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Physica C 419 (2005) 13–17
PHYSICA C
www.elsevier.com/locate/physc

Exact commutation relations for the Cooper pair operators and the problem of two interacting Cooper's pairs

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Received 14 July 2004; accepted 19 November 2004
Available online 19 December 2004

Abstract

The analysis of trilinear commutation relations for the Cooper pair operators reveals that they correspond to the modified parafermi statistics of rank $p = 1$. Two different expressions for the Cooper pair number operator are presented. We demonstrate that the calculations with a Hamiltonian expressed via pairon operators is more convenient using the commutation properties of these operators without presenting them as a product of fermion operators. This allows to study problems in which the interactions between Cooper's pairs are also included. The problem with two interacting Cooper's pairs is resolved and its generalization in the case of large systems is discussed.

Keywords: Cooper's pair commutation relations; Pairing interactions; Strongly correlated electron systems

1. Introduction

It is well-known that the theory of the low temperature superconductivity was created by Bardeen, Cooper, and Schrieffer (BCS) [1] only after Cooper [2] had shown that two electrons interacting above the Fermi sea of non-interacting electrons can couple in a stable pair, if the interaction resulting from virtual exchange of phonons is attractive near the Fermi surface. As was demonstrated in a more sophisticated study [3], in full agreement with the Cooper assumption, the largest binding energy of the Cooper pair corresponds to electrons with the opposite momenta and spins. In the second quantization formalism, the operators of creation, b_k^+, and annihilation, b_k, of Cooper's pair in a state $(\mathbf{k}\alpha, -\mathbf{k}\beta)$, are defined as simple products of the electron creation and annihilation operators, $c_{k\sigma}^+$ and $c_{k\sigma}$, satisfying the fermion commutation relations,

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doi:10.1016/j.physc.2004.11.025

$$b_k^+ = c_{k\alpha}^+ c_{-k\beta}^+,\qquad b_k = c_{-k\beta} c_{k\alpha}. \tag{1}$$

Let us call these operators, following Schrieffer [3], as 'pairon' operators.

The Cooper pair has the total spin $S = 0$. Hence, in accordance with the Pauli principle, the wave functions describing the Cooper pair system have the boson permutation symmetry, that is, they are symmetric under permutations of pairs. But the pairon operators (1) do not obey the boson commutation relations [1,3]. It is easy to show by direct calculation. Namely,

$$[b_k, b_{k'}^+]_- = [b_k^+, b_{k'}^+]_- = [b_k, b_{k'}]_- = 0 \quad \text{for } k \neq k', \tag{2}$$

$$[b_k, b_k^+]_- = 1 - \hat{n}_{k\alpha} - \hat{n}_{-k\beta}, \tag{3}$$

$$(b_k^+)^2 = (b_k)^2 = 0, \tag{4}$$

where $\hat{n}_{k\alpha} = c_{k\sigma}^+ c_{k\sigma}$ is the electron number operator. As follows from Eqs. (2)–(4), for $k \neq k'$ the Cooper pairs are bosons, while for $k = k'$ they do not obey the boson commutation relations, although they obey the Pauli principle and have the fermion occupation numbers for one-particle states.

Thus, the pairon operators may not be considered neither as the Bose operators, nor as the Fermi operators. This is the reason that the problem with the model Hamiltonian of the BCS theory

$$H = \sum_k \varepsilon_k b_k^+ b_k + \sum_{k',k} V_{kk'} b_{k'}^+ b_k \tag{5}$$

cannot be directly solved by transforming Hamiltonian (5) to the diagonalized form

$$H = \sum_n \varepsilon_k' B_k^+ B_k \tag{6}$$

by means of some unitary transformation

$$B_n = \sum_k u_{nk} b_k, \quad B_n^+ = \sum_k u_{nk}^* b_k^+. \tag{7}$$

The unitary transformation is canonical only for the Bose or Fermi operators. In general case, it is not canonical; it does not preserve the commutation properties of the operators transformed. Therefore, practically all calculations in the BCS approach were performed using the fermion properties of electron operators forming the Cooper pair.

In this paper we analyze the commutation relations for the pairon operators and reveal that they correspond to the modified parafermi statistics of rank $p = 1$. The general expression for the Cooper pair number operator is analyzed and it is proved that the same expression as for the boson (fermion) number operator can be also used in the pairon case. We demonstrate that the calculations with a Hamiltonian expressed via the pairon operators more convenient to perform using the commutation properties of these operators without presenting them as a product of fermion operators. This allows to study problems in which the interactions between Cooper's pairs are also included. The solution of the simplest problem with two interacting Cooper's pairs is presented.

