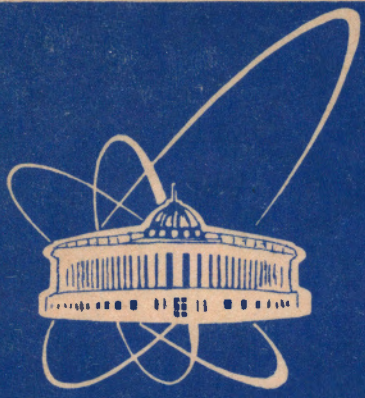

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна



E17-96-465

V.A.Moskalenko, D.F.Digor[1], L.A.Dogotaru[2], I.G.Porcescu[1]

# NEW DIAGRAM TECHNIQUE FOR PERIODIC ANDERSON MODEL

Submitted to «Journal of Superconductivity»

[1]Institute of Applied Physics, Moldova Academy of Sciences, Chisinau, Moldova

[2]Technical University of Moldova, Chisinau, Moldova

1996

# 1. Introduction

The systems with strong electronic correlations, showing unusual thermodynamic, magnetic, transport and superconducting properties are of great interest now. Among them, are the heavy fermion compounds, the copper oxides, in which high-$T_c$ superconductivity was discovered and other materials. Their microscopically quantum - theoretical investigation can be done using the periodic Anderson Model (PAM) [1]. We shall discuss the simplest form of this model with the Hamiltonian

$$H = H_c^0 + H_f^0 + H_{int} \tag{1}$$

$$H_c^0 = \sum_{\mathbf{k},\sigma} (\epsilon(\mathbf{k}) - \mu) c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma};$$

$$H_f^0 = \sum_{i,\sigma} (E_f - \mu) f_{i\sigma}^+ f_{i\sigma} + U \sum_i f_{i\uparrow}^+ f_{i\uparrow} f_{i\downarrow}^+ f_{i\downarrow};$$

$$H_{int} = \frac{V}{\sqrt{N}} \sum_{i,\mathbf{k},\sigma} [c_{\mathbf{k}\sigma}^+ f_{i\sigma} e^{i\mathbf{k}\mathbf{R}_i} + f_{i\sigma}^+ c_{\mathbf{k}\sigma} e^{-i\mathbf{k}\mathbf{R}_i}] \tag{2}$$

were $c_{\mathbf{k}\sigma}^+ (c_{\mathbf{k}\sigma})$ -are creation (annihilation) operators of conduction electrons with wave vector k ,energy $\epsilon(\mathbf{k})$, band width $W$ and spin $\sigma$; $f_{i\sigma}^+ (f_{i\sigma})$- the corresponding operators for localized on site $i$ $f$-electrons. $U$- is on-site Coulomb repulsion of $f$ - electrons, $\mu$-chemical potential of the system. The local $f$ - orbitals with site energy $E_f$ are single site hybridized through $V$ with conduction electron states.

The PAM is rather complicated many-body problem and obtaining of some general relations and properties of the renormalized Green's function is useful.

The properties of PAM were discussed in a large number of papers [2-14] where the influence of Coulomb repulsion $U$ and hybridization $V$ on ground state and energy spectrum of quasiparticles of the system, the existence of mixed valence of electrons, the phase transitions of them were investigated and different approaches and approximations were proposed.

In this paper the thermodynamic perturbation theory is developed for the system with Hamiltonian (1) supposing that hybridization Hamiltonian is a perturbation. In zero order approximation $f$-electrons are considered localized and Hubbard [15] operators $X_i^{nm}$ are used to diagonalize Hamiltonian $H_f^0$.

$$c_{i\sigma} = X_i^{0,\sigma} + \sigma X_i^{-\sigma,2}; f_{i\sigma}^+ = X_i^{\sigma,0} + \sigma X_i^{2,-\sigma}; H_f^0 = \sum_{i,\alpha} E_\alpha X_i^{\alpha,\alpha} \tag{3}$$

where index $\alpha$ enumerates four on site electron states: without electrons, with one electron having $\sigma$ spin and with two electrons of opposite spins. Their energy are:

$$E_0 = 0; E_\sigma = E_f - \mu; E_2 = U + 2(E_f - \mu).$$

Conduction electrons in this approximation are considered free and determined by the wave vectors k , spins $\sigma$ and band energy $\epsilon(\mathrm{k})$. The grand partition function of the system in zero approximation is factorized by wave vectors for conduction and by sites $i$ for localized electrons. In such a way the statistical averages with this partition function are calculated for $c$ -electrons by making use of Wick theorem for the products of $c$ -electron operators. But for the statistical average of localized $f$ -electron operator products the generalized Wick theorem proposed in papers [16-18] is employed. This last theorem is based on the conception of many particles irreductible Green's functions or Kubo cumulants which appear in realization of these averages.

