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Phase Diagram of the BCS–Hubbard Model in a Magnetic Field

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We propose an extended BCS–Hubbard model and investigate its ground state phase diagram in an external magnetic field. By mapping the model onto a model of spinless fermions coupled with conserving Z_2 variables which are mimicked by pseudospins, the model is shown to be exactly solvable along the symmetric lines for an arbitrary on-site Hubbard interaction on the bipartite lattice. In the zero field limit, the ground states exhibit an antiferromagnetic order of pseudospins. In the large field limit, on the other hand, the pseudospins are fully polarized ordered. With the increase of the applied field, a first-order phase transition occurs between these kinds of phases when the on-site Coulomb interaction is less than a critical value $U_{\rm c}$. Above this critical $U_{\rm c}$, a novel intermediate phase emerges between the fully polarized and antiferromagnetic phases. The ground states in this phase are macroscopically degenerate, like in a spin ice, and the corresponding entropy scales linearly with the lattice size at zero temperature.

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Strongly correlated systems, such as high-$T_{\rm c}$ superconductors,[1,2] non-Fermi liquids[3,4] and quantum spin liquids,[5–9] have attracted great interests in recent decades. In these systems, the electron-electron interaction is so strong that the conventional mean-field approximations are no longer applicable. In one dimension, the physical properties of the Hubbard, the Heisenberg and other fundamental models of condensed matter physics can be well understood with the bosonization,[10–12] the Bethe Ansatz[13,14] and other non-perturbative methods. This leads to a thorough understanding of many interesting phenomena, such as the spin-charge separation[15–18] and the Mott physics.[19,20] However, in higher dimensions, there are not many analytical tools that can be used, and exact solutions are available only in very limited cases.

Recently, inspired by the Kitaev honeycomb model, an exactly solvable BCS–Hubbard model on a bipartite lattice in an arbitrary dimension was introduced by Chen *et al.*[21] This model adds a p-wave pairing term to the Hubbard model. It could be reduced to a non-interacting fermion model coupled with quenched Z_2 gauge fields. An extension of this BCS–Hubbard model was introduced by Ezawa[22] to include a Kane–Mele spin-orbit coupling term on the honeycomb lattice. A topological superconducting state was found in the Haldane–BCS–Hubbard model on a honeycomb lattice by Miao *et al.*[23]

In this Letter, we generalize the BCS–Hubbard model to include (a) a spin flip hopping term, (b) a p-wave pairing term by two electrons with opposite spins, and (c) an external magnetic field, and show that this model is exactly solvable along the symmetric lines where the hopping integrals become equal to the corresponding pairing amplitudes. This generalization broadens the range of the integrability of the BCS–Hubbard model and enriches its phase diagram. We solve the model on the symmetric lines and determine the phase diagram of the ground states.

Model. Our model is defined on a bipartite lattice, which can be divided into two sublattices, denoted as A and B, where sites in one sublattice only interact with sites in the other sublattice. The model Hamiltonian reads

$$H = H_1 + H_2 + H_3 + H_4, \tag{1}$$

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where

$$H_1 = \sum_{\langle ij\rangle\sigma} \left(t_1 c^\dagger_{i\sigma} c_{j\sigma} + t_2 c^\dagger_{i\sigma} c_{j\bar{\sigma}}\right) + \text{h.c.}, \tag{2}$$

$$H_2 = \sum_{\langle ij\rangle\sigma} \left(\varDelta_1 c^\dagger_{i\sigma} c^\dagger_{j\sigma} + \varDelta_2 c^\dagger_{i\sigma} c^\dagger_{j\bar{\sigma}}\right) + \text{h.c.}, \tag{3}$$

$$H_3 = U \sum_l \left(c^\dagger_{l\uparrow} c_{l\uparrow} - \frac{1}{2}\right)\left(c^\dagger_{l\downarrow} c_{l\downarrow} - \frac{1}{2}\right), \tag{4}$$

$$H_4 = -ih \sum_l \left(c^\dagger_{l\uparrow} c_{l\downarrow} - c^\dagger_{l\downarrow} c_{l\uparrow}\right). \tag{5}$$

