Singlet pairing in the 2D Hubbard model

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Abstract

By use of the composite operator method we show that the 2D single-band Hubbard model exhibits superconducting solution. In particular, we consider singlet pairing and we show that both s-wave and d-wave symmetries are possible solutions of the model. Calculations of the order parameters and critical temperatures are presented as functions of the interaction intensity and particle density.

Keywords: Hubbard model; Superconductivity; Singlet pairing

1. Introduction

Since the discovery of high-\(T_c\) superconducting copper oxides by Bednorz and M\"uller, many efforts have been devoted to understanding the mechanism and the nature of high-\(T_c\) superconductors. It has been believed that a new mechanism is operating in these systems. Even if at present there is no consensus on the symmetry of the order parameter, there is evidence that it is d_{x^2-y^2}\textsuperscript{1, 2} rather than s-wave and this suggests an electronic mechanism for pairing rather than the original BCS phonon-mediated one. In this paper we study the possibility of the superconducting solution of the 2D Hubbard model by means of the composite operator method\textsuperscript{[3]}. In the framework of the static approximation we derive a set of self-consistent equations which give a complete solution of the model. We show that both s-wave and d-wave symmetries are possible solutions of the model.

2. The formalism

A convenient set for the study of the Hubbard model

\[ H = \sum_{i<j} t_{ij} c^\dagger(i) \cdot c(j) + U \sum_i n_i(i)n_i(i) - \mu \sum_i c^\dagger(i) \cdot c(i) \]

is given by the Hubbard operators in the Nambu representation. Therefore, we introduce the doublet composite field

\[ \psi(i) = \begin{pmatrix} \xi(i) \\ \eta(i) \end{pmatrix}, \]

where

\[ \xi(i) = \begin{pmatrix} \xi_x(i) \\ \xi_y(i) \end{pmatrix}, \quad \eta(i) = \begin{pmatrix} \eta_x(i) \\ \eta_y(i) \end{pmatrix} \]

with

\[ \xi_x(i) = c_x(i)[1 - c^\dagger_x(i)c(i)] \]

and

\[ \eta_x(i) = c_x(i)c^\dagger_x(i)c(i). \]

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In the static approximation [4] the Fourier transform \( S(k, \omega) \) of the retarded thermal Green's function
\[
S(i, j) = \langle R[\psi(i)\psi^\dagger(j)] \rangle
\]
is given by
\[
S(k, \omega) = \frac{1}{\omega - \varepsilon(k)} l(k)
\]
where \( \varepsilon(k) = m(k)l^{-1}(k) \), \( l(k) \) and \( m(k) \) are the Fourier transforms of the matrix:
\[
l(i, j) = \langle \{\psi(i), \psi^\dagger(j)\} \rangle_{E.T.}
\]
and
\[
m(i, j) = \left\{ \frac{\partial}{\partial t}, \psi^\dagger(j) \right\}_{E.T.}
\]
A straightforward calculation gives the expressions of the \( l(k) \) and \( m(k) \) matrices which contain the following set of parameters:
\[
\Delta \equiv \langle c_i(i)c_i(i) \rangle,
\]
\[
s \equiv \langle \xi_i^a \xi_i^a \rangle - \langle \eta_i \eta_i^* \rangle,
\]
\[
s_1 \equiv 2\langle \xi_i^a \xi_i^a \rangle + \langle \eta_i \eta_i \rangle + \langle \eta_i \xi_i^a \rangle,
\]
\[
s_2 \equiv 2\langle \eta_i \eta_i \rangle + \langle \eta_i \xi_i^a \rangle + \langle \xi_i \eta_i \rangle,
\]
\[
p_{ij} = -\langle c_i(i)c_i(i)c_i^\dagger(j)c_i^\dagger(j) \rangle
+ \langle c_i^\dagger(i)c_i(i)c_i^\dagger(j)c_i(j) \rangle
+ \langle c_i^\dagger(i)c_i(i)c_i^\dagger(j)c_i(j) \rangle,
\]
\[
f_{ij} = \langle c_i^\dagger(i)c_i(i)c_i^\dagger(j)c_i(j) \rangle
- \langle c_i^\dagger(j)c_i(j)c_i(i)c_i(i) \rangle,
\]
where operators like \( c^a(i) \) denote the operators on the first neighbour sites. By making use of equations of motion and symmetry considerations it is possible to derive a closed set of self-consistent equations both for the case of s- and d-wave symmetry. Referring to a forthcoming paper for details of computations, in this note we present some results for the order parameter and the critical temperature. In the case of s-wave solution, the order parameter \( \Delta \) is reported in Fig. 1 as a function of the reduced temperature \( T/t \) for

\[\begin{array}{c}
\text{Fig. 1. The order parameter } \Delta, \text{ for s-wave solution, as a function of the reduced temperature } T/t \text{ for } U/t = 2, 3, 4. \text{ The particle density has been fixed as } n = 0.4.
\end{array}\]

\[\begin{array}{c}
\text{Fig. 2. The reduced critical temperature } T_c/t \text{ as a function of } n \text{ for } U/t = 3 \text{ in the case of s-wave solution.}
\end{array}\]

\[\begin{array}{c}
\text{Fig. 3. The reduced critical temperature } T_c/t \text{ as a function of } n \text{ for } U/t = 2, 3, 4 \text{ for d-wave solution.}
\end{array}\]
the order parameter is defined by \( f = f_{ij} \) for \( R_i - R_j = ( \pm a, 0 ) \). This quantity is reported in Fig. 4 as a function of \( T/t \) for \( U/t = 2, 3, 4 \) and \( n = 0.75 \).

In conclusion, in the static approximation, we have obtained a fully self-consistent superconducting solution for the 2D Hubbard-model and we have shown that d-wave superconductivity occurs with a maximum value of \( T_c \) in the range of 20–70 K for different values of the Coulomb interaction.

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**References**