behavior and the phase transition boundary depends crucially on the spectrum given by the density of states \( \rho_{p/q}(E) \) and is determined by the denominator of the summand in the spherical constraint equation of Eq. (17). Specifically, when \( [1/G(k = 0, \omega = 0)] = 0 \), where \( G(k, \omega) \) is the Fourier transformed order parameter correlation of Eq. (16), the system displays a critical point at

\[
\lambda_0 - \epsilon_{p/q}^{\text{max}} E_J + [W_{\ell}(\omega = 0)]^{-1} = 0,
\] (21)

where \( \epsilon_{p/q}^{\text{max}} \) is the maximum value of the spectrum described by the density of states (19). This fixes the saddle point value \( \lambda \): with the onset of the phase transition saddle point value of the Lagrange multiplier \( \lambda \) “sticks” to that value at criticality (\( \lambda = \lambda_0 \)) and stays constant in the whole low temperature phase.

**IV. PHASE DIAGRAMS**

By substituting the value of \( \lambda_0 \) from Eq.(21) into (20), after performing the summation over Matsubara frequencies, one obtains the \( T \to 0 \) limit the result

\[
1 = P \int_{-\infty}^{+\infty} d\xi \rho_{p/q}(\xi) \sqrt{\frac{E_C}{2(\lambda_0 + 2E_C - \xi E_J)}} \left[ \text{sign} \left( 4q_x \frac{E_C}{E_J} + \frac{\sqrt{2(\lambda_0 + 2E_C - \xi E_J)E_C}}{E_J} \right) \right. \\
- \left. \text{sign} \left( 4q_x \frac{E_C}{E_J} - \frac{\sqrt{2(\lambda_0 + 2E_C - \xi E_J)E_C}}{E_J} \right) \right],
\] (22)

where \( P \) denotes the principal value of the integral. The charging energy for the two-dimensional square lattice may be explicitly written as

\[
E_C = \frac{1}{2} e^2 [C^{-1}]_{rr} \\
[C^{-1}]_{rr} = \lim_{N \to \infty} \frac{1}{N} \sum_k \frac{1}{C_0 + 4C_1 - 2C_1(\cos k_x + \cos k_y)} \\
= \frac{2}{\pi(C_0 + 4C_1)} K \left( \frac{4C_1}{C_0 + 4C_1} \right),
\] (23)

where \( K(x) \) is the elliptic integral of the first kind\(^{25}\) (see also Eq.(A5) in Appendix). Furthermore, we introduce the charging energy parameters \( E_0 = \frac{1}{2} e^2 C_0^{-1} \) and \( E_1 = \frac{1}{2} e^2 C_1^{-1} \) related to the island and junction capacitances. We fist examine the ground state phase diagram for a number of rational values of the flux piercing the array without charge frustration (\( q_x = 0 \)). We give in Fig.1 a graph showing the ground state phase diagram as a function of island-to-junction charging energy for various rational flux numbers.
The charge frustration $q_x$ may serve as a control parameter distinguishing between ordered and non-ordered states. The energy difference for two charge states in each grain of the JJA with $n$ and $n+1$ extra electrons may be reduced by changing $q_x$. As a consequence the effects of a finite charging energy $E_C$ are weakened and the superconducting region in the phase diagram turns out to be enlarged. The dependence of Josephson to the total charging energy $E_J/E_C$ is shown in Fig.2 for a number of rational fluxes. The behavior shown in in Fig.2 is readily understood by realizing that the Hamiltonian (1) is periodic in $q_x$ with period unity. this implies that the phase diagram should be similarly periodic, repeating at each integer number.\textsuperscript{14}

