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SUPEREXCHANGE INTERACTION AND SUPERCONDUCTIVITY IN HUBBARD MODEL

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ԳԵՐՓՈԽԱՆԱԿԱՅԻՆ ՓՈԽԱԶԴԵՑՈՒԹՅՈՒՆԸ ԵՎ ԳԵՐՀԱՂՈՐԴԱԿԱՆՈՒԹՅՈՒՆԸ ՀԱԲԱՐԴԻ ՄՈԴԵԼՈՒՄ

Գտնված է մի ունիտար ձևափոխություն, որը թույլ է տալիս ցանկացած նշանով ներատոմային փոխազդեցություն ունեցող հաբարդի մոդելի համար ստանալ նոր քվազիմասնիկների՝ սպինոնների, դուբլոնների և հոլոնների միջոցով արտահայտված արդյունավետ մի համիլտոնյան: Տարածության չափողականությունից անկախ, t^2/U մշգրտությամբ ստացված է երկատոմ մոլեկուլի մշգրիտ լուծման հետ համընկնող հայզենբերգի արդյունավետ համիլտոնյանը: Ցույց է տրված, որ $U > 0$ դեպքում ստացված համիլտոնյանը համընկնում է հայզենբերգի սպինների գերփոխանակային փոխազդեցության մոդելի հետ, իսկ $U < 0$ դեպքում՝ լիցքավորված դուբլոնների ու հոլոնների գերփոխանակային փոխազդեցության հետ: Գտնված է երկատոմ մոլեկուլի և գծային անվերջ շղթայի ընկալունակությունը արտաքին մագնիսական դաշտում և հաշվված են ֆերոմագնիսական վիճակին անցման կրիտիկական դաշտը: Հայզենբերգ-Հզինգի մոդելի շրջանակներում, երբ $U < 0$, որում հաշվի է առնված հարևան կենտրոններից էլեկտրոնների կուլոնյան վանումը ($V > 0$), ուսումնասիրված է մեկ ատոմին ընկնող էլեկտրոնների թվից կախված գերհաղորդականության վիճակին անցման հնարավորությունը:

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СУПЕРОБМЕННОЕ ВЗАИМОДЕЙСТВИЕ И СВЕРХПРОВОДИМОСТЬ В МОДЕЛИ ХАББАРДА

Найдено унитарное преобразование, позволяющее получить для модели Хаббарда с произвольным знаком внутриатомного взаимодействия (U) эффективный гамильтониан в терминах новых квазичастиц - спинонов, дублонов и голонов. Вне зависимости от размерности пространства с точностью до t^2/U получен эффективный гамильтониан Гайзенберга, совпадающий с точным решением двухатомной молекулы. Показано, что при $U > 0$ полученный гамильтониан совпадает с моделью Гайзенберга с суперобменным взаимодействием спинов, а при $U < 0$ - суперобменным взаимодействием заряженных голонов и дублонов. Найдена восприимчивость двухатомной молекулы и бесконечной линейной цепочки атомов во внешнем магнитном поле и рассчитаны критические поля перехода в ферромагнитное состояние. В рамках XXY модели Гайзенберга-Изинга с $U < 0$, учитывающей кулоновское отталкивание $V > 0$ электронов на соседних центрах, исследовалась возможность перехода в сверхпроводящее состояние в зависимости от числа электронов на атомы.

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SUPEREXCHANGE INTERACTION AND SUPERCONDUCTIVITY IN HUBBARD MODEL

A unitary transformation has been found which allows one to obtain for the Hubbard model with an arbitrary sign of intratomic interaction (U) an effective hamiltonian in terms of new quasi-particles - spinons, doublons and holons. Irrespective of space dimension, an effective Heisenberg hamiltonian with an accuracy up to t^2/U coinciding with exact solution of diatomic molecule is obtained. It is shown that at $U > 0$ the obtained hamiltonian coincides with the Heisenberg model with superexchange interaction of spinons, and at $U < 0$ - with superexchange interaction of charged holons and doublons. Susceptibility of a diatomic molecule and infinite linear atomic chain in the external magnetic field is found and critical fields of transition to ferromagnetic state are calculated. In the framework of Heisenberg-Ising XXY model with $U < 0$ that takes account of Coulomb repulsion, $V > 0$, of electrons on neighbour centres there was investigated a possibility of transition to superconductivity state versus the number of electrons per atom, n.

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Introduction

As known from the experiments [1] , in high-temperature superconductors (HTSC) based on oxide ceramics the correlation length ξ turns out to be comparable with the lattice parameter, which is by one-two orders of magnitude less than in usual superconductors [2] . The X-ray structural analysis of these compounds points out that they contain one, two and three planes of CuO_2, and this correlates with the values of their critical temperatures of superconductivity (SC) transition equal approximately to 40 K, 80 K and 120 K, respectively [3] . So long as the interplanar distances in them are larger than the lattice parameter in the plane, these systems can be considered as two-dimensional or quasi-two-dimensional.

High critical temperatures of SC transition, T_c , and the large effective masses of electrons, $m \sim 10 m_e$ point out an essentially local character of interaction of the electrons with each other and with the lattice.

The band theory approach turned out inapplicable as to describe the HTSC properties, since the ground state of "pure" La_2CuO_4 and $YBa_2Cu_3O_6$ contrary to predictions of this theory are antiferromagnetics and semiconductors. And these facts were theoretically explained in systems with strong electron correlations.

As shown below, in strong-correlated systems of La_2CuO_4 we are able to separate the spin degrees of freedom from the charge ones as well as to describe the system in terms of new quasi-particles - spin-carrying spinons and charge-carrying doublons and holons.

The analysis of X-ray spectra near the absorption edge is indicative of the presence of mainly two-valence state of copper Cu^{2+} with electron configuration d^9 in the system [4]. The states of Cu^+ with an extra electron are by energy much higher ($U \sim 5 - 10$ eV). This allows us to describe the copper atoms by the Hubbard model [5] with strong Coulomb repulsion (U) on the centre.

The model of resonating valence bonds (RVB) [6] describing the spin fermi-liquid turned out to be rather fruitful to study a behavior of electrons of copper sublattice. At one electron per atom the ground state of the system of resonating spinon pairs turns out to be a singlet (a quantum analog of antiferromagnetism) [7,8] . The low-lying triplet excitations are separated from the quasi-ion ones by the Mott-Hubbard gap $\sim U$ [9] .

