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ЕРЕВАНСКИЙ ФИЗИЧЕСКИЙ ИНСТИТУТ
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CHARGE FLUCTUATIONS AND SUPERCONDUCTIVITY IN THE HUBBARD MODEL WITH ATTRACTION

Ереванский Физический
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ԼԻՑՔԱՅԻՆ ԽՈՏՈՐՈՒՄՆԵՐ ԵՎ ԳԵՐՀԱՂՈՐԴԱԿԱՆՈՒԹՅՈՒՆ՝ ՀԱԲԱՐԴԻ ՄՈԴԵԼՈՒՄ ՁԳՈՂԱԿԱՆՈՒԹՅԱՄԲ

Ուսումնասիրված է Հաբարդի ընդհանրացված մոդելը՝ ձգողականությամբ՝ մեկ կենտրոնում և կուլոնյան փոխազդեցությամբ՝ տարբեր կենտրոններում։ Ստացվել է արդյունավետ համիլտոնյան, որը նկարագրում է Հայզենբերգի քվանտային հակաֆերոմագնիսը մագնիսական դաշտում։ Ինքնահամաձայնեցված դաշտի մոտավորությամբ՝ Δ կարգի ոչ-անկյունագծային գերհաղորդիչ պարամետրի և η լիցքային կարգավորման պարամետրի հաշվառմամբ՝ ստացվել են վերլուծական արտահայտություններ հավասարակշռության կորերի համար՝ կրիտիկական ջերմաստիճանի և թթվածնի ատոմի էլեկտրոնների n թվի փուլային դիագրամի վրա։ Ցույց է տրված Հայզենբերգ-Իզինգի համիլտոնյանի և երկգոտի անսպին ֆերմիոնների մոդելի համապորությունը, որտեղ գերհաղորդականությունը գոյություն ունի թթվածնի վալենտականության խոտորումների շնորհիվ։

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1. Introduction

Appearance of high-temperature superconductors (HTSC) raised a keen interest to investigation of new non-traditional mechanisms of superconductivity (SC). Among other approaches quite realistic is the model that takes into account conductivity of small-radius polarons and the possibility of their paring with formation of bipolarons [1]. Measurements of heat capacity γ, magnetic susceptibility χ, where at a constant γ/χ ratio the density of states increases, indicate a strong interaction of electrons with a lattice (λ). This can be directly connected with polaronic narrowing of conduction band [2].

The thermopower data also indicate existence of a narrow band and are in a good agreement with the polaron model in a normal state. A direct evidence to existence of electron-phonon interaction in these materials can be obtained from the results of measurements of the isotope effect, thermal conductivity, Ramon spectra, elastic constants and Debye-Waller factor for the oxygen component. In particular, an anomalous softening of phonon modes (ω_0) below critical temperature T_c has been established from measurements of the Young module and sound velocity. Naturally, one is tempted to connect the mechanism of SC of lanthanum and yttrium ceramics with the non-magnetic mechanism of interaction characteristic of, e.g., $BaPb_{1-x}Be_xO_3$ which does not contain any magnetic atoms. Additional evidences to existence of polarons in normal state are obtained from measuring the characteristic properties of frequency dependence of electron conductivity $\sigma(\omega)$ in CuO_2 planes. Small amplitude at zero frequency that corresponds to ~5% of total strength of oscillators, indicates conductivity of small-radius polarons.

The integral of electron transition, t, of 2p-electrons of oxygen atoms through an intermediate copper atom is strongly suppressed by the Frank-Condon effect $t=\tilde{t}\exp(-E_p/\omega_0)$, where E_p is polaron coupling energy g^2/ω_0. But in the optical region, at $\omega\sim 2g^2/\omega_0\sim 0.5$ eV there is a peak, the intensity of which increases with dopant concentration. This testifies to an essential contribution to conductivity of these frequencies of fast electron transitions without phonon relaxation.

The assumption on increasing effective mass allows us to explain unusual temperature effects in conductivity, susceptibility and thermal capacity. Existence of compounds that display n- and p-type conductivity at changing composition, is another important peculiarity.

2.The Effective Hamiltonian of Hubbard Model.

Interaction of 2p-electrons with uniform b_{ij} lattice deformation $H_{e-ph}=\lambda \sum_{<ij>}(n_i+n_j)(b^+_{ij}+b_{ij})$ together with elasticity energy $\omega_0 \sum b^+_{ij} b_{ij}$ leads to polaron coupling into small bipolarons. The scenario of bipolaron formation for the light oxygen component in CuO_2 plane is based on an assumption of possibility of a local coupling of two holes on the same oxygen ion O^{--} (a doubly occupied site - a doublon) [4], which leads to formation of neutral oxygen O^0 (an empty site - a holon).