V. SUMMARY

We have studied the ground phase diagram in quantum two-dimensional Josephson junction arrays, using the spherical model approximation with exactly evaluated density of states for two-dimensional lattice with rational magnetic flux $f = p/q$ for a number of values $f = 1/q$. One of the most important issues in these systems is the role of the charging energy on the phase coherence transition. The detailed phase boundaries crucially depend on the ratio of the junction-to-self- capacitances, $C_1/C_0$ as well as on the magnetic and charge frustration. In arrays which are in the superconducting state at $f = 0$ but with the value $E_C/E_J$ close to the critical value, a magnetic filed can be used to drive the array into the insulating state (see, Fig.1). It is interesting to compare the calculated values of $E_C/E_J$ for $f = 0$ and $f = 1/2$ with the experiments:\textsuperscript{5} the measured critical value $E_C/E_J$ close to $T = 0$ is about a factor 0.7 lower than the zero field value. This is to be compared with the value 0.88 found for $T = 0$ in the present paper. Note that the critical value of $E_C/E_J$ is greater than for others commensurate values $f = 1/q$ which suppress the superconducting state substantially. We found that the effect of this supression is considerably larger than that which comes from the mean-field analysis of JJA with magnetic flux (for comparison see, e.g. Ref. 14). Closing we note that a reliable comparison with experiments presumably will still require incorporating into the model several other ingredients as, e.g, disorder and dissipation. These are topics to be considered in the future.

APPENDIX A: DENSITY OF STATES FOR 2D SQUARE LATTICE IN A RATIONAL–FLUX CASE

If one uses the Landau gauge, $A = B(0, x, 0)$ than the dispersion $\epsilon(k)$ for a square lattice of spacing $a$ with flux $\phi = Ba^2/\Phi_0 \equiv p/q$ with is given by:\textsuperscript{24}

$$\det \begin{pmatrix} M_1 & -e^{ik_x a} & 0 & \ldots & 0 & -e^{-ik_x a} \\ -e^{-ik_x a} & M_2 & -e^{ik_x a} & \ddots & \ddots & 0 \\ 0 & -e^{-ik_x a} & M_3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & -e^{ik_x a} & 0 \\ 0 & \ddots & \ddots & -e^{ik_x a} & M_{q-1} & -e^{ik_x a} \\ -e^{ik_x a} & 0 & \ldots & 0 & -e^{-ik_x a} & M_q \end{pmatrix} = 0 \quad (A1)$$
where
\[ M_n = -2 \cos (k_y a + 2\pi \phi_n) - \epsilon(k). \] (A2)

Equation (A2) is known as Harper’s equation and has been studied extensively. If integers \( p \) and \( q \) are chosen to represent the flux (with no common factor in \( p \) and \( q \)), then the dependence on the wave vector always appears through the generalized structure factor \( \gamma_n = \cos(nk_x a) + \cos(nk_y a) \). The density of states \( \rho_p^q(E) \) given by the Eq.(19) can be obtained by computing energy bands \( \epsilon(k) \) from the eigenvalue equation (A1). The calculation of the exact density of states is straightforward, although for large values of \( q \) may only be done numerically. However, for a number of \( q \) values of interest it can be done analytically with a closed–form expression for \( \rho_p^q(E) \) as end result. Below we list these cases.

1. \( f = 0 \)

In the case of zero magnetic field the density of states for the square two–dimensional lattice reads simply
\[ \rho(E) = \int_{\pi/a}^{\pi/a} \frac{d^2k}{(2\pi)^2} \delta \left[ E - \gamma_1(k) \right]. \] (A3)

Performing the integration over the wave-vectors we obtain (see, Fig.3)
\[ \rho_{2D}(E) = \frac{1}{\pi^2} K \left[ \sqrt{1 - \left( \frac{E}{2} \right)^2} \right] \Theta \left( 1 - \frac{|E|}{2} \right) \] (A4)

where
\[ K(x) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - x^2 \sin^2 \phi}} \] (A5)

is the elliptic integral of the first kind and
\[ \Theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x \leq 0 \end{cases} \] (A6)

the unit step function.