## 2. Perturbation theory

The evolution operator of the thermodynamic perturbation theory is

$$U(\beta) = T\exp(-\int_0^\beta H_{int}(\tau)d\tau) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}T(H_{int}(\tau_1)...H_{int}(\tau_n)) \qquad (4)$$

The free energy of the system is equal:

$$F = F_0 - \frac{1}{\beta}\ln\langle U(\beta)\rangle_0; F_0 = -\frac{1}{\beta}\ln Tr\{e^{-\beta(H_c^0+H_f^0)}\} \qquad (5)$$

The average $\langle U(\beta)\rangle_0$ can be obtained taking into account only the even $n = 2m$ degrees of perturbation theory because of the structure of $H_{int}$ multiplies. Then in a such product of $2m$ multiplies there are in total $4m$ operators. Only the operator structures which have m operators $c, \bar{c}, f, \bar{f}$ of each kind must be considered in the future because other operator combinations have zero statistical averages. The number of such structures is equal to $C_{2m}^m$ and changing the indices $i, \mathrm{k}, \sigma$ of summing and of $\tau$ integration, we can prove that all of them are equivalent. Taking one of such operator structure and multiplying by $C_{2m}^m$ after dividing on $(2m)!$ we obtain

$$\langle U(\beta)\rangle_0 = 1 + \sum_{m=1}^{\infty}\frac{V^{2m}}{N^m(m!)^2}\sum_{i_1\mathrm{k}_1\sigma_1}...\sum_{i_{2m},\mathrm{k}_{2m},\sigma_{2m}}\int d\tau_{1...}\int d\tau_{2m}$$

$$\langle T\bar{c}_{\mathrm{k}_1\sigma_1}(\tau_1)...\bar{c}_{\mathrm{k}_m\sigma_m}(\tau_m)c_{\mathrm{k}_{m+1}\sigma_{m+1}}(\tau_{m+1})...c_{\mathrm{k}_{2m}\sigma_{2m}}(\tau_{2m})\rangle_0 *$$

$$\langle Tf_{i_1\sigma_1}(\tau_1)...f_{i_m\sigma_m}(\tau_m)\bar{f}_{i_{m+1}}(\tau_{m+1})...\bar{f}_{i_{2m}\sigma_{2m}}(\tau_{2m})\rangle_0 *$$



$$\exp\{i(\mathrm{k}_1\mathrm{R}_1 + ... + \mathrm{k}_m\mathrm{R}_m - \mathrm{k}_{m+1}\mathrm{R}_{m+1} - ... - \mathrm{k}_{2m}\mathrm{R}_{2m})\} \qquad (6)$$

The statistical average of conduction electron operators calculated by using Wick theorem gives us the sum of $m!$ member each of them equal to the product of $m$ free conducting electron propagators $G^{c(0)}$.

By changing all, above mentioned, indices we can prove that all of them are equivalent and m! additional multiplier appears in the numerator of (6).

So we have

$$\langle U(\beta)\rangle_0 = 1 + \sum_{m=1}^{\infty}\frac{V^{2m}}{N^m m!}\sum_{i_1\mathrm{k}_1\sigma_1}...\sum_{i_{2m},\mathrm{k}_{2m},\sigma_{2m}}\int d\tau_{1...}\int d\tau_{2m}$$

$$\langle T\bar{c}_{\mathrm{k}_1\sigma_1}(\tau_1)c_{\mathrm{k}_{2m}\sigma_{2m}}(\tau_{2m})\rangle_0...\langle T\bar{c}_{\mathrm{k}_m\sigma_m}(\tau_m)c_{\mathrm{k}_{m+1}\sigma_{m+1}}(\tau_{m+1})\rangle_0 *$$

