Strong-Weak Coupling Self-Duality in the Two-Dimensional Quantum Phase Transition of $p + ip$ Superconducting Arrays

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The 2D quantum phase transition that occurs in a square lattice of Josephson-coupled $p \pm ip$ superconductors is an example of how four-body interactions in $d = 2$ reproduce nonperturbative effects caused by two-body interactions in $d = 1$. The ordered phase has an unconventional "bond order" of the local T-breaking variable. This problem can be analyzed using an exact self-duality; this duality in classical notation is the 3D generalization of the Kramers-Wannier duality of the 2D Ising model, and there are similar exact dualities in dimensions $d \geq 3$. We discuss the excitation spectrum and experimental signatures of the ordered and disordered phases, and the relationship between our model and previously studied behavior of 2D boson models with four-boson interactions.

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Many topical problems in condensed matter physics are described by effective Hamiltonians with explicit three- or four-body interaction terms, even though the underlying Coulomb interaction between particles is only a two-body interaction. An example is the Pfaffian state of paired composite fermions in the fractional quantum Hall effect [1], which is the exact ground state of a three-body interaction [2]; this state has been observed at $\nu = \frac{5}{2}$ [3]. Regular Josephson-junction arrays of a $p + ip$ superconductor such as Sr_2RuO_4 can be modeled by a multiple-spin lattice Hamiltonian [4], as can several models of frustrated magnetism [5] and superconductivity [6]. This Letter considers quantum effects on a classical four-spin Hamiltonian as an improved model of a $p + ip$ superconducting array, and presents several exact results on the resulting 2D quantum phase transition.

This analysis is based on an exact strong-weak coupling self-duality for multiple-spin interactions in high dimensions, generalizing the Kramers-Wannier duality [7] of the classical Ising model in 2D or the quantum Ising chain in 1D. This higher-dimensional self-duality continues recent developments [6,8] showing that phenomena that occur with two-body interactions in one quantum dimension, such as spin-charge separation, can also be realized by three- or four-body interactions in two quantum dimensions. Superconducting arrays and frustrated magnets are important examples of this physics because they can generate three-, four-, or six-spin interactions without two-spin interactions, essentially because of unusual symmetries. There are many known dualities in $d > 2$ that relate a strong-coupling regime of one model to a weak-coupling regime of another model, e.g., the duality between the 3D Ising model and 3D $\mathbb{Z}_2$ lattice gauge theory, but self-dualities are quite rare in $d > 2$ [9].

We start from the following classical model of Ising spins on a square lattice:

$$\beta E = -K \sum_{\square} s_1^{\square} s_2^{\square} s_3^{\square} s_4^{\square}, \tag{1}$$

where $s_i^{\square} = \pm 1$, $i = 1, \ldots, 4$ are Ising variables at the four corners of one face of the lattice, and the sum is over all faces. This model was recently introduced [4] to understand the effects of frustrating geometric phases in a square array of superconducting grains where each grain has either $p + ip$ or $p - ip$ order: the state of grain i is described by both a phase ϕ_i and an Ising variable $s_i = \pm 1$ that determines the order parameter $p + is_i p$.

The same geometric phases that led to the experimental determination of d order in the cuprates [10,11] lead to frustration of the superconductivity unless each plaquette of four grains has an even number of Ising $+1$ spins (and an even number of -1 spins) [4]. The phase Φ acquired by a Cooper pair moving around a plaquette is determined by the states $s_i = \pm 1$ of the four grains at corners $i = 1, \ldots, 4$: $\Phi = \frac{\pi}{2}(s_1 + s_2 + s_3 + s_4)$. This phase is equivalent to zero if the plaquette has an even number of $+1$ spins, and otherwise equivalent to π, which generates the local energy in (1) proportional to $s_1 s_2 s_3 s_4$. Josephson weak links [12] have been made in superfluid He^3, and in one phase the symmetries of the weak link break the symmetry group down to $p \pm ip$.

