phys. stat. sol. (b) **220**, 493 (2000)

Subject classification: 67.90.+z; 74.20.–z; 74.72.Jt; S10.15

Theoretical Study of Hole-Pair System in a Periodical Lattice

O. NAVARRO (a, b) and I. G. KAPLAN (a, c)

(a) Instituto de Investigaciones en Materiales, UNAM, Apartado Postal 70-360, 04510 México D.F., Mexico

(b) Laboratoire d'Etudes des Propiétés Electroniques des Solides, CNRS, B.P. 166, 38042 Grenoble Cedex 9, France

(c) Instituto de Física, UNAM, Apartado Postal 20-364, 01000 México D.F., Mexico

(Received November 1, 1999)

We investigate the statistics of the coupled hole pairs in a crystal lattice in high T_c superconductors, following the previously developed approach for the collective charge state (holon). The exact commutation relations for the hole pair operators correspond to a modified parafermi statistics of rank M' (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 M' pairs. Even in the absence of dynamic interaction, the system of hole pairs is characterized by some immanent interaction (kinematic interaction), which depends on the hole-pairs concentration. In spite of the kinematic interaction, there is no statistical prohibition on the Bose-Einstein condensation of coupled hole pairs.

Introduction Contrary to the conventional (low temperature) superconductivity, the charge carriers in the high-T_c cuprates are positive. Although some important aspects of the physical origin of this cuprates remain controversial, a set of characteristic features is well established. It is found that the pairing is between holes instead of electrons with a short coherence length. The other important peculiarity of the cuprate superconductivity is its anisotropy.

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]. Theoretical models which consider the local interactions seem appropriate to describe the short-range electron or hole pairing. The Hubbard model is one of the simplest and general models expressed in terms of local interactions and used to study the many-body aspects of the electronic properties in solids.

The single-band extended Hubbard Hamiltonian (EHH) can be written as [1, 2]

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j \,, \tag{1}$$

where t is the hopping integral, $t > 0$, $\langle i, j\rangle$ denotes nearest-neighbor sites, $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ being $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. It is important to mention that in principle the on-site, U, and inter-site, V, interaction terms are positive because they are direct Coulomb integrals between charges with the same sign. However, U and V could be negative if attractive indirect interactions through phonons or other type of excitations are included and they are stronger than the direct Coulomb repulsion.

When a particle–hole transformation [2] is made in the EHH, $c^{+}_{i,\sigma} \rightarrow h_{i,\sigma}$, the Hamiltonian becomes

$$H = (U + 2ZV)\,(N - \sum_{i,\sigma} n^{\mathrm{h}}_{i,\sigma}) + t \sum_{\langle i,j\rangle,\sigma} h^{+}_{j,\sigma} h_{i,\sigma} + U \sum_{i} n^{\mathrm{h}}_{i,\uparrow} n^{\mathrm{h}}_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n^{\mathrm{h}}_{i} n^{\mathrm{h}}_{j}\,, \tag{2}$$

where N is the total number of sites, Z is the lattice coordination number, $h^{+}_{i,\sigma}(h_{i,\sigma})$ is the hole creation (annihilation) operator, and $n^{\mathrm{h}}_{i} = n^{\mathrm{h}}_{i,\uparrow} + n^{\mathrm{h}}_{i,\downarrow}$ with $n^{\mathrm{h}}_{i,\sigma} = h^{+}_{i,\sigma} h_{i,\sigma}$. The first term in equation (2) only contributes to a shift in the total energy, and so the holes can be also described via the Hubbard Hamiltonian. However, there are two crucial differences between the electron and the hole cases: the density of holes is $1 - n$ in terms of the electron density n and the sign of the hopping matrix is opposite, which is irrelevant for the band structure of a bipartite lattice. The latter is a network that can be divided into two sublattices such that the first nearest-neighbors to one site of a sublattice belong to the other sublattice, like the square and simple cubic lattices. For a nonbipartite lattice (e.g., the triangular and face center cubic lattices), there are some peculiar behaviors of the electronic instabilities [3]. For instance, a strong-coupling analysis on a triangular lattice indicates that the charge density wave state cannot be formed for any band filling due to frustration [4].

As we already mentioned, usually holes are considered as fermion particles with spin $1/2$ and positive charge. But in real systems holes are located on many-electron atoms or molecules and can have different values of spin S. For example, holes in the CuO_2 planes in high T_c cuprates oxides have $S = 0$, the so-called Zhang-Rice singlet [5, 6]. In this study, we consider holes as positively charged atoms (molecules) with $S = 0$, or as spinless quasiparticles in the second quantization formalism.