Here, $c_{l\sigma}$ is the annihilation operator of electron with spin σ at site l. In this study, we use i and j to represent the sites on A and B, respectively; $\langle ij\rangle$ indicates that i and j are nearest neighboring sites; t_1 and t_2 are the hopping integrals without and with spin flip, respectively. H_2 is the triplet pairing term. Two paired electrons can be in one of the three basis states of a spin triplet, whose z-component of the total spin, S_z, equals 1, 0, and -1, respectively. $\varDelta_1$ and $\varDelta_2$ are the pairing amplitudes, corresponding to the pairing states with $S_z = \pm 1$ and 0, respectively. H_3 is the on-site Hubbard interaction. H_4 is the Zeeman interaction of electrons imposed by an external magnetic field applied along the y-axis. The BCS–Hubbard model, first introduced by Chen *et al.*, contains just the t_1, $\varDelta_1$ and U terms. For simplicity, we still call it the BCS–Hubbard model.

In the symmetric case where the hopping constants become strongly correlated with the pairing amplitudes, i.e., $\varDelta_1 = t_1$ and $\varDelta_2 = t_2$, it can be shown that the above Hamiltonian is equivalent to a model of spinless fermions interacting only with static Z_2 site-variables.[23] For each given configuration of these Z_2 variables, the model is described by a Hamiltonian of non-interacting fermions. This reduces a complex quantum many-body problem to a single-particle one, which allows us to solve this model on large lattice systems. Hence this model is quasi-exactly solvable.

In this work, we discuss the solution for the symmetric case only. Let us start by introducing the Majorana fermion representation of electrons,

$$c_{l\uparrow} = \frac{\gamma_{l1} + i\gamma_{l2}}{2}, \qquad c_{l\downarrow} = \frac{\gamma_{l3} + i\gamma_{l4}}{2}. \tag{6}$$

The electron operators at each site are decomposed into four Majorana fermion operators $\gamma_{i\eta}$ ($\eta = 1, 2, 3, 4$). In this representation, the Hamiltonian becomes

$$\begin{aligned} H_{\rm s} =& -i \sum_{\langle ij\rangle} [t_1(\gamma_{i2}\gamma_{j1} + \gamma_{i4}\gamma_{j3}) \\ &+ t_2(\gamma_{i2}\gamma_{j3} + \gamma_{i4}\gamma_{j1})] - \frac{U}{4}\sum_l \gamma_{l1}\gamma_{l2}\gamma_{l3}\gamma_{l4} \\ &+ \frac{ih}{2}\sum_l (\gamma_{l1}\gamma_{l3} + \gamma_{l2}\gamma_{l4}). \end{aligned} \tag{7}$$

We add a subscript s to emphasize that this is the Hamiltonian along the symmetric line. In this Hamiltonian, only half of the Majorana modes, namely the even Majorana modes, γ_{i2} and γ_{i4}, on sublattice A, and odd Majorana modes, γ_{j1} and γ_{j3}, on sublattice B, emerge in the first two terms. The other two Majorana modes, i.e., γ_{i1} and γ_{i3} on the A sublattice and γ_{j2} and γ_{j4} on the B sublattice, do appear in the other terms of $H_{\rm s}$. It should be noticed that these operators always appear in pairs. This suggests that

$$D_l = i\gamma_{l1}\gamma_{l3}\delta_{l\in A} + i\gamma_{l2}\gamma_{l4}\delta_{l\in B} \tag{8}$$

is a conversing operator. Indeed, it is straightforward to show that D_l commutes with $H_{\rm s}$. Thus the values of $\{D\}_N = (D_1, \dots D_N)$ on the whole lattice are conserved, N is the lattice size. D_l is a Z_2 operator because $D_l^2 = 1$. It takes two values $D_l = \pm 1$, which can be effectively regarded as the two eigenvalues of an $S = 1/2$ pseudospin operator.

