Original Paper

phys. stat. sol. (b) **242**, No. 9, 1793 – 1796 (2005) / **DOI** 10.1002/pssb.200461754

Statistical properties of the Cooper pair operators

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Received 11 October 2004, revised 8 April 2005, accepted 8 April 2005
Published online 17 June 2005

PACS 05.30.Fk, 05.30.Jp, 74.20.Fg

The Cooper pair has the total spin $S = 0$. So, in accordance with the Pauli principle, the wave functions describing the Cooper pair system should have the boson permutation symmetry, but the pairon operators (Cooper's pair operators) do not obey the boson commutation relations. The pairon operators may not be considered neither as the Bose operators, nor as the Fermi operators. In this work, we analyze the statistical properties and the commutation relations for the pairon operator and reveal 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 pair are also included. The problem of two interacting Cooper's pairs is discussed.

1 Introduction

As is now well established, 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 $(k\alpha, -k\beta)$, are defined as simple products of the electron creation and annihilation operators, $c_{k\sigma}^+$ and $c_{k\sigma}$, satisfying the fermion commutation relations,

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

Let us call these operators, following Schrieffer [1], 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, 2]. It is easy to show by direct calculation. Namely,

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

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

where $\hat{n}_{k\sigma} = c_{k\sigma}^+ c_{k\sigma}$ is the electron number operator. As follows from Eqs. (2)–(3), for $k \neq k'$ the Cooper pairs are bosons, while for $k = k'$ they do not obey the boson commutation relations. It can be shown that they obey the Pauli principle and have the fermion occupation numbers for one-particle states.

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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 cannot be directly solved by transforming it to the diagonalized form by means of some unitary transformation. 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 [3].

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.

$$\left[b_k, b_k^+\right]_- = 1 - c_{k\alpha}^+ c_{k\alpha} - c_{-k\beta}^+ c_{-k\beta} \; . \tag{4}$$

To operate with the pairon operators, the commutation relations for these operators must not 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

$$\left[\left[b_k^+, b_{k'}\right]_-, b_{k''}^+\right]_- = 2\delta_{kk'}\delta_{kk''} b_k^+ \; , \tag{5}$$

$$\left[\left[b_k^+, b_{k'}\right]_-, b_{k''}\right]_- = -2\delta_{kk'}\delta_{kk''} b_k \; . \tag{6}$$

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. (5), instead of the two presented Kroneker symbols there is one, namely, $\delta_{k'k''}$, and in relations corresponding to Eq. (6), $\delta_{kk'}$ is absent. Thus, the pairon operators satisfy some modified parafermi statistics of rank $p = 1$ (the latter because of the Fermi occupation numbers).

As follows from the definition of the particle number operator $\hat{N}_k$, $\hat{N}_k |N_k\rangle = N_k |N_k\rangle$. For the boson and fermion number operators, the well-known expression $\hat{N} = a_k^+ a_k$ 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

$$\hat{N}_k = \tfrac{1}{2}([a_k^+, a_k]_- + p) \, , \tag{7}$$

for the case of pairons $p = 1$. Using Eq. (3) it is easy to show that Eq. (7) is equivalent to

$$\hat{N}_k = \tfrac{1}{2}(\hat{n}_{k\alpha} + \hat{n}_{-k\beta}) \, . \tag{8}$$

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. (8) follows that the expression $\hat{N}_k = b_k^+ b_k$ 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 general case

$$\hat{n}_{k\alpha}\hat{n}_{-k\beta} \neq \tfrac{1}{2}(\hat{n}_{k\alpha} + \hat{n}_{-k\beta}) \, . \tag{9}$$

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. (9) is equal to its right-hand part. Thus,

$$\tfrac{1}{2}(\hat{n}_{k\alpha}+\hat{n}_{-k\beta})=b_k^+b_k\,, \tag{10}$$

and from Eqs. (8) and (10) follows that although Cooper's pairs are neither bosons nor fermions, for the operators of their number, the traditional form $\hat{N}_k=b_k^+b_k$ can be used.

The substitution of $\hat{n}_{k\alpha}+\hat{n}_{-k\beta}=2b_k^+b_k$, into the commutation relation (3) transforms it into

$$\left[b_k,b_k^+\right]_-=\left(1-2b_k^+b_k\right)\quad\text{or}\quad\left[b_k,b_k^+\right]_+=1\,. \tag{11}$$

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

The Eqs. (2) and (11) can be combined into one commutation relation

$$\left[b_k,b_{k'}^+\right]_-=\delta_{kk'}\left(1-2b_k^+b_k\right). \tag{12}$$

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

$$b_k\left|0\right\rangle=0,\qquad b_kb_{k'}^+\left|0\right\rangle=\delta_{kk'}\left|0\right\rangle. \tag{13}$$

The relations (12) and (13) are sufficient for performing calculations using only the pairon operators.