After a canonical transformation that excludes linear deformation, we obtain the generalized effective Hubbard model

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

where the parameters $\tilde{t},\tilde{U},\tilde{V}$ appear to be renormalized

$$t=\tilde{t}\exp\left(-\frac{(z-1)\lambda^2}{\omega_0^2}\right); \quad U=\tilde{U}-\frac{2z\lambda^2}{\omega_0}; \quad V=\tilde{V}-\frac{2\lambda^2}{\omega_0}.$$

It is seen that when $V<0$, $|V|\gg t$ and $U\gg t$, there can be formed bipolarons on the neighbouring sites. But in the case when $U<0$ and $|U|\gg t$, formation of local pairs on separate sites is advantageous. Below we shall find conditions of crystalization and SC of local pairs.

Considering now the Hubbard operators X_i^{ab} and using the canonical transformation [8] at an arbitrary sign of U,

$$T = \prod_i \exp\left[1/2(B^+_{ij}-B_{ij})\ \mathrm{arctg}\ 4t/U\right] \qquad (2)$$

the term $2t(B^+_{ij}+B_{ij})$ in (1) is omitted, where

$$B_{ij} = 1/2 \sum_\sigma \sigma (X_i^{\sigma 0} X_j^{-\sigma 2} + X_j^{\sigma 0} X_i^{-\sigma 2}) \qquad (3)$$

$$\tau_{ij} = \sum_\sigma (X_i^{\sigma 0} X_j^{0\sigma} + X_j^{2-\sigma} X_i^{-\sigma 2}) \qquad (4)$$

and the effective Hamiltonian which allows for only two neighboring center interactions, is obtained with an accuracy up to $t^2/U\ll 1$ in the unrestricted Hilbert space $H_{0,1,2}$

$$H = -t \sum_{<ij>} (\tau^+_{ij}+\tau_{ij}) - 4t^2/U \sum_{<ij>} (B_{ij}B^+_{ij} - B^+_{ij}B_{ij}) + U\sum_i X_i^{22} \qquad (5)$$

where

$$B_{ij}B^+_{ij} = \frac{1}{2}\left(\frac{\bar{n}_i\bar{n}_j}{2} - 2\vec{S}_i\vec{S}_j\right),\quad B^+_{ij}B_{ij} = \frac{1}{2}\left(\frac{\bar{m}_i\bar{m}_j}{2} - 2\vec{L}_i\vec{L}_j\right)$$

$$\bar{n}_i = \sum_\sigma X_i^{\sigma\sigma},\quad S_i^z = \frac{1}{2}\sum_\sigma \sigma X^{\sigma\sigma},\quad S_i^+ = X_i^{\sigma-\sigma},\quad S_i^- = X_i^{-\sigma\sigma}$$

$$\bar{m}_i = \sum_{\alpha=0,2} X_i^{\alpha\alpha},\quad 2L_i^z = X_i^{00}-X_i^{22},\quad L_i^+ = X^{20},\quad L_i^- = X^{02}.$$

The projection of (5) at $U<0$ on the states with only empty and doubly occupied states on the restricted Hilbert space $H_{0,2}$ with $X^{00}+X^{22}=1$ (X^{00} and X^{22} are the operators of the number of holons and doublons, respectively) with regard to the term V in (1) yields an isotropic Heisenberg-Ising Hamiltonian for the pseudospins $L^z=1-m_i/2$, $L_i^+=\sigma C_{i\sigma}^+ C_{i-\sigma}^+$:

$$H = \sum_{<ij>} J_\perp L_i^z L_j^z - J_\parallel/2 \sum_{<ij>} (L_i^+ L_j^- + L_i^- L_j^+) - \tilde{H} \sum_i L_i^z \qquad (6)$$

where

$$J_\perp = 4V_{ij} + 2t^2/|U|, \quad J_\parallel = 2t^2/|U|, \ \tilde{H} = |U| - \mu .$$

The Ising term in (6) also takes into account the next nearest-neighbor interaction. The operators satisfy the well-known permutation conditions for the spins $[L^+, L^-]=2L^z$; $[L^\pm, L^z]=\pm L^\pm$; $[L^+, L^-]=1$.