2. Statistics of Cooper's pairs

As was discussed in the introduction, the pairon operators, Eq. (1), obey boson commutation relations only in the case of different momenta. For equal momenta, the right-hand part of commutation relation (3) contains the products of fermion operators that reflects the fermion structure of pairon operators.

$$[b_k, b_k^+]_- = 1 - c_{k\alpha}^+ c_{k\alpha} - c_{-k\beta}^+ c_{-k\beta}. \tag{8}$$

To operate with the pairon operators, the commutation relations for these operators do not have to include other kinds of operators. One of the ways to achieve this goal is to calculate trilinear commutation relations, as it is formulated in the parastatistics [4], for a short description see Refs. [5,6].

The direct calculation leads to the following trilinear commutation relations

$$\left[[b_k^+, b_{k'}]_-, b_{k''}^+\right]_- = 2\delta_{kk'}\delta_{kk''} b_k^+, \tag{9}$$

$$\left[[b_k^+, b_{k'}]_-, b_{k''}\right]_- = -2\delta_{kk'}\delta_{kk''} b_k. \tag{10}$$

These relations coincide with the trilinear commutation relations of the parafermi statistics for $k = k' = k''$. For different k, k' and k'' the relations are different. In the parafermi statistics in relations corresponding to Eq. (9) instead of the two presented Kroneker symbols there is one, namely, $\delta_{k'k''}$; and in relation corresponding to Eq. (10), $\delta_{kk'}$ is absent. Thus, the pairon operators satisfy some modified parafermi statistics of the rank $p = 1$. The latter follows from Eq. (4), since for the parastatistics of rank p

$$(a_k^+)^N \mid 0\rangle \neq 0 \quad \text{for } N \leqslant p, \tag{11}$$

$$(a_k^+)^{p+1} \mid 0\rangle = 0. \tag{12}$$

As follows from the definition of the particle number operator $\widehat{N}_k$

$$\widehat{N}_k \mid N_k\rangle = N_k \mid N_k\rangle. \tag{13}$$

For the boson and fermion number operators the well-known expression $\widehat{N} = a_k^+ a_k$ is valid. But it is quite not evident that the same expression is valid for the pairon number operator. In the parafermi statistics, the particle number operator is defined as

$$\widehat{N}_k = \frac{1}{2}\left([a_k^+, a_k]_- + p\right), \tag{14}$$

for pairons $p = 1$ and

$$\widehat{N}_k = \frac{1}{2}\left([b_k^+, b_k]_- + 1\right). \tag{15}$$

As follows from the trilinear commutation relations (9) and (10), the operator (15) satisfies the commutation relations for the particle number operator that were established earlier for bosons and fermions, see Ref. [7],

$$[\widehat{N}_k, b_k^+]_- = b_k^+, \tag{16}$$

$$[\widehat{N}_k, b_k]_- = -b_k. \tag{17}$$

It is easy to check that for fermions, Eq. (15) is equivalent to the standard expression $\hat{n}_k = c_k^+ c_k$. Let us study it in the pairon case.

Using Eq. (3), the expression for the pairon number operator (15) can be written as

$$\widehat{N}_k = \frac{1}{2}(\hat{n}_{k\alpha} + \hat{n}_{-k\beta}). \tag{18}$$

This is quite natural that the number of Cooper's pairs is two times less than the number of electrons forming pairs. It can be proved that from Eq. (18) follows that the expression $\widehat{N}_k = b_k^+ b_k$ may be also used for the pairon number operators. Let us do it.

The product $b_k^+ b_k$ is equal to the product of the fermion number operators $\hat{n}_{k\alpha}\hat{n}_{-k\beta}$, but in the general case

$$\hat{n}_{k\alpha}\hat{n}_{-k\beta} \neq \frac{1}{2}(\hat{n}_{k\alpha} + \hat{n}_{-k\beta}). \tag{19}$$

Pairons operators possess the fermions occupation numbers, $n_{k\alpha}$ and $n_{-k\beta}$ equal to 0 or 1, in this case, and only in this case, the left-hand part of Eq. (19) is equal to its right-hand part. Thus,

$$\frac{1}{2}(\hat{n}_{k\alpha} + \hat{n}_{-k\beta}) = b_k^+ b_k \tag{20}$$

and from Eqs. (18) and (20) follows that although Cooper's pairs are neither bosons nor fermions, for the operators of their number, the traditional form $\widehat{N}_k = b_k^+ b_k$ can be used.

If one substitutes the equality

$$\hat{n}_{k\alpha} + \hat{n}_{-k\beta} = 2b_k^+ b_k, \tag{21}$$

into the commutation relation (3), it transforms into

$$[b_k, b_k^+]_- = (1 - 2b_k^+ b_k) \tag{22}$$

or

$$[b_k, b_k^+]_+ = 1. \tag{23}$$

Thus, for equal k, the pairon operators obey the fermion commutation relations, while for different k, they obey the boson commutation relations.