The classical model (1) also describes the two-dimensional "right-angle water" ice model [13] and maps onto to a case of the eight-vertex model [4,14]. Note that (1) is not ordinary 2D $\mathbb{Z}_2$ gauge theory, where the sum is over bond variables σ_i around each face. The overall symmetry group is much smaller for (1): $\mathrm{Vol}(G') = 2^{N_x + N_y}$ rather than the full gauge group $\mathrm{Vol}(G) = 2^{N_x N_y}$ of $\mathbb{Z}_2$ gauge theory. The problem (1) has a one-dimensional ground-state degeneracy $2^{N_x + N_y}$ even with no physical boundary (e.g., on a torus). The model can be solved in the thermodynamic limit for all K: its free energy per face is just $\beta f = -\log(2\cosh K)$, since all

the face variables can be chosen independently. The model is equivalent to the 1D Ising model and has no phase transition.

The model becomes quantum mechanical in the presence of a transverse magnetic field:

$$H = -K\sum_{\square}\sigma_1^z\sigma_2^z\sigma_3^z\sigma_4^z - h\sum_i \sigma_i^x. \tag{2}$$

Here again the K interaction is around a plaquette but now the spin is a quantum spin-half and the σ are Pauli matrices. In the superconducting array realization, the magnetic field h corresponds to tunneling between the two order parameters $p \pm ip$, which will in the limit of strong tunneling induce a single real order parameter p_x. Application of pressure in Sr_2RuO_4 is found experimentally to drive the system toward a real p state [15], but the explanation of this effect is unclear. The model (2) is clearly one of the simplest possible 2D lattice quantum Hamiltonians with four-spin interactions. The main weakness of the model (2) is that in the real system at low T there is a long-ranged vortex-vortex interaction between frustrated plaquettes [4]; the Hamiltonian (2) corresponds to treating the core energy of a vortex but not its interaction with other vortices, as might be appropriate at higher temperatures.

We now show that the quantum model (2) has a phase transition at zero temperature when K/h is exactly one. For simplicity we will give the model's self-duality here in its classical form; the same duality can be shown directly in the quantum model (2) and interchanges K and h [16]. The 3D anisotropic classical model

$$\beta E = -\tilde{K}\sum_{\square} s_1^{\square}s_2^{\square}s_3^{\square}s_4^{\square} - J_z\sum_b s_1^b s_2^b, \tag{3}$$

where $\square$ ranges over all plaquettes in the xy planes, and b ranges over all bonds in the z direction (Fig. 1), will be shown to have a phase transition along the line

$$\sinh 2\tilde{K}\sinh 2J_z = 1. \tag{4}$$

The connection between coupling constants in the classical model and in the quantum model is standard [17]:

$$\tilde{K} = aK, \qquad e^{-2J_z} = \tanh(ah), \qquad T = \frac{1}{Ma}, \tag{5}$$

where a is the lattice spacing and M the number of sites in the z direction of the classical model, and T is the temperature in the quantum case.

The quantum-classical mapping becomes exact in the limits $T \to 0$, $a \to 0$, and $M \to \infty$. Knowing the phase transition line in the classical model (4) fixes the quantum transition because in the above limits

$$\sinh 2\tilde{K}\sinh 2J_z \to \tilde{K}e^{2J_z} = K/h = 1. \tag{6}$$

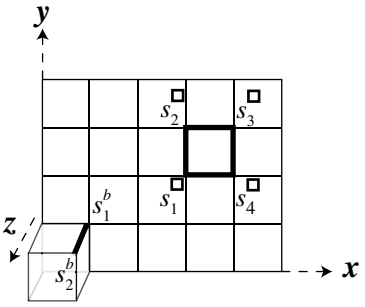

FIG. 1. The classical anisotropic 3D problem that describes the quantum critical point of the model (2). The two types of interactions (shaded bonds) are plaquette interactions in the planes normal to $\hat{\mathbf{z}}$, and bond interactions along $\hat{\mathbf{z}}$.

