Rigorous eta -pairing ground state in an extended Hubbard model

1995 J. Phys. A: Math. Gen. 28 3417

(http://iopscience.iop.org/0305-4470/28/12/015)

J. Phys. A: Math. Gen. 28 (1995) 3417–3420. Printed in the UK

Rigorous η-pairing ground state in an extended Hubbard model

Z J Wang, X M Qiu and X B Zhou
Southwestern Institute of Physics, PO Box 432, Chengdu 610041, People's Republic of China

Received 1 August 1994

Abstract. In this paper we show the existence of η-pairing and off-diagonal long-range order (ODLRO) in the ground state of an extended Hubbard model with $N_\uparrow - N_\downarrow = 1$, where $N_\uparrow$ and $N_\downarrow$ are the occupation numbers of up and down spins, for connected bipartite lattices.

The concept of ODLRO was proposed and showed its relevance to superconductivity and superfluidity three decades ago [1]. Therefore, it is very important to rigorously show some non-trivial interacting-electron models possessing ODLRO. Recently, the ground-state ODLRO was proved for the strong-coupling limit of the attractive-U Hubbard model [2, 3] and for some one-dimensional models [4]. The resulting ODLRO state was related to the so-called η-pairing state of Yang [5]. More recently, Shen and Qiu [6] have demonstrated that the attractive-U Hubbard model on some bipartite lattices Λ possesses ODLRO in the ground state with a finite range of the electron filling factor.

In this paper we study the extended negative-U Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} C_{i\sigma}^\dagger C_{j\sigma} - U \sum_i (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) + \sum_{ij\sigma\tau} W_{ij} n_{i\sigma} n_{j\tau} \qquad (1)$$

where $C_{i\sigma}^\dagger (C_{i\sigma})$ is the creation (annihilation) operator of the electron with spin σ at site i, $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$ is the electron number operator, the hopping matrix elements are t_{ij}, U the on-site interaction of electrons and W_{ij} the inter-site interaction of electrons. After extending Tasaki's theorem [7] on the existence of ferromagnetism in the large positive-U Hubbard model with precisely one hole, we prove, strictly, that there exists η-pairing in the ground state of the extended large negative-U Hubbard model (1) through a particle–hole transformation.

We start by considering the Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} C_{i\sigma}^\dagger C_{j\sigma} + U \sum_i (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) + \sum_{ij\sigma\tau} W_{ij} [n_{i\sigma} n_{j\tau} - 2 n_{i\sigma} n_{j-\sigma} + (n_{i\uparrow} - n_{i\downarrow}) + (n_{j\uparrow} - n_{j\downarrow}) + 1] \qquad (2)$$

where the meaning of the parameters is the same as that in model (1). The latter four terms in the square brackets represent our extension to Tasaki's model.

We introduce the spin operators

$$S^+ = (S^-)^\dagger = \sum_i C_{i\uparrow}^\dagger C_{i\downarrow}$$

$$S^z = \frac{1}{2}\sum_i (n_{i\uparrow} - n_{i\downarrow}) \tag{3}$$

$$\mathbf{S}^2 = (S^z)^2 + \frac{1}{2}(S^+S^- + S^-S^+)$$

where the eigenvalues of $\mathbf{S}^2$ are $S(S+1)$. It is easy to show that $\mathbf{S}^2$ and S^z commute with the Hamiltonian (2) respectively. Hence, $\mathbf{S}^2$ and S^z are conserved quantities of model (2).

Theorem. Consider model (2) with $t_{ij} \geqslant 0$, $W_{ij} \leqslant 0$, $U = \infty$ and the electron number $N_e = N - 1$, where N is the total number of sites. The lattice Λ satisfies the connectivity condition. Then, the ground state has $S = S_{max} = (N-1)/2$ and is unique except for the trivial N-fold degeneracy.

Remark 1. Two states $|i, \sigma\rangle$ and $|j, \tau\rangle$ are said to be directly connected to each other if $\langle j, \tau|t_{ij}(C_{i\uparrow}^\dagger C_{j\uparrow} + C_{i\downarrow}^\dagger C_{j\downarrow})|i, \sigma\rangle \neq 0$. A finite lattice Λ satisfies the connectivity condition if all the states $|i, \sigma\rangle$ with the same value of S^z are connected to each other [7]. Nagaoka [8] has demonstrated that when t_{ij} is non-vanishing for the nearest neighbour (i, j) only, the connectivity condition is satisfied in the square lattice, triangular lattice and some regular three-dimensional lattices (such as the simple-cubic, the body-centred-cubic and the face-centred-cubic lattice).

Remark 2. According to Tasaki, if U is finite but sufficiently large, the theorem mentioned above holds.