As we showed in Ref. [7], the holes in a crystal lattice can be described as spinless particles with the paulion properties

$$\begin{aligned} &[b_n, b^{+}_{n'}]_{-} = [b_n, b_{n'}]_{-} = [b^{+}_{n}, b^{+}_{n'}]_{-} = 0 \quad \text{for} \quad n \neq n'\,, \\ &[b_n, b^{+}_{n}]_{+} = 1\,; \qquad [b_n, b_n]_{+} = [b^{+}_{n}, b^{+}_{n}]_{+} = 0\,, \end{aligned} \tag{3}$$

the operators acting on different sites obey the Bose commutation relations while the operators acting on one site obey the Fermi commutation relations. Similar properties are valid for electron and spin excitation operators in crystal lattices [8, 9].

In the absence of interaction between holes, the model Hamiltonian for an arbitrary lattice with one type of holes can be written as follows:

$$H = \varepsilon_0 \sum_{n} b^{+}_{n} b_n + \sum_{n,n'} M_{nn'} b^{+}_{n} b_{n'}\,, \tag{4}$$

where b^{+}_{n}, b_n are the hole creation and annihilation operators, respectively; ε_0 is the energy of the hole creation in a lattice and $M_{nn'}$ is the so called hopping integral, characterizing the efficiency of charge transfer (hopping) from site n to site n'. According to the theory of resonance interaction (see Section 1.2.3 in [10]), the hopping integral can be expressed by the resonance integral in the form

$$M_{nn'} = \langle \Psi_0(A^{+}_{n'})\, \Psi_0(A_n) |\, V_{\mathrm{int}}\, | \Psi_0(A_{n'})\, \Psi_0(A^{+}_{n}) \rangle\,, \tag{5}$$

where $\Psi_0(A_n)$ and $\Psi_0(A^{+}_{n})$ are the ground-state many-electron wave functions for neutral and ionized atoms (monomers) located at site n. In the case of one-electron wave

function the expression (5) has the same physical sense as the hopping integral in the Hubbard Hamiltonian, cf. Ref. [11].

When a hole–hole interaction is included, the Hamiltonian in site representation is

$$H = \varepsilon_0 \sum_n b_n^+ b_n + \sum_{nn'} M_{nn'} b_n^+ b_{n'} + \sum_{nn'} V_{nn'} b_n^+ b_{n'}^+ b_{n'} b_n \,, \tag{6}$$

where $V_{nn'}$ is the hole–hole interaction term. We consider the case of one hole per site, so we have not a term similar to the U term in Eq. (2). Let us assume that the interaction between holes is attractive, so they can form coupled hole pairs.

Some Properties of the Hole-Pair System 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. Suppose that 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 $M' = M/m$, where m is the number of sites in the region of localization of two coupled holes, see Fig. 1.

The hole pair operators a_t^+ and a_t obey the same commutation relation, Eq. (3), as the hole operators, so they describe paulion particles (note: the same is true for the Cooper pair operators, see Ref. [12], Eqs. (2.21), although they are constructed from delocalized fermion operators). Using the pair operators, the model Hamiltonian for hole pairs can be presented as

$$H = \sum_t \varepsilon_{\mathrm{p}} a_t^+ a_t + \sum_{tt'} \overline{M}_{tt'} a_t^+ a_{t'} \,, \tag{7}$$

where the hole–hole interaction energy is included as a self-energy, $\varepsilon_{\mathrm{p}} = 2\varepsilon_0 + V_0$, V_0 is the attractive potential between holes which we assume to be the same for all pairs, like in the BCS theory, and $\overline{M}_{tt'}$ is the hopping integral for a coupled hole pair moving as a whole entity.

Let us consider some aspects of the many-pair problem. The Hamiltonian (7) can be transformed by some unitary transformation

$$A_{\mathbf{q}} = \frac{1}{\sqrt{M'}} \sum_t u_{\mathbf{q}t} a_t \,; \qquad A_{\mathbf{q}}^+ = \frac{1}{\sqrt{M'}} \sum_t u_{\mathbf{q}t}^* a_t^+ \tag{8}$$

to the diagonalized form in quasi-momentum space

$$H = \sum_{\mathbf{q}} \varepsilon_{\mathbf{q}} A_{\mathbf{q}}^+ A_{\mathbf{q}} \,, \tag{9}$$

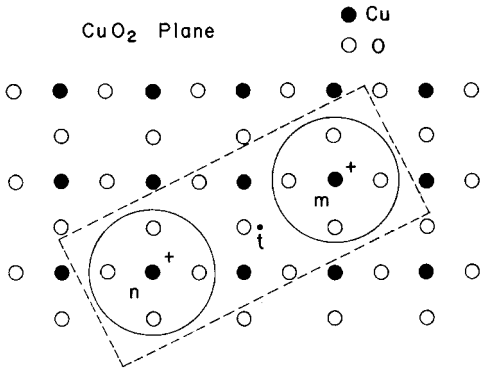

Fig. 1. Coupled hole pair on the CuO_2 plane in high-T_c superconductors ceramics

where, for a lattice of one atom (molecule) per cell, the pair energy is given by

$$\varepsilon_{\mathbf{q}} = \varepsilon_{\mathrm{p}} + \sum_{t'(\neq t)} \overline{M}_{tt'} \exp\left[i\mathbf{q} \cdot (\mathbf{r}_t - \mathbf{r}_{t'})\right]. \tag{10}$$