The Hamiltonian is block diagonal according the values of these quasispin variables $\{D\}_N$. This allows us to reduce $H_{\rm s}$ into a quadratic Hamiltonian of fermions. To see this more clearly, let us introduce a set of fermion operators on the two sublattices,

$$a_i = \frac{1}{2}(\gamma_{i2} + {\rm i}\gamma_{i4}), \qquad a_j = \frac{1}{2}(\gamma_{j1} + {\rm i}\gamma_{j3}). \tag{9}$$

In terms of these spinless fermion operators, the Hamiltonian can be expressed as

$$\begin{aligned} H_{\rm s} =& \sum_{\langle ij\rangle} \left[2it_1\left(a^\dagger_j a_i - a^\dagger_i a_j\right) - 2t_2\left(a_i a_j + a^\dagger_j a^\dagger_i\right)\right] \\ &+ \sum_l \left[\left(h - \frac{U}{2}D_l\right)\left(a^\dagger_l a_l - \frac{1}{2}\right) + \frac{h}{2}D_l\right]. \end{aligned} \tag{10}$$

This is an effective BCS mean-field Hamiltonian in the presence of a site-dependent Z_2 potential determined by $\{D\}_N$. It can also be written in a matrix form

$$H_{\rm s} = \varPsi^\dagger M \varPsi. \tag{11}$$

Here, $\varPsi^\dagger = (a_1^\dagger, \dots, a_N^\dagger, a_1, \dots, a_N)$ is a $2N$-dimensional Nambu spinor. M is a matrix defined by

$$M = \begin{pmatrix} \alpha & \beta \\ -\beta & -\alpha^T \end{pmatrix}, \tag{12}$$

where both α and β are $N \times N$ matrices. Moreover, α is a hermitian matrix and β is a real and antisymmetric matrix.

If V is an eigenvector of M with eigenvalue ω, it is straightforward to show that $V' = XV^*$ is also an eigenvector of M with an eigenvalue $-\omega$. Here

$$X = \begin{pmatrix} 0 & I_N \\ I_N & 0 \end{pmatrix}, \tag{13}$$

and I_N is the N-dimensional identity matrix. Hence the eigenvalues of M emerge in pairs. Suppose ω_i ($i = 1, \ldots N$) to be the N non-negative eigenvalues of $H_{\rm s}$, then the ground state energy per site is

$$E_0 = -\frac{1}{N}\sum_{i=1}^{N}\omega_i. \tag{14}$$

The ground state of $H_{\rm s}$ depends on the configuration of pseudospins $\{D\}_N$. The applied magnetic field tends to polarize all the pseudospins. In the strong field limit $|h| \to \infty$, $\{D\}_N$ are fully polarized and form a fully polarized pseudospin state in which $D_l = 1$ or $D_l = -1$ if $h < 0$ or $h > 0$. In the limit $h \to 0$, on the other hand, the pseudospins are antiferromagnetic ordered, where D_l takes opposite values on the two sublattices. In this case, the ground state is at least doubly degenerate because D_l can take value 1 in either of the two sublattices. In these two special limits, the Hamiltonian Eq. (10) can be analytically solved in the thermodynamic limit. The ground state energy per site of the fully polarized state with $D_l = 1$, $E_{\rm FP}$, and the antiferromagnetic ordered state, $E_{\rm AFM}$, are given by the formulas

$$E_{\rm FP} = -4\int_0^{\frac{\pi}{2}}\frac{dk_x}{\pi}\frac{dk_y}{\pi}f_{0,\frac{U}{4}-\frac{h}{2}}(k_x,k_y) + \frac{h}{2}, \tag{15}$$

$$E_{\rm AFM} = -4\int_0^{\frac{\pi}{2}}\frac{dk_x}{\pi}\frac{dk_y}{\pi}f_{\frac{U}{4},\frac{h}{2}}(k_x,k_y), \tag{16}$$

where

$$f_{a,b}(x,y) = \eta_{a,b}(\cos x + \cos y) + \eta_{a,b}(\cos x - \cos y), \tag{17}$$

and

$$\eta_{a,b}(x) = \max\left(\sqrt{a^2 + 4t_1^2x^2}, \sqrt{b^2 + 4t_2^2x^2}\right). \tag{18}$$

