*Краткие сообщения ОИЯИ №2[28]-88 JINR Rapid Communication No.2[28]-88*
УДК 538.945

# ON THE RVB THEORY OF HIGH-$T_c$ SUPERCONDUCTIVITY

Nguyen Van Hieu, Nguyen Ai Viet

The high-$T_c$ superconductivity of a nearly half-filled electron system in a two-dimensional square lattice with the Hubbard Hamiltonian is studied in the strong repulsion limit by means of the self-consistent field method. Besides the superconducting order parameter the self-consistent effective Hamiltonian contains some physical parameters which are the normal vacuum averages of the products of two quasifermion operators. The system of equations for all these parameters of the model is derived. The possible itinerant antiferromagnetism of the mobile holes is also considered.

The investigation has been performed at the Institute of Physics, Hanoi, Vietnam.

## К теории высокотемпературной сверхпроводимости с резонирующей валентной связью

Нгуен Ван Хьеу, Нгуен Аи Вьет

Высокотемпературная сверхпроводимость почти наполовину заполненной электронной системы в двумерной квадратной решетке с гамильтонианом Хаббарда изучается в пределе сильного отталкивания при помощи метода самосогласованного поля. Наряду со сверхпроводящим параметром порядка самосогласованный эффективный гамильтониан содержит некоторые физические параметры, представляющие собой нормальные вакуумные средние произведений двух квазифермионных операторов. Выводится система уравнений для всех этих параметров модели. Возможный антиферромагнетизм проводящих дырок также рассматривается.

Работа выполнена в Институте физики, Ханой, Вьетнам.

The problem of high-$T_c$ superconductivity was studied theoretically during many years /1/. Since the experimental discovery of high-$T_c$ superconducting materials /2/ the well-known models of high-$T_c$ superconductivity as well as the newly proposed ones with different physical mechanisms were widely discussed /3,4/. Many of them have a common feature: the essential mechanism of the superconductivity is the strong electron correlation due to the strong on-site repulsion of electrons. The simplest model of this type is the Anderson resonating valence bond (RVB) theory [4] of a nearly half-filled electron system with the Hubbard Hamiltonian [5]. In deriving the equations for the order parameters of this model [4] Baskaran, Zou and Anderson (BZA) have introduced the electron concentration into the Hamiltonian in a phenomenological manner. Moreover, besides the order parameters considered by BZA there exist other physical parameters of the system which also must be taken into account in any self-consistent theory. On the other hand, the simplest RVB model with the Hubbard Hamiltonian proposed by Anderson is the essential part of many high-$T_c$ superconductivity models with the strong electron correlation. Therefore it is necessary to generalize the reasonings of BZA and provide a more systematic and complete theoretical study of the above simplest RVB model. This will be done in the present work.

We study the two-dimensional electron system in a square lattice with the Hubbard Hamiltonian in the limit of the very strong on-site repulsion of electrons and derive the effective Hamiltonian acting within the Hilbert subspace of states with non-doubly occupied sites. The latter can be considered as the total Hamiltonian of the system of holes in the nearly half-filled electron system. To apply the famous self-consistent field method of Bogolubov [6] for studying this system it is necessary to introduce the vacuum averages of all products of two fermion operators. They are the physical parameters of the system. We are interested also in the coexistence of the superconductivity and the itinerant antiferromagnetism of the system of mobile holes. For that purpose we divide the original square lattice into two square sublattices and assume that the vacuum averages of the same product of two operators at the sites of different sublattices may be different. By means of the self-consistent field theory reasonings we then derive the system of equations for all physical parameters of the system including the order parameters studied by BZA. One of the physical parameters of the system — the hole concentration — automatically appears in the effective Hamiltonian in a self-consistent manner, and the derived system of equations permits one to study the hole concentration dependence of the energy gap and the superconducting transition temperature, in particular.

The physical assumptions of the model have been stated and discussed in Refs.[4]. We start from the Hubbard Hamiltonian for a two-dimensional electron system in a square lattice R with the hopping integral t and the strong on-site repulsion potential U

$$H = -t \sum_{\sigma} \sum_{<ij>} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

where $c_{i\sigma}$ and $c^+_{i\sigma}$ are the destruction and creation operators for the electron with spin projection $\sigma = \uparrow, \downarrow$ at the site i,

$$n_{i\sigma} = c^+_{i\sigma} c_{i\sigma} ,$$

$\langle ij \rangle$ denote all possible pairs of nearest neighbours. By means of a suitable canonical transformation /7/ excluding the transitions from the Hilbert subspace of the states without doubly occupied sites to the complementary one in the lowest order in t/U, and the orthogonal projection onto the above Hilbert subspace

