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A NEW APPROACH TO THE THEORY OF STRONGLY CORRELATED SYSTEMS

V.A.Moskalenko,
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia
Institute of Applied Physics, Moldova Academy of Sciences, Chisinau 2028, Moldova

P.Entel,
Theoretische Physik, Gerhard-Mercator-Universität Duisburg, 47048 Duisburg, Germany

D.F.Digor,
Institute of Applied Physics, Moldova Academy of Sciences, Chisinau 2028, Moldova

M.I.Vladimir
Technical University, Chisinau 2000, Moldova

A new diagrammatic method for the investigation of the properties of strongly correlated electron systems is formulated. The method is used in order to handle the strong Coulomb on-site repulsion of the electrons of unfilled inner ion shells of transition and rare earth metals. The new elements of this diagram technique are the many-particle on-site irreducible Green's functions, which contain all the essential spin and charge fluctuations of this system. The infinite sum of such contributions essentially determines the correlation function $Z(\mathbf{x}, \mathbf{x}')$ which is used to formulate the Dyson equation for renormalized one-particle Green's function. The summing of a class of diagrams permits us to close the equations which determine $Z(\mathbf{x}, \mathbf{x}')$ function and to discuss Mott–Hubbard and superconducting phase transitions of the system. The influence of strong electron-phonon interaction on the phase transitions is discussed.

1. INTRODUCTION

The theory of strongly correlated electron systems has been of great interest for Prof. N.N.Bogoliubov, who in the middle of the fortieth years [1] elaborated the theory of polar state of the metals using the perturbation theory for nonorthogonality integral of ion eigenfunctions. In zero order approximation when nonorthogonality integrals were omitted Prof. N.N.Bogoliubov obtained the Hamiltonian of metals now called as Hubbard Hamiltonian and also he proposed some generalization of it. Prof. N.N.Bogoliubov interest to this problem has been renewed [2–7] in the last period of his life thanks to the discovery of high T_c superconductivity in oxides materials and intensive discussion of the theoretical aspects of this phenomenon.

We shall address our investigation to some models of strongly correlated electron systems. The simplest from them is the so-called one-band Hubbard [8] model which supposes that at sites i of the crystal lattice with coordinates $\mathbf{R}_i$ there are ions of transition or rare earth metals with unfilled shells. The electrons of these shells have the strong on-site Coulomb repulsion U and make transitions between the lattice sites with the hopping integral $t(\mathbf{R}_i - \mathbf{R}_j)$.

The electron correlations have a strong influence on the magnetic, thermal and transport properties of the materials with such electron structure. They play an important role for our understanding of the properties of high-temperature superconductors.

The corresponding Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}^0 + \mathcal{H}_{int}, \tag{1}$$

where

$$\begin{aligned} \mathcal{H}^0 &= \sum_i \mathcal{H}_i^0, \qquad & \mathcal{H}_i^0 &= -\mu \sum_\sigma n_{i\sigma} + U n_{i\uparrow} n_{i\downarrow}, \\ \mathcal{H}_{int} &= \sum_{i,j,\sigma} t(j-i) c_{j\sigma}^\dagger c_{i\sigma}, \qquad & n_{i\sigma} &= c_{i\sigma}^\dagger c_{i\sigma}, \end{aligned} \tag{2}$$

in which μ is the chemical potential of the system, $c_{i\sigma}^\dagger, c_{i\sigma}$ — the electron operators.

2. EXPANSION THEORY FROM THE ATOMIC LIMIT

The problem is now to deal properly with the impact of electronic correlations on the system properties. This can be done best by using Green's functions provided one finds a key to deal with the spin and charge degrees of freedom. Since we have included the Coulomb term in zero order, conventional perturbation theory of quantum statistical mechanics is not an adequate tool because it relies on the ability to expand the partition function about the noninteracting state. Instead, projection or Hubbard operators are necessary to diagonalize H^0 which prevents the use of traditional Wick's theorem and conventional Feynman expansion of the thermodynamic perturbation theory. It was Hubbard who had first proposed a graphical expansion for correlated electrons about atomic limit in power of the hopping integrals, whereby thermal averages are expanded into sums of products of Kubo cumulants [8]. Each term of the expansion can be represented by a graph consisting of a series of vertices, each of it corresponds to a cumulant factor, and a series of lines joining the vertices which represent the hopping integrals. The resulting expression for the free energy was given in terms of connected vacuum diagrams. Because of the complicated algebraically structure of the operators, this approach remained unused for some time. This