More generally, $\{D\}_N$ is neither fully nor antiferromagnetic polarized. To characterize the ground state phase diagram, we introduce the following two order parameters of pseudospins,

$$D^{(+)} = \frac{1}{N}\sum_l D_l, \quad D^{(-)} = \frac{1}{N}\Big|\sum_l (-1)^l D_l\Big|. \tag{19}$$

The states with $D^{(+)} = \pm 1$ and $D^{(-)} = 0$ correspond to the two fully polarized states. The state with $D^{(+)} = 0$ and $D^{(-)} = 1$, on the other hand, corresponds to an antiferromagnetic state.

For a given pseudospin configuration $\{D\}_N$, the Hamiltonian can be diagonalized on a lattice whose size is as large as 10^5. In order to determine the ground state in an arbitrarily given parameter regime, we must scan a large portion of the full configuration space of pseudospins. As the number of the pseudospin configurations grows exponentially with the lattice size, an accurate determination for the spin configuration of the ground state is feasible only on small lattices.

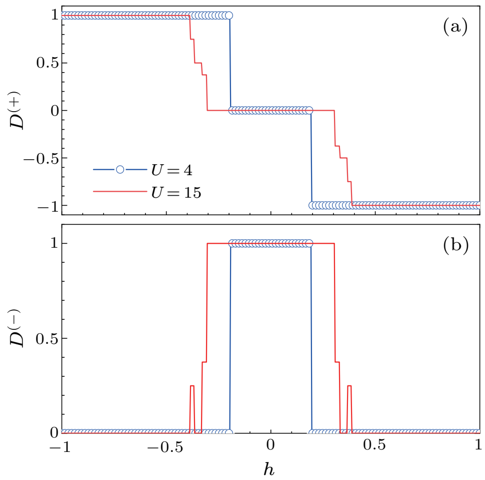

Fig. 1. Field dependence of the pseudospin order parameters $D^{(+)}$ and $D^{(-)}$ for the symmetric BCS–Hubbard model with $t_1 = 1$ and $t_2 = 0.5$.

Phase Diagram. We now explore the phase diagram of the symmetric BCS–Hubbard model on the square lattice. It is simple to show that $H_{\rm s}$ is invariant under the following transformation

$$a_i \to i a_{i+\delta}^\dagger, \quad a_j \to -i a_{j+\delta}^\dagger, \quad D_l \to -D_l, \tag{20}$$

if the direction of the magnetic field h is changed to $-h$. Here δ takes one of the values $(\hat{x}, -\hat{x}, \hat{y}, -\hat{y})$. This transformation swaps the two sublattices. It implies that the phase diagram is symmetric with respect to $h = 0$, only the values of D_l are reversed if the direction of the applied field is reversed. In the case the pairing term in $H_{\rm s}$ vanishes, $t_2 = 0$, it is simple to show that $H_{\rm s}$ is also invariant under the following on-site transformation

$$a_l \to i a_l^\dagger, \quad a_l^\dagger \to -i a_l, \quad D_l \to -D_l, \quad h \to -h. \tag{21}$$

In the discussion below, we set $t_1 = 1$ as the unit of energy.