The partition function of the above model is

$$\begin{aligned} Z &= \sum_{\{s\}} e^{-\beta E} \\ &= \sum_{\{s\}}\prod_{\square}[(\cosh\tilde{K} + s_1^{\square}s_2^{\square}s_3^{\square}s_4^{\square}\sinh\tilde{K}) \\ &\quad \times \prod_b (\cosh J_z + s_1^b s_2^b \sinh J_z)]. \end{aligned} \tag{7}$$

Introduce face variables $k_{\square} = 0, 1$ and bond variables $k_b = 0, 1$, and define $c_0 = \cosh\tilde{K}$, $c_1 = \sinh\tilde{K}$, $d_0 = \cosh J_z$, $d_1 = \sinh J_z$. Then

$$Z = \sum_{\{s\}}\sum_{k_{\square}}\sum_{k_b}\left\{\left[\prod_{\square} c_{k_{\square}}(s_1^{\square}s_2^{\square}s_3^{\square}s_4^{\square})^{k_{\square}}\right]\times\left[\prod_b d_{k_b}(s_1^b s_2^b)^{k_b}\right]\right\}. \tag{8}$$

Now the spin sum can be evaluated: for each spin the result is 2 if the spin is raised to an even power, and 0 otherwise. Z is a constrained sum over the k variables:

$$Z = 2^N {\sum_{k_{\square},k_b}}' \left(\prod_{\square} c_{k_{\square}}\right)\left(\prod_b d_{k_b}\right). \tag{9}$$

Here $N = N_x N_y N_z$ is the total number of sites. Each site of the original lattice appears via 4 face terms and 2 bond terms. The constraint is that the sum of the six k variables be an even number for every site.

Now introduce dual variables to solve the constraint. The dual spins σ are located at the centers of the fundamental cubes of the original cubic lattice. For a site i of the original lattice, its four neighboring spacelike faces are pierced by four vertical bonds of the dual lattice, and for each piercing bond b of the dual lattice fix the relation $k_{\square} = \frac{1}{2}(1 - \sigma_1^b\sigma_2^b)$. Each of the two vertical bonds b containing site i pierces a spacelike face $\square$ of the dual lattice, and we set $k_b = \frac{1}{2}(1 - \sigma_1^{\square}\sigma_2^{\square}\sigma_3^{\square}\sigma_4^{\square})$.

These variables satisfy the constraint since the eight dual lattice sites $\sigma_1, \ldots, \sigma_8$ around an original site satisfy

$$k_{\square 1} + k_{\square 2} + k_{\square 3} + k_{\square 4} + k_{b1} + k_{b2} = 3 - \frac{1}{2}(\sigma_1\sigma_2\sigma_3\sigma_4 + \sigma_5\sigma_6\sigma_7\sigma_8 + \sigma_1\sigma_5 + \sigma_2\sigma_6 + \sigma_3\sigma_7 + \sigma_4\sigma_8) \equiv 0 \bmod 2. \tag{10}$$

This holds if all spins are up, and flipping any spin changes the sum by an even number. Next we need to find how many dual spin configurations correspond to one configuration of the k variables. The answer is just the size of the gauge group $\mathrm{Vol}(G') = 2^{N_x+N_y}$, since once the dual spin configuration is set on a spacelike plane, the vertical bonds fix the configuration everywhere else.

The last step is to calculate the dual couplings. Writing

$$c_k = k \sinh\tilde{K} + (1-k)\cosh\tilde{K}, \tag{11}$$

for a face $\square$ of the original lattice, pierced by Ising bond b in the dual problem,

$$\begin{aligned} c_{k_\square} &= \frac{1+\sigma_1^b\sigma_2^b}{2}\cosh\tilde{K} + \frac{1-\sigma_1^b\sigma_2^b}{2}\sinh\tilde{K} \\ &= \frac{e^{\tilde{K}}}{2}(1+\sigma_1^b\sigma_2^b\tanh J_z^*) = \frac{1}{\sqrt{2\sinh 2J_z^*}} e^{J_z^*\sigma_1^b\sigma_2^b}, \end{aligned} \tag{12}$$

where $\tanh J_z^* = e^{-2\tilde{K}}$. By the same process

$$d_{k_b} = \frac{1}{\sqrt{2\sinh 2\tilde{K}^*}} e^{\tilde{K}^*\sigma_1^\square\sigma_2^\square\sigma_3^\square\sigma_4^\square}, \tag{13}$$

with $\tanh\tilde{K}^* = e^{-2J_z}$.