The next correction to the Hamiltonian is of the order of t^4/U^3 and corresponds to the interaction of the next nearest neighbor pseudospins. It can be exactly shown [8] that at any filling at $U>0$ the Hamiltonian (1) is reduced by a canonical transformation to the complete effective Hamiltonian which contains all possible combinations of linked operators $B_{ij}^+ B_{ij} B_{jk}^+ B_{jk}$, and so on. However, in the case with $t/U \ll 1$, which we consider in the lowest-order approximation, we can restrict ourselves to considering the Hamiltonian (6).

3. Phase Diagram in attractive Hubbard Model.

The pseudo-spin flop corresponds to adding two electrons (a doublon) to the system. The doublon complies with the projection $L_i^z=-1/2$, and the holon - with $L_i^z=+1/2$. For a simple square lattice for oxygen atoms on the plane of CuO introduce

anomalous averages for the off-diagonal order parameter $\Delta = <X_i^{02}>$ which describes the Bose condensate of Kosterlitz-Thouless type and the parameter $\eta = <X_i^{00}> - <X_j^{00}>$, which describes the charge order of oxygen ions with different valence. At half filling ($\tilde{H}=0$), for $d>3$ dimensionality as a result of AF ordering of spins in the z direction, the ground state turns out a mixed one - SC coexists with CDW. But for $d=2$ SC is lacking in the isotropic Heisenberg model [9]. In contrast to this, in the XY model ($J_\perp=0$) Kosterlitz-Thouless transition with $T_c/J_\parallel z = n(2-n)$ is possible.

At deviation from half filling ($\tilde{H} \neq 0$) the "magnetic" field disturbs the symmetry, which leads to XY Heisenberg models. So, the problem of arising charge ordering and SC in the Hubbard model with attraction is reduced to the AF anisotropic Heisenberg model in external magnetic field. Under definite conditions there exists the Kosterlitz-Thouless transition with a power-law drop of correlation functions.

It is convenient to turn again to the Hubbard operators:

$$H - \mu n = -\frac{J_\perp}{2} \sum_{<ij>} (X_i^{22} X_j^{00} + X_i^{00} X_j^{22}) - \frac{J_\parallel}{2} \sum_{<ij>} (X_i^{20} X_j^{02} + X_i^{02} X_j^{20}) - \mu \sum_i X_i^{00} + U \sum_i X_i^{22} \qquad (7)$$

In the main field approximation for two alternative sublattice systems we obtain the following Hamiltonian:

$$H = -\mu(X_1^{00} + X_2^{00}) - U(X_1^{22} + X_2^{22}) - \frac{J_\perp}{2}(n_{d2} X_1^{00} + n_{d1} X_2^{00}) - \frac{J_\perp}{2}(n_{h2} X_1^{22} + n_{h1} X_2^{22}) - \frac{J_\parallel}{2}(\Delta_2 X_1^{02} + \Delta_1 X_2^{20} + \Delta_2 X_1^{20} + \Delta_1 X_2^{02}) \qquad (8)$$

where

$$\Delta_{1,2} = <X_{1,2}^{20}>; \quad n_{h1,2} = <X_{1,2}^{00}>; \quad n_{d1,2} = <X_{1,2}^{22}> . \qquad (9)$$

Using the canonical u,v Bogolubov transformation $S_n = u_n - v_n$ $(X_n^{20} - X_h^{02})$ turn to new quasi-particle operators:

$$Y_h^{00} = S_n X_n^{00} S_n^{-1} = u_n^2 X_n^{00} + v_n^2 X_n^{22} + u_n v_n (X_n^{20} + X_n^{02}) \qquad (10)$$

where the parameters u and v are obtained from the condition of vanishing of the term before the off-diagonal part $(Y^{20} + Y^{02})$

$$u_1 v_1 \tilde{\mu}_2 = J_\parallel z \Delta_2 (u_1^2 - v_1^2) \qquad (11)$$

$$u_2 v_2 \tilde{\mu}_1 = J_\parallel z \Delta_1 (u_2^2 - v_2^2) \qquad (12)$$

where

$$\tilde{\mu}_1 = -\mu + U + J_\perp z (n - \eta - 1) \qquad (13)$$

$$\tilde{\mu}_2 = -\mu + U + J_\perp z (n + \eta - 1) \qquad (14)$$

$$H_{eff} = \sum_{n=1,2} E_n^+ Y_n^{00} + \sum_{n=1,2} E_n^- Y_n^{22} \qquad (15)$$

where

$$E^\pm_{1,2} = \frac{\tilde{\mu}_{2,1}}{2} \pm (\tilde{\mu}^2_{2,1} + 4 J_\parallel^2 z^2 \Delta^2_{2,1})^{1/2} - U - J_\perp z\, n_{h2,1} \qquad (16)$$