$$\langle Tf_{i_1\sigma_1}(\tau_1)...f_{i_m\sigma_m}(\tau_m)\bar{f}_{i_{m+1}\sigma_{m+1}}(\tau_{m+1})...\bar{f}_{i_{2m}(\sigma_{2m})}(\tau_{2m})\rangle_0 *$$

$$\exp\{i(\mathrm{k}_1\mathrm{R}_1 + ... + \mathrm{k}_m\mathrm{R}_m - \mathrm{k}_{m+1}\mathrm{R}_{m+1} - ... - \mathrm{k}_{2m}\mathrm{R}_{2m})\} \qquad (7)$$

where

$$G^{c(0)}(\mathrm{k}_1\sigma_1\tau_1|\mathrm{k}_2\sigma_2\tau_2) = -\langle Tc_{\mathrm{k}_1\sigma_1}(\tau_1)\bar{c}_{\mathrm{k}_2\sigma_2}(\tau_2)\rangle_0.$$

The equation (7) has the form of the perturbation theory for Hubbard model if the hopping of the $f$ -electrons of this last model is considered as a perturbation:

$$H_{int} = -\sum_{ij\sigma}t(j-i)f_{j\sigma}^+ f_{i\sigma}$$

In (7) the instantaneous matrix elements $t(i-j)$ of Hubbard model are replaced by dynamically propagators $G^{c(0)}$ multiplied by $V^2$

In the next the generalized Wick theorem of [16-18] is used. For $m = 1$ the average $\langle f_1\bar{f}_2\rangle_0$ is free propagator for localized and strong interacting $f$ -electrons

$$G^{f(0)}(\mathrm{k}_1\sigma_1\tau_1|\mathrm{k}_2\sigma_2\tau_2) = -\langle Tf_{\mathrm{k}_1\sigma_1}(\tau_1)\bar{f}_{\mathrm{k}_2\sigma_2}(\tau_2)\rangle_0$$

For $m = 2$ the average is equal [16-18]

$$\langle Tf_1f_2\bar{f}_3\bar{f}_4\rangle_0 = \langle Tf_1\bar{f}_4\rangle_0\langle Tf_2\bar{f}_3\rangle_0 -$$

$$-\langle Tf_1\bar{f}_3\rangle_0\langle Tf_2\bar{f}_4\rangle_0 + \langle 12|\bar{3}\bar{4}\rangle_0^{ir} \qquad (8)$$

where $1 = (i_1, \sigma_1, \tau_1)$

$$\langle 12|\bar{3}\bar{4}\rangle_0^{ir} = G_2^{(0)ir}(i_1\sigma_1\tau_1, i_2\sigma_2\tau_2|i_3\sigma_3\tau_3, i_4\sigma_4\tau_4) =$$

$$= \delta_{i_1 i_2}\delta_{i_1 i_3}\delta_{i_1 i_4} G_2^{(0)ir}(\sigma_1\tau_1, \sigma_2\tau_2|\sigma_3\tau_3, \sigma_4\tau_4);$$

$$G_2^{(0)ir}(\sigma_1\tau_1, \sigma_2\tau_2|\sigma_3\tau_3, \sigma_4\tau_4) =$$

$$= \langle T f_{\sigma_1}(\tau_1) f_{\sigma_2}(\tau_2)\bar{f}_{\sigma_3}(\tau_3)\bar{f}_{\sigma_4}(\tau_4)\rangle_0 - \langle T f_{\sigma_1}(\tau_1)\bar{f}_{\sigma_4}(\tau_4)\rangle_0 *$$

$$*\langle T f_{\sigma_2}(\tau_2)\bar{f}_{\sigma_3}(\tau_3)\rangle_0 + \langle T f_{\sigma_1}(\tau_1)\bar{f}_{\sigma_3}(\tau_3)\rangle_0$$

$$\langle T f_{\sigma_1}(\tau_1)\bar{f}_{\sigma_4}(\tau_4)\rangle_0 \qquad (9)$$

All the quantities of right hand of equation (8) are one-site ones. They depend on spin indices and $\tau$ variables and are independent of site indices. $G_2^{(0)ir}$ is the two particles irreducible Green function or the Kubo cumulant. When Coulomb interaction is zero such functions don't exist.