Now we combine the above results: the number of bonds parallel to $\hat{\mathbf{z}}$ and the number of spacelike faces are both $N = N_xN_yN_z$, so we have up to boundary terms

$$Z(\tilde{K}, J_z) = \frac{Z(\tilde{K}^*, J_z^*)}{\mathrm{Vol}(G')\sinh(2J_z^*)^{N/2}\sinh(2\tilde{K}^*)^{N/2}}. \tag{14}$$

More precisely, we have shown that in the limit $N \to \infty$,

$$\begin{aligned} \frac{\log Z(\tilde{K}, J_z)}{N} &= \frac{\log Z(\tilde{K}^*, J_z^*)}{N} - \frac{1}{2} \\ &\quad \times \log\sinh(2\tilde{K}^*) - \frac{1}{2}\log\sinh(2J_z^*). \end{aligned} \tag{15}$$

The duality relation for the couplings is

$$\sinh(2J_z^*) = \frac{1}{\sinh(2\tilde{K})}, \quad \sinh(2\tilde{K}^*) = \frac{1}{\sinh(2J_z)}. \tag{16}$$

This determines the entire phase boundary line in the $(\tilde{K}, J_z)$ plane. It also shows that there is a hidden symmetry between the couplings $\tilde{K}$ and J_z. The same construction leads to an exact duality of the 4D model with eight-spin interactions around spacelike cubes, plus a bond interaction in the fourth dimension; and similarly for any $d \geq 2$. The self-dual point is $\tilde{K} = J_z = K_c = \frac{1}{2} \times \log(1+\sqrt{2})$. If there is only one phase transition in the model at finite coupling, it must be at the self-dual line. The self-duality of this model is similar to the classical anisotropic self-dual Villain $\mathbb{Z}_N$ models studied in [9].

We remark that the model can be solved if the system has only one row of spacelike plaquettes: the bond variables $b_x = s_{x,1}s_{x,2}$ become spins in an anisotropic 2D Ising model, and with $e^{2J'} = \cosh 2J_z$,

$$\frac{\log Z_{N_x\times 2\times N_z}(\tilde{K}, J_z)}{N_xN_z} = \frac{\log Z^{2DI}_{N_x\times N_z}(2\tilde{K}, J')}{N_xN_z}. \tag{17}$$

If there is a single second-order transition in the 3D classical model, then there is a second-order transition at $K = h$ in the quantum model. The spontaneous order that develops across the transition is unconventional "bond order." At $h = 0$, the ground states all have long-range order along every row of the vertical bond $\sigma_i^z\sigma_{i+\hat{y}}^z$, and of horizontal bonds along each column. Another way to describe the $h = 0$ ordered state is using the Wilson operator for the product of spins around a loop $\mathcal{L}$,

$$W(\mathcal{L}) = \prod_{i\in\mathcal{L}}\sigma_i^z. \tag{18}$$

In any ground state, $\langle W(\mathcal{L})\rangle = 1$. We will use bond order below to make a connection between the order parameter and the excitation spectrum. The two orders are connected since a closed loop contains an even number of bonds from each row and column.

A Peierls-type argument can be used to show that there is an ordered phase of the classical 3D model at low temperature, and hence at least one phase transition. We have performed Monte Carlo and high-temperature series calculations to check whether the above model has a single second-order phase transition (which must then lie at the self-dual point K_c). The results are consistent with this picture, but the single-spin Monte Carlo algorithm becomes very slow close to criticality, as in [18].

The high-temperature series proves that this model does not have the same free energy per site as an Ising model, as might have been suspected since the classical 2D model with face interactions (1) has the same free energy per site as the 1D two-spin Ising model. The first terms for the classical symmetric model ($\tilde{K} = J_z$) are

$$\begin{aligned} c &= T\frac{\partial s}{\partial T} = -T\frac{\partial^2 F}{N(\partial T)^2} \\ &= 2\tilde{K}^2 - 2\tilde{K}^4 + 94\tilde{K}^6/3 + O(\tilde{K}^8). \end{aligned} \tag{19}$$

This differs from the $d \geq 2$ two-spin Ising model at order $\tilde{K}^4$ and the $d = 1$ two-spin Ising model at order $\tilde{K}^6$.