To gain a heuristic picture on the ground state phase diagram, we diagonalize the Hamiltonian $H_{\rm s}$ for all possible pseudospin configurations on the 4×4 lattice. From the numerical results, we find that the phase diagram is divided into two parts in the small and large U regions, separated by the on-site interaction roughly at $U \sim 8$. Figure 1 shows the field dependence of $D^{(+)}$ and $D^{(-)}$ in the ground states of $H_{\rm s}$ in these two regions, exemplified using the results obtained at $U = 4$ and $U = 15$. In the small U case, two full-polarization phases with $D^{(+)} = \pm 1$ and $D^{(-)} = 0$ and one antiferromagnetic phase $D^{(+)} = 0$

and $D^{(-)} = 1$, which is sandwiched between the two full-polarization phases, are discovered in the ground states. There is a first-order transition between either of full-polarization phases and the antiferromagnetic phase.

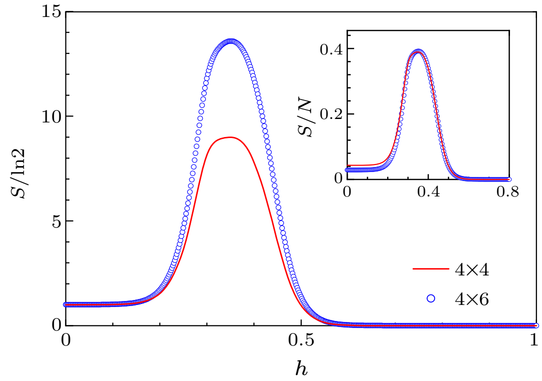

Fig. 2. Field dependence of the entropy S at zero temperature for the symmetric BCS–Hubbard model on the $N = 4\times 4$ and 4×6 lattices. The inset is the entropy density S/N at zero temperature. Here, $t_2 = 0.5$ and $U = 15$.

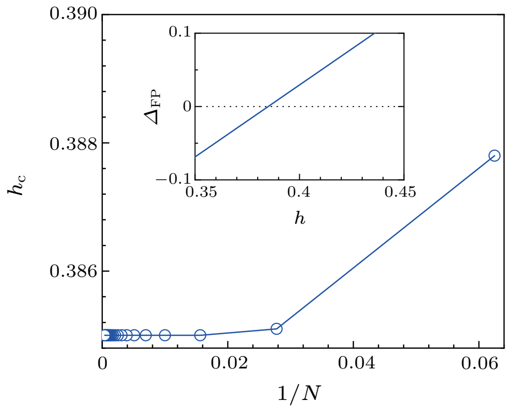

Fig. 3. Critical field h_c between the intermediate and full-polarization phases as a function of the inverse of the lattice size for the symmetric BCS–Hubbard model with $t_2 = 0.5$ and $U = 15$. The inset shows how $\Delta_{\rm FP}$ varies with h on the 40×40 lattice. $\Delta_{\rm FP}$ becomes zero at the critical field h_c.

In the large U case, an intermediate phase emerges between the antiferromagnetic and full-polarization phases in either the positive or the negative magnetic field side. The values of $D^{(+)}$ are finite but less than 1 in this intermediate phase. To further elucidate the nature of this intermediate phase, we evaluate the entropy of the system at zero temperature, which is determined by the ground state degeneracy. Figure 2 shows the zero-temperature entropy S as a function of the applied field for the symmetric BCS–Hubbard model with $U = 15$ on the 4×4 and 4×6 lattices. The ground state is non-degenerate in the full-polarization phase. The corresponding entropy is zero. In the intermediate and antiferromagnetic phases, the ground states become degenerate. In the antiferromagnetic phase, the ground states are doubly degenerate so that the entropy is $\ln 2$. In the intermediate phase, the ground states are highly degenerate. As the entropy density is almost lattice size independent (see the inset of Fig. 2), it suggests that the intermediate phase is macroscopically degenerate and the entropy scales linearly with N in the thermodynamic limit.

