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Superconductor-insulator transition in frustrated Josephson-junction arrays on a honeycomb lattice

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Abstract. The zero-temperature superconductor to insulator transition is studied in a self-charging model of Josephson-junction arrays on a honeycomb lattice in an external magnetic field corresponding to f flux quantum per plaquette. Path integral Monte Carlo simulations of the equivalent (2+1)-dimensional classical model are used to study the phase transition and critical behavior. For $f = 1/3$, the transition is first order. For $f = 0$ and $f = 1/2$, the transition is second order and the corresponding correlation length exponents are estimated from finite-size scaling.

1. Introduction

The superconductor to insulator transition in Josephson junction arrays have attracted considerable interest [1, 2, 3, 4, 5, 6, 7, 8, 9, 10] as a physical realization of a quantum phase transition. Such arrays can currently be fabricated in any desired geometry both in one and two dimensions (2D) [4] as a lattice of superconducting grains coupled by the Josephson or proximity effect and with well-controlled parameters. When charging effects due to the small capacitance of the grains or junctions dominate over the Josephson coupling, strong quantum fluctuations of the phase of the superconducting order parameter may drive the system into an insulating phase at zero temperature leading to a superconductor to insulator transition as a function of the ratio of charging energy to the Josephson coupling. In presence of an external magnetic field, frustration effects lead to distinct universality classes which can depend on the geometry of the array. For a Josephson-junction array on square lattice, the universality class of these transitions have already been investigated in detail numerically [10, 11], both in relation to experiments [3, 4] and theoretical predictions [7, 8, 13]. However, for a Josephson-junction array on a honeycomb lattice the superconductor to insulator transition has not been investigated in detail. Such array is particularly interesting as a simple model [14] for ultra-thin superconducting films with a triangular pattern of nanoholes [15]. This system undergoes a superconductor to insulator transition for decreasing thickness with properties very sensitive to the applied magnetic field, which is the analog of the transition in the superconducting array for increasing ratio of the charging energy to the Josephson coupling at different frustration parameters.

In this work, we study the zero-temperature superconductor to insulator transition in a self-charging model of Josephson-junction arrays in an external magnetic field corresponding to f flux quantum per plaquette. Path integral Monte Carlo simulations of the equivalent (2+1)-dimensional classical model are used to study the phase transition and critical behavior. For


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$f = 1/3$, we find that the transition is first order. For $f = 0$ and $f = 1/2$, the transition is second order and the corresponding correlation length exponents are estimated from finite-size scaling.

2. Model and simulation

We consider a Josephson-junction array on a honeycomb lattice as illustrated in Fig. 1, where charging effects are dominated by the capacitance to the ground of each grain [1, 6], and described by the Hamiltonian

$$\mathcal{H} = -\frac{E_c}{2}\sum_r \left(\frac{d}{d\theta_r}\right)^2 - E_J \sum_{<rr'>} \cos(\theta_r - \theta_{r'} - A_{rr'}). \quad (1)$$

The first term in Eq. (1) describes quantum fluctuations induced by the charging energy $E_c = 4e^2/C$ of a non-neutral superconducting grain located at site r, where e is the electronic charge and C is the effective capacitance to the ground of the grain, while the second term is the usual Josephson-junction coupling between nearest-neighbor grains described by phase variables θ_r. The effect of the applied magnetic field appears through the bond variables $A_{rr'} = (2\pi/\Phi_o)\int_r^{r'} A \cdot dr$, where $\mathbf{A}$ is the vector potential due to the external magnetic field $\mathbf{B}$ and the gauge-invariant sum around an elementary cell of the array is given by $\sum_{rr'} A_{rr'} = 2\pi f$ with $f = \Phi/\Phi_o$ defining the frustration parameter, which corresponds to the number of flux quanta per plaquette. This model is periodic in f with period $f = 1$.