The first two components of (8) are of Wick type but the last one is a new contribution conditioned by strong electronic correlations. For $m = 3$ the existing statistical average $\langle T f_1 f_2 f_3 \bar{f}_4 \bar{f}_5 \bar{f}_6\rangle_0$ contains 3! Wick contributions each of them equal to the product of three propagators $G^{f(0)}$. Then there are 9 contributions each of them equal to the product of propagator $G^{f(0)}$ and one irreductible two particles Green's function and there is also one contribution equal to three particles irreductible Green's function $G_3^{(0)ir}$.

In general case of statistical average of $2m$ $f$-operators the generalized Wick theorem gives us $m!$ components of Wick type, each of them equal to the product of $m$ propagators, and then there are the sum of products of different kind of Kubo cumulants, organized in such way that the number of particles in all these cumulants is equal to $m$. The sign of all these contributions is determined by the number of permutations of Fermi $f$-operators which is necessary to obtain the given cumulant structure.

Some of vacuum diagrams are shown in Fig.1. Here the thin directed full line is the $G^{f(0)}$ propagator and a directed dotted line is $G^{c(0)}$ one. The point of the diagram contains hybridization $V$. 1.a diagram is the simplest connected one but 1.b diagram is disconnected one. More complicated connected diagrams are 1.d,1.c ones. The analysis of the vacuum diagram's structure gives us the equation

$$\langle U(\beta)\rangle_0 = 1 + \sum_{n=1}^{\infty} \frac{[\langle U(\beta)\rangle_0^c]^n}{n!} = \exp[\langle U(\beta)\rangle_0^c] \qquad (10)$$

where $\langle U(\beta)\rangle_0^c$ is the connected part of all vacuum diagrams. This equation is the very well known theorem of connected diagrams of statistical physics.



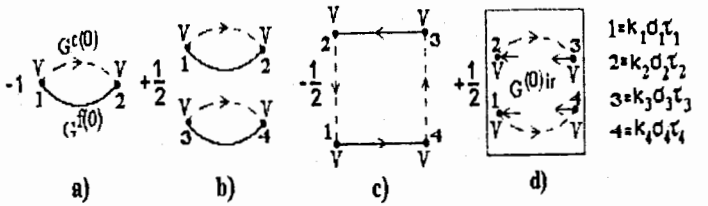


Fig. 1

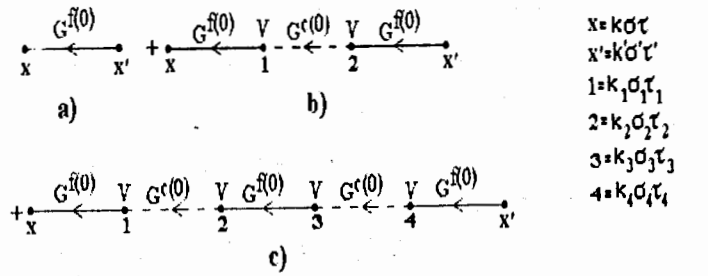


Fig. 2

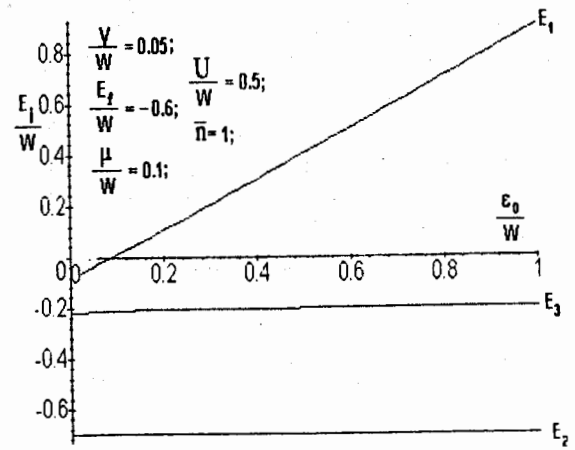


Fig. 3

## 3. One particle Green's functions

We shall discuss now the renormalized $f$-electron one particle Green's function:

$$G^{ff}(\mathbf{x}\sigma\tau|\mathbf{x}'\sigma'\tau') = -\langle T f_{\mathbf{x}\sigma}(\tau) f_{\mathbf{x}'\sigma'}(\tau') U(\beta)\rangle_0^c \qquad (11)$$

where index c points out that only connected propagator diagrams must be considered.

