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Exactly solvable pairing model for superconductors with $p_x + ip_y$-wave symmetry

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We present the exact Bethe ansatz solution for the two-dimensional BCS pairing Hamiltonian with $p_x + ip_y$ symmetry. Using both mean-field theory and the exact solution we obtain the ground-state phase diagram parametrized by the filling fraction and the coupling constant. It consists of three phases that are denoted weak-coupling BCS, weak pairing, and strong pairing. The first two phases are separated by a topologically protected line where the exact ground state is given by the Moore-Read pfaffian state. In the thermodynamic limit the ground-state energy is discontinuous on this line. The other two phases are separated by the critical line, also topologically protected, previously found by Read and Green. We establish a duality relation between the weak and strong pairing phases, whereby ground states of the weak phase are "dressed" versions of the ground states of the strong phase by zero energy (Moore-Read) pairs and characterized by a topological order parameter.

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In 1957, Bardeen, Cooper, and Schrieffer[1] (BCS) published an epoch defining paper giving a microscopic explanation of the properties of superconducting metals at low temperatures. The model was based on a reduced Hamiltonian which describes the pairing interaction between conduction electrons. The original study of the BCS model was formulated in the grand-canonical ensemble and solved with a mean-field approximation. In 1963 Richardson[2] derived the exact solution of the reduced BCS Hamiltonian with s-wave symmetry in the canonical ensemble. This solution was largely unnoticed until its rediscovery in the theoretical studies of ultrasmall metallic grains in the 1990s, where it was employed to understand the crossover between the fluctuation dominated regime and the fully developed superconducting regime (for a review see Ref. 3). The exact solution for the s-wave BCS model is related to the Gaudin spin Hamiltonians, and their integrability can be understood in the general framework of the quantum inverse scattering method.[4,5] These later developments allowed for an exact computation of various correlators,[4,6,7] and led to generalizations of the Richardson-Gaudin models with applications to condensed matter and nuclear physics.[3,8]

In this Rapid Communication we analyze the two-dimensional (2D) BCS model where the symmetry of the pairing interaction is $p_x + ip_y$ (hereafter referred to as $p+ip$). The Hamiltonian of the model is

$$H = \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \frac{G}{4m} \sum_{\mathbf{k} \neq \mathbf{k}'} (k_x - ik_y)(k'_x + ik'_y) c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger c_{-\mathbf{k}'} c_{\mathbf{k}'}, \tag{1}$$

where $c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger$ are destruction and creation operators of 2D spinless or polarized fermions with momentum $\mathbf{k}$, m is their mass, and G is a dimensionless coupling constant which is positive for an attractive interaction. The $p+ip$ model has attracted considerable attention due to the connection with the Moore-Read (MR) pfaffian state arising in the quantum Hall effect at filling fraction 5/2,[9] which has been proposed to support non-Abelian anyons allowing for topological quantum computation.[10,11] Motivated by these considerations, concrete proposals for engineering the $p+ip$ form of the pairing interaction have been formulated in the context of cold Fermi gases.[12,13] Here we will study the model through the exact Bethe ansatz solution. We remark that exact solvability holds independent of the choice for the ultraviolet cutoff, which we denote as ω, and independent of the distribution of the momenta $\mathbf{k}$. In particular this means that a one-dimensional system is obtained by simply setting all $k_y = 0$. Unless stated otherwise, all discussions below deal with finite particle numbers in a finite-sized system.

Using the standard mean-field theory approach Read and Green (RG) showed[14] the existence of a second-order phase transition governed by the chemical potential μ. Adopting the terminology of Ref. 14, this transition takes place between a weak pairing phase ($\mu > 0$), the ground state (GS) of which behaves as the Moore-Read pfaffian state at long distances, and a strong pairing phase (for $\mu < 0$). The spectrum of Bogolioubov quasiparticles is gapless at $\mu = 0$. The GS of the weak pairing phase also has a nontrivial topological structure in $\mathbf{k}$ space, as shown by Volovik.[15] However in the mean-field analysis the weak pairing GS is continuously connected to the weak-coupling BCS GS.[14]

Our goal is to re-examine the properties of the $p+ip$ model. Through this study we will achieve the following. (i) From the mean-field results the ground-state phase diagram will be determined, comprising of the weak-coupling BCS, weak pairing, and strong pairing phases; ii) a duality relation between the weak pairing and strong pairing phases will be shown to exist; iii) from the Bethe ansatz solution the duality will be formulated in terms of a dressing relation involving zero energy MR pairs; iv) dressing of the vacuum will be seen to give the boundary line between weak-coupling BCS and weak pairing phases, representing a zeroth-order quantum phase transition when the thermodynamic limit is taken (cf. Ref. 16 for analogous zeroth-order thermal phase transitions); v) and the weak pairing phase will be shown to have a nontrivial topological structure, related to the dressing operation, which will be quantified by a winding number.