Contrary to that the interaction of electrons on oxygen atoms has an attractive nature, which may be due to both local interaction of electrons with the lattice and the attractive

mechanism of chemical nature [10] connected with hole polarization of occupied electron p-shell [11] . This may be the cause of the fact that the oxygen atoms form two relatively stable configurations O^{--} and O. In what follows we compare them with charged quasi-ion states - holons and doublons.

The mentioned peculiarities of the HTSC electron structure can be taken into account in the Hubbard model with Coulomb interaction on the neighbour centres V:

$$H = E_o \sum_{i\sigma} C^+_{i\sigma} C_{i\sigma} - t \sum_{\langle ij\rangle\sigma} C^+_{i\sigma} C_{j\sigma} + U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + V \sum_{\langle ij\rangle} (n_i - 1)(n_j - 1) \qquad (1)$$

where the integral of transition t represents indirect transitions of electrons from oxygen to oxygen via the intermediate copper atom, or from copper to copper via oxygen, and parameter U is positive for the copper sublattice and negative for the oxygen one. In t^2/U approximation the result turns out to be independent of space dimensions and coincides with the exact solution for the diatomic molecule studied in Section 1.

In Section 2 we have obtained an effective hamiltonian for the infinite linear chain and studied the system response to the external magnetic field.

In Section 3 the superconductivity properties of the system are studied.

1. The hamiltonian of a diatomic molecule in the Hubbard model has a form:

$$H = E_o \sum_{\sigma} (C^+_{1\sigma} C_{1\sigma} + C^+_{2\sigma} C_{2\sigma}) - t \sum_{\sigma} (C^+_{1\sigma} C_{2\sigma} + C^+_{2\sigma} C_{1\sigma}) + \frac{U}{2} \sum_{\sigma} (n_{1\sigma} n_{2-\sigma} + n_{2\sigma} n_{2-\sigma}) \qquad (1')$$

here the first term is the electron coupling energy in the atom, the second term is kinetic energy with the integral of transition t, the last term is the intratomic interaction of two electrons which can be both positive and negative.

It is convenient in (1) to turn to Hubbard operators [5] :

$$C_{i\sigma} = X_i^{o\sigma} + \sigma X_i^{-\sigma 2}$$

$$C_{i\sigma}^{+} = X_i^{\sigma o} + \sigma X_i^{2-\sigma} \qquad (2)$$

From the anticommutation relation of C^+ and C we obtain:

$$\sum_{\sigma} X_i^{\sigma\sigma} + \sum_{\alpha} X_i^{\alpha\alpha} = 1 \qquad (3)$$

where summation in (3) goes over $\sigma = \pm 1$ and $\alpha = 0,2$ (0 for holons and 2 for doublons). Hamiltonian (1) takes the form:

$$H = E_o \sum_{\sigma} (X_1^{\sigma\sigma} + X_2^{\sigma\sigma}) - t(\tau_{12}^{+} + \tau_{12}) - 2t(B_{12}^{+} + B_{12}) + (U + 2E_o)(X_1^{22} + X_2^{22}) \qquad (4)$$

wherein we introduced notations:

$$\tau_{ij} = \sum_{\sigma} (X_i^{\sigma o} X_j^{o\sigma} + X_j^{2-\sigma} X_i^{-\sigma 2})$$

$$B_{ij} = \frac{1}{2} \sum_{\sigma} \sigma (X_i^{\sigma o} X_j^{-\sigma 2} + X_j^{\sigma o} X_i^{-\sigma 2}) \qquad (5)$$

Applying to (4) the canonical transformation

$$T = \exp\left\{ \frac{1}{2} (B_{12}^{+} - B_{12}) \operatorname{arctg} \frac{4t}{U} \right\} \qquad (6)$$

and getting rid of the linear over B term in (4) we finally obtain an effective hamiltonian

$$H = E_o \sum_{\sigma} (X_1^{\sigma\sigma} + X_2^{\sigma\sigma}) - t(\tau_{12} + \tau_{12}^{+}) + \varepsilon(U)(B_{12} B_{12}^{+} - B_{12}^{+} B_{12}) + (U + 2E_o)(X_1^{22} + X_2^{22}), \qquad (7)$$

where

$$\varepsilon(U) = \frac{U}{2} - \operatorname{sign}(U) \sqrt{\frac{U^2}{4} + 4t^2} \,. \qquad (8)$$

In the states with one electron per atom n=1 ($\delta = \frac{N_e - N}{N} = 0$) the term with τ vanishes. Fig.1 shows the spectrum of spinons (S) and doublon-holons (d-h) at n=1.

The normalized singlet spin wave function Ψ_1^S and its eigenvalue E_S have the forms:

$$\Psi_1^S = B_1 B_1^{+} = \frac{1}{2} \sum_{\sigma\sigma'} \sigma\sigma' X_1^{\sigma\sigma'} X_2^{-\sigma-\sigma'}, \qquad E_S = \varepsilon(U) + 2E_o \qquad (9)$$

Similarly, the triplet spinon state with the energy $E = 2E_o$ is described by the operator functions:

$$\Psi_2^S = X_1^{\sigma\sigma} X_2^{\sigma\sigma}$$

$$\Psi_3^S = X_1^{-\sigma-\sigma} X_2^{-\sigma-\sigma} \qquad E = 2E_o \qquad (10)$$

$$\Psi_4^S = \frac{1}{2} \sum_{\sigma\sigma'} X_1^{\sigma\sigma'} X_2^{-\sigma-\sigma'}$$

For the doublon-holon (d-h) singlet charge state (q) we obtain the following expressions:

$$\Psi_1^q = \frac{1}{2} \sum_{\alpha\alpha'} \tilde{\alpha}\tilde{\alpha}' X_1^{\alpha\alpha'} X_2^{-\bar{\alpha}\bar{\alpha}'} \qquad E_{\Psi_1} = 2E_o + U \qquad (11)$$

$$\varphi_2^q = B_{12}^+ B_{12} = \frac{1}{2}\sum_{\alpha\alpha'} X_1^{\alpha\alpha'} X_2^{\bar\alpha\bar\alpha'} \qquad E_{\varphi_2} = 2E_0 + U - \varepsilon(U) \qquad (12)$$

$$\alpha = 0,2 \;; \qquad \bar\alpha = 2,0 \;; \qquad \tilde\alpha, \tilde\alpha' = 1,-1 \;.$$

The degenerate states of the diatomic molecule with 1 electron per atom are not presented in Fig.1. The eigenstate is described by operators $\tau^+\tau$ and $\tau\tau^+$, different in parity, with eigenvalues t and -t, respectively.