diagrammatic approach was reformulated in a systematic way for the single band Hubbard model and some other its modifications by Slobodyan and Stasyuk [9], and independently by Zaitsev [10] and Ivanov [11] and further developed by Izyumov [12]. These authors proposed a regular diagrammatic procedure based on the properties of Hubbard operators giving rise to a variety of diagrammatic vertices and zero order Green's functions. The technique of these authors is based on the disentanglement of the nondiagonal Hubbard operators in the chronological averages of the perturbation expansion. This is difficult to handle since one has to deal with operators of different statistics and complex structure. The diagrams are also complicated and depend on the operator to be disentangled first (as do the results). On the other hand, such phenomena as metal insulator, magnetic and superconducting transition, respectively, require partial summation of the diagrams. Therefore, it appeared to us more appropriate to develop a diagrammatic technique which uses more simple creation and annihilation operators for electrons at all intermediate stages of the theory [13,14]. Only at the final stage of the investigation, when local quantities have to be calculated, projection operators are used. Our perturbation theory as the theory of previous authors, is formulated in the interaction representation by using grand canonical ensemble averages of chronological products of interactions. These averages are reduced to n-particle Matsubara Green's functions of the atomic system. These functions can be factorized into independent local averages by using a generalization of Wick's theorem (GWT) which takes into account the strong local correlations (for details see Refs. 13,14). The GWT differs from traditional Wick's theorem by the appearance of additional contributions which contain new irreducible on-site many-particle Green's functions. These functions have the structure of Kubo cumulants and are entirely conditioned by the presence of strong Coulomb repulsion between the localized electrons. When the Coulomb repulsion is zero, these functions vanish identically. These irreducible n-particle Green's functions are diagonal with respect to their site indices, but they can have different time and spin labels. These new functions contain all spin and charge fluctuations of the Hubbard model. The diagrammatic rules were formulated in Refs. 13–15. The novelty of our diagram technique is:

1. The GWT allows to generate all contributions of the perturbation expansion for correlated electron systems by using at the same time the simple algebra of usual Fermion operators instead of the algebra of projection operators. Projection operators are only used at the final stage of the calculation. The new irreducible diagrams which appear in the expansion contain all spin and charge fluctuations. They mainly determine the renormalization of propagators of correlated systems as well as possible phase transitions. This technique exhibits only one kind of vertex, one localized electron Green's function and only one irreducible n-particle Green's function. Previous diagrammatical formulations contain a variety of such quantities.

2. We have proved the validity of the linked-cluster theorem for the present expansion of the Hubbard model as well as the existence of a Dyson type of equation for the delocalized one-particle Green's function. The Dyson equation contains irreducible Green's functions which are gathered together in the correlation function Z (for details see Refs. 13–15) which is the sum of connected irreducible Green's function; Z is the main element of the renormalization process of delocalization. The simplest Z function is expressed by the two-particle function representing the sum of 24 chronologically ordered functions, each of it corresponds to a product of four Hubbard operators. This type of Z function and the resulting Dyson equation (see Eqs. (6)–(8) below) have not been introduced in the previous expansions for correlated electrons [9–12,20].

3. Our diagram technique permits the summation of special class of diagrams, thereby allowing one to investigate the Mott–Hubbard or superconducting phase transition. The diagram technique has been elaborated firstly for the Hubbard model but it can be used for other model systems of correlated electrons like the impurity and lattice Anderson model [16-19].

A GWT for chronological averages of products of electron operators was formulated later by Metzner [20]. Metzner proposed a linked-cluster expansion around the atomic limit and established diagrammatic rules for the Green's function and the contribution to the free energy. The author did not derive the Dyson equation for the renormalized one-particle Green's function and the properties and the role of the new correlation function comparable to our correlation function Z was not established. In spite of similarity to our work, the diagrams in his approach are quite different: The n-particle cumulant is represented by a 2n-valent point vertex with attached n-entering and n-living lines, whereas in our approach such a cumulant or irreducible Green's function is represented by a rectangle with $2n$ vertices with n-entering and n-leaving arrows (see Izyumov [12]). The rectangle contours the vertices with the same site index but different time and spin labels. In addition Metzner investigated the limit of high lattice dimensions. Generalizing Metzner's procedure to include the Dyson equation, Crao and Gusmao have subsequently investigated the metal-insulator transition by using the irreducible Green's function to one-loop order [21].