Before presenting the exact solution of the Hamiltonian we first extend the mean-field results reported in Ref. 14. The BCS order parameter associated to Eq. (1) is

$$\hat{\Delta} = \frac{G}{m}\sum_{\mathbf{k}} (k_x + ik_y)\langle c_{-\mathbf{k}}c_{\mathbf{k}}\rangle \tag{2}$$

in terms of which Hamiltonian (1) can be approximated as (up to an additive constant)

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \frac{1}{4}\sum_{\mathbf{k}} [\hat{\Delta}(k_x - ik_y)c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger + \text{h.c.}], \tag{3}$$

where $\xi_{\mathbf{k}}=\mathbf{k}^2/2m-\mu/2$ and $\mu/2$ is the chemical potential. This Hamiltonian can be diagonalized by a Bogoliubov transformation. The gap $\Delta=|\hat{\Delta}|$ and chemical potential are the solutions of the equations

$$\sum_{\mathbf{k}\in\mathbf{K}_+} \frac{\mathbf{k}^2}{\sqrt{(\mathbf{k}^2-\mu)^2+\mathbf{k}^2\Delta^2}} = \frac{1}{G}, \tag{4}$$

$$\mu\sum_{\mathbf{k}\in\mathbf{K}_+} \frac{1}{\sqrt{(\mathbf{k}^2-\mu)^2+\mathbf{k}^2\Delta^2}} = 2M - L + \frac{1}{G}, \tag{5}$$

where we have set that $m=1$, L is the total number of energy levels, and M is the number of Cooper pairs. The set $\mathbf{K}_+$ denotes the set of momenta where $k_x>0$ and any k_y so that we avoid overcounting of energy levels. The mean-field expression for the GS energy is [accounting for the constant term missing in Eq. (3)]

$$E = \frac{1}{2}\sum_{\mathbf{k}\in\mathbf{K}_+} \mathbf{k}^2\left(1 - \frac{2\mathbf{k}^2+\Delta^2-2\mu}{2\sqrt{(\mathbf{k}^2-\mu)^2+\mathbf{k}^2\Delta^2}}\right). \tag{6}$$

Projection of the grand-canonical GS wave function onto a fixed number of M pairs gives

$$|\psi\rangle = \left[\sum_{\mathbf{k}\in\mathbf{K}_+} g(\mathbf{k})c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger\right]^M |0\rangle, \tag{7}$$

where $g(\mathbf{k})=[2E(\mathbf{k})-\mathbf{k}^2+\mu]/[(k_x+ik_y)\hat{\Delta}^*]$ and $E(\mathbf{k})$ is the quasiparticle energy spectrum,

$$E(\mathbf{k}) = \frac{1}{2}\sqrt{(\mathbf{k}^2-\mu)^2+\mathbf{k}^2\Delta^2}. \tag{8}$$

Note that the spectrum is gapless at $\mu=0$ as $|\mathbf{k}|\to 0$. Furthermore, the behavior of $g(\mathbf{k})$ as $\mathbf{k}\to 0$ depends on the sign of μ,[14]

$$g(\mathbf{k}) \sim \begin{cases} k_x - ik_y, & \mu<0, \\ 1/(k_x+ik_y), & \mu>0. \end{cases} \tag{9}$$

In real space (7) takes the form of a pfaffian,

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_{2M}) = \mathcal{A}[g(\mathbf{r}_1-\mathbf{r}_2)\ldots g(\mathbf{r}_{2M-1}-\mathbf{r}_{2M})], \tag{10}$$

where $\mathcal{A}$ denotes the antisymmetrization of the positions and $g(\mathbf{r})$ is the Fourier transform of $g(\mathbf{k})$. We will refer to the case $\mu=0$ as the RG state. For $\mu>0$ the large distance behavior is $g(\mathbf{r})\sim 1/(x+iy)$, which asymptotically reproduces the MR state.[14]