The critical field that separates the fully polarization and intermediate phases is determined by the difference

$$\Delta_{\rm FP}(h) = E_{\rm FP,1}(h) - E_{\rm FP}(h), \tag{22}$$

between the energy of the fully polarized state, $E_{\rm FP}$, and that of the state in which one pseudospin is flipped with respect with the fully polarized state, $E_{\rm FP,1}$. Since the fully polarized state is translation invariant, this flipped pseudospin could be at the origin or any other lattice site. $\Delta_{\rm FP}$ is positive in the fully polarized or negative in intermediate phase. It becomes zero exactly at the critical point. Figure 3 shows how the critical field h_c so determined varies with the lattice size for $U = 15$. By extrapolation, we obtain the value in the thermodynamic limit.

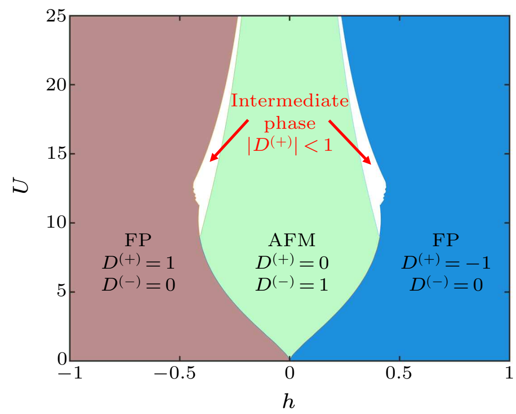

Fig. 4. Phase diagram of the symmetric BCS–Hubbard model with $t_2 = 0.5$. FP represents the full-polarization phases of pseudospins with $D^{(+)} = \pm 1$ and $D^{(-)} = 0$. AFM is the antiferromagnetic phase of pseudospins with $D^{(-)} = 1$ and $D^{(+)} = 0$. Between the AFM and either FP phase there is a glass-like intermediate phase. The ground state is doubly degenerate in the AFM phase and macroscopically degenerate in the intermediate phase.

Similarly, the critical field separating the antiferromagnetic phase from the intermediate one is determined by the energy difference between the antiferromagnetic state and the state in which one of the pseudospin in the antiferromagnetic state is flipped. Again, this flipped pseudospin could be located at any lattice site due to the translation invariance of the antiferromagnetic state in each sublattice and equivalence of two sublattices.

Figure 4 shows the typical phase diagram of the ground states for H_s in the thermodynamic limit. This phase diagram is symmetric with respect to the applied field, but all the pseudospins change sign if h

is changed to $-h$. In other words, there is a one-to-one correspondence between the ground states in the positive and negative h systems with opposite pseudospins.

The intermediate phase results from the interplay between the Coulomb interaction and the applied field. Inside this phase, we find that the charge excitation gap in the pseudo-fermion channel does not change much with the increase of the lattice size. This suggests that there may be a finite excitation gap to remove or add an "a" fermion from or to a ground state in a given pseudospin configuration in this phase. On the other hand, since the the ground states are macroscopically degenerate in the intermediate phase, there is no gap for flipping a pair of opposite pseudospins, hence the pseudospin excitation gap is zero. If one can add an interaction to lift all the degeneracy of the ground states but preserve the charge excitation gap of pseudo-fermions in this intermediate phase, the system is likely to become a quantum spin liquid.

In summary, we have extended the exactly solvable BCS–Hubbard model, first proposed by Chen *et al.*,[21] to include a spin-flip hopping term a corresponding p-wave pairing term, and an external magnetic field term. We show that the extended model can also be reduced to a model of non-interacting fermions coupled with quenched Z_2 fields of pseudospins in the symmetric limit. We solve this model both analytically and numerically, and determine the ground state phase diagram of it on the square lattice. In the absence of the applied field, the pseudospins are antiferromagnetically ordered in the doubly degenerate ground states. The applied magnetic field enriches the phase diagram. With the increase of the applied field, a first-order phase transition from the antiferromagnetic ordered states to a fully polarized ordered state of pseudospins occurs in the weak coupling region where the Coulomb interaction $U \lesssim 8$. In the strong coupling region, a novel intermediate phase emerges between the antiferromagnetic and full-polarization phases of pseudospins in the ground states. The ground states in this intermediate phase are macroscopically degenerate, like in a spin ice.

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