Exact Demonstration of η Pairing in the Ground State of an Attractive-U Hubbard Model

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We show that the recently discovered η-pairing scheme combined with the Nagaoka-Thouless picture for itinerant ferromagnetism leads to a new type of superconductivity in the attractive-U Hubbard model in the sector $0<(N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow) \ll 1$, where $N_\uparrow$ and $N_\downarrow$ are the occupation numbers of up and down spins. This result holds for all dimensionalities $d \gtrsim 2$.

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The BCS theory of superconductivity[1] and the concept of off-diagonal long-range order[2] (ODLRO) have been well established in theoretical physics for over two decades now. However, there does not exist a nontrivial interacting-electron model for which such an order can be rigorously established. Very recently, Yang[3] discovered a class of eigenstates of the Hubbard Hamiltonian[4] which have the property of ODLRO, but can be shown to be of very high energy compared to the global ground state.[5] Following his notation we will call these η-paired states. In this paper we wish to show that there is an exact mapping between the Nagaoka-Thouless[6] picture of ferromagnetism in the repulsive-U Hubbard model and η pairing in the attractive-U Hubbard model. Therefore, just as the completely ferromagnetic state is the ground state for the repulsive large-U Hubbard model slightly off half filling, the η-pairing state is the ground state for the attractive large-U Hubbard model in the slightly spin-polarized state.

Many years ago Nagaoka[6] demonstrated that the ground state of the repulsive large-U Hubbard model with exactly one electron less than half filling was a fully aligned ferromagnet in any finite system for a variety of two- and three-dimensional lattices. Whether this leads to a thermodynamic ferromagnetic phase is not rigorously established. In fact, this has been a subject of various numerical[7] and variational[8] studies in the past few years. It is believed, though, that such a phase is obtained for sufficiently large U over a wide range of electron concentration. Using the symmetries of the Hubbard model outlined by Yang and Zhang,[9] which includes the well-known mapping[10] between the repulsive- and attractive-U Hubbard models, we show that this ferromagnetic phase for the repulsive-U model slightly away from half filling maps onto an η-paired superconductor for an attractive-U model in the presence of a small spin asymmetry for bipartite lattices in arbitrary dimensions $d \gtrsim 2$. The mapping is exact, and hence for $N_\uparrow - N_\downarrow = 1$ we have rigorously shown that the ground state has ODLRO.

The half-filled Hubbard model is given by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) . \quad (1)$$

Yang and Zhang have shown that this model has two sets of commuting SU(2) symmetries. The first is characterized by the generators

$$\eta = \sum_i (-1)^i c_{i\downarrow} c_{i\uparrow} , \qquad \eta = J_x - iJ_y,\ \ \eta^\dagger = J_x + iJ_y,\ \ J_z = \tfrac{1}{2}(N-M) , \quad (2)$$

where we assume a bipartite lattice and $(-1)^i$ is -1 for one sublattice and $+1$ for the other. Here M is the number of lattice sites and N is the number of particles. The second has the generators

$$\zeta = \sum_i c_{i\uparrow} c_{i\downarrow}^\dagger , \qquad \zeta = J_x' - iJ_y',\ \ \zeta^\dagger = J_x' + iJ_y',\ \ J_z' = \tfrac{1}{2}(N_\uparrow - N_\downarrow) . \quad (3)$$

Large values of the spin quantum number j' correspond to ferromagnetism, whereas large values of the j quantum number are related to a staggered off-diagonal long-range order and superconductivity. Under a particle-hole transformation for one spin species, $c_{l\downarrow}^\dagger \to (-1)^l c_{l\downarrow}$, which maps the repulsive-U Hubbard model to an attractive one, the role of the two sets of SU(2) generators is interchanged. This mapping also takes the chemical potential in the repulsive case to a spin-polarizing field[11] in the attractive case. Thus the Nagaoka-Thouless state, which occurs at large repulsive U and nonzero chemical potential μ, corresponds to an η-paired superconductor for large attractive U and a nonzero spin-polarizing field.

A closer investigation shows that the XY ordering of the Nagaoka ferromagnet corresponds to ODLRO and superconductivity, whereas ZZ ordering corresponds to phase separation, where the electron *density* becomes inhomogeneous. Thus the full rotational symmetry of the

TABLE I. Summary of the mappings between the positive- and negative-U Hubbard models. All operators in the $-U$ and $+U$ columns are interchanged under the mapping $c_{i\downarrow}^\dagger \rightarrow (-1)^i c_{i\downarrow}$. Here $n_i = n_{i\uparrow} + n_{i\downarrow}$ is the total charge on a site. The spin on a site is $m_i = n_{i\uparrow} - n_{i\downarrow}$. Also, $\eta_i = c_{i\downarrow}c_{i\uparrow}$, and $\zeta_i = c_{i\uparrow}c_{i\downarrow}^\dagger$.