Finding the eigenfunctions and eigenenergies, we obtain the free-energy functional

$$F = -T \ln z_0 \qquad (17)$$

$$z_0 = \sum_{a,b} \exp(-\beta(E_1^a + E_2^b)) \qquad (18)$$

$$\tilde{\mu} = -\mu + U + J_\perp z (n-1) \qquad (19)$$

where n is the number of holes (holons) on the neighboring sites. The self-consistent system of equations for Δ, η, μ has the form:

$$\frac{J_\parallel z}{z_0} \left\{ \sum_{a,b} \exp(-\beta(E_1^a + E_2^b)) (E_1^{a^{-1}} + E_2^{b^{-1}}) \right\} + 4 = 0 \qquad (20)$$

$$\frac{1}{z_0} \left\{ \sum_{a,b} \exp(-\beta(E_1^a + E_2^b)) (\tilde{\mu}_1 E_1^{a^{-1}} - \tilde{\mu}_2 E_2^{b^{-1}}) \right\} + 4\eta = 0 \qquad (21)$$

$$\frac{1}{4 z_0} \left\{ \sum_{a,b} \exp(-\beta(E_1^a + E_2^b)) (\tilde{\mu}_1 E_1^{a^{-1}} + \tilde{\mu}_2 E_2^{b^{-1}}) \right\} + 1 - n = 0 \qquad (22)$$

Simultaneous solving of the system (20)-(22) yields a system of equations for $\eta = 0$, which defines the equilibrium line between "pure" SC and a mixed phase

$$2\theta = 2x / \ln((1+x)/(1-x)) \qquad (23)$$

$$2\theta = \frac{g(1-n)^2 (x^2 - 1)}{(g-1)x^2 - g(1-n)^2} \qquad (24)$$

where $x = ((1-n)^2 + 4\Delta^2)^{1/2}$ and $g = J_\perp / J_\parallel$, $\theta = T / z J_\parallel$. This system essentially differs from that obtained in [5]. From (20)-(22) at $\Delta = 0$ we obtain the equilibrium line which represents itself the interface of the MS and CDW phases

$$\theta = 2g\eta / \ln\left[\frac{2\eta + \eta^2 + n(2-n)}{-2\eta + \eta^2 + n(2-n)}\right] \qquad (25)$$

$$\theta = 2M / \ln\left[\frac{-\eta^2 + (2-n)^2}{-\eta^2 + n^2}\right] \qquad (26)$$

where

$$M = 1/2 \left[1 - n + ((1-n)^2 + 4g\eta^2 (g-1))^{1/2}\right].$$

It is easy to be convinced that near n~1 the function of the charge ordering critical temperature has the form $T_c = gn(2-n)/2$

At distinction from the SC state (Fig.1a,b) at $I_\parallel > I_\perp$ in the system, together with a pure SC state there is a region with charge density wave (CDW) as well as a mixed state (MS). Dependence of T_c near n~0 (2) is logarithmic $\vartheta = (1-n)/\ln((2-n)/n)$ like in the bipolaronic SC mechanism [5] and complies with the Bose condensation of holons (doublons). Near n~1 the CDW-MS interface is defined by:

$$\theta = -(g - (g(g-1))^{1/2}) / \ln((1-n)/2) \qquad (27)$$

Such analytical dependence near n~1 is in a qualitative agreement with the results obtained in the 2d Heisenberg model calculated by the Monte Carlo method [10]. Figs.1a,b show the critical temperature of transition into SC and CDW states as a function of the electron number density per oxygen atom, n, at different values of $g=J_{\perp}/J_{\parallel}$. Here we show also the type of carriers (n and p) in different phases. It is easy to find the critical point n^{*}, at which all 4 phases (normal (N), CDW, SC, MS) coexist, which differs from that obtained in [5].

$$1/g = (2-n^{*})n^{*} \ln((2-n^{*})/n^{*}) /2(1-n^{*}) \quad (28)$$

The value n^{**} determines the beginning ($\Delta=0$, $\eta\to0$) of the MS phase

$$n^{**}_{1,2}=1 \pm (1- 1/g)^{1/2} \quad (29)$$

The analytical function of the interface of the SC and MS phases near n^{**} has the form:

$$n = n^{**} - (1-n^{**}) \exp(-1/\theta)/\theta \quad (30)$$

From (20)-(22) we conclude, that the values of η, Δ and μ at any magnitude of the constant g are smooth functions of n and T, and that the phase interfaces are the equilibrium lines of the II-order phase transitions.