At n=1, using the conditions of completeness (3) and electron number conservation:

$$\sum_{\sigma,i} X_i^{\sigma\sigma} + 2\sum_i X_i^{22} = 2$$

the normalized vacuum function $|0\rangle$ of diatomic molecule can be taken as

$$|0\rangle = |2_1 0_2\rangle + |0_1 2_2\rangle + |\uparrow_1 \downarrow_2\rangle + |\downarrow_1 \uparrow_2\rangle + |\uparrow_1 \uparrow_2\rangle + |\downarrow_1 \downarrow_2\rangle$$

The ground state $\Psi_1^s|0\rangle$ with n=1 is, just like the linear chain ground state, a singlet. Due to strong quantum fluctuations, the average value of spin on one centre in the state is zero:

$$\langle \vec S_1 \rangle = \langle 0|\Psi_1^s \vec S_1 \Psi_1^s|0\rangle = 0. \qquad (13)$$

And the average value of the operator S^z which is the integral of motion commuting with (4) is

$$\langle S_1^z \rangle = \langle 0|\Psi_1^s S_1^z \Psi_1^s|0\rangle = S(S+1) = \frac{3}{4} \qquad (14)$$

Although the average spin $\langle S_1\rangle = 0$ because of fluctuations, nevertheless the correlation function that characterizes the nearest order turns out equal to:

$$\langle S_1 S_2 \rangle = \langle 0|\Psi_1^s \vec S_1 \vec S_2 \Psi_1^s|0\rangle = -\frac{3}{4}. \qquad (15)$$

This is in agreement with the result obtained by Lieb and Wu [12] at n=1 for the linear chain which remains a dielectric at all interaction constants U (RVB-S-state of the linear chain). Such a behavior, apparently, is due to the appearance of quantum ferromagnetic with strong fluctuations characterized by $\langle S_1\rangle = 0$ but with correlation functions $\langle S_0 S_j\rangle = (-1)^j/j$ slightly decreased with increasing j. The classical Neel state with alternating spins $\Psi_N = X_1^{\sigma\sigma} X_2^{-\sigma-\sigma}|0\rangle$ is an eigenvector of operator S^z but is not an eigenfunction of the hamiltonian (4). And the average value in state Ψ_N is

$$\Psi_N H \Psi_N = \frac{\varepsilon(U)}{2} + 2E_0 \qquad (16)$$

The Neel energy turns out to be larger than the energy of the ground state E_S by the magnitude of $\frac{\varepsilon(U)}{2}$.

At sign variation in U the inversion $\Psi_1 \leftrightarrow \Psi_2$ takes place. At $U > 0$ the ground state with n=1 is a singlet Ψ_1^s with energy (9). In a crystal (in linear chain) it may be comparable with the resonance valence bonds of the neighbour pairs of spinons (RVB-S). And at $U < 0$ the ground state also is a singlet φ_2^q with energy (12) and corresponds to the resonance of charged dipole pairs (RVB-Q).

In what follows it will be convenient to pass over to spin

operators using the connection between the Hubbard operators (X) and spinon operators:

$$X^{\sigma-\sigma} = \bar{C}_\sigma^+ \bar{C}_{-\sigma} = S^+$$
$$X^{\sigma\sigma} = \bar{C}_\sigma^+ \bar{C}_\sigma = \bar{n}_\sigma (1-n_{-\sigma}) n_\sigma \qquad (17)$$
$$\bar{C}_\sigma^+ = X^{\sigma 0} = C_\sigma^+ (1-n_{-\sigma})$$

Operators $X^{\sigma 0}$ satisfy the anticommutation relations $\{X_i^{\sigma 0} X_j^{-\sigma 0}\}_+ = 0$ which hold at $i=j$ too; this implies that the centre may contain no more than one spinon.

Operator BB^+ with eigenvalues 0 and 1 in (7) at n=1 and $U > 0$ (in the absence of holons and doublons) can be readily expressed through the spin operators of spinon:

$$B_{12} B_{12}^+ = \frac{1}{2}\left(\frac{\bar{n}_1 \bar{n}_2}{2} - 2\vec{S}_1 \vec{S}_2\right), \qquad (18)$$

where

$$\bar{n} = \sum \bar{n}_\sigma \quad \text{and} \quad S^z = \frac{1}{2}\sum \sigma \bar{n}_\sigma, \; S^+ = \bar{C}_\sigma^+ \bar{C}_{-\sigma}, \; S^- = \bar{C}_{-\sigma}^+ \bar{C}_\sigma$$

Hence the effective hamiltonian (7) at n=1 and $U > 0$ is reduced to the Heisenberg one with a constant $\varepsilon(U)$ equal to energy of singlet ground state of diatomic molecule:

$$H = \left(\frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t^2}\right)\left(\frac{1}{4} - \vec{S}_1 \vec{S}_2\right) + 2E_0 \qquad (19)$$

Fig.2 shows the character of variation of superexchange Anderson interaction [6] versus the value of U/t.

At $t/U \ll 1$ the exact expansion yields $\varepsilon(U) = -\frac{4t^2}{U}$ whose value is less than the result of [6] by a factor of two,

and of [13] by a factor of four.

At n=1 and $U < 0$, as shown in Fig.1, the ground state is a singlet with energy $-\left(\frac{|U|}{2} + \sqrt{\frac{U^2}{4} + 4t^2}\right)$. Here also it is convenient to turn from Hubbard operators to pseudospin operators of holons and doublons L using the connection

$$L^+ = X^{20} = d_i^+ h_i = \sigma C_\sigma^+ C_{-\sigma}^+; \qquad L^- = X^{02} \qquad (20)$$

$$X^{22} = d^+ d = n_\sigma n_{-\sigma}; \quad X^{00} = h^+ h = (1-n_\sigma)(1-n_{-\sigma}), \qquad (21)$$

where the create operators of doublons (d^+) and holons (h^+) are expressed through electron operators:

$$d^+ = \frac{\sigma}{\sqrt{2}}\left(n_{-\sigma} C_\sigma^+ - n_\sigma C_{-\sigma}^+\right), \qquad (22)$$

$$h^+ = \frac{1}{\sqrt{2}}\left(C_{-\sigma}(1-n_\sigma) + C_\sigma(1-n_{-\sigma})\right) \qquad (23)$$