	$-U$ model	$+U$ model	
Up occupation	$n_{i\uparrow}$	$n_{i\uparrow}$	Up occupation
Down occupation	$n_{i\downarrow}$	$1-n_{i\downarrow}$	Down hole occupation
Kinetic energy	$-t\sum_{ij\sigma}(c_{i\sigma}^\dagger c_{j\sigma}+c_{j\sigma}^\dagger c_{i\sigma})$	$-t\sum_{ij\sigma}(c_{i\sigma}^\dagger c_{j\sigma}+c_{j\sigma}^\dagger c_{i\sigma})$	Kinetic energy
Potential energy	$-U\sum_i(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})$	$+U\sum_i(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})$	Potential energy
Spin-polarizing field	$h\sum_i m_i$	$\mu\sum_i n_i$	Chemical potential
Charge-density wave	$S_{\rm cdw}=\sum_{ij}(-1)^{i+j}n_i n_j$	$S_{\rm af}^{ZZ}=\sum_{ij}(-1)^{i+j}m_i m_j$	Antiferromagnet (ZZ)
$k=0$ superconductivity	$P_s=\sum_{ij}\eta_i^\dagger\eta_j$	$S_{\rm af}^{+-}=\sum_{ij}(-1)^{i+j}\zeta_i^\dagger\zeta_j$	Antiferromagnet (XY)
Density fluctuations	$C=\sum_{ij}n_i n_j$	$S_{\rm f}^{ZZ}=\sum_{ij}m_i m_j$	Ferromagnet (ZZ)
η pairing	$P_\eta=\sum_{ij}(-1)^{i+j}\eta_i^\dagger\eta_j$	$S_{\rm f}^{+-}=\sum_{ij}\zeta_i^\dagger\zeta_j$	Ferromagnet (XY)

$U>0$ ferromagnetic state translates into the possibility of coexisting superconductivity and phase separation in the negative-U Hubbard model. This exact mapping is analogous to the corresponding relation between the charge-density-wave order and usual zero-momentum superconductivity and the ZZ and XY *antiferromagnetic* order. These relations are summarized in Table I.

This new superconductivity is different from the ordinary one in the following sense. Including the possibility of phase separation, the order parameter has the symmetries of a Heisenberg ferromagnet, whereas in the usual superconductivity it is of the XY type. The former corresponds to a conserved order parameter (a good quantum number) while the latter corresponds to a nonconserved one. It is likely that in any real system the delicate symmetry of the Hubbard model will not be obtained due to the long-range nature of the Coulomb interactions. This will make it unfavorable for the system simultaneously to phase separate and superconduct, thus reducing the symmetry of the order parameter for the superconducting case to that of an XY ferromagnet. Since the XY ferromagnet and the antiferromagnet are related by a gauge symmetry, we expect many physical properties to be similar to conventional pairing. To the extent that further-neighbor interactions are small, there may still be large-scale density fluctuations in such a system. Finally, the pair-field order parameter is staggered here, corresponding to pairing at momentum π. This is in contrast to the usual case, where the pairing occurs at zero momentum.

To conclude, in this paper we have shown the exact correspondence between the Nagaoka-Thouless ferromagnet and the η-paired superconductor. The exact range of parameters over which ferromagnetism is obtained is currently a subject of intense research. Thus the same applies to superconductivity. The precise relevance of this type of superconductivity to experiments remains to be explored.

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[5]In the Hubbard model the number of up and down spin particles are separately conserved. In the particle-hole symmetric notation [see Eq. (1)] the global ground state corresponds to $N_\uparrow/M = N_\downarrow/M = 1/2$, where M is the number of sites in the problem. This result follows from the two theorems of E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989), and the symmetries considered in this paper. Lieb also showed that in a finite system there is a gap to all excitations. It is believed that in the thermodynamic limit this gap closes, giving rise to antiferromagnetic order for $U>0$ and charge-density-wave order for $U<0$. However, for $U>0$ a gap remains to charged excitations and for $U<0$ to spin excitations. Thus the $U>0$ non-half-filled case and $U<0$ spin-polarized case can be in a different phase from this global ground state. It is this new phase, which was argued to be ferromagnetic (for $U>0$) by Nagaoka, which is argued to be superconducting (for $U<0$) in this paper.

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[11]By a spin-polarizing field, we mean a field which changes the relative occupation of up and down spins (see Table I).