4. Ground State Properties

At T=0 we obtain the ground state energy:

$$E = ((\tilde{\mu}_1-\tilde{\mu}_2)-((\tilde{\mu}_1+4\Delta^2 J_{\parallel} z^2)^{1/2}+(\tilde{\mu}_1+4\Delta^2 J_{\parallel} z^2)^{1/2})/2 + 2U-J_{\perp}zn \quad (31)$$

The corresponding equations of self-consistency have the form:

$$\tilde{\mu}_1(\tilde{\mu}_1^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2} + \tilde{\mu}_2(\tilde{\mu}_2^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2} = 2(1-n). \quad (32)$$

$$(\tilde{\mu}_1^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2} + (\tilde{\mu}_2^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2} = 2/J_{\parallel} z \quad (33)$$

$$\tilde{\mu}_1(\tilde{\mu}_1^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2}+ \tilde{\mu}_2(\tilde{\mu}_2^2+4\Delta^2 J_{\parallel}^2 z^2)^{-1/2} = -2\eta . \quad (34)$$

Solving the system (32)-(35) we find the dependence of μ, Δ, η on n (Figs.3,4):

$$2\tilde{\mu}/J_{\parallel} z = (1-n) \pm ((1-n)^2 + g(g-1)\eta^2)^{1/2} \quad (35)$$

To the right from the point A and to the left from the point B the dependence of Δ and η on n is linear and square-root, respectively

$$\Delta \simeq (n^{**}-n)\, g(2g-3)(g-1)^{-1/2}\, 2^{-7/2} + \Delta^{**} \quad (36)$$

$$\eta = (n^{**}-n)^{1/2} (g(g-1))^{-1/4} \quad (37)$$

The value of $\Delta=\Delta^{**}$ at $n=n^{**}$ is defined as:

$$\Delta^{**} = 1/2\, (J_{\parallel}/J_{\perp})^{1/2} \quad (38)$$

Near n~1 the dependence of the parameters Δ and η is inverse:

$$\Delta = g(2g-1)(1-2(g^2-g)^{1/2})(g^2-g)^{-1/2} (g^{1/2}+(g-1)^{1/2})^{-1}(1-n)^{1/2} \quad (39)$$

$$\eta = 1 - 0.5(2g-1)(1-n)(g(g-1))^{-1/2} \quad (40)$$

The interface between the SC and M phases is defined by (29) and is shown in Fig.4 by the solid curve. The interface between the SC and M phases obtained in [5]

$$(2-n)n=(1+(1-n)^2)/g \quad (41)$$

is also presented in Fig.4 by a dotted curve for comparison. It is seen that in our case the pure SC phase is more preferable and it occupies a larger area on the phase diagram. The charge ordered phase in the ground state is realized only at n=1, which is shown by the heavy vertical line in Fig.5.

5.Conclusion

The approximation (8) has a simple physical interpretation of the results, provided the analogy of the model (7) with the mixed valence system for two-band s-f model with Coulomb repulsion of s-f spinless fermions is used ($n_s+n_f=1$) [12]

$$H=\sum_i E_1 a_i^+ a_i + \sum_i E_2 f_i^+ f_i + g \sum_{<ij>} a_i^+ a_i f_j^+ f_j \qquad (42)$$

where E_1 and E_2 are the energy of s and f levels, respectively. Then in the modified mean-field approximation we must take into account the anomalous averages $V=<a_i^+ f_j>$ (which describe the effective hybridization term of s and f levels) and the normal averages $n_f=<f_i^+ f_i>$ and $n_s=<a_i^+ a_i>$

$$H=\sum (E_1+gn_f) a_i^+ a_i + \sum (E_2+gn_s) f_i^+ f_i + g\tilde{V} \sum_{<ij>} (a_i^+ f_j + h.c) \qquad (43)$$

It is easy to see that the hybridization term corresponds to $J_{\parallel}\Delta(X^{20}+X^{02})$ in (8) and describes the "mixing" of holons and doublons which corresponds to fluctuations of valence of oxygen ions. The Coulomb interaction brings to non-equality of $J_{\parallel}$ and $J_{\perp}$ and in the s-f model corresponds to the electron-lattice interaction, which renormalized the parameter g in the first two terms. The difference $E=E_1-E_2$ between the two levels corresponds to the external magnetic field in (6) (for half filling E=0). It is easy to see, that for arbitrary values of E, g, g_1 the mixed valence V=0 (except for E=0, when V=0) is realized in the system. At $g_1 \geq g$ for an alternating (bipartite) lattice there exists a non-uniform mixed valence ($n_{si}-n_{sj} \neq 0$) with CDW. In contrast to the case when $g_1<g$, we have a homogeneous solution with $n_{si}=n_{sj}$. Therefore, such analogy allows to connect the nature of HTSC with the physics of the phenomenon of mixed oxygen valence.