Proof of the theorem. Following the method of Tasaki we define the basis state as

$$|i, \alpha\rangle = (-1)^i C_{1\sigma_1}^\dagger C_{2\sigma_2}^\dagger \cdots C_{i-1\sigma_{i-1}}^\dagger C_{i+1\sigma_{i+1}}^\dagger \cdots C_{N\sigma_N}^\dagger |0\rangle$$

where i denotes the position of the unique hole, and $\alpha = \{\sigma_j\}_{j\neq i}$ is a multi-index describing the spin of each electron. $|0\rangle$ is the vacuum state which satisfies $C_{i\sigma}|0\rangle = 0$ for any i, σ.

Let $|\Psi\rangle = \sum_{i,\alpha} \psi_{i,\alpha}|i, \alpha\rangle$ be an arbitrary normalized state. Let us define a state $|\Phi\rangle$ with $S = S_{max}$ as $|\Phi\rangle = \sum_i \varphi_i|i, \{\uparrow\}\rangle$ where $\varphi_i = (\sum_\alpha |\psi_{i,\alpha}|^2)^{1/2}$ and the multi-index $\{\uparrow\}$ indicates that all the electrons have upward spin. When $t_{ij} \geqslant 0$ and $W_{ij} \leqslant 0$ we find

$$\langle\Psi| - \tfrac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - \tfrac{1}{2})|\Psi\rangle = \langle\Phi| - \tfrac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - \tfrac{1}{2})|\Phi\rangle \tag{4}$$

$$\langle\Psi|W_{ij}\sum_{\sigma\tau}(n_{i\sigma}n_{j\tau} + 1)|\Psi\rangle = \langle\Phi|W_{ij}\sum_{\sigma\tau}(n_{i\sigma}n_{j\tau} + 1)|\Phi\rangle. \tag{5}$$

Since

$$\langle\Psi| - 2W_{ij}\sum_\sigma n_{i\sigma}n_{j-\sigma}|\Psi\rangle = -2W_{ij}\sum_{k\neq i,j;\alpha(\sigma_i=-\sigma_j)} |\psi_{k,\alpha}|^2 \geqslant 0$$

and

$$\langle\Phi| - 2W_{ij}\sum_\sigma n_{i\sigma}n_{j-\sigma}|\Phi\rangle = 0$$

then

$$\langle\Psi| - 2W_{ij}\sum_{\sigma} n_{i\sigma}n_{j-\sigma}|\Psi\rangle \geqslant \langle\Phi| - 2W_{ij}\sum_{\sigma} n_{i\sigma}n_{j-\sigma}|\Phi\rangle. \tag{6}$$

Because

$$\begin{aligned}\langle\Psi|W_{ij}(n_{i\uparrow} - n_{i\downarrow} + n_{j\uparrow} - n_{j\downarrow})|\Psi\rangle &= \langle\Psi|W_{ij}[(n_{i\uparrow} + n_{i\downarrow}) + (n_{j\uparrow} + n_{j\downarrow}) - 2(n_{i\downarrow} + n_{j\downarrow})]|\Psi\rangle \\ &= W_{ij}\Bigg(\sum_{k\neq i;\alpha}|\psi_{k\alpha}|^2 + \sum_{k\neq j;\alpha}|\psi_{k\alpha}|^2\Bigg) \\ &\quad - 2W_{ij}\Bigg(\sum_{k\neq i;\alpha(\sigma_i=\downarrow)}|\psi_{k\alpha}|^2 + \sum_{k\neq j;\alpha(\sigma_j=\downarrow)}|\psi_{k\alpha}|^2\Bigg) \\ &\geqslant W_{ij}\Bigg(\sum_{k\neq i;\alpha}|\psi_{k\alpha}|^2 + \sum_{k\neq j;\alpha}|\psi_{k\alpha}|^2\Bigg)\end{aligned}$$

and

$$\begin{aligned}\langle\Phi|W_{ij}(n_{i\uparrow} - n_{i\downarrow} + n_{j\uparrow} - n_{j\downarrow})|\Phi\rangle &= W_{ij}\Bigg(\sum_{k\neq i}|\varphi_k|^2 + \sum_{k\neq j}|\varphi_k|^2\Bigg) \\ &= W_{ij}\Bigg(\sum_{k\neq i;\alpha}|\psi_{k\alpha}|^2 + \sum_{k\neq j;\alpha}|\psi_{k\alpha}|^2\Bigg)\end{aligned}$$

then

$$\langle\Psi|W_{ij}(n_{i\uparrow} - n_{i\downarrow} + n_{j\uparrow} - n_{j\downarrow})|\Psi\rangle \geqslant \langle\Phi|W_{ij}(n_{i\uparrow} - n_{i\downarrow} + n_{j\uparrow} - n_{j\downarrow})|\Phi\rangle. \tag{7}$$