The solution of Eqs. (4) and (5) for L energy levels and M number of pairs can be classified, with the corresponding phase diagram given in Fig. 1 parametrized by the filling fraction $x=M/L$ and the rescaled coupling constant $g=GL$. We now demonstrate how the topological aspects of the phase diagram can be deduced in a transparent manner. From Eq. (5) we see that $\mu=0$ imposes the relation $x_{\mathrm{RG}}=(1-g^{-1})/2$. This result is completely independent of the momentum distribution and choice of cutoff, reflecting the topological nature of the transition discussed in Ref. 14; i.e., the boundary line is protected from perturbations of the system which alter the distribution of the momenta. Furthermore we identify a second topological boundary by setting $\mu=\Delta^2/4$, which from Eq. (6) gives $E=0$, again independent of the momenta. Using Eqs. (4) and (5) it is found that this occurs when $x_{\mathrm{MR}}=1-g^{-1}$. Later we will show that in this instance the GS is a discrete analog of the MR state mentioned earlier, which in the thermodynamic limit is exactly the MR state.

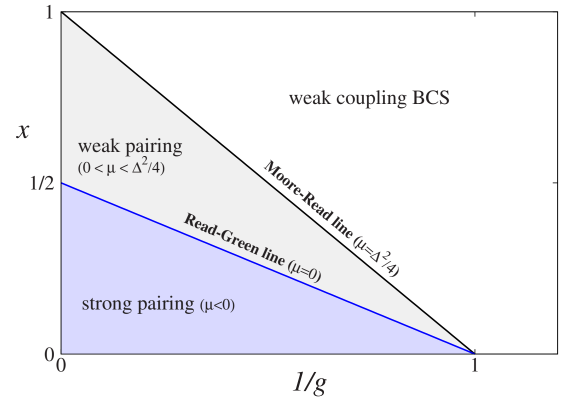

FIG. 1. (Color online) Ground-state phase diagram of the $p+ip$ model in terms of the inverse coupling $1/g$ and filling fraction $x=M/L$. Phase boundaries are given by the Read-Green line ($\mu=0$) and the Moore-Read line ($\mu=\Delta^2/4$) (Ref. 17). The phase boundaries are independent of the choice of the momentum distribution and independent of the ultraviolet cutoff.

A further notable $\mathbf{k}$-independent property of the phase diagram is the existence of a "duality" between a point (g,x_I) in the weak pairing regime and another point (g,x_{II}) in the strong pairing regime related by

$$x_I + x_{II} = x_{\mathrm{MR}} \equiv 1 - \frac{1}{g}, \tag{11}$$

which necessarily can only hold for rational values of g. In the mean-field analysis this duality means that the corresponding solutions are related by $\mu_I=-\mu_{II}$ and $\Delta_I^2-2\mu_I=\Delta_{II}^2-2\mu_{II}$ such that the GS energies satisfy $E_I=E_{II}$ according to Eq. (6). The RG state is self-dual, whereas the MR state is dual to the vacuum. This duality is apparent in the exact solution where it will be shown to be related to a dressing operation mentioned in the introduction.

The detailed derivation of the exact Bethe ansatz solution will be presented elsewhere. Here we simply mention that the technical aspects follow the derivation of the s-wave model solution through the quantum inverse scattering method, as described in Refs. 4 and 5. The only fundamental difference is that the R-matrix solution of the Yang-Baxter

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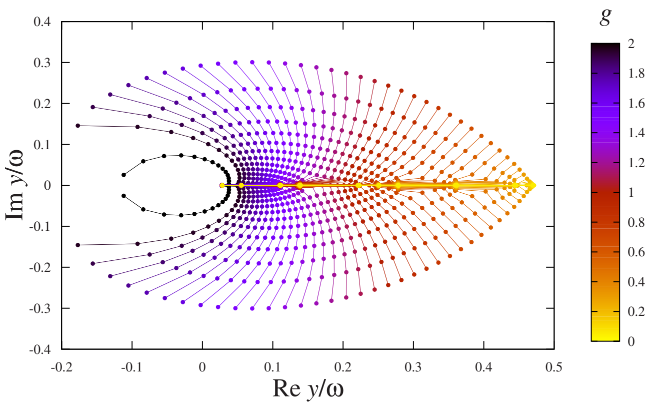

FIG. 2. (Color online) Numerical solutions for the ground-state roots $y_j (j=1,\ldots,M)$ of the BAEs [Eq. (13)] with $M=31$, $L=62$, and $0<g<1.99$. For this range of couplings the system is in the weak-coupling BCS phase. The maximal pairing energy (the cutoff) is denoted ω. At the critical coupling $g=2$ (MR line) all the roots collapse to the origin (not shown).

equation used to solve the $p+ip$ model is the trigonometric *XXZ* solution, in contrast to the rational *XXX* solution used for the s-wave model.