2. \( f = \frac{1}{2} \)

For the square lattice with the half-flux quantum per plaquette the Harper’s equation (A2) reads
\[ \epsilon^2(k) - 2\gamma_2 - 4 = 0 \] (A7)

so that the energy dispersion has two branches:
\[ \epsilon(k) = \begin{cases} -\sqrt{4 + 2 (\cos 2k_1 + \cos 2k_2)} & \text{if } E \in [-2\sqrt{2}; 0] \\ +\sqrt{4 + 2 (\cos 2k_1 + \cos 2k_2)} & \text{if } E \in [0; 2\sqrt{2}] \end{cases} \] (A8)

Integrating over the wave vectors belonging to the Brillouin zone we obtain from Eq.(A3) with the help of the formula (A4)

\[ \rho_{1/2}(E) = \frac{|E|}{2} \rho_{2D} \left( \frac{E^2 - 4}{2} \right) \Theta \left( 8 - E^2 \right) \] (A9)

Fig.4 gives the plot of the density (A9).

3. \( f = \frac{1}{3} \)

For \( p/q = 1/3 \) the Harper's equation is now of cubic form

\[ \epsilon^3(k) - 6\epsilon(k) + 2\gamma_3 = 0 \] (A10)

and its roots give the dispersion of the energy

\[ \epsilon(k) = \begin{cases} \frac{1 + i\sqrt{3}}{(-\gamma_3 + \sqrt{-8 + \gamma_3^2})^{\frac{1}{3}}} & \text{if } E \in \langle -1 - \sqrt{3}; -2 \rangle \\ \frac{i}{2} \left( i + \sqrt{3} \right) \left( -\gamma_3 + \sqrt{-8 + \gamma_3^2} \right)^{\frac{1}{3}} & \text{if } E \in \langle 1 - \sqrt{3}; -1 + \sqrt{3} \rangle \\ \frac{1}{2} \left( 1 + i\sqrt{3} \right) \left( -\gamma_3 + \sqrt{-8 + \gamma_3^2} \right)^{\frac{1}{3}} & \text{if } E \in \langle 1 + \sqrt{3}; \rangle \\ \frac{2 + \left( -\gamma_3 + \sqrt{-8 + \gamma_3^2} \right)^{\frac{2}{3}}}{(-\gamma_3 + \sqrt{-8 + \gamma_3^2})^{\frac{1}{3}}} & \text{if } E \in \langle 2; 1 + \sqrt{3} \rangle \end{cases} \] (A11)

The density of states then becomes (see, Fig.5)

\[ \rho_{1/2}(E) = \frac{1}{2} \rho_{2D} \left[ \frac{E(E^2 - 6)}{2} \right] \left| \sqrt{(E^2 - 8)(E^2 - 2)} \right| x \times \] (A12)

\[ \times \left\{ \left| x^2 - 2 \right|^{-1} \left[ \Theta(E + 1 + \sqrt{3}) - \Theta(E + 2) \right] + \\ + \left| x^2 + 2 \right|^{-1} \left[ \Theta(E - 1 + \sqrt{3}) - \Theta(E) \right] + \\ + \left| x^2 + 2 \right|^{-1} \left[ \Theta(E) - \Theta(E - 1 + \sqrt{3}) \right] + \\ + \left| x^2 - 2 \right|^{-1} \left[ \Theta(E - 2) - \Theta(E - 1 - \sqrt{3}) \right] \right\} , \] (A13)

where

\[ x(E) = \frac{1}{2} \left( E^3 - 6E + \sqrt{E^2(E^2 - 6)^2 - 32} \right) . \] (A15)
4. $f = \frac{1}{4}$

The matrix formula (A2) produces now a four order polynomial equation for the dispersion $\epsilon(k)$.

$$\epsilon^4(k) - 8\epsilon^2(k) - 2\gamma_4 + 4 = 0 \quad (A16)$$

Because the Eq.() is in fact bi-quadratic with respect to $\epsilon(k)$ its roots can be readily found:

$$J(k) = \begin{cases} 
-\sqrt{4 + \sqrt{2}6 + \gamma_4} & \text{if } E \in \left(-\sqrt{4 + 2\sqrt{2}}; -2\sqrt{2}\right) \\
-\sqrt{4 - \sqrt{2}6 + \gamma_4} & \text{if } E \in \left(-\sqrt{4 - 2\sqrt{2}}; 0\right) \\
+\sqrt{4 - \sqrt{2}6 + \gamma_4} & \text{if } E \in \left(0; \sqrt{4 - 2\sqrt{2}}\right) \\
+\sqrt{4 + \sqrt{2}6 + \gamma_4} & \text{if } E \in \left(2\sqrt{2}; \sqrt{4 + 2\sqrt{2}}\right)
\end{cases}. \quad (A17)$$