Equation (11) can be transformed by using the arguments of the previous section. In such a way we obtain

$$G^{ff}(x|x') = G^{f(0)}(x|x') - \sum_{m=1}^{\infty} \frac{V^{2m}}{N^m m!} \int d\tau_1 ... \int d\tau_{2m} \sum_{i_1 \mathbf{k}_1 \sigma_1} ...$$

$$... \sum_{i_{2m}\mathbf{k}_{2m}\sigma_{2m}} \langle T\bar{c}_1 c_{2m}\rangle_0 * ... \langle T\bar{c}_m c_{m+1}\rangle_0 * \langle T f_x \bar{f}_{x'} f_1 ...$$

$$... f_m \bar{f}_{m+1} ... \bar{f}_{2m}\rangle_0 \exp\{i(\mathbf{k}_1\mathbf{R}_1 + ... + \mathbf{k}_m\mathbf{R}_m - \mathbf{k}_{m+1}\mathbf{R}_{m+1} -$$

$$- ... - \mathbf{k}_{2m}\mathbf{R}_{2m})\} \qquad (12)$$

Here $x$ and $x'$ indices of $f$ -operators stand for $\mathbf{x}\sigma\tau$ and $\mathbf{x}'\sigma'\tau'$ correspondingly. The other indices of $f$ - operators are of the same kind, for example $1 = i_1\sigma_1\tau_1$ but for $c$ -electron operators we have $1 = \mathbf{k}_1\sigma_1\tau_1$ and so on. The existence of the exponents gives us the possibility to use also local presentation for $c$ -electron quantities or wave vector presentation for $f$ -operators.

If in the last statistical average of (12) we take into account only Wick type contributions we obtain the chain type diagrams shown in Fig.2.Here all the irreducible Green's functions were omitted. All this diagrams are weak connected because they can be divided in two parts by cutting one line.

All these diagrams can be summed up by using Fourier-presentation. We obtain Hubbard I approximation for Dyson equation:

$$G^{ff}_\sigma(\mathbf{k}|i\omega_n) = G^{f(0)}_\sigma(i\omega_n)(1 + V^2 G^{c(0)}(\mathbf{k}|i\omega_n) G^{ff}_\sigma(\mathbf{k}|i\omega_n));$$

$$G^{ff}_\sigma(\mathbf{k}|i\omega_n) = [G^{f(0)}_\sigma(i\omega_n)^{-1} - V^2 G^{c(0)}(\mathbf{k}|i\omega_n)]^{-1};$$

In this approximation it is easy to obtain also the Dyson equation for renormalized conduction electron Green's function $G^{cc}_\sigma(\mathbf{k}|i\omega_n)$. Free electron propagators are



$$G^{cc(0)}_\sigma(\mathbf{k}|i\omega_n) = (i\omega_n - \epsilon_0)^{-1}; \epsilon_0 = \epsilon(\mathbf{k}) - \mu$$

$$G^{f(0)}_\sigma(i\omega_n) = \frac{1-\bar{n}_{-\sigma}}{i\omega_n - \epsilon_1} + \frac{\bar{n}_{-\sigma}}{i\omega_n - \epsilon_2}; \epsilon_1 = E_f - \mu; \epsilon_2 = U + E_f - \mu;$$

$$\bar{n} = \langle \bar{f}_\sigma f_\sigma\rangle_0 = \{\exp(-\beta\epsilon_1) + \exp[-\beta(\epsilon_1+\epsilon_2)]\}\{1+$$

$$2\exp(-\beta\epsilon_1) + \exp[-\beta(\epsilon_{1+}\epsilon_2)]\}^{-1}.$$

The energy spectrum of quasiparticles is determined by equation:

$$(E - \epsilon_0) - V^2[(1-\bar{n})/(E-\epsilon_1) + \bar{n}/(E-\epsilon_2)] = 0.$$