In order to study the phase transition, it is convenient to use an imaginary-time path-integral formulation of the model [2]. In this formulation, the 2D quantum problem of Eq. (1) maps into a (2+1)D classical statistical mechanics problem with the extra dimension corresponding to the imaginary-time direction. The time axis τ can be discretized in slices $\Delta\tau$ and the ground state energy of the quantum model corresponds to the reduced free energy of the classical model, per unit length in the imaginary time direction. After re-scaling the time slices appropriately in order to get space-time isotropic couplings, the resulting classical partition function is given by $Z = Tr_{\{\theta\}} e^{-H}$ where the reduced classical Hamiltonian can be defined as

$$\begin{aligned} H = \quad & -\frac{1}{g}[\sum_{\tau,j} \cos(\theta_{\tau,j} - \theta_{\tau+1,j}) \\ & + \sum_{<ij>,\tau} \cos(\theta_{\tau,i} - \theta_{\tau,j} - A_{ij})]. \end{aligned} \quad (2)$$

In the above equation, j and τ label the spatial and time directions, respectively, and the ratio of the charging energy to the Josephson coupling $g = (E_c/E_J)^{1/2}$ plays the role of an effective temperature in the 3D classical model. This classical Hamiltonian can be viewed as a frustrrated XY model on a layered honeycomb lattice.

We carry out MC simulations using the 3D classical Hamiltonian in Eq. (2) regarding g as a temperature-like parameter and employing the exchange MC method (parallel tempering) [16]. In this method, many replicas of the system with different couplings g in a range above and below the critical point are simulated in parallel and the corresponding configurations are allowed to be exchanged with a probability distribution satisfying detailed balance. Simulations are performed in system sizes with equal spatial and time linear length L. This choice of the aspect ratio of the system assumes implicitly that the dynamic critical exponent z characterizing the superconductor to insulator transition is close to $z \sim 1$. In general, a quantum phase transition is characterized by intrinsic anisotropic scaling with different diverging correlation lengths ξ and ξ_τ in the spatial and time directions [2], respectively, related by the dynamic exponent z as $\xi_\tau \propto \xi^z$. Our choice is justified by the observation that the best data collapse implied by the scaling behavior discussed below is obtained for $z \sim 1$.

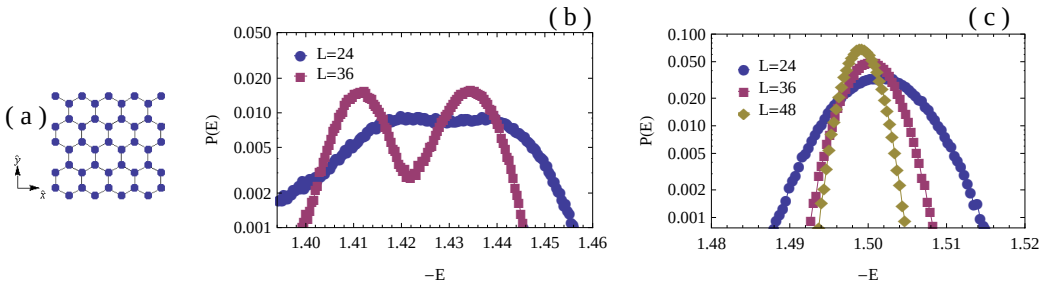


Figure 1. (a) Josephson-junction array on a honeycomb lattice. Filled circles represent superconducting grains and the lines the Josephson junctions. (b) and (c) Probability distribution of the energy $-E$ near the transition for different system sizes L in the equivalent $(2+1)$D classical model of Eq. (2), for (b) f=1/3 and (c) f=1/2.