One can readily be convinced that these pseudoboson operators on different centres satisfy the anticommutation relations:

$$\{d_1^+, d_2\}_+ = 0 \qquad \{h_1^+, h_2\} = 0 \qquad (24)$$

Using the relationship for the number of doublons and holons

$$d^+ d + h^+ h = M \qquad (25)$$

and introducing the operator of pseudospin component

$$d_i^+ d_i - h_i^+ h_i = Q_i = 2L_i^z \qquad (26)$$

the operator B^+B can be presented as

$$B_{12}^{+} B_{12} = \frac{1}{2}\left(\frac{M_1 M_2}{2} - 2L_1^z L_2^z + L_1^+ L_2^- + L_1^- L_2^+\right). \qquad (27)$$

The eigenvalue of operator $B_{12}^{+} B_{12}$ in state φ_1^q is unity. If now we make invariant transformation of pseudospin (20), (21), (26) at a given centre with its turn at 180° around the z axis, which corresponds to transitions $L^{\pm} \to -L^{\mp}$ and $L^z \to L^z$, then we'll obtain from (23) an expression:

$$B_{12}^{+} B_{12} = \frac{1}{2}\left(\frac{M_1 M_2}{2} - 2\vec{L}_1 \vec{L}_2\right) \ldots \qquad (28)$$

Hamiltonian (7) at $U < 0$ can be written in the equivalent form that resembles the isotropic Heisenberg spin exchange (19):

$$H = -\left(-\frac{|U|}{2} + \sqrt{\frac{U^2}{4} + 4t^2}\right)\frac{1}{2}\left(\frac{M_1 M_2}{2} - 2\vec{L}_1 \vec{L}_2\right) - U. \qquad (29)$$

Knowing the eigenvalues of energy (9), (12) we'll find out a statsum:

$$Z = e^{-\frac{E_s}{T}} + 3e^{-\frac{E_t}{T}} + e^{-\frac{E_{g_1}}{T}} + e^{-\frac{E_{g_2}}{T}} \qquad (30)$$

whence the thermodynamic quantities can readily be determined.

To study magnetic properties of the system, we apply an external homogeneous magnetic field $H \parallel z$ in the direction of quantization axis z.

Then the field action is reduced to the addition of Zeeman term to (4):

$$H_z = \frac{1}{2} g\mu H \sum_{i=1,2} \sigma C_{i\sigma}^{+} C_{i\sigma} = \frac{1}{2} g\mu H \sum_{i=1,2} \sigma X_i^{\sigma\sigma} \qquad (31)$$

It can be readily shown that the (31) is not transformed under unitary transformation diagonalizing the (4); therefore, the spectrum of singlet states (9), (11), (12) turns out to be the same as in the absence of magnetic field. Whereas the triplet state splits into φ_2^s, φ_3^s and φ_4^s states with energies $-\frac{\mu g H}{2}$, $\frac{1}{2}\mu g H$ and 0, respectively. Therefore, at critical fields $\bar{H}_c$, equal to coupling energy of singlet state

$$g\mu \bar{H}_c = \sqrt{U^2 + 16t^2} - U \qquad (32)$$

the transition from the ground state $\Psi_1^s|0\rangle$ to ferromagnetic state $\Psi_2^s = X_1^{\sigma\sigma} X_2^{\sigma\sigma}|0\rangle$ turns out to be energy-advantageous. At $U < 0$ the relevant transition to ferromagnetic state occurs at high fields:

$$g\mu H_c = |U| + \sqrt{U^2 + 16t^2} \qquad (33)$$

with increasing U, $\bar{H}_c$ falls off, and H_c grows.

Now we turn to the consideration of a linear triatomic molecule.

By a transformation similar to (6), the initial hamiltonian at n=1 along with the spin-exchange interaction consisting of the product of even number of B operators also contains terms with three B operators. Applying to the obtained hamiltonian a repeated unitary transformation

$$S = \prod_i \exp\left\{c\left(B_{i,i+1}^{+} B_{i+1,i+2} B_{i+1,i+2}^{+} - \text{h.c.}\right)\right\} \qquad (34)$$

we'll find out parameter C from the condition of exclusion of terms consisting of a product of three B operators. Finally

we'll obtain that the effective hamiltonian on the states with n=1 contains only even number of B operators:

$$H = J_1 \sum_{\langle ij \rangle} B_{ij} B_{ij}^{+} + J_2 \sum_{ijk} (B_{ij} B_{ij}^{+} B_{jk} B_{jk}^{+} + \text{a.c.}) \qquad (35)$$

$$+ J_3 \sum B_{ij} B_{ij}^{+} B_{jk} B_{jk}^{+} B_{ij} B_{ij}^{+}$$

Turning in a usual way to spin operators we'll obtain along with the antiferromagnetic Heisenberg exchange between the nearest neighbours also the ferromagnetic exchange between those next to the nearest neighbours:

$$H = \varepsilon_1 \sum_{i=1,2} (S_i \; S_{i+1} - \tfrac{1}{4}) + \varepsilon_2 (S_1 S_3 - \tfrac{1}{4}) \qquad (36)$$

From the result one can readily conclude that at small t/U both ε_1 and ε_2 are proportional to t^2/U and t^4/U^3, respectively, and the sign of ε_1 is opposite to the sign of ε_2. For the closed triatomic molecule ε_2 is proportional to t^2/U.

Expanding over the small parameter t/U with an accuracy to t^3/U^3 we'll obtain the result of Ref. [14].

Just like in the case of a diatomic molecule, here we can find a spectrum and eigenfunctions of hamiltonian (34).