$$P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) ,$$

we obtain the following effective Hamiltonian acting only within this Hilbert subspace

$$H = P \{ -t \sum_\sigma \sum_{\langle ij \rangle} c^+_{i\sigma} c_{j\sigma} - J \sum_{\langle ij \rangle} \sum_{\langle \ell j \rangle} \times$$

$$\times (c^+_{i\uparrow} c^+_{j\downarrow} - c^+_{i\downarrow} c^+_{j\uparrow})(c_{j\downarrow} c_{\ell\uparrow} - c_{j\uparrow} c_{\ell\downarrow}) \} P, \tag{2}$$

$$J = \frac{4t^2}{U} .$$

Let us consider a nearly half-filled electron system with the given Hamiltonian (1). In the limit of large U the states with doubly occupied sites form very high upper energy bands, and the main effect of the electron correlation — due to the presence of the repulsion term in the Hubbard Hamiltonian — is to prevent the electron hopping from the single occupied sites into the doubly occupied ones. In this case the nearly half-filled electron system behaves like a system of holes with a low concentration. The total Hamiltonian of this system of holes is obtained directly from the expression (2) by considering $c_{i\sigma}$ and $c^+_{i\sigma}$ as the creation and destruction operators for the holes with the opposite spin projection:

$$c_{i\uparrow} = h^+_{i\downarrow}, \quad c_{i\downarrow} = h^+_{i\uparrow}, \quad c^+_{i\uparrow} = h_{i\downarrow}, \quad c^+_{i\downarrow} = h_{i\uparrow} .$$

Thus the problem to be studied is the superconductivity of the system with following total Hamiltonian

$$H_h = P \{ t \sum_\sigma \sum_{\langle ij \rangle} h^+_{i\sigma} h_{j\sigma} - J \sum_{\langle ij \rangle} \sum_{\langle \ell j \rangle} \times$$
$$\times (h^+_{i\uparrow} h^+_{j\downarrow} - h^+_{i\downarrow} h^+_{j\uparrow})(h_{j\downarrow} h_{\ell\uparrow} - h_{j\uparrow} h_{\ell\downarrow}) \} P. \tag{3}$$

Note that the quasifermion operators

$$P h_{i\sigma} P, \qquad P h^{+}_{i\sigma} P$$

do not satisfy the usual canonical anticommutation relations while the hole operators $h_{i\sigma}$ and $h^{+}_{i\sigma}$ do satisfy. Therefore it is very convenient to use the total Hamiltonian in the form (3).

Now we apply the self-consistent field method to the system with the Hamiltonian (3). Each product of 4 quasifermion operators is then replaced by a linear combination of the products of two operators with coefficients being the vacuum averages of the products of two remaining operators taken with the appropriate sign $\pm 1$. Among the non-zero vacuum averages there are three main physical parameters:

$$n = \sum_{\sigma} \langle P h^{+}_{i\sigma} h_{i\sigma} P \rangle ,$$

$$p = \sum_{\sigma} \sum_{i \in D_j} \langle P h^{+}_{i\sigma} h_{j\sigma} P \rangle , \qquad (4)$$

$$\tilde{n} = \sum_{\sigma} \sum_{i \in D_j} \sum_{\ell \in D_j} \langle P h^{+}_{i\sigma} h_{\ell\sigma} P \rangle ,$$

where $D_j$ denotes the set of all 4 sites i which are the nearest neighbours of the site j. We are interested also in the itinerant antiferromagnetism of the mobile holes. For this purpose we imagine that the original square lattice R is composed by two square sublattice $R^{I}$ and $R^{II}$ with the same lattice constant

$$R = R^{I} \cup R^{II} ,$$

and introduce the constants

$$n^{I,II}_{\sigma} = \langle P h^{+}_{i\sigma} h_{i\sigma} P \rangle \qquad \text{for } i \in R^{I,II} ,$$

$$\tilde{n}^{II,I}_{\sigma} = \sum_{i \in D_j} \sum_{\ell \in D_j} \langle P h^{+}_{i\sigma} h_{\ell\sigma} P \rangle \qquad \text{for } j \in R^{I,II} . \qquad (5)$$