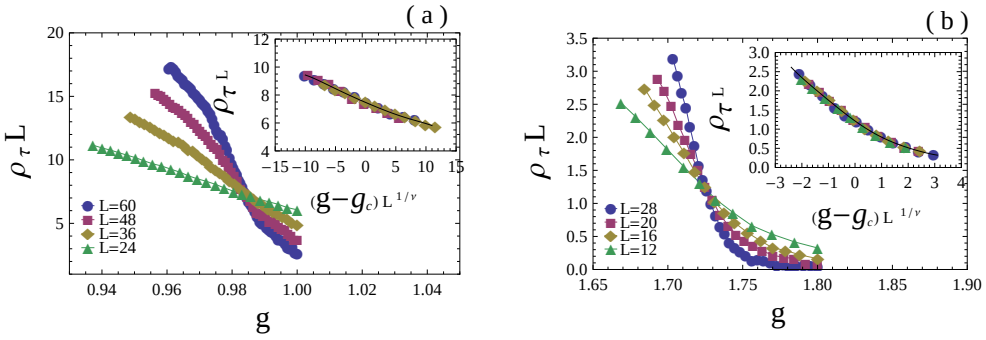


Figure 2. (a) Phase stiffness in the imaginary time direction ρ_τ for $f = 1/2$. Inset: scaling plot for data near the transition and systems sizes $L \geq 36$ with $g_c = 0.9837$ and $\nu = 0.51$. b) Phase stiffness ρ_τ for $f = 0$. Inset: corresponding scaling plot for data near the transition with $g_c = 1.7255$ and $\nu = 0.66$.

3. Numerical results and discussion

We first determine the nature of the transition by examining the histogram of the probability distribution for the energy density near the transition. As can been seen from Fig. 2, double maxima appears for $f = 1/3$, indicating that there are two coexisting phases corresponding to a first order transition. On the other hand, for $f = 1/2$, such feature is absent indicating that the transition is continuous. In the absence of the external magnetic field, $f = 0$, one expects that the superconductor-insulator transition is in the universality class of the 3D classical XY model, for which the correlation length exponent is well known. For $f = 1/2$, however, the critical behavior is unknown. Below, we verify the expected scaling behavior for the continuous transitions and obtain an estimate of the critical exponents.

To locate the superconductor-insulator transition at the critical coupling g_c and determine the critical exponents, we have performed MC calculations of the phase stiffness ρ_τ in the time direction and the finite-size correlation lengths ξ and ξ_τ measuring the spatial and time decay of the phase-correlation function for $g \geq g_c$. In the superconducting phase ρ_τ should be finite, reflecting the existence of phase coherence, while in the insulating phase it should vanish in the thermodynamic limit. For a continuous phase transition, the phase stiffness should satisfy the finite-size scaling form

$$\rho_\tau L = F(L^{1/\nu}\delta g), \tag{3}$$

where $F(x)$ is a scaling function and $\delta g = g - g_c$. This scaling form implies that data for the quantity $\rho_\tau L$ as a function of g, for different system sizes L, should cross at the critical coupling

g_c. Moreover, a scaling plot of $\rho_\tau L \times L^{1/\nu}\delta g$ sufficiently close to g_c should collapse on to the same curve if ν is chosen correctly. Fig. 2a shows the behavior of $\rho_\tau L$ as a function of g for different system sizes L, when $f = 1/2$. The transition point g_c is located where the curves cross. In the inset of Fig. 2a, we show a scaling plot of the data close to the transition for the largest system sizes ($L = 36 - 60$) according to the scaling form of Eq. (3), which provides the estimates $g_c = 0.9837(5)$ and $\nu = 0.51(6)$. For comparison, in Fig. 2b we show similar results for the unfrustrated case, $f = 0$, which gives the estimates $g_c = 1.7255(5)$ and the correlation length exponent $\nu = 0.66(4)$ in good agreement with the known result for the 3D XY model [18], $\nu = 0.671$. Note that the critical coupling $g_c(f = 1/2)$ is significantly smaller than $g_c(f = 0)$

We have also investigated the scaling behavior of the finite-size correlation lengths in the $\hat{x}$ direction ξ and in the time direction ξ_τ. The correlation length in the finite system can be obtained from a second moment calculation using the correlation function as [17]

$$\xi(L) = \frac{1}{2\sin(k_0/2)}[S(0)/S(k_0) - 1]^{1/2}, \tag{4}$$

where $S(k)$ is given by the Fourier transform of the phase correlation function $C(r)$ and k_0 is the smallest nonzero wave vector in the finite system. As in the previous work in absence of quantum fluctuations [14], it is convenient to define the correlation function in terms of the overlap order parameter $q(j) = \exp(i\theta_j^1 - i\theta_j^2)$, where 1 and 2 denote two independent copies of the system, with same parameters g and f in the model of Eq. (2). For a continuous transition, the finite-size correlation length $\xi(L, g)$ should satisfy the scaling form