As a result the density of states becomes

$$\rho_{\frac{1}{4}}(E) = \frac{|E^2 - 4|}{2} \rho_{2D} \left(\frac{E^4 - 8E^2 + 4}{2}\right) \times$$

$$\times \left\{ \sqrt{4 + |E^2 - 4|} \left[\Theta \left(8 - E^2\right) - \Theta \left(4 + 2\sqrt{2} - E^2\right)\right] + \sqrt{4 - |E^2 - 4|} \Theta \left(4 - 2\sqrt{2} - E^2\right) \right\}. \quad (A18)$$

In Fig. 6 we have plotted the density of states given by Eq.(A19).

5. $f = \frac{1}{6}$

The Harper’s equation (A2) now is given by

$$\epsilon^6(k) - 12\epsilon^4(k) + 24\epsilon^2(k) - 2\gamma_6 - 4 = 0 \quad (A20)$$

which is a bi–cubic equation for the dispersion parameter $\epsilon(k)$. Although the solutions of Eq.(A20) can be found analytically the result is quite involved so that we refrain form reproducing it here. However, the resulting density of states (see, Fig.7) can be put in a closed–form expression as follows:

$$\rho_{\frac{1}{6}}(E) = 2^{-\frac{3}{2}} \rho_{2D} \left(\frac{E^6 - 12E^4 + 24E^2 - 4}{2}\right) \left|x^\frac{1}{3}\sqrt{7}\right| \times$$

$$\times \left\{ \frac{2}{x} \right\}^\frac{1}{2} \sqrt{\frac{x^\frac{1}{3} + 4 \cdot (2x)^\frac{2}{3} + 8 \cdot 2^\frac{2}{3}}{(2x^2)^\frac{2}{3} - 16}} \left[\Theta \left(5 + \sqrt{21} - E^2\right) - \Theta \left(6 + 2\sqrt{3} - E^2\right)\right]$$

$$+ \left[\sqrt{4 \cdot 2^\frac{2}{3} - (2x^\frac{1}{3})^{-1} \left[\frac{2^\frac{1}{2} \left(1 - i\sqrt{3}\right) x^\frac{2}{3} + 16 \left(1 + i\sqrt{3}\right)}{2^\frac{1}{2} \left(1 - i\sqrt{3}\right) x^\frac{2}{3} - 16 \left(1 + i\sqrt{3}\right)}\right]\Theta \left(5 - \sqrt{21} - E^2\right)$$

$$\right\}.$$
\[
\sqrt{4 \cdot 2^\frac{3}{2} - (2x^\frac{1}{3})^{-1} \left[ \frac{16 \left( 1 - i\sqrt{3} \right) + 2^\frac{1}{2} \left( 1 + i\sqrt{3} \right) x^\frac{2}{3}}{16 \left( 1 - i\sqrt{3} \right) - 2^\frac{1}{2} \left( 1 + i\sqrt{3} \right) x^\frac{2}{3} \right]}
\times \left[ \Theta(6 - 2\sqrt{3} - E^2) - \Theta(2 - E^2) \right],
\]
where
\[
\begin{align*}
x(E) &= E^6 - 12E^4 + 24E^2 + 32 + \sqrt{y} \\
y(E) &= \left( E^4 - 8E^2 + 8 \right)^2 \left( E^4 - 8E^2 - 16 \right)^2.
\end{align*}
\]
FIGURES

FIG. 1. Zero temperature phase diagram for two-dimensional Josephson junction array on a square lattice in magnetic field as a function of charging energies related to self-capacitance ($E_0$) and mutual capacitance ($E_1$), (normalized by the Josephson coupling energy $E_J$) for different values of the flux ratio $f$. The inset shows closeup of the plot for $f = 0$ and $f = 1/2$. The superconducting (insulating) phase is located above (below) each curve.