2. In the case of infinite linear chain for which we have the expression for the ground state energy, using the transformation similar to (6) we obtain:

$$T = \prod_i \exp\left\{ \frac{1}{2} (B_{i,i+1}^{+} - B_{i,i+1}) \operatorname{arctg} \frac{4t}{U} \right\} \qquad (37)$$

Using the anticommutation relations for the Hubbard operators

$$\left\{ H_i^{\sigma 0}, H_j^{0\sigma} \right\} = 0 ; \; \left\{ H_i^{2-\sigma}, H_j^{-\sigma 2} \right\} = 0 ; \; \left\{ X_i^{\sigma 0}, X_j^{-\sigma 2} \right\} = 0 ; \; \left\{ H_i^{2-\sigma}, X_j^{0\sigma} \right\} = 0$$

we obtain

$$B_{ij} B_{ij}^{+} B_{jk} B_{jk}^{+} B_{ij} B_{ij}^{+} = \tfrac{1}{4} B_{ij} B_{ij}^{+} \sum_{\sigma} X_k^{\sigma\sigma}$$

$$\left\{ B_{ij} B_{ij}^{+}, B_{jk} B_{jk}^{+} \right\} = \tfrac{1}{2} (B_{ij} B_{ij}^{+} + B_{jk} B_{jk}^{+} - B_{ik} B_{ik}^{+}) \qquad (38)$$

$$(S_i S_j)^2 = \frac{3}{16} - \frac{1}{2} (S_i S_j) \qquad i \neq j$$

The effective hamiltonian on states with one electron per atom can be presented as a polynomial by operators $B_{ij} B_{ij}^{+}$. Expressing $B_{ij} B_{ij}^{+}$ through spin ones by means of (18) we'll obtain an effective spin hamiltonian where along with the Heisenberg interaction of nearest neighbours there are also farther ones.

The form of the complete effective hamiltonian will be discussed in detail in our subsequent work, where the correlators $\langle S_i S_k \rangle$ will be calculated too.

In the limit of small $t/U \ll 1$, restricting ourselves to the second-order terms on this parameter, we write out expressions that contain only two- and three-centre interactions:

$$H = E_0 \sum_{i\sigma} X_i^{\sigma\sigma} + (U + 2E_0) \sum_i X_i^{22} - t \sum_{ij} (\tau_{ij}^{+} + \tau_j) \qquad (39)$$

$$-\frac{4t^2}{U}\sum_i \left(B_{i,i+1}B^+_{i,i+1} + [B^+_{i,i+1}, B_{i+1,i+2}] + [B^+_{i+1,i+2}, B_{i,i+1}]\right)$$

$$-\frac{t^2}{U}\sum_i \left(B^+_{i,i+1}\, B_{i+1,i+2}\, X^{22}_{i+1} + h.c.\right)$$

The projection of (39) on the state with one electron per atom, n=1, leads to the Heisenberg-Anderson superexchange interaction

$$H = -\frac{4t^2}{U}\sum_i B_{i,i+1}B^+_{i,i+1} = \frac{4t^2}{U}\sum (S_i S_{i+1} - \frac{1}{4}) + O\left(\frac{t^3}{U^3}\right) \qquad (40)$$

Thus, up to t^2/U terms, the infinite chain hamiltonian is equal to the sum of hamiltonians of all diatomic molecules.

The energy of the ground state (40), according to [15] is

$$\frac{E}{N} = -\frac{4t^2}{U}\ln 2 \qquad (41)$$

The same result can be obtained directly from the expansion of the exact value of the ground state for the one-dimensional Hubbard model [12]:

$$\frac{E_o}{N} = -4t\int_0^\infty \frac{J_0(x)J_1(x)\,dx}{x(1+\exp(x|U|/t))} = -\frac{4t^2}{U}\ln 2 + \frac{9t^4}{U^3}\zeta(3) + O\left(\frac{t^4}{U^4}\right) \qquad (42)$$

where $\zeta(x)$ is the Riemann function.

For the infinite chain with the accuracy up to terms t^4/U^4 we obtain an expression for the spin hamiltonian:

$$H_{eff} = \left(\frac{4t^2}{U} - \frac{16t^4}{U^3}\right)\sum_i (S_i S_{i+1} - \frac{1}{4}) \qquad (43)$$

$$+\frac{4t^4}{U^3}\sum_i (S_i S_{i+2} - \frac{1}{4})$$

With the accuracy up to t^4/U^3 the infinite chain hamiltonian is equal to the sum of hamiltonians of all triatomic molecules.

Note, that at deviation of n from unity in (39) apart from the kinetic term linear in t, because of the degeneracy of the ground state there also arises three-centre superexchange interaction (the last four terms) of the order of t^2/U.

Compare the energy of the infinite chain ground state with energies E_K for: a) classical Neel antiferromagnetic $\frac{E_N}{N} = -\frac{t^2}{U}$; b) $\frac{N}{2}$ of non-interacting diatomic molecules $E/N = -2t^2/U$.

The values of relative deviation of energy from the exact value of E_o

$$\alpha = \frac{E_o - E_K}{E_o} \qquad (44)$$

are given in the table:

	α
AF	$\frac{\ln 2 - 0{,}25}{\ln 2} = 0{,}63$
RVB-2	$\frac{\ln 2 - 0{,}5}{\ln 2} = 0{,}14$

Comparing at $U/t \ll 1$ the ground state energy of infinite chain

Correspondingly we'll find nonlinear susceptibility $\chi = \frac{\partial M}{\partial H}$:

$$\chi = \frac{g\mu}{2}\frac{dm}{dH} = \frac{(g\mu)^{3/2}}{\pi\sqrt{2}\sqrt{J(H_c - H)}} \qquad (52)$$

which in a rootwise way diverges near $H_c = 8t^2/U$ transforming into ferromagnetic state.

Comparing this critical field with (32) we can see that with an accuracy up to t^2/U there is complete coincidence in the values of critical fields of transition to ferromagnetic state for a diatomic molecule and infinite chain.

The critical field H_c of transition to ferromagnetic state is positive, and hence the state with a maximum spin is not the ground state of linear chain. This conclusion is in agreement with the theory of Lieb and Mattis on the properties of one-dimensional system in normal state.

It is of interest to study the response of the system in weak fields near the singlet ground state with $N_\uparrow = N_\downarrow \left(\eta = \frac{1}{2}\right)$ at energy $E\left(\frac{1}{2}, \frac{1}{2}, U\right)$. Using now the expansion $E\left(\frac{1}{2}-S, \frac{1}{2}+S, U\right)$ near $\eta = \frac{1}{2} - S$ from equations (45)-(49) in a similar way at n=1 $(Q = \pi)$ with an accuracy up to t^2/U we'll obtain:

$$E\left(\tfrac{1}{2}-S, \tfrac{1}{2}+S, U\right) - E\left(\tfrac{1}{2}, \tfrac{1}{2}, U\right) = \frac{8\pi^2 t^2 S^2}{U} + O\left(\frac{1}{\ln|S|}\right) \qquad (53)$$

Correspondingly we'll find susceptibility

$$\chi = \frac{g^2\mu^2}{\pi^2}\,\frac{U}{4t^2} \qquad (54)$$

If we put U=0, we'll find susceptibility of ideal Fermi gas,

$$\chi = g^2\mu^2/4T$$

At negative $U < 0$ we have a set of integral equations similar to (45)-(49) from which we obtain the following expansion for $E\left(\frac{1}{2}-S, \frac{1}{2}+S, U\right)$ in low fields near the singlet ground state at $t/U \ll 1$:

$$\Delta E\left(\tfrac{1}{2}-S, \tfrac{1}{2}+S, U\right) = -(4t + |U|)S + \frac{8\pi^2}{3}\,\frac{t^2 S^3}{U} + O(S^4) \qquad (55)$$

The magnetization turns to zero at $\mu H_c < |U| + 4t$.