Despite the fact that each Cooper's pair has the total spin $S = 0$, the pairons are not bosons, because for equal momenta k they behave as fermions. However, for different k, the pairons obey the Bose–Einstein statistics and can occupy one energy level, that is, they can undergo the phenomenon of the Bose–Einstein condensation. However, all electrons composed into the condensed Cooper pairs must have different momenta k.

The Eqs. (2) and (22) can be combined into one commutation relation

$$[b_k, b_{k'}^+]_- = \delta_{kk'}(1 - 2b_k^+ b_k). \tag{24}$$

The application of pairon operators to the vacuum state follows from their definition, Eq. (1),

$$b_k \mid 0\rangle = 0, \quad b_k b_{k'}^+ \mid 0\rangle = \delta_{kk'} \mid 0\rangle. \tag{25}$$

The relations (24) and (25) are sufficient for performing calculations using only the pairon operators.

3. Generalized model Hamiltonian and the problem with two interacting Cooper's pairs

Let us add to the BCS Hamiltonian the term describing the interaction among Cooper's pairs. The generalized model Hamiltonian is

$$H = 2\sum_k \epsilon_k b_k^\dagger b_k - \sum_{k,k'}{}' V_{k,k'} b_{k'}^\dagger b_k + \frac{1}{2}\sum_{k_1',k_2'}{}' \sum_{k_1'',k_2''}{}' V_{k_1'k_2',k_1''k_2''} b_{k_1''}^\dagger b_{k_2''}^\dagger b_{k_1'} b_{k_2'} \tag{26}$$

where primes in sums denote that $k \neq k'$, $k_1' \neq k_2'$ and $k_1'' \neq k_2''$. The other restriction is concern with the potential energy of interpair interaction in which $k_1'' \neq k_1'$ and $k_2'' \neq k_2'$. While according to the Cooper model, $V_{k,k'} > 0$, the sign of $V_{k_1'k_2',k_1''k_2''}$ is not restricted, it can be both positive for a repulsive interpair interaction and negative for an attractive interaction.

In general, the variational wave function of the system with N pairs can be presented as

$$|\Psi(1,2,\ldots,N)\rangle = \sum_{k_1,k_2,\ldots,k_N}{}' \alpha(k_1,k_2,\ldots,k_N) \times b_{k_1}^+ b_{k_2}^+ \ldots b_{k_N}^+ \mid 0\rangle, \tag{27}$$

where $k_1 \neq k_2 \neq \cdots \neq k_N$ because of the fermion condition (4), or it can be presented in the BCS form, which is not as precise as the variational function (27) but easier for calculations.

$$|\Psi(1,2,\ldots,N)\rangle = \prod_{k=1}^{N}(u_k + v_k b_k^+) \mid 0\rangle. \tag{28}$$

As an illustration of operations with the Cooper pair operators using their properties (24) and (25), we consider the model of two interacting pairs described by the BCS wave function

$$|\Psi(1,2)\rangle = \prod\nolimits_{k_{j=1}}^{2}(u_{k_j} + v_{k_j} b_{k_j}^\dagger) \mid 0\rangle = \Big(u_{k_1}u_{k_2} + u_{k_1}v_{k_2}b_{k_2}^\dagger + u_{k_2}v_{k_1}b_{k_1}^\dagger + v_{k_1}v_{k_2}b_{k_1}^\dagger b_{k_2}^\dagger\Big) \mid 0\rangle. \tag{29}$$

Following the BCS theory, we assume in the general Hamiltonian (26) that the interaction energies do not depend upon the value of moments.

$$H = 2\sum_k \epsilon_k b_k^\dagger b_k - V_0 \sum_{k,k'}{}' b_{k'}^\dagger b_k + \frac{V_1}{2}\sum_{k_1',k_2'}{}' \sum_{k_1'',k_2''}{}' b_{k_1''}^\dagger b_{k_2''}^\dagger b_{k_1'} b_{k_2'}. \tag{30}$$

Using the properties of Cooper's pair operators, Eqs. (24) and (25), we calculate the expectation value for the energy $W = \langle\Psi(1,2)|H|\Psi(1,2)\rangle$ with the Hamiltonian (30) and wave function (29). The results is

$$W = 2v_{k_1}^2\epsilon_{k_1} + 2v_{k_2}^2\epsilon_{k_2} - 2V_0 u_{k_1}v_{k_1}u_{k_2}v_{k_2} + V_1 v_{k_1}^2 v_{k_2}^2. \tag{31}$$

