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# Statistics of hole pairs in a crystal lattice

Oracio Navarro*, Ilya G. Kaplan

*Instituto de Investigaciones en Materiales, Univ. Nacional Autonoma de Mexica, A.P. 70-360, 04510, México D.F., Mexico*

**Abstract**

The system of coupled hole pairs in a crystal lattice is studied. The exact commutation relations for the hole pair operators correspond to a modified parafermi statistics of rank $\bar{M}$ ($\bar{M}$ is the number of sites in a "superlattice" formed by centers of mass for each hole pair), i.e. one state can be occupied by up to $\bar{M}$ pairs. Even in the absence of dynamic interaction, the system of hole pairs is characterized by some immanent interaction (kinematic interaction). In spite of the kinematic interaction, there is no statistical prohibitions on the Bose–Einstein condensation of coupled hole pairs. © 2000 Elsevier Science B.V. All rights reserved.

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In contrary to the conventional (low temperature) superconductivity, the charge carriers in the high $T_c$ cuprates are positive. The holes are usually described as fermions and the Hamiltonian in the second quantization formalism is constructed from operators obeying the Fermi anticommutation relations [1]. As we showed in Ref. [2], the holes in a crystal lattice can be described as spinless particles with the paulion properties:

$$[b_n, b_{n'}^+]_- = [b_n, b_{n'}]_- = [b_n^+, b_{n'}^+]_- = 0 \quad \text{for } n \neq n',$$

$$[b_n, b_n^+]_+ = 1, \quad [b_n, b_n]_+ = [b_n^+, b_n^+]_+ = 0, \tag{1}$$

the operators acting on different sites obey the Bose commutation relations while the operators acting on one sites obey the Fermi commutation relations. Similar properties are valid for electron and spin excitations operators in crystal lattices [3,4]

In this report we discuss statistical properties of hole pairs and physical consequences from it. The Hamiltonian for holes in site representation is

$$H = \varepsilon_0 \sum_n b_n^+ b_n + \sum_{nn'} M_{nn'} b_n^+ b_{n'} + \sum_{nn'} V_{nn'} b_n^+ b_{n'}^+ b_{n'} b_n, \tag{2}$$

where $\varepsilon_0$ is the hole energy, $M_{nn'}$ is the hopping integral and $V_{nn'}$ is the hole–hole interaction term. Let us assume that the interaction between holes is attractive, so they can form coupled hole pairs. For one-pair problem, using Hamiltonian (2) in momentum space, we obtain the same result for the binding energy as that one for the Cooper pair. Let us consider some aspects of the many-pair problem.

In site representation, the hole pair creation and annihilation operators can be introduced as $a_t^+ = b_n^+ b_m^+$ and $a_t = b_m b_n$, respectively, where $t$ denotes the location point of the center of mass of the coupled hole pair, which not necessarily coincides with a crystal lattice site. The location points $t$ form a "superlattice". If we denote the number of sites in the original lattice by $M$, then the number of sites in the "superlattice" is given by $\bar{M} = M/m$, where $m$ is the number of sites in the region of localization of two coupled holes.

It can be shown that the hole pair operators $a_t^+$ and $a_t$ obey the same commutation relation, Eq. (1), as the hole operators, so they describe paulion particles (note: the same is true for the Cooper pair operators, see Ref. [5, Eqs. (2.21)], although the latter are constructed from delocalized fermion operators). Using the pair operators, the model Hamiltonian for hole pairs can be presented as

$$H = \sum_t \varepsilon_p a_t^+ a_t + \sum_{tt'} \bar{M}_{tt'} a_t^+ a_{t'}, \tag{3}$$

where the hole–hole interaction energy is included as a self-energy, $\varepsilon_p = 2\varepsilon_0 + V_0$, $V_0$ is the attractive potential

* Corresponding author. Tel.: 52-5-6224626; fax: 52-5-6161251.

*E-mail address:* navarro@servidor.unam.mx (O. Navarro)

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between holes which we assume to be the same for all pairs, like in the BCS theory, and $\bar{M}_{tt'}$ is the hopping integral for a coupled hole pair moving as a whole entity.

Hamiltonian (3) can be transformed by some unitary transformation:

$$A_q = \frac{1}{\sqrt{\bar{M}}}\sum_t u_{qt} a_t, \quad A_q^+ = \frac{1}{\sqrt{\bar{M}}}\sum_t u_{qt}^* a_t^+ \tag{4}$$

to the diagonalized form in quasi-momentum space

$$H = \sum_q \varepsilon_q A_q^+ A_q. \tag{5}$$

Since the operators $a_t$ and $a_t^+$ are neither bosons nor fermions, transformation (4) is not canonical, in other words, it does not preserve the commutation properties. As we proved in Ref. [2], the operators (4) obey the modified parafermi statistics of rank $\bar{M}$ with trilinear commutation relations. This statistics was introduced by Kaplan in 1976 [3]. From this follows that one state in $\boldsymbol{q}$-space can be occupied by up to $\bar{M}$ hole pairs. The number of hole pairs cannot be larger than the number $\bar{M}$ of sites in the "superlattice". Thus, there are no statistical prohibitions on the Bose–Einstein condensation phenomenon in a system of coupled hole pairs.

Second important consequence from the parafermi properties of the operators (4): Hamiltonian (5) does not describe independent quasiparticles. Although it has no dynamical interaction terms, it always contain an immanent interaction, named kinematic interaction [6], whose magnitude depends on the deviation of quasiparticle statistics from the Bose (Fermi) statistics. The expectation value of Hamiltonian (5) in the state with $N$ hole pairs with the same $\boldsymbol{q}$, $|N_q\rangle$, can be calculated as it was performed for holes in Ref. [2] and is equal to

$$E(N_q) = \left\langle N_q \Big| \sum_{q'} \varepsilon_{q'} A_{q'}^+ A_{q'} \Big| N_q \right\rangle = N\left[\varepsilon_q + \frac{(N-1)}{\bar{M}}(\bar{\varepsilon} - \varepsilon_q)\right], \tag{6}$$

where $\bar{\varepsilon} = (1/(\bar{M}-1))\sum_{q' \neq q} \varepsilon_{q'}$ is the mean energy of the hole-pair band. The second term in Eq. (6) describes the kinematic interaction and depends on the concentration of hole pairs.

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