We again set $m=1$. The exact eigenstates of the Hamiltonian with M fermion pairs are given by

$$|\psi\rangle = \prod_{j=1}^{M} C(y_j)|0\rangle, \quad C(y) = \sum_{\mathbf{k}\in \mathbf{K}_+} \frac{k_x - ik_y}{\mathbf{k}^2 - y} c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger}, \tag{12}$$

where the rapidities $y_j, j=1,\ldots,M$ satisfy the Bethe ansatz equations (BAEs)

$$\frac{q}{y_j} + \frac{1}{2}\sum_{\mathbf{k}\in\mathbf{K}_+} \frac{1}{y_j - \mathbf{k}^2} - \sum_{l\neq j}^{M} \frac{1}{y_j - y_l} = 0, \tag{13}$$

with $2q=1/G-L+2M-1$. The total energy of state (12) is given by

$$E = (1+G)\sum_{j=1}^{M} y_j. \tag{14}$$

Numerical solutions of the Bethe ansatz equations indicate that there are no unpaired fermions in the GS when the fermion number is even. In Fig. 2 we present numerical GS solution of Eq. (13). This solution is obtained starting from the initial condition $y_j \to (1+G)\mathbf{k}^2 (j=1,\ldots,M)$ as $G\to 0$, with the $\mathbf{k}$ chosen to fill the Fermi sea. As g increases, the roots y_j closest to the Fermi level become complex pairs. When g approaches the MR line the roots bend toward the origin (as shown in Fig. 2) and at the value $g^{-1}=1-x$ all the roots collapse onto the origin (not shown). At larger values of g one enters the weak pairing phase where all the roots are nonzero, except at some rational values of g where a fraction of the roots collapses again. Finally, in the strong pairing regime all the roots become real and they belong to an interval on the negative real axis.

Looking closer at the weak pairing phase, one can check that the M_W roots y_j can be split into M_0 vanishing roots and M_S nonzero roots provided that

$$\frac{M_0}{L} + 2\frac{M_S}{L} = 1 - \frac{1}{g}. \tag{15}$$

Moreover the M_S nonzero roots satisfy BAE (13) in the strong pairing region. Altogether this implies that given an eigenstate, say $|S\rangle$, in the strong pairing regime then one can dress it with M_0 MR pairs [as given by Eq. (15)] obtaining an eigenstate $|W\rangle$ in the weak pairing phase with the same energy; i.e.,

$$H|S\rangle = E|S\rangle \Rightarrow H|W\rangle = H[C(0)]^{M_0}|S\rangle = E|W\rangle.$$

Noticing that the filling fraction of the strong pairing state is $x_S=M_S/L$ and that of the weak pairing state is $x_W=(M_0+M_S)/L$, we find that Eq. (15) coincides with duality relation (11). The physical picture we obtain from this discussion is that the fermion pairs forming the GS in the weak pairing phase are of two types: the strong localized pairs with negative energy and the delocalized MR pairs with zero energy. This picture is substantially different from projected mean-field wave function (7), which is more akin to a condensate of Cooper pairs in the same one-particle state. An exception to this occurs on the MR line, where the projected mean-field and exact wave functions are identical. We see from Eq. (12) that when all roots of the Bethe ansatz equations are zero, the GS is a discrete analog of the MR state with zero energy in agreement with mean-field theory.