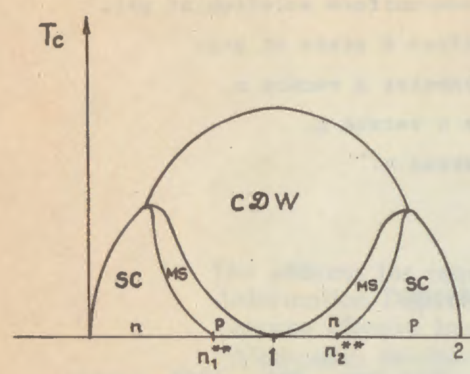

Fig.1

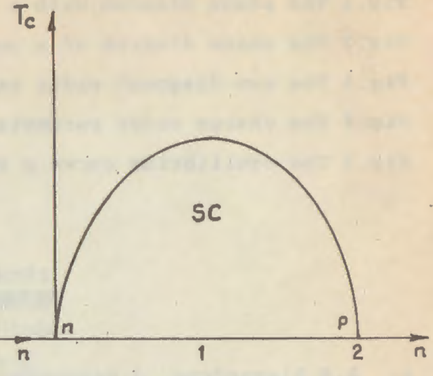

Fig.2

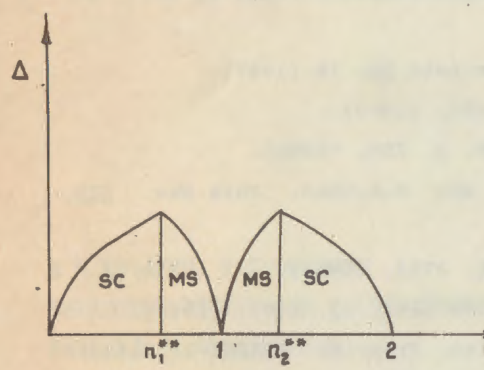

Fig.3

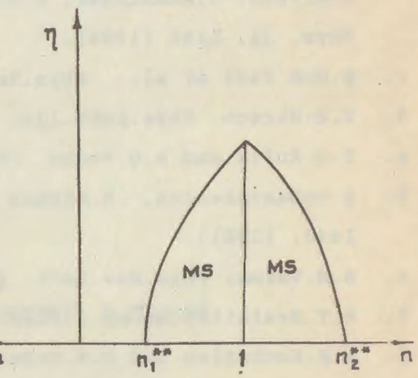

Fig.4

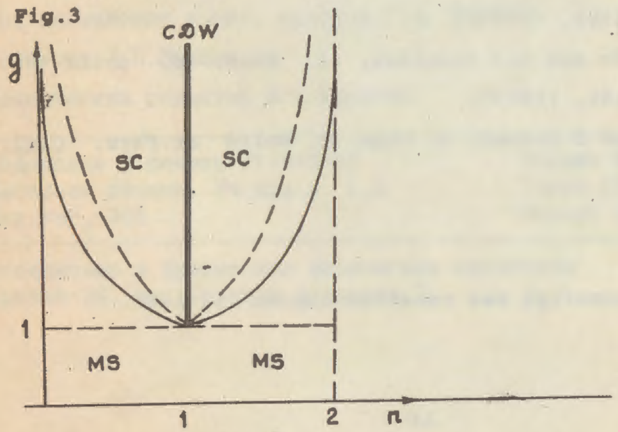

Fig.5

Figure Captions

Fig.1 The phase diagram with a non-uniform solution at g>1.

Fig.2 The phase diagram of a uniform S state at g<1.

Fig.3 The non-diagonal order parameter Δ versus n.

Fig.4 The charge order parameter η versus n.

Fig.5 The equilibrium curve g versus n.

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ЗАРЯДОВЫЕ ФЛУКТУАЦИИ И СВЕРХПРОВОДИМОСТЬ В МОДЕЛИ ХАББАРДА С ПРИТЯЖЕНИЕМ

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