By a minimization procedure respect to v_{k_1} and v_{k_2} using the Lagrange multiplicators, the following definitions

$$\Delta_{k_1} \equiv V_0 u_{k_2}v_{k_2}; \quad \Delta_{k_1}' \equiv V_1 v_{k_2}^2, \tag{32}$$

$$\Delta_{k_2} \equiv V_0 u_{k_1}v_{k_1}; \quad \Delta_{k_2}' \equiv V_1 v_{k_1}^2 \tag{33}$$

and introducing

$$E_{k_1}' = \sqrt{\left(\epsilon_{k_1} + \frac{\Delta_{k_1}'}{2}\right)^2 + \Delta_{k_1}^2}; \quad E_{k_2}' = \sqrt{\left(\epsilon_{k_2} + \frac{\Delta_{k_2}'}{2}\right)^2 + \Delta_{k_2}^2} \tag{34}$$

we obtain that

$$v_{k_1}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{k_1} + \frac{\Delta_{k_1}'}{2}}{E_{k_1}'}\right); \quad u_{k_1}^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{k_1} + \frac{\Delta_{k_1}'}{2}}{E_{k_1}'}\right), \tag{35}$$

$$v_{k_2}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{k_2} + \frac{\Delta_{k_2}'}{2}}{E_{k_2}'}\right); \quad u_{k_2}^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{k_2} + \frac{\Delta_{k_2}'}{2}}{E_{k_2}'}\right), \tag{36}$$

and

$$u_{k_1}v_{k_1} = \frac{1}{2}\left\{1 + \frac{\left(\epsilon_{k_1} + \frac{\Delta_{k_1}'}{2}\right)}{E_{k_1}'^2}\right\}^{1/2} = \frac{\Delta_{k_1}}{2E_{k_1}'}. \tag{37}$$

The calculation of the quasiparticle excitation energy results in

$$E'_k = \sqrt{\left(\epsilon_k + \frac{\Delta'_k}{2}\right)^2 + \Delta_k^2}. \tag{38}$$

Thus, the quantities introduced by Eq. 34 and entered into Eqs. (35)–(37) have the physical sense as the quasiparticle excitation energies.

Using, as in the BCS theory, the approximations

$$\begin{aligned} \Delta_{k_1} &= \Delta_{k_2} = \Delta, \\ \Delta'_{k_1} &= \Delta'_{k_2} = \Delta', \\ \epsilon_{k_1} &\simeq \epsilon_{k_2} = \epsilon \end{aligned} \tag{39}$$

we obtain the explicit expressions for the parameters Δ' and Δ

$$\Delta' = V_1 \frac{V_0 - 2\epsilon}{2V_0 + V_1}, \tag{40}$$

$$\Delta = \sqrt{\left(\frac{V_0}{2}\right)^2 - \left\{\epsilon + \frac{V_1}{2}\left(\frac{V_0 - 2\epsilon}{2V_0 + V_1}\right)\right\}^2} \tag{41}$$

In the expression for E'_k and u_k^2 and v_k^2, as well, the electron energy enters with the additive term $\Delta'_k/2$. According to Eq. 40, this term depends upon the interactions energies V_1 and V_0, and it disappears when $V_1 = 0$. Thus, one can say that the interpair interaction leads to the renormalization of the electron energy.

For comparison with the BCS theory, we have to neglect the interaction between pairs, $V_1 = 0$. With this condition, expressions for u_k^2, v_k^2 and E_k are reduced to the BCS expressions. But in the case of Δ (Eq. 41), it is not so, it is reduced to

$$\Delta = \sqrt{\left(\frac{V_0}{2}\right)^2 - \epsilon^2}. \tag{42}$$

This formula differs from the exponential expression for the energy gap in the BCS theory. The difference is connected with the fact that in a system with a finite number of particles, the distances between the energy levels are also finite, there is a discrete set of energy levels. The approximation $\epsilon_{k_1} = \epsilon_{k_2} = \epsilon$, Eq. (39), is valid only for systems with $N \gg 1$, for which the energy spectrum is continuous and after integration one obtains the exponential dependence as in the BCS theory.

Finally, it is important to mention that the two-pairon system was considered as an illustration of applying the commutation relation for pairons, Eq. (24). The employment of pairon operators b_k^+, b_k in place of presenting them as product of fermion operators reduces twice the number of operators in the Hamiltonian. For instance, for the two-pairon system the interaction term contains four pairon operators instead of eight fermion operators.

Let us note that the two interacting pairon problem has been solved exactly. The real physical problem for N interacting pairons with $N \to \infty$ is very complicated and can be solved only approximately. For its solution one should, similar to the BCS theory, consider the interacting pairons in the nearest neighborhood of the Fermi level and take into account an approximation similar to that given by Eq. (39), so the summation over k can be replaced by an integration.

Acknowledgments

This work was partially supported by grants from CONACYT (México) 41226-F and from UNAM through IN102203.

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