The Hubbard model for 2- and 3-dimensional cases has a form:

$$H = -t\sum_{\vec{l},\vec{\Delta},\sigma} C^{+}_{\vec{l}\sigma}\, C_{\vec{l}+\vec{\Delta}\sigma} + U\sum_{i\sigma} n_{\vec{l}\sigma}\, n_{\vec{l}-\sigma} \qquad (56)$$

where summation in the first term of (55) goes over all nearest neighbour atoms of the lattice. Hamiltonian (56) rewritten in Hubbard operators can with an accuracy up to t^2/U^2 via canonical transformation be reduced to Heisenberg exchange interaction of spins:

$$H = -\frac{t}{2}\sum_{i\Delta\sigma}\left(X_i^{\sigma 0} X_{i+\Delta}^{0\sigma} + X_{i+\Delta}^{\sigma 0} X_i^{0\sigma}\right) - \frac{2t^2}{U}\sum_{i\Delta}\left(B_{i,i+\Delta} B^{+}_{i,i+\Delta} - B^{+}_{i,i+\Delta} B_{i,i+\Delta}\right) \qquad (57)$$

where summation in (57) is carried out over all nearest neighbours. At one electron per atom the 1-st term in (57) is zero. In hole formation, along with the nonzero first term there also arise, just like in (39), terms of the order of t^2/U that represent three-centre interaction. Clearly, at sufficiently large U the three-centre interactions can be neglected, and the main contribution to the ground state energy will be made only by terms written out in (57).

In order to find out the ground state energy (57), we solve the Schrodinger equation, $H = E\Psi$, where the test wave

function is to be searched for in the form:

$$\Psi = \sum_i C_i X_i^{o\sigma} |0\rangle \qquad (58)$$

So long as the wave functions of the ground and excited states are mutually orthogonal,

$$\langle 0 | X_i^{o\sigma} | 0 \rangle = 0 \qquad (59)$$

then from (58) we obtain a completeness condition, $\sum C_i^2 = 1$.
The Schrodinger equation will take the form:

$$\left\{ -\frac{t}{2} \sum_{i\Delta\sigma} \left(X_i^{\sigma o} X_{i+\Delta}^{o\sigma} + h.c \right) - \frac{2t^2}{U} \sum_{i\Delta} \left(B_{i,i+\Delta} B_{i,i+\Delta}^{+} - B_{i,i+\Delta}^{+} B_{i,i+\Delta} \right) \right\} \Psi = E\Psi \qquad (60)$$

Acting in the left-hand side of (60) by operator $X^{\sigma' o}$ we'll come to the following secular equation for a homogeneous solution:

$$\sum_{\Delta} C_{i+\Delta} = \lambda C_i \quad , \qquad \lambda = \frac{\bar{E}}{tT} \qquad (61)$$

where we introduce notations:

$$\bar{E} = E - \frac{2t^2}{U}\Phi$$

$$T = - \frac{\sum_{\sigma} \langle 0 | X_{i+\Delta}^{\sigma\sigma'} X_i^{\sigma'\sigma} | 0 \rangle}{\langle 0 | X_i^{\sigma'\sigma'} | 0 \rangle} \qquad (62)$$

$$\Phi = \frac{\sum_{i'\Delta} \langle 0 | B_{i',i'+\Delta} B_{i',i'+\Delta}^{+} X_i^{\sigma'\sigma} | 0 \rangle}{\langle 0 | X_i^{\sigma\sigma'} | 0 \rangle}$$

Quantity T in (62) is simply expressed through spin operators:

$$T = -\langle 0 | \frac{1}{4} + \frac{S_i^z + S_j^z}{2} + (\bar{S}_i \bar{S}_j) | 0 \rangle \qquad (63)$$

In the limit $U \to \infty$ for a closed chain consisting of N atoms it can be shown that the maximal by absolute magnitude eigenvalue of λ is 2. For a square lattice on the plane the maximum eigenvalue of λ is 4. The values 2, 4, etc. coincide with the number of nearest neighbours in the lattice. One may be convinced that for an arbitrary lattice with nearest neighbours interaction the ground state energy is simply expressed through the coordinate number z:

$$E = z t T - \frac{2t^2}{U}\Phi \qquad (64)$$

The result (64) is in good agreement with the homogeneous solution of Nagaoka in the presence of one hole [16].

3. As is well known, La- and Y-based ceramics display superconductivity properties only at their doping. New mechanisms of high-temperature superconductivity (HTSC) in oxide ceramics based on an exclusive role of oxygen in these compounds are at present under discussion in the literature [11] . Experimental data point out that oxygen in them is in two stable electron configurations (valence states) - neutral oxygen, O (below called a holon, h) and O^{--} with occupied p-shell (called a doublon, d) with close energies. One-electron (spinon) excitations of O^{--} due to transition of an electron from the ion O^{--} or on a neutral oxygen O are in energy considerably higher than (U) and form unstable configurations [10] :

$$2O_2^{-} = 2O^{--} + O_2 \qquad (65)$$

In "pure" La_2CuO_4 compounds the number of holons is equal to the number of doublons. Doping leads to violation of this equality, which, to our opinion, is just the reason of superconductivity. Note, that the observed antiferromagnetic ordering in a "pure" La_2CuO_4 at low temperatures we associate with the copper sublattice, whereas the charge density wave is to be observed on the oxygen sublattice.

Although the problem outwardly seems to be symmetric relative to doublon-holon replacement, nevertheless, as mentioned by Hirsch, the hole-particle symmetry is broken when taking account of the polarization of p-shell electrons by a hole, which is just the reason of instability (1) and results in effective attraction of electrons on the centre ($U < 0$). The attraction may be intensified by strong electron-phonon interaction which leads to renormalization of the intratomic interaction constant.