Since the operators a_t and a_t^+ are neither bosons nor fermions, the transformation (8) is not canonical, in other words, it does not preserve the commutation properties. As we proved in Ref. [7], the operators (8) obey the modified parafermi statistics of rank M' with trilinear commutation relations. This statistics was introduced by Kaplan in 1976 [8] for molecular exiton and magnon systems. According to its properties, one state in $\mathbf{q}$-space can be occupied by up to M' hole pairs. The number of hole pairs cannot be larger than the number 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.

Another important consequence from the parafermi properties of the operators (8) is that the Hamiltonian (9) does not describe independent quasiparticles. Although it has no dynamical interaction terms, it always contains an immanent interaction, named kinematic interaction [13], whose magnitude depends on the deviation of quasiparticle statistics from the Bose (Fermi) statistics.

For the case of N hole-pairs with the same $\mathbf{q}$, the wave function is given by

$$|N_{\mathbf{q}}\rangle = C_N (A_{\mathbf{q}}^+)^N |0\rangle. \tag{11}$$

Using this state vector it can be calculated the expectation value of the Hamiltonian (9), as it was performed for holes in Ref. [7], it is equal to

$$E(N_{\mathbf{q}}) = \langle N_{\mathbf{q}}| \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}'} A_{\mathbf{q}'}^+ A_{\mathbf{q}'} |N_{\mathbf{q}}\rangle = N\left[\varepsilon_{\mathbf{q}} + \frac{(N-1)}{M'} (\overline{\varepsilon} - \varepsilon_{\mathbf{q}})\right], \tag{12}$$

where $\overline{\varepsilon} = \frac{1}{M'-1} \sum_{\mathbf{q}' \neq \mathbf{q}} \varepsilon_{\mathbf{q}'}$ is the mean energy of the hole-pair band. The second term in (12) describes the kinematic interaction and depends on the concentration of hole pairs.

Conclusions We have studied the statistical properties of the collective hole-pair states in a periodical lattice using the exact trilinear commutation relations for the pair operators. As was shown, the hole-pairs obey the modified parafermi statistics of rank M', where M' is the number of lattice sites on which the pair can be created, i.e. one state can be occupied by up to M' pairs. The number of hole-pairs cannot be larger than the number M' of sites. Thus, there is no statistical prohibition on the Bose-Einstein condensation phenomenon in a hole-pair system.

The second important conclusion of this study is that, in general, the system of dynamically non-interacting hole-pairs cannot be considered as an ideal gas. In the hole-pair system, the immanent interaction and coupling of all states of the pair band (the so called kinematic interaction) is always present. The magnitude of the kinematic interaction is proportional to the hole-pair concentration, $\frac{N}{M'}$, and has the same order as the corrections for the non-Bose behavior in the commutation relations for the pair operators.

Acknowledgement This work was partially supported by grants from DGAPA-UNAM IN108697 and IN109998 and by CONACyT 25582-E. One of us (O.N.) wants to thank CONACyT and DGAPA-UNAM for a sabbatical fellowship.

References

[1] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[2] M. W. Long, The Hubbard Model (Recent Results), Ed. M. Rasetti, World Scientific Publ. Co., Singapore 1991 (p. 1).
[3] L. A. Perez, O. Navarro, and C. Wang, Phys. Rev. B **53**, 15389 (1996).
[4] R. R. dos Santos, Phys. Rev. B **48**, 3976 (1993).
[5] F. S. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[6] I. G. Kaplan, J. Soullard, J. Hernandez-Cobos, and R. Pandey, J. Phys.: Condensed Matter **11**, 1049 (1999).
[7] I. G. Kaplan and O. Navarro, J. Phys.: Condensed Matter **11**, 6187 (1999).
[8] I. G. Kaplan, Theor. Math. Phys. **27**, 466 (1976).
[9] B. A. Nguen and N. C. Hoang, J. Phys.: Condensed Matter **2**, 4127 (1990).
[10] I. G. Kaplan, Theory of Molecular Interactions, Elsevier Publ. Co., Amsterdam 1986.
[11] J. E. Hirsch, Phys. Rev. B **48**, 3327 (1993).
[12] J. R. Schrieffer, Theory of Superconductivity, Addison-Wesley Publ. Co., Redwood City 1988.
[13] F. Dyson, Phys. Rev. **102**, 1217 (1956).