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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 Müller, 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 $d_{x^2-y^2}$ [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 [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.

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2. The formalism

A convenient set for the study of the Hubbard model

$$H = \sum_{ij} t_{ij} c^\dagger(i)\cdot c(j) + U\sum_i n_\uparrow(i)n_\downarrow(i) - \mu\sum_i c^\dagger(i)\cdot c(i)$$

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

$$\xi(i) = \begin{pmatrix} \xi_\uparrow(i) \\ \xi_\downarrow^\dagger(i) \end{pmatrix}, \qquad \eta(i) = \begin{pmatrix} \eta_\uparrow(i) \\ \eta_\downarrow^\dagger(i) \end{pmatrix}$$

with

$$\xi_\sigma(i) = c_\sigma(i)[1 - c^\dagger_{-\sigma}(i)c_{-\sigma}(i)]$$

and

$$\eta_\sigma(i) = c_\sigma(i)c^\dagger_{-\sigma}(i)c_{-\sigma}(i).$$

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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:

$$l(i,j) = \langle\{\psi(i), \psi^{\dagger}(j)\}\rangle_{\mathrm{E.T.}}$$

and

$$m(i,j) = \left\langle \left\{ \mathrm{i}\frac{\partial\psi(i)}{\partial t}, \psi^{\dagger}(j) \right\} \right\rangle_{\mathrm{E.T.}}$$

A straightforward calculation gives the expressions of the $l(k)$ and $m(k)$ matrices which contain the following set of parameters:

$$\Delta \equiv \langle c_{\uparrow}(i)c_{\downarrow}(i)\rangle,$$

$$s \equiv \langle \xi_{\downarrow}^{\alpha}\xi_{\downarrow}^{\dagger}\rangle - \langle \eta_{\downarrow}\eta_{\downarrow}^{\dagger}\rangle,$$

$$s_1 \equiv 2\langle \xi_{\uparrow}\xi_{\downarrow}^{\alpha}\rangle + \langle \xi_{\uparrow}\eta_{\downarrow}^{\alpha}\rangle + \langle \eta_{\uparrow}\xi_{\downarrow}^{\alpha}\rangle,$$

$$s_2 \equiv 2\langle \eta_{\uparrow}\eta_{\downarrow}^{\alpha}\rangle + \langle \eta_{\uparrow}\xi_{\downarrow}^{\alpha}\rangle + \langle \xi_{\uparrow}\eta_{\downarrow}^{\alpha}\rangle,$$

$$p_{ij} = -\langle c_{\uparrow}(i)c_{\downarrow}(i)c_{\downarrow}^{\dagger}(j)c_{\uparrow}^{\dagger}(j)\rangle + \langle c_{\downarrow}^{\dagger}(i)c_{\downarrow}(i)c_{\downarrow}^{\dagger}(j)c_{\downarrow}(j)\rangle + \langle c_{\downarrow}^{\dagger}(i)c_{\uparrow}(i)c_{\uparrow}^{\dagger}(j)c_{\downarrow}(j)\rangle,$$

$$f_{ij} = \langle c_{\downarrow}^{\dagger}(i)c_{\downarrow}(i)c_{\downarrow}(j)c_{\uparrow}(j) - \langle c_{\uparrow}^{\dagger}(j)c_{\uparrow}(j)c_{\uparrow}(i)c_{\downarrow}(i)\rangle,$$

where operators like $c^{\alpha}(i)$ 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 fourthcoming 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 Δ is reported in Fig. 1 as a function of the reduced temperature T/t for

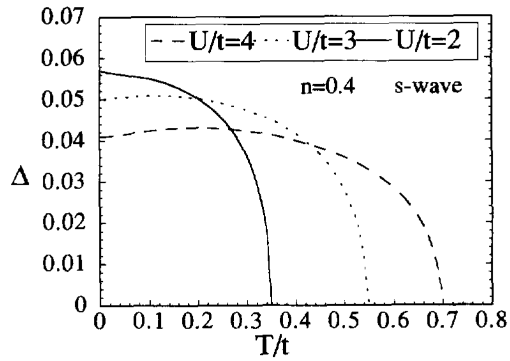

Fig. 1. The order parameter Δ, for s-wave solution, as a function of the reduced temperature T/t for $U/t = 2, 3, 4$. The particle density has been fixed as $n = 0.4$.

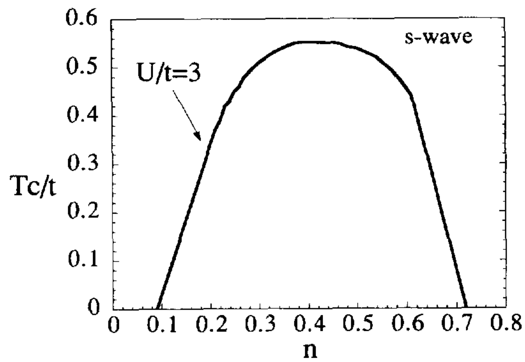

Fig. 2. The reduced critical temperature T_c/t as a function of n for $U/t = 3$ in the case of s-wave solution.

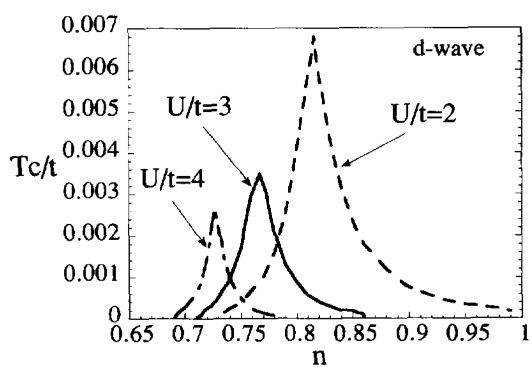

Fig. 3. The reduced critical temperature T_c/t as a function of n for $U/t = 2, 3, 4$ for d-wave solution.

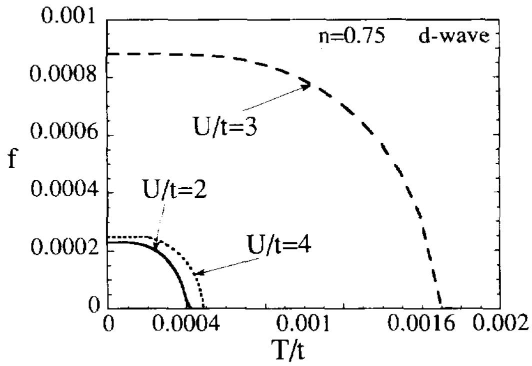

Fig. 4. The order parameter f as a function of the reduced temperature T/t for different values of $U\backslash t = 2, 3, 4$ and $n = 0.75$ in the case of d-wave solution.

$U/t = 2, 3, 4$. The particle density has been fixed as $n = 0.4$. The reduced critical temperatureT_c/t, as a function of n, is shown in Fig. 2, for the value of $U/t = 3$. Figs. 1 and 2 show that the s-wave solution of the Hubbard model has a very high unrealistic critical temperature. In the case of d-wave,T_c/t, reported in Fig. 3, is sharply peaked at an optimum doping depending on the ratio U/t and its values are more reasonable. For d-wave solution 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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