Finally, since

$$\langle\Psi|t_{ij}\sum_{\sigma} C^{\dagger}_{i\sigma}C_{j\sigma}|\Psi\rangle = \sum_{\alpha,\tau}(-t_{ij})\bar{\psi}_{j\tau}\psi_{i\alpha} \tag{8.1}$$

and

$$\langle\Phi|t_{ij}\sum_{\sigma} C^{\dagger}_{i\sigma}C_{j\sigma}|\Phi\rangle = (-t_{ij})\bar{\varphi}_j\varphi_i \leqslant \sum_{\alpha,\tau}(-t_{ij})\bar{\psi}_{j\tau}\psi_{i\alpha} \tag{8.2}$$

then

$$\langle\Psi|t_{ij}\sum_{\sigma} C^{\dagger}_{i\sigma}C_{j\sigma}|\Psi\rangle \geqslant \langle\Phi|t_{ij}\sum_{\sigma} C^{\dagger}_{i\sigma}C_{j\sigma}|\Phi\rangle. \tag{8.3}$$

Here, the sum in expressions (8) has been over α, τ such that the two states $|i,\alpha\rangle$ and $|j,\tau\rangle$ are directly connected and we have used the Schwarz inequality to obtain the inequality (8.2). These expressions imply that the expectation of the energy of the state $|\Phi\rangle$ is never larger than that of the original state $|\Psi\rangle$. Then, among the ground states there exists at least N states with $S = S_{\max} \equiv (N-1)/2$ by taking $|\Psi\rangle$ as one of the ground states and using the global SO(3) symmetry of the system. Alternatively, by examining Tasaki's proof of the uniqueness of the ground state, it follows that the uniqueness of our theorem holds. □

It is well known that the repulsive- and attractive-U Hubbard model can be interchanged by means of a particle–hole transformation [9] which means $C_{i\uparrow} \rightarrow (-1)^i C_{i\uparrow}^\dagger$ and $C_{i\downarrow} \rightarrow C_{i\downarrow}$ in the present case. We now perform this transformation on model (2). We further assume a bipartite lattice and that $(-1)^i$ is -1 for one sublattice and $+1$ for the other. Under this transformation, model (2) is mapped onto model (1). It follows from our theorem that when $t_{ij} \geqslant 0$, $W_{ij} \leqslant 0$, $U = \infty$ and $N_e = N - 1$, then *model (2) has a* ferromagnetic ground state. It is well known that the ferromagnetic order of model (2) in the x and y directions can be mapped onto staggered BCS ODLRO through the transformation mentioned above. This corresponds to the relation

$$S^{\pm} = \sum_{ij} \xi_i^\dagger \xi_j \rightarrow P_c = \sum_{ij} \eta_i \eta_j^\dagger \tag{9}$$

where $\xi_i = C_{i\uparrow} C_{i\downarrow}^\dagger$, and $\eta_i = (-1)^i C_{i\uparrow} C_{i\downarrow}$ is the η-pairing operator. The z direction of the ferromagnetic order maps to phase separation. This mapping also maps the electron number $N_\uparrow + N_\downarrow = N - 1$ onto $N_\uparrow - N_\downarrow = 1$.

In summary, we have demonstrated that there exists η-pairing in model (1). The map is exact and, hence, we have exactly proven that the extended Hubbard model (1) with $N_\uparrow - N_\downarrow = 1$ has η-pairing for large enough U; this corresponds to ODLRO and superconductivity in the ground state on connected bipartite lattices.

References

[1] Yang C N 1962 *Rev. Mod. Phys.* **34** 694
[2] Singh R R P and Scalettar R T 1991 *Phys. Rev. Lett.* **66** 3203
[3] Rojo A G, Sofo J O and Balseiro C A 1990 *Phys. Rev.* B **42** 10241
Tian G S 1992 *Phys. Rev.* B **45** 3145
[4] Fye R M 1993 *Phys. Rev.* B **47** 1113
[5] Yang C N 1989 *Phys. Rev. Lett.* **63** 2144
[6] Shen S Q and Qiu Z M 1993 *Phys. Rev. Lett.* **71** 4238
[7] Tasaki H 1989 *Phys. Rev.* B **40** 9192
[8] Nagaoka Y 1965 *Solid State Commun.* **3** 409; 1966 *Phys. Rev.* **147** 392
[9] Robaszkicz S, Micnas R and Chao K A 1981 *Phys. Rev.* B **23** 1447
Shiba H 1972 *Prog. Theor. Phys.* B **48** 2171
Emiery V J 1976 *Phys. Rev.* B **14** 1989