For large values of Coulomb interaction $U \to \infty$ three energetic branches are:

$$E_{1,2}(\mathbf{k}) = [\epsilon_0 + \epsilon_1 \pm \sqrt{(\epsilon_0-\epsilon_1)^2 + 4V^2(1-\bar{n})}]/2+$$

$$+\frac{V^2\bar{n}}{2\epsilon_2}[1 \pm (\epsilon_0-\epsilon_1)/\sqrt{(\epsilon_0-\epsilon_1)^2 + 4V^2(1-\bar{n})}] + o(1/U^2);$$

$$E_3(\mathbf{k}) = \epsilon_2 + V^2\bar{n}/\epsilon_2 + o(1/U^2)$$

The chemical potential of the system with $N_e$ ellectrons is determined from

$$(1/\beta)\sum_{\omega_n}\sum_{\mathbf{k}\sigma}[G^{ff}_\sigma(\mathbf{k}|i\omega_n) + G^{cc}_\sigma(\mathbf{k}|i\omega_n)]\exp(i\omega_n 0^+) = N_e.$$

This equation is reduced to

$$\sum_\sigma\sum_{\mathbf{k}}\{A_\sigma(\mathbf{k})/[\exp(\beta E_{1\sigma}) + 1] + B_\sigma(\mathbf{k})/[\exp(\beta E_{2\sigma} + 1]+$$

$$+C_\sigma(\mathbf{k})/[\exp(\beta E_{3\sigma}) + 1]\} = N_e$$

where in the limit of large $U$ value $U \to \infty$ these coefficients are

$$A_\sigma(\mathbf{k}) \approx 1 - \bar{n}v^2(\mathbf{k}); B_\sigma \approx 1 - \bar{n}u^2(\mathbf{k}); C_\sigma(\mathbf{k}) \approx \bar{n};$$

where

$$u^2(\mathbf{k}) = \frac{1}{2}\left[1 + (\epsilon_0-\epsilon_1)/\sqrt{(\epsilon_0-\epsilon_1)^2 + 4V^2(1-\bar{n})}\right]$$

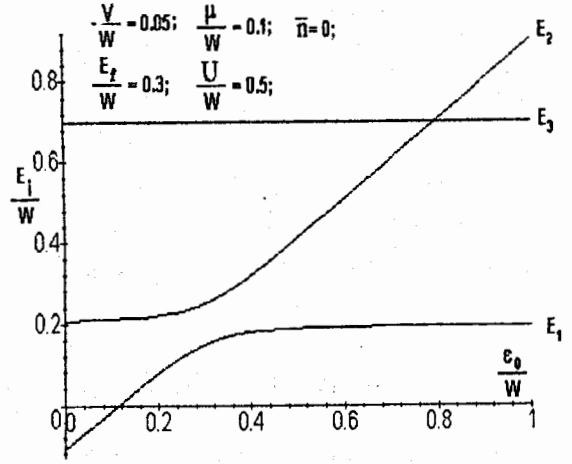


Fig. 4

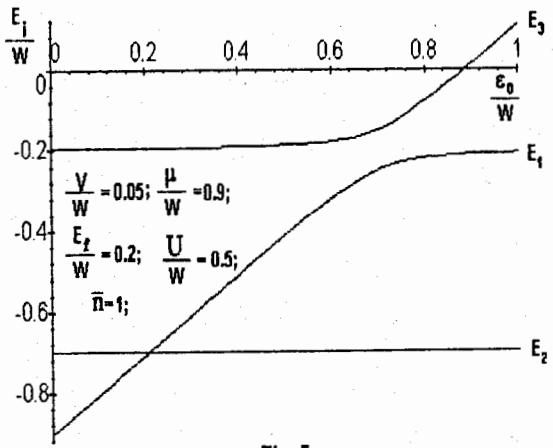


Fig. 5



$$v^2(\mathrm{k}) = [1 - (\epsilon_0 - \epsilon_1)/\sqrt{(\epsilon_0 - \epsilon_1)^2 + 4V^2(1-\bar{n})}]/2.$$

In this limit there are two subbands with energy gap between them. The sum of the widths of these two subbands is equal to the width $W$ of bare conduction band but the distance between the bottom of the lower subband and the top of the upper subband is equal to $W$ plus the width of energy gap.

The dependence of the electron number on the chemical potential of the system have been obtained also. For example, in the case when the chemical potential is situated into the lower subband this dependence is

$$\frac{N_e}{2N} = \frac{(\mu + W/2)}{W} + \frac{V^2(1-\bar{n})}{(E_f - \mu)W}$$

Because the local initial level $E_f$ is situated in the energy gap of this renormalized system in our case of zero temperature $E_f - \mu > 0$ we have the average $\bar{n} = 0$. When $\mu$ is higher than the top of the upper subband $N_e = 3N$.