A simplest model for the oxygen subsystem is the Hubbard model with attraction which also takes account of the Coulomb interaction on the neighbour centres (1).

Turning to Hubbard operators and using the completeness condition (3), the (1) can be reduced to the form (up to terms of the order of t^2/U):

$$H = \frac{2t^2}{U}\sum_{<ij>}(B_{ij}^{+}B_{ij} - B_{ij}B_{ij}^{+}) + V\sum_{<ij>}Q_i^z Q_j^z - t\sum_{ij}(\tau_{ij} + \tau_{ij}^{+}) \qquad (66)$$

where

$$Q_i = X_i^{00} - X_i^{22} \qquad (67)$$

and where we put $E_o = U/2$ for we consider holon and doublon

energies the same.

Projecting (66) on the states with even number of electrons we obtain:

$$H = -\frac{2t^2}{U}\sum_{<ij>}(X_i^{22}X_j^{00} + X_i^{00}X_j^{22} + X_i^{02}X_j^{20} + X_i^{20}X_j^{02}) \qquad (68)$$

$$+ V\sum_{<ij>}(X_i^{22} - X_i^{00})(X_j^{22} - X_j^{00}) + U\sum_i X_i^{22}$$

The terms of the order of t^2/U represent the holon-doublon superexchange which is similar to spinon superexchange at $U > 0$ responsible for the occurence of resonating valence bonds (RVB) [6] .

Here we neglected spinon excitations and put

$$X_i^{00} + X_i^{22} = 1 \qquad (69)$$

After the rotation in the isotropic space we'll obtain an effective hamiltonian:

$$H = \sum_{<ij>}(J_\perp L_i^z L_j^z - J_\parallel/2(L_i^{+}L_j^{-} + L_i^{-}L_j^{+})) \qquad (70)$$

$$J_\perp = 4V + \frac{4t^2}{U}\ , \qquad J_\parallel = \frac{4t^2}{U}$$

where

$$L_i^z = \frac{1}{2}(X_i^{22} - X_i^{00}) \qquad (71)$$

$$L_i^{+} = \sigma C_{i\sigma}^{+} C_{i-\sigma}^{+} \qquad (72)$$

$$L_i^{-} = \sigma C_{i-\sigma} C_{i\sigma} \qquad (73)$$

Thus, the problem is reduced to the XXY Heisenberg-Ising model with anisotropic interaction of pseudospins.

Concerning this model, one can make the following qualitative quite strict conclusions:

1. At n=1 the number of holes is equal to the number of doublons ($n_h = n_d = \frac{1}{2}$) and at $J_\perp \gg J_\parallel$, irrespective of the space dimensionality $d > 1$ charge density wave with alternating holons and doublons is established in the system (Wigner crystallization). One can readily see that hamiltonian (70) is invariant under sign variation of $J_\parallel$.

2. The nonzero averages of z projections of pseudospins, $\langle L_i^z \rangle \neq 0$, lead to the establishment of charge density wave, and the ordering of their xy components, $\langle L_i^{\pm} \rangle = \Delta \neq 0$, results in superconductivity.

3. Addition of a pair of holes to the system corresponds to a flip of one pseudospin, which results in occurence of spin excitations separated from the ground state by the gap Δ_0 which for the one-dimensional case is $\Delta_0 = 4\pi \exp\left(-\frac{\pi^2}{2}\sqrt{J_\parallel}/\sqrt{2(J_\perp - J_\parallel)}\right)$. At small concentration of holes, $n_h \ll 1 - n/2$, on the background of doublons one may neglect the interaction $J_\perp$.

4. At $J_\perp > J_\parallel$ in the vicinity of $n \leqslant 1$ there are formed complexes of holons which in the one-dimensional case represent trimers, and in two-dimensionality - clusters of five holons aligned in the form of a cross. The trimer may decay into two non-interacting dimers (diholons) which represent two domain walls (soliton-antisoliton). In two-dimensionality the cluster is stable due to confinement: in case of the collapse of the complex the motion of fragments leads to pseudospins

flipping along the whole trajectory of motion, and correspondingly, to the energy loss proportional to the length. At $J_\perp > J_\parallel$ owing to pseudospin fluctuations the initial symmetry is restored in the system. In virtue of the fact that these complexes are of Bose type (subject to Pauli principle), the occurence of charged holon condensate with a gap in the spectrum leading to superconductivity is possible.

5. At small concentration of holons ($n \leqslant 1$) at arbitrary relation of $J_\perp$ and $J_\parallel$ constants the formation of a complex consisting of a holon surrounded by doublons leading to their effective repulsion turns out to be energy-advantageous. Ferromagnetic ordering of doublons in the xy plane leads to a homogeneous solution and to superconductivity of holons.

The above statements can be obtained in the framework of model (70). Using the self-consistent field approximation for the case of $J_\perp < J_\parallel$ and $n_h \ll 1$ and introducing anomalous averages $\Delta = \langle X^{20} \rangle$ that describe the Bose condensate and $n_h = \langle X^{00} \rangle$ - the mean number of holons per atom, we'll obtain the effective hamiltonian at $n \leqslant 2$:

$$H - \mu n = -\mu \sum_i X_i^{22} - J_\perp \sum_i (n_h X_i^{00} + (1 - n_h) X_i^{22}) \tag{74}$$

$$- J_\parallel \Delta \sum_i (X_i^{20} + X_i^{02}) + J_\perp n_h (1 - n_h) + J_\parallel \Delta^2$$

Via canonical u-v Bogolyubov transformation

$$S = u - v (X^{20} - X^{02}) \tag{75}$$

we'll pass over to new quasi-particles that describe the condensate:

$$Y^{oo} = SX^{oo}S^{-1} = u^2X^{oo} + v^2X^{22} + uv(X^{02} + X^{20})$$
$$Y^{22} = SX^{22}S^{-1} \qquad (76)$$

and so on.