We assume that

$$n^{I}_{\uparrow} = n^{II}_{\downarrow} , \quad n^{I}_{\downarrow} = n^{II}_{\uparrow} , \quad \tilde{n}^{I}_{\uparrow} = \tilde{n}^{II}_{\downarrow} , \quad \tilde{n}^{I}_{\downarrow} = \tilde{n}^{II}_{\uparrow} , \qquad (6)$$

and set

$$m = n^{I}_{\uparrow} - n^{I}_{\downarrow} = -(n^{II}_{\uparrow} - n^{II}_{\downarrow}) ,$$

$$\tilde{m} = \tilde{n}^{I}_{\uparrow} - \tilde{n}^{I}_{\downarrow} = -(\tilde{n}^{II}_{\uparrow} - \tilde{n}^{II}_{\downarrow}) . \qquad (7)$$

The physical parameters (4) and (7) automatically appear in the self-consistent effective Hamiltonian of the system of holes. Besides the normal vacuum averages (4) and (5) we introduce also the anomalous one $\Delta$,

$$\frac{1}{2}\Delta = \sum_{i \in D_j} \langle P(c^+_{i\uparrow} c^+_{j\downarrow} - c^+_{i\downarrow} c^+_{j\uparrow}) P \rangle, \tag{8}$$

which is the superconducting order parameter. By applying the famous Bogolubov transformation to diagonalize the self-consistent effective Hamiltonian we can derive the system of equations for the physical quantities n, $\tilde{n}$, p, m, $\tilde{m}$ and $\Delta$.

To formulate the final results we introduce following notations:

$$\gamma(\bar{k}) = \sum_{i \in D_j} e^{i(\bar{R}_i - \bar{R}_j)\bar{k}}, \tag{9}$$

$\bar{R}_i$ and $\bar{R}_j$ being the coordinate vectors of the sites i and j,

$$\epsilon(\bar{k}) = -\frac{1}{2} J [ n\gamma(\bar{k})^2 + \tilde{n} ], \tag{10}$$

$$\delta(\bar{k}) = (Jp - t)\gamma(\bar{k}), \tag{11}$$

$$\mu(\bar{k}) = \frac{1}{2}[ m\gamma(\bar{k})^2 + \tilde{m} ], \tag{12}$$

$$\Delta(\bar{k}) = -J\Delta\gamma(\bar{k}), \tag{13}$$

$$\xi_{\alpha,\beta}(\bar{k}) = \epsilon(\bar{k}) \pm [ J^2_{\mu}(\bar{k})^2 + \delta(\bar{k})^2 ]^{1/2}, \tag{14}$$

$$E_{\alpha,\beta}(\bar{k}) = \{[\xi_{\alpha,\beta}(\bar{k}) - E_F]^2 + \Delta(\bar{k})^2\}^{1/2}, \tag{15}$$

$$\Phi[E_{\alpha,\beta}(\bar{k})] = \frac{1}{2}[1 + \mathrm{th}\frac{E_{\alpha,\beta}(\bar{k})}{2T}] + \frac{\xi_{\alpha,\beta}(\bar{k}) - E_F}{2E_{\alpha,\beta}(\bar{k})}[1 - \mathrm{th}\frac{E_{\alpha,\beta}(\bar{k})}{2T}], \tag{16}$$

$E_F$ being the Fermi energy. It is easy to verify that

$$\lim_{\Delta\to o} \Phi[E_{\alpha,\beta}(\bar{k})] = f[\xi_{\alpha,\beta}(\bar{k})], \tag{17}$$

where $f[\xi]$ is the usual Fermi distribution function at temperature T

$$f[\xi] = [1 + e^{\frac{\xi - E_F}{T}}]^{-1}. \tag{18}$$

Denote by N the number of sites; by $\sum_{\bar{k}}$, the sum over the Brillouin zone of each sublattice $R^I$ or $R^{II}$. We have following system of equations

$$n = \frac{2}{N} \sum_{\bar{k}} \{\Phi[E_\alpha(\bar{k})] + \Phi[E_\beta(\bar{k})]\}, \tag{19}$$

$$m = -\frac{2J}{N} \sum_{\bar{k}} \frac{\mu(\bar{k})}{[J^2\mu(\bar{k})^2 + \delta(\bar{k})^2]^{1/2}} \{\Phi[E_\alpha(\bar{k})] - \Phi[E_\beta(\bar{k})]\}, \tag{20}$$

$$p = -\frac{2}{N} \sum_{\bar{k}} \frac{\gamma(\bar{k})\,\delta(\bar{k})}{[J^2\mu(\bar{k})^2 + \delta(\bar{k})^2]^{1/2}} \{\Phi[E_\alpha(\bar{k})] - \Phi[E_\beta(\bar{k})]\}, \tag{21}$$