In order to conclude the comparison to other work, we would like to mention that there are alternative ways to formulate a perturbation theory, which are based on the contour integral representation of the partition and correlation function. This technique makes use of the resolvent expansion allowing to introduce a self-energy operator similar to the self-energy in Feynman perturbation theory. For an overview of this method and its applications we refer to the review of Bickers [22].

Finally in connection with the problem of valence fluctuations we would like to mention that Grewe and Keiter have formulated a Goldstone-type of expansion of the partition function (Brillouin–Wigner type of perturbation theory) around the

atomic limit which, however, requires a regularizing procedure of the self-energy [23]. Along similar lines but without the concept of statistical quasiparticles, is the work of Kuromoto [24]. These formulations are in close analogy to the standard Green's function method but without making use of the linked-cluster theorem.

3. AVERAGES OF ELECTRON OPERATORS

We start by introducing the temperature Green's function for the electrons defined by

$$\mathcal{G}(\mathbf{x},\sigma,\tau|\mathbf{x}',\sigma',\tau') = -\langle T\,\widehat{c}_{\mathbf{x}\sigma}(\tau)\widehat{\overline{c}}_{\mathbf{x}'\sigma'}(\tau')\rangle_{\mathcal{H}}, \tag{3}$$

where $\mathbf{x},\mathbf{x}'$ are the site indices and τ,τ' stand for the imaginary time with $0 < \tau < \beta$, where β is the inverse temperature of the system; T is the time ordering operator. The operators with hats are defined in the Heisenberg representation with the original Hamiltonian (1)

$$\widehat{c}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau}c_{\mathbf{x}\sigma}e^{-\mathcal{H}\tau}, \quad \widehat{\overline{c}}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau}c^{\dagger}_{\mathbf{x}\sigma}e^{-\mathcal{H}\tau},$$

and statistical averaging $\langle\ldots\rangle_{\mathcal{H}}$ is done with the density operator of the grand canonical ensemble, $e^{-\beta\mathcal{H}}/\mathrm{Tr}\,e^{-\beta\mathcal{H}}$. As usual, $\overline{c}_{\mathbf{x}\sigma}(\tau)$ is not the adjoint of $c_{\mathbf{x}\sigma}(\tau)$ as long as τ is real. But interpreted as a complex variable, τ may be analytically continued to a pure imaginary value $\tau = it/\hbar$.

The corresponding Green's function of the Hubbard model is in the interaction representation given by

$$\mathcal{G}(\mathbf{x},\sigma,\tau|\mathbf{x}',\sigma',\tau') = -\frac{\langle T\,c_{\mathbf{x}\sigma}(\tau)\overline{c}_{\mathbf{x}'\sigma'}(\tau')U(\beta)\rangle_0}{\langle U(\beta)\rangle_0}, \tag{4}$$

where the evolution operator $U(\beta)$ is given by

$$U(\beta) = T\exp\left(-\int_0^{\beta} d\tau\,\mathcal{H}_{int}(\tau)\right). \tag{5}$$

The statistical averaging is now carried out with respect to the zero-order density matrix of the localized electrons.

The sum of strongly connected diagrams (i.e., those which cannot be divided into two parts by cutting a single hopping line) which contain irreducible Green's functions of all kinds in the perturbation expansion of Eq. (5), determines the special function $Z(x|x')$ (for details see Refs. 13,14,15). This function contains all charge and spin correlations. It allows us, together with the mass operator

which is in our case the hopping matrix element, to formulate the Dyson equation for the one-electron Green's function [13–15]

$$\mathcal{G}(x|x') = \Lambda(x|x') + \sum_{1,2} \Lambda(x|1)t(1-2)\mathcal{G}(2|x'), \tag{6}$$

where

$$\Lambda(x|x') = \mathcal{G}^{(0)}(x|x') + Z(x|x'), \tag{7}$$

$$t(x-x') = \delta(\tau-\tau')\, t(\mathbf{x}-\mathbf{x}'). \tag{8}$$

Here x stands for $\mathbf{x}, \sigma, \tau$ and the sum is over the discrete indices including the integration over τ. Using the Fourier representation for these quantities gives us the following form of the Dyson equation for the renormalized one-electron Green's function,

$$\mathcal{G}_\sigma(\mathbf{k}|i\omega_n) = \frac{1}{\Lambda_\sigma^{-1}(\mathbf{k}|i\omega_n) - \varepsilon(\mathbf{k})}. \tag{9}$$

Here ω_n stands for the Matsubara frequency $\omega_n = (2n+1)\,\pi/\beta$.