The calculated values of the renormalized quasiparticle energies as function of $\epsilon_0/W$ for T=0 and different values of the main parameters of the theory are shown in Figures 3-6. The origin of the energy is at the bottom of the bare conduction electron band. The bare energy band of conduction electrons can remain unsplitted by the hybridization energy (Fig. 3.), can be splitted in two subbands (Figs.4-5) or in general case can be splitted in three subbands (Fig.6.).

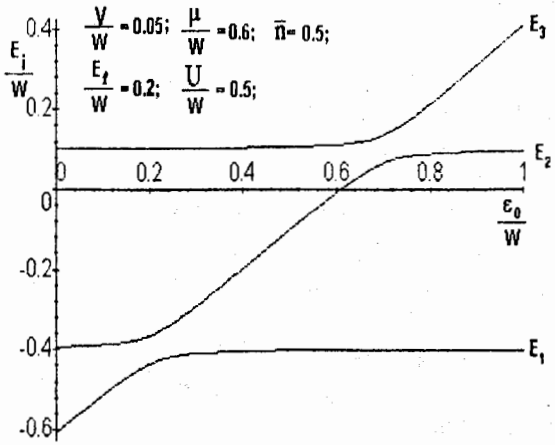


Fig. 6

The first situation is realized when one of the following inequalities hold:
a) $E_f + U < 0$; b) $E_f > W$; c) $W - U < E_f < 0$;
The appearance of two subbands is realized at the conditions:
$0 < \mu < E_f$ or $E_f + U < \mu < W$
and the last situation takes place when

$$0 < E_f < \mu < E_f + U < W.$$

## Conclusions

The approach we have described provides a general framework to investigate the properties of the systems with strong electron correlations. This new diagramm method of investigation admit the next discussion of the role of the spin and charge correlations on the system many-particle properties by taking into account many-particle one-site irreducible Green functions. The numerical results we have presented illustrate the general features of the three branches of energy spectrum in Hubbard I approximation as a function of the $\epsilon_0/W$ at different values of main theory parameters of the theory.

## Acknowledgements

Financial support from Soros foundation is gratefully acknowledged. Authors thank Prof. N.M.Plakida for very useful discussion and support.

[1] P.W. Anderson, Phys. Rev. **124**, 41 (1961).
[2] H.I. Leder and B.Mühlschlegel , Z.Physik B **29**, 341 (1978).
[3] P. Coleman, Phys. Rev. B **29**, 3035 (1984).
[4] J. Callway et al., Phys. Rev. B **38**, 2583 (1988).
[5] J. Callway, L. Tan and H. Zheng, Phys. Rev. B **50**, 1369 (1994).
[6] T.M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985).
[7] R.Blankenbecler, J.R.Fulco, W.Gill, D.I.Scalapino, Phys. Rev. Lett.**58**, 411 (1987).
[8] K.Yamoto, K.Ueda, Jur. Phys. Soc. Japan **59**, 3284 (1990).
[9] K.Yamada and K.Yosida, 1981. Electron correlation and magnetism in narrow-band systems ed. T.Morya, Berlin Springer, p.210.



[10] B. Möller and P. Wölfle, Phys. Rev. B **48**, 10320 (1993).
[11] E. Halvorsen and Q. Czycholl, Jour. Phys. Condens. Matter. **8**, 1775 (1996).
[12] A. Kuzemsky. International Centre For Theoretical Physics IC/93/336
[13] A. Kuzemsky and J.C.Parlebas and H. Bec, Physica A**198**, 606 (1993).A.Kuzemsky. Rapid Communication JINR Dubna. 3/60/1993.
[14] B.H.Brandow,Phys.Rev. B**33**, 215 (1986).
[15] J. Hubbard, Proc. Roy. Soc. A**276**, 233 (1963).
[16] M.I. Vladimir and V.A. Moskalenko, Teor.Matem.Fiz. **82**,428 (1990).
[17] S.I. Vacaru, M.I. Vladimir and V.A. Moskalenko, Teor.Matem.Fiz. **85**, 248 (1990).
[18] N.N. Bogoliubov and V.A. Moskalenko, Dokl, Akad. Nauk SSSR **136**, 1107 (1991).

Received by Publishing Department
on December 14, 1996.