$$\tilde{n} = \frac{2}{N} \sum_{\bar{k}} \gamma(\bar{k})^2 \{\Phi[E_\alpha(\bar{k})] + \Phi[E_\beta(\bar{k})]\}, \tag{22}$$

$$\tilde{m} = -\frac{2J}{N} \sum_{\bar{k}} \frac{\gamma(\bar{k})^2 \mu(\bar{k})}{[J^2\mu(\bar{k})^2 + \delta(\bar{k})^2]^{1/2}} \{\Phi[E_\alpha(\bar{k})] - \Phi[E_\beta(\bar{k})]\}, \tag{23}$$

$$1 = \frac{2J}{N} \sum_{\bar{k}} \gamma(k)^2 \{\frac{1}{E_\alpha(\bar{k})} \,\mathrm{th}\, \frac{E_\alpha(\bar{k})}{2T} + \frac{1}{E_\beta(\bar{k})} \,\mathrm{th}\, \frac{E_\beta(\bar{k})}{2T}\}. \tag{24}$$

In the limit $\Delta \to 0$, $m \to 0$, $\tilde{m} \to 0$ the relations (19), (21) and (22) form a system of equations determining the physical parameters n, $\tilde{n}$ and p in terms of the given constants t, J and $E_F$. At very low hole concentration

$$p \approx 4n, \qquad \tilde{n} \approx 16n.$$

This result shows that it is necessary to introduce the physical parameters n and $\tilde{n}$ together with the order parameter p of BZA. With the given values of n, $\tilde{n}$ and p the relations (20) and (23) at the limit $\Delta \to 0$ form a system of equations for the antiferromagnetism parameters m and $\tilde{m}$ of the normal system of holes. For a low concentration of hole there exists only the trivial zero solution

$$m = \tilde{m} = 0.$$

Thus the itinerant antiferromagnetism of the normal system of low density mobile holes does not exist. With the given values of n, $\tilde{n}$ and p equation (24) determines the dependence of the energy gap and the superconducting transition temperature on these physical parameters.

The physical implications of the system of equations (19)-(24) will be studied in a subsequent work.

The authors would like to express their sincere appreciation to Academician N.N.Bogolubov and Professor V.G.Kadyshevsky for the interest in this work and the stimulating discussions.

*REFERENCES*

1. Ginzburg V.L., Kirzhnitz D.A. Problem of High Temperature Superconductivity, M., Nauka, 1977.
2. Bednorz J.G., Muller K.A. — Z.Phys., 1986, v. B64, N. 2, p.189-193;
   Chu C.W., Hor P.H., Meng P.L., Gao L., Huang Z.J., Wang Y.Q. — Phys.Rev.Lett., 1987, v.58, N.4, p.405-407.
3. Plakida N.M., Aksenov V.L., Drechler S.L. — Europhys. Lett., 1987, v.4, N.11, p.1309-1314;
   Emery V.J. — Phys.Rev.Lett., 1987, v.58, N. 26, p.2194-2797;
   Parameter R.H. — Phys.Rev.Lett., 1987, v.58, N. 8, p.923-925;
   Rice T.M. — Z.Phys., 1987, v. B67, N.2, p.141-145;
   Kresin V.Z. — Solid State Commun., 1987, v.63, N.8, p.725-727;
   Aoki H., Kamimura — Solid State Commun., 1987, v. 63, N. 7, p.665-669;
   Kuramoto Y., Watanabe T. — Solid State Commun., 1987, v. 63, N.9, p.821-825;
   Kukuyama H., Yosida K. — Japan J. App. Phys., 1987, v. 26, N.4, p.L371-L373;
   Ohkawa F.J. — Japan J. App. Phys., 1987, v.26, N.5, p.L652-L654;
   Kamimura H. — Japan J. App. Phys., 1987, v. 26, N.5, p.L627-L630.
4. Anderson P.W. — Science, 1987, v. 235, N. 4793, p.1196-1198;
   Baskaran G., Zou Z., Anderson P.W. — Solid State Commun., 1987, v. 63, N.11, p.973-976.
5. Hubbard J. — Proc. Roy. Soc., 1963, v. A276, N.1365, p.238-257.

6. Bogolubov N.N. Selected Works. Kiev, Naukova Dumka, 1969.
7. Hirsch J.E. — Phys.Rev.Lett., 1985, v.54, N.12, p.1317-1320; Gros C., Joynt R., Rice T.M. — Z.Phys., 1987, v. B68, N.4, p.425-432.

Received on February 9, 1988.