3 Two interacting Cooper's pairs

As an illustration of operations with the Cooper pair operators using their properties (12) and (13), we consider the model of two interacting pairs described by the BCS wave function

$$\left|\Psi(1,2)\right\rangle=\prod_{k_{j=1}}^{2}(u_{k_j}+v_{k_j}b_{k_j}^\dagger)\left|0\right\rangle=(u_{k_1}u_{k_2}+u_{k_1}v_{k_2}b_{k_2}^\dagger+u_{k_2}v_{k_1}b_{k_1}^\dagger+v_{k_1}v_{k_2}b_{k_1}^\dagger b_{k_2}^\dagger)\left|0\right\rangle. \tag{14}$$

Following the BCS theory, we assume that the interaction energies do not depend upon the value of moments, so the Hamiltonian is given by

$$H=2\sum_k\varepsilon_kb_k^\dagger b_k-V_0\sum_{k,k'}{}'b_{k'}^\dagger b_k+\frac{V_1}{2}\sum_{k_1',k_2'}{}'\sum_{k_1'',k_2''}{}'b_{k_1''}^\dagger b_{k_2''}^\dagger b_{k_1'}b_{k_2'}\,. \tag{15}$$

Calculation of the expectation value for the energy $W=\left\langle\Psi(1,2)\right|H\left|\Psi(1,2)\right\rangle$ gives

$$W=2v_{k_1}^2\varepsilon_{k_1}+2v_{k_2}^2\varepsilon_{k_2}-2V_0u_{k_1}v_{k_1}u_{k_2}v_{k_2}+V_1v_{k_1}^2v_{k_2}^2\,, \tag{16}$$

and by a minimization procedure respect to v_{k_1} and v_{k_2} using the following definitions

$$\Delta_{k_1}\equiv V_0u_{k_2}v_{k_2}\,;\qquad\Delta_{k_1}'\equiv V_1v_{k_2}^2\,, \tag{17}$$

$$\Delta_{k_2}\equiv V_0u_{k_1}v_{k_1}\,;\qquad\Delta_{k_2}'\equiv V_1v_{k_1}^2\,, \tag{18}$$

we obtain that

$$v_k^2=\frac{1}{2}\left(1-\frac{\varepsilon_k+\dfrac{\Delta_k'}{2}}{E_k'}\right);\qquad u_k^2=1-v_k^2\,, \tag{19}$$

$$E_k'=\sqrt{\left(\varepsilon_k+\frac{\Delta_k'}{2}\right)^2+\Delta_k^2}\,. \tag{20}$$

It can be shown that E_k' is the quasiparticle exitation energy. As in the BCS theory, using the approximations

$$\begin{aligned} &\Delta_{k_1} = \Delta_{k_2} = \Delta\,, \\ &\Delta_{k_1}' = \Delta_{k_2}' = \Delta'\,, \\ &\varepsilon_{k_1} \simeq \varepsilon_{k_2} = \varepsilon\,, \end{aligned} \tag{21}$$

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

$$\Delta' = V_1 \frac{V_0 - 2\varepsilon}{2V_0 + V_1}\,, \tag{22}$$

$$\Delta = \sqrt{\left(\frac{V_0}{2}\right)^2 - \left\{\varepsilon + \frac{V_1}{2}\left(\frac{V_0 - 2\varepsilon}{2V_0 + V_1}\right)\right\}^2}\,. \tag{23}$$

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. (22), this term depends upon the interaction 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. This renormalization is proportional to the interaction potential V_1 between pairs. On the other hand, the interpair interaction leads to an augmentation of the gap, which is according to Eq. (20) equal to $\sqrt{\Delta_k^2 + (\Delta_k'/2)^2}$, the interpair interaction increases the energy of creating the excited quasiparticle.

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. 23), it is not so, it is reduced to

$$\Delta = \sqrt{\left(\frac{V_0}{2}\right)^2 - \varepsilon^2}\,. \tag{24}$$

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 $\varepsilon_{k_1} = \varepsilon_{k_2} = \varepsilon$, Eq. (21), 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.

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

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