$$\xi/L = G(L^{1/\nu}\delta g), \tag{5}$$

where $G(x)$ is a scaling function. Similar scaling form applies to the correlation length ξ_τ in the time direction. According to this scaling form, curves of $\xi(L, g)/L$ as a function of g, for different system sizes L, should cross at the critical coupling g_c and a scaling plot of $\xi(L, g)/L \times L^{1/\nu}\delta g$ sufficiently close to g_c should collapse on to the same curve. Figs. 3 shows the finite-size behavior of the correlation lengths ξ_τ and ξ scaled by the system size L as function of g, for $f = 1/2$. The curves for the largest systems cross at the same point, demonstrating that there is a continuous transition. In the insets of Figs. 3a and 3b, we show a scaling plot of the data according to the scaling form of Eq. (5), which provides the estimates $g_c = 0.9836(5)$ and $\nu = 0.44(5)$, and $g_c = 0.9845(5)$ and $\nu = 0.48(5)$, respectively. These alternative estimates and the value obtained from the phase-stiffness scaling are in reasonable agreement, within the errorbars, leading to the final result $\nu = 0.48(4)$.

4. Conclusions

We have studied the superconductor to insulator transition in a self-charging model of Josephson-junction arrays on a honeycomb lattice in an external magnetic field corresponding to f flux quantum per plaquette. The model can be physically as two-dimensional arrays of weakly coupled superconducting grains and ultra-thin superconducting films with a triangular pattern of nanoholes [14, 15]. From Path integral Monte Carlo simulations of the equivalent (2+1)-dimensional classical model we found that for $f = 1/3$, the superconductor to insulator transition for increasing ratio g of the charging energy to the Josephson coupling is first order. For $f = 0$ and $f = 1/2$, the transition is second order and the corresponding correlation length exponents are estimated from finite-size scaling. Since the critical coupling $g_c(f = 1/2)$ is significantly smaller than $g_c(f = 0)$, magnetoresistance measurements in the insulating side near the $f = 0$ transition should display oscillations with minima at integer values $f = n$ and maxima at $f = n + 1/2$. This is in fact observed experimentally at low temperatures in superconducting films with a triangular pattern of nanoholes [15]. The $f = 1/2$ case is of particular interest

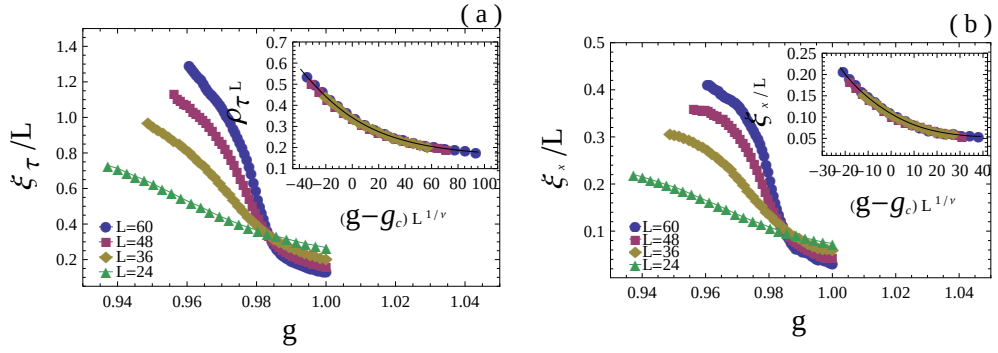


Figure 3. (a) Behavior of the scaled correlation length in the time direction ξ_τ/L for $f = 1/2$, for different systems sizes L. Inset: scaling plot for data near the transition and systems sizes $L \geq 36$ with $g_c = 0.9836$ and $\nu = 0.44$. b) Behavior of the scaled correlation length in the $\hat{x}$ spatial direction ξ_x/L for $f = 1/2$. Inset: corresponding scaling plot with $g_c = 0.9845$ and $\nu = 0.48$.

because even without charging effects, geometrical frustration and thermal fluctuations leads to an unusal phase transition as function of temperature, which is still not well understood [14, 19]. It should also be interesting to investigate the universal resistivities at the transition for $f = 1/2$ and $f = 0$ in comparison to the results obtained earlier for the same model defined on a square lattice [7, 11].

5. Acknowledgments

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