FIG. 2. Ground state phase diagram of the square JJA as a function of the total charging energy ($E_C$, normalized by the Josephson coupling $E_J$) and the charge frustration parameter $q_x$. The inset shows closeup of the plot for $f = 0$ and $f = 1/2$. The insulating phase is located within each lobe.

FIG. 3. Density of states $\rho(E)$ for two-dimensional square lattice.

FIG. 4. Density of states for two-dimensional square lattice with one-half of the magnetic flux quantum per plaquette.

FIG. 5. Density of states for 2D square lattice in the magnetic field for the flux ratio $f = 1/3$.

FIG. 6. Density of states for 2D square lattice in the magnetic field for the flux ratio $f = 1/4$.

FIG. 7. $\rho(E)$ for 2D square lattice in the magnetic field for the flux ratio $f = 1/6$ (depicted for positive argument $E$ only, to reveal details of the band structure.)
REFERENCES

1 E. Simanek, Phys. Rev B 32, 500 (1985); Inhomogeneous Superconductors (Oxford University Press, New York, 1994).
2 E. Simánek, Phys. Rev. B 32, 500 (1985); see also E. Simánek, in Inhomogeneous Superconductors (Oxford University Press, 1994).
3 J. G. Kissner and U. Eckern, Z. Phys. B 91, 155 (1993)
4 C. Rojas and J. V. José, Phys. Rev. B 54, 12361 (1996).
5 H. S. J. van der Zant, W. J. Elion, L. J. Geerlings and J. E. Mooij Phys. Rev. B 54, 10081 (1996)
6 J. A. Hertz, Phys. Rev. B 14, 1165 (1976); for a recent review see, S. L. Sondhi, S. M. Girvin, J. P. Carini and D. Shahar Rev. Mod. Phys. 69, 315 (1997).
7 R. Fazio and G. Schöll, Phys. Rev. B 43, 5307 (1991).
8 E. Roddick and D. Stroud, Phys. Rev. B 48, 16 600 (1993)
9 G. Grignani, A. Mattoni, P. Sodano, and A. Trombettoni, Phys. Rev. B 61, 11 676 (2000).
10 R. T. Scalettar, G. G. Batrouni and G. T. Zimany, Phys. Rev. Lett. 66, 3144 (1991).
11 E. Granato, J. M. Kosterlitz, and M. P. Nightingale, Physica B 222, 226 (1996).
12 B. J. Kim, J. Kim, S. Y. Park, and M. Y. Choi Phys. Rev B 56, 395 (1997).
13 B. J. Kim, G. S. Jeon, M.-S. Choi, and M. Y. Choi Phys. Rev B 58, 14524 (1998).
14 C. Bruder, R. Fazio, A. Kampf, A. van Otterlo and G. Schöll, Physica Scripta, 42, 139 (1992).
15 J. K. Freericks and H. Monien Phys. Rev. B 53, 2691 (1996).
16 M. V. Simkin, Phys. Rev. B 44, 7074 (1991)
17 S. Kim and M. Y Choi, Phys. Rev. B 41, 111 (1990).
18 A. D. Zaikin, J. Low.Temp. Phys. 80, 223 (1990).
19 S. Doniach, Phys. Rev. B 24, 5063 (1981).
20 D. Das and S. Doniach, Phys. Rev. B 60, 1261 (1999).
21 H. Kleinert, Path Integrals in Quantum Mechanics, Statistics and polymer Physics (World Scientific, Singapore 1990)
22 T.K. Kopeć and J. V. José, Phys. Rev. B 60, 7473 (1999).
23 P. G. Harper, Proc. Physc. Soc. London Sect. A 68, 674 (1955)
24 Y. Hasegawa, P. Lederer, T.M. Rice, and P.B. Wiegmann, Phys. Rev. Lett. 68 (1989).
25 M. Abramovitz and I. Stegun, Handbook of Mathematical Functions (Dover, New York, 1970).
This figure "Fig2.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1
This figure "Fig3.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1
This figure "Fig4.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1
This figure "Fig5.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1
This figure "Fig6.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1
This figure "Fig7.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0301212v1