The resultant effective hamiltonian will take the form:

$$H = Y^{22}(u^2(J_\perp(1-2n_h)-\mu) - J_\perp(1-n_h) + 2J_\parallel \Delta uv)$$
$$+ Y^{oo}(v^2(J_\perp(1-2n_h)-\mu) - J_\perp(1-n_h) - 2J_\parallel \Delta uv) + J_\perp n_h(1-n_h) + J_\parallel \Delta^2$$

where $\Delta = uv$, and u and v are found from the conditions:

$$(u^2 - v^2)\Delta + uv(1-2n_h) = 0 \; ; \quad uv(\mu + J_\perp(1-2n_h)) = J_\parallel \Delta(u^2 - v^2) \qquad (77)$$

From the condition of holon number conservation we find:

$$n_h = -\frac{\partial \mathcal{E}}{\partial \mu} = u^2 \qquad (78)$$

The system of self-consistent equations allows a nontrivial solution for parameter $\Delta = \sqrt{n_h(1-n_h)}$. The critical temperature of the superconductivity transition is determined from the zero condition: $\Delta(T_c) = 0$

$$T_c = \frac{2t^2}{U}(1-2n_h) \Big/ \ell n\left(\frac{1-n_h}{n_h}\right) \qquad (79)$$

Fig.3 shows T_c as a function of n at various values of parameters. The behavior of the system essentially varies at $J_\perp \geqslant J_\parallel$ in the vicinity of n=1, when the charge density wave is established in the system (solid curve in the figure).

Simple account of correlations in terms of the density-density type does not suppress the transition temperature in the vicinity of n=1 [17] . Here, as will be shown in our subsequent work, in order to take this effect into account, it becomes necessary to turn to double-sublattice system and introduce anomalous averages on each sublattice. Acting as before, we'll find that under these conditions at n = 1 are strictly zero and grow at deviation of n from unity (see Fig.3, dotted line).

Note, that at $J_\perp < J_\parallel$ the co-existence of weakened charge density wave and superconductivity Bose-condensate with $\Delta \neq 0$ is possible. This phase represents amorphous charged glass with strong superconductivity correlations.

The "pure" La_2CuO_4 we refer to the point n=1 in Fig.3, it corresponds to alternating holons and doublons on oxygen sublattice, with the charge density wave of maximum amplitude. The doping by strontium or oxygen in $La_{2-x}Sr_xCuO_{4-y}$ leads to a decrease in the number of electrons ($n < 1$) and correspondingly T_c increases up to its maximum value and then decreases down to zero at n=0. Such a behavior is observed in a number of compounds based on yttrium and lanthanum. High critical temperatures of transition here are provided by large values of t^2/U , just as in the RVB systems with spinons [6] .

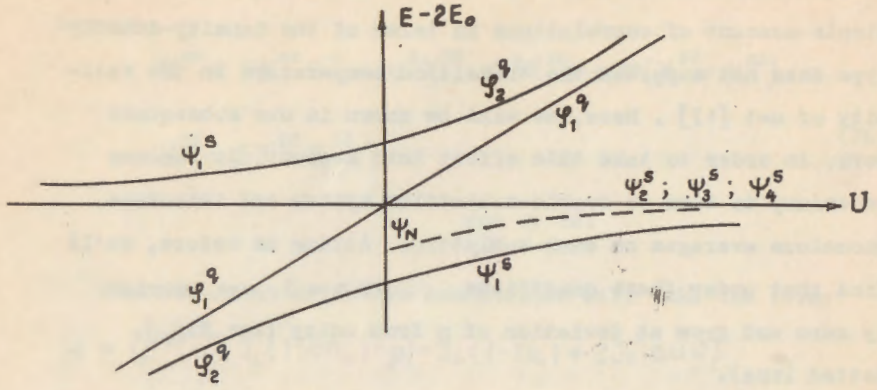

Fig.1

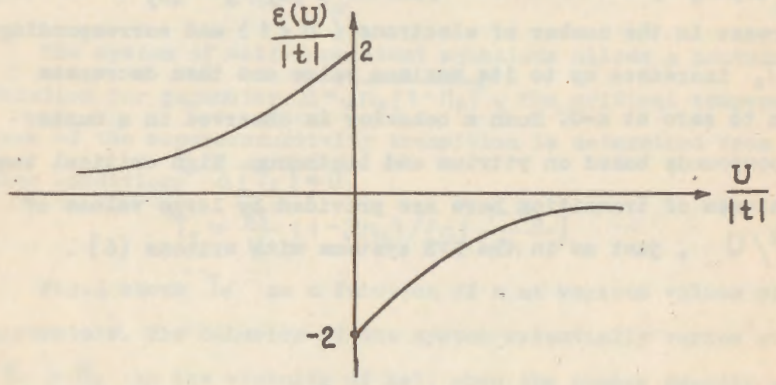

Fig.2

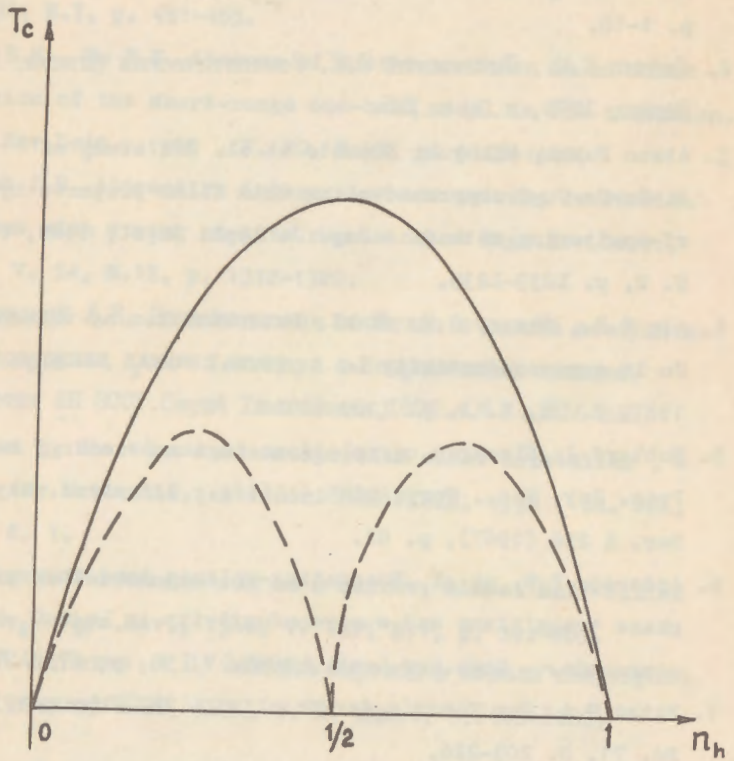

Fig.3

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