As was shown previously, [3, 7, 24] the Dyson equation in the case of superconductivity is of the form,

$$\mathcal{G}_{\sigma\sigma}(\mathbf{k}|i\omega_n) = \frac{\Lambda_\sigma(\mathbf{k}|i\omega_n)[1-\Lambda_{-\sigma}(-\mathbf{k}|-i\omega_n)\,\varepsilon(-\mathbf{k})]}{D_\sigma(\mathbf{k}|i\omega_n)} - \frac{\varepsilon(-\mathbf{k})\,Y_{\sigma-\sigma}(\mathbf{k}|i\omega_n)\,\overline{Y}_{-\sigma,\sigma}(\mathbf{k}|i\omega_n)}{D_\sigma(\mathbf{k}|i\omega_n)}, \tag{10}$$

$$\mathcal{F}_{\sigma,-\sigma}(\mathbf{k}|i\omega_n) = \frac{Y_{\sigma,-\sigma}(\mathbf{k}|i\omega_n)}{D_\sigma(\mathbf{k}|i\omega_n)}, \tag{11}$$

$$\overline{F}_{-\sigma,\sigma}(\mathbf{k}|i\omega_n) = \frac{\overline{Y}_{-\sigma,\sigma}(\mathbf{k}(i\omega_n)}{D_\sigma(\mathbf{k}|i\omega_n)}, \tag{12}$$

where

$$D_\sigma(k|i\omega_n) = [1-\varepsilon(\mathbf{k})\Lambda_\sigma(\mathbf{k}|i\omega_n)]\;[1-\varepsilon(-\mathbf{k})\Lambda_{-\sigma}(-\mathbf{k}|-i\omega_n)] + \varepsilon(\mathbf{k})\,\varepsilon(-\mathbf{k})\,Y_{\sigma,-\sigma}(\mathbf{k}|i\omega_n)\,\overline{Y}_{-\sigma,\sigma}(\mathbf{k}|i\omega_n), \tag{13}$$

$$\Lambda_\sigma(\mathbf{k}|i\omega_n) = \mathcal{G}_\sigma^{(0)}(i\omega_n) + Z_\sigma(\mathbf{k}|i\omega_n). \tag{14}$$

Equations (10)–(12) contain two superconducting irreducible contributions $Y_{\sigma,-\sigma}$ and $\overline{Y}_{-\sigma,\sigma}$, besides the function Z_σ which also exists in the normal state. The first two new quantities are the order parameters of the superconducting state, which describe the pairing correlations of electrons with opposite spins.

The three irreducible functions, Z_σ, $Y_{\sigma,-\sigma}$, and $\overline{Y}_{-\sigma,\sigma}$, stand for infinite sums of diagrams which contain irreducible many-particle Green's functions.

In order to obtain a closed set of equations, we will restrict ourselves to a class of rather simple diagrams which, however, contain the most important spin, charge, and pairing correlations.

The analytical structure of the equations behind the diagrams is of the following form,

$$Z(\mathbf{x}\sigma\tau|\mathbf{x}'\sigma'\tau') = -\delta_{\mathbf{x},\mathbf{x}'} \sum_{\substack{\mathbf{1,2}\\ \sigma_1,\sigma_2}} t(\mathbf{1}-\mathbf{x})\, t(\mathbf{x}-\mathbf{2}) \int_0^\beta \int_0^\beta d\tau_1 d\tau_2$$
$$\times\, \mathcal{G}_2^{(0)\,ir}(\sigma,\tau;\sigma_1,\tau_1|\sigma_2,\tau_2;\sigma',\tau')\; \mathcal{G}_{\sigma_2\sigma_1}(\mathbf{2}-\mathbf{1}|\tau_2-\tau_1), \qquad (15)$$

$$Y(\mathbf{x},\sigma,\tau|\mathbf{x}',-\sigma',\tau') = -\frac{\delta_{\mathbf{x},\mathbf{x}'}}{2} \sum_{\substack{\mathbf{1,2}\\ \sigma_1,\sigma_2}} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2\, t(\mathbf{x}-\mathbf{1}) t(\mathbf{x}-\mathbf{2})$$
$$\times\, \mathcal{G}_2^{(0)\,ir}(\sigma,\tau;-\sigma',\tau'|\sigma_1,\tau_1;-\sigma_2,\tau_2)\; \mathcal{F}_{\sigma_1,-\sigma_2}(\mathbf{1}-\mathbf{2}|\tau_1-\tau_2), \qquad (16)$$

where $\mathcal{G}_2^{(0)\,ir}(\sigma,\tau;-\sigma',\tau'|\sigma_1,\tau_1;-\sigma_2,\tau_2)$ is the simplest irreducible Green's function (for detailes see Ref. 24). The equation for $\overline{Y}_{-\sigma,\sigma}$ can be written down in analogy to the last one. If we Fourier transform the last two equations and consider only the spin-singlet channel of superconductivity, $\sigma' = \sigma$, we obtain,

$$Z_\sigma(i\omega) = -\frac{1}{\beta N} \sum_{\substack{\mathbf{k}\\ \omega_1,\sigma_1}} \varepsilon^2(\mathbf{k})\, \mathcal{G}_{\sigma_1}(\mathbf{k}|i\omega_1)\, \widetilde{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;\sigma_1,i\omega_1|\sigma_1,i\omega_1;\sigma,i\omega), \quad (17)$$

$$Y_{\sigma,-\sigma}(i\omega) = -\frac{1}{2\beta N} \sum_{\substack{\mathbf{k}\\ \omega_1,\sigma_1}} \varepsilon(\mathbf{k})\, \varepsilon(-\mathbf{k})\, \mathcal{F}_{\sigma_1,-\sigma_1}(\mathbf{k}|i\omega_1)$$
$$\times\, \widetilde{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;-\sigma,-i\omega|\sigma_1,i\omega_1;-\sigma_1,-i\omega_1). \quad (18)$$

From the equation for $Z_\sigma(i\omega)$ in (17) we can obtain an expression for $\Lambda_\sigma(i\omega)$,

$$\Lambda_\sigma(i\omega) = \mathcal{G}_\sigma^{(0)}(i\omega) - \frac{1}{\beta N} \sum_{\mathbf{k},\omega_1} \frac{\varepsilon^2(\mathbf{k})}{D_\sigma(\mathbf{k}|i\omega_1)} \Big[\Lambda_\sigma(i\omega_1)\big(1-\varepsilon(-\mathbf{k})\Lambda_{-\sigma}(-i\omega_1)\big)$$
$$-\,\varepsilon(\mathbf{k})\, Y_{\sigma-\sigma}(i\omega_1)\, \overline{Y}_{-\sigma\sigma}(i\omega_1)\Big] \widetilde{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;\sigma,i\omega_1|\sigma,i\omega_1;\sigma,i\omega)$$
$$-\,\frac{1}{\beta N} \sum_{\mathbf{k},\omega_1} \frac{\varepsilon^2(-\mathbf{k})}{D_\sigma(\mathbf{k}|i\omega_1)} \Big[\Lambda_{-\sigma}(-i\omega_1)\big(1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega_1)\big)$$
$$-\,\varepsilon(-\mathbf{k})\, Y_{\sigma,-\sigma}(i\omega_1)\, \overline{Y}_{-\sigma,-\sigma}(i\omega_1)\Big]$$
$$\times\, \widetilde{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;-\sigma,-i\omega_1|-\sigma,-i\omega_1;\sigma,i\omega). \quad (19)$$

The equations (18) and (19) together with ones for the one- and two-particle irreducible Green's functions determine completely the properties of the normal and the superconducting phases. But in spite of the approximations involved, this system of equations is rather complicated and numerical solutions have not yet been obtained so far. These equations have to be completed by the definition of the chemical potential μ of the system:

$$\frac{1}{\beta} \sum_{\substack{\mathbf{k} \\ \omega_n, \sigma}} \mathcal{G}_\sigma(\mathbf{k}|i\omega_n)\, e^{i\omega_n o^+} = N_e, \tag{20}$$

where N_e is the electron number.

Some analytical solutions of these equations are accessible in the case when the electron number is equal to the lattice sites number $N (N_e = N)$. In this case of half-filling, the chemical potential is known: $\mu = U/2$, and the antisymmetry property

$$\begin{aligned