The quantum model (2) has an infinite but nonextensive set of conservation laws: along any one of the N_y rows, say $\mathcal{R}$, the product

$$\hat{O}_{\mathcal{R}} = \prod_{i\in\mathcal{R}}\sigma_x^i \tag{20}$$

commutes with the Hamiltonian (2), and similarly for each of N_x columns. These $N_x + N_y$ conserved quantities are related to the ground-state degeneracy in the ordered state. There are $2^{N_x+N_y}$ sectors of the theory, labeled by the eigenvalues of the operators (20). In the large-h phase, there is a single ground state invariant under $N_x + N_y$ transformations that each act on all the spins in one row or

column via

$$\sigma_x \to \sigma_x, \qquad \sigma_y \to -\sigma_y, \qquad \sigma_z \to -\sigma_z. \tag{21}$$

At the transition $K = h$ in the thermodynamic limit, these symmetries are spontaneously broken and there are $2^{N_x+N_y}$ degenerate ground states once $K > h$. In a finite system, there is no spontaneous symmetry breaking and ground-state degeneracy on the ordered side $K > h$ will be split by an amount exponentially small in $\min(N_x, N_y)$. The breaking of these many symmetries at a single transition occurs because of the infinite number of conservation laws. In the language of hard-core bosons, the charge along each row or column is conserved modulo 2, just as in the Bose metal model discussed in [6].

Now we consider the excitation spectrum in the two phases of the quantum model. Recall the familiar quantum Ising chain ($d = 1$) [17]: the lowest excitation in the ordered phase with periodic boundary conditions is to flip one spin from the ground state, so the first excited state contains two bad bonds. These two bad bonds can be separated into two kinks, with a string of flipped spins between them. In the large h limit, all the spins point along $\hat{\mathbf{x}}$ and the one-particle state is a flipped spin with momentum and kinetic energy, with

$$\epsilon_k = Kh[2 - 2/h\cos(k) + O(1/h^2)]. \tag{22}$$

For our model in 2D, in the large K limit the system stays near the ground state manifold, and the first excited state locally connected to the ground state is obtained by flipping one spin. This flipped spin results in four bad plaquettes (or four $\mathbb{Z}_2$ vortices). As in the $d = 1$ case, this excitation can disintegrate into four fractional excitations, which become four vertices of a rectangle with all the interior spins flipped.

The large-h limit requires more attention. In the $\hat{\mathbf{x}}$ basis, it is clear that the single flipped spin is nondispersive because of the $\mathbb{Z}_2$ conservation laws. The single flipped spin in the large-h limit is equivalent via duality to a single bad plaquette in the large-K limit. Instead, the lowest mobile state is a flipped bond: the flipped bond can hop in one direction, the direction perpendicular to the bond, and its dispersion relation is the same as that in the $d = 1$ case (22). These one-particle states can scatter off each other, and because they hop unidirectionally, this kind of scattering is very similar to 1D scattering. The ordered state at small h is a condensation of bonds.

Direct experimental observation of the order-parameter state of a superconducting grain is currently possible only for isolated superconducting grains. However, there are several experimental signatures of the bond ordering predicted above, even though in the ground state the system has no frustrating fluxes and hence is uniform from the superconducting point of view. The gapless fluctuations near the transition will modify the specific heat and transport in the system: transport will be attenuated near the critical point by scattering off the fluctuations, while specific heat will show a peak. The true spin action in a $p + ip$ superconducting array is more complicated and includes long-ranged interactions between frustrated plaquettes [4], but it has the same gauge symmetries as (2). If grain orders could be measured at the array boundary, the directionality of the predicted bond ordering would be seen, and the Ising variables of each neighboring pair of grains develop a symmetry-breaking correlation at the transition.

An unresolved question is whether (2) is a free-fermion model like 1D quantum Ising. We have not found additional conservation laws beyond ordinary symmetries and the infinitely many $\mathbb{Z}_2$ laws described above. A solution of this 2D quantum model would give further insight into the physics of explicit four-point interactions.

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