We reiterate that until now all our analyses have been in the context of finite-sized systems, and in particular the topological (i.e., $\mathbf{k}$ independent) nature of duality (11) is not dependent on taking the thermodynamic limit. In going to the thermodynamic limit we take $L,M\to\infty$, $G\to 0$ with $x=M/L$ and $g=GL$ fixed. A peculiar feature of the MR line is the discontinuity of the GS energy $E(g,x)$ in the thermodynamic limit as the filling fraction x approaches the value $x_{\rm MR}$ from the weak pairing region. To derive this result, for finite L we take the one-pair state and dress it to give the dual GS in the weak pairing region. The filling x_I of the dressed state is given by Eq. (11), setting $x_{II}=1/L$, i.e., $x_I=x_{\rm MR}-1/L$, which approaches $x_{\rm MR}=1-1/g$ as $L\to\infty$. Since the MR pairs carry no energy, the GS energy of the dressed state coincides with the one-pair energy. To compute this energy we consider the BAE for one Cooper pair and take the continuum limit [i.e., Eq. (13) with $M=1$]. Settting $\epsilon=\mathbf{k}^2$ and ω as the cutoff, for simplicity we take the momentum distribution to be that for free particles in two dimensions; i.e., $\rho(\epsilon)=\omega^{-1}$. This leads to

$$L - \frac{1}{G} - 1 = \sum_{\mathbf{k}\in\mathbf{K}_+} \frac{y}{y-\mathbf{k}^2} \Rightarrow 1 - \frac{1}{g} = y\int_0^{\omega} \frac{d\epsilon}{\omega}\frac{1}{y-\epsilon}.$$

This equation has a unique negative energy solution $y<0$ satisfying

$$1 - \frac{1}{g} = \frac{y}{\omega}\log\left(\frac{y}{y-\omega}\right),$$

which we denote as $y=\mathcal{E}(g)$. From here one derives the aforementioned discontinuity on the MR line $x_{\rm MR}=1-g^{-1}$,

$$\lim_{L\to\infty} E(g,x_l) = \mathcal{E}(g) \neq E(g,x_{\mathrm{MR}}) = 0,$$

which may be described as a zeroth-order quantum phase transition. This is a rare example of a zeroth-order quantum phase transition in a many-body system. We have also numerically analyzed the excited states on the MR line obtained by blocking the energy levels which are occupied by unpaired electrons. These excitations have a gap whose value agrees with the mean-field result, suggesting that only the RG line is gapless, consistent with mean-field theory predictions.

As mentioned in the introduction, the mean-field solution shows that the weak pairing phase has a nontrivial topological structure in $\mathbf{k}$ space.[14,15] This structure can be characterized by the winding number w of the mean-field wave function $g(\mathbf{k})=g_x(\mathbf{k})+ig_y(\mathbf{k})$, and it is given by,

$$w = \frac{1}{\pi}\int_{\mathbb{R}^2} dk_x dk_y \frac{\partial_{k_x} g_x \partial_{k_y} g_y - \partial_{k_y} g_x \partial_{k_x} g_y}{(1+g_x^2+g_y^2)^2}. \tag{16}$$

One finds that $w=0$ for $\mu<0$ (i.e., strong pairing phase), while $w=+1$ for $\mu>0$ (i.e., weak pairing and weak-coupling BCS phases).[14,15] The existence of an exact solution of the model calls for a generalization of w applicable to the many-body wave function of the model $\psi(\mathbf{k}_1,\ldots,\mathbf{k}_M)$, where $\mathbf{k}_i(i=1,\ldots,M)$ are the distinct momenta of the pairs. This generalization consists of replacing $g(\mathbf{k})$ in Eq. (16) by $\psi(\mathbf{k}+\mathbf{c}_1,\ldots,\mathbf{k}+\mathbf{c}_M)$, where $\mathbf{c}_j \neq \mathbf{c}_l \forall j,l$ are a set of distinct constants. With this definition we find that w vanishes for the exact ground-state wave function except in the weak pairing region where it coincides with the number of MR pairs. Hence w provides a nontrivial topological order parameter for the weak pairing phase which is zero in the other two phases.

In summary, we have provided the exact Bethe ansatz solution for the BCS model with $p+ip$ pairing. Using this we have investigated the ground-state phase diagram, whose structure is richer than previously supposed. We have found that the weak pairing region is dual to the strong pairing region, with the duality being encoded in a dressing transformation between GS of the two phases by means of zero energy MR pairs. The MR state obtained by dressing the vacuum is the exact GS on a line in the phase diagram. The MR line separates the weak pairing and weak-coupling BCS regions, and while the gap does not vanish on it, the GS energy is discontinuous in the thermodynamic limit. We have also found a topological order parameter that characterizes the weak pairing phase. An important future issue is to explore how vortices (e.g., see Ref. 10) can be incorporated into a similar model to the one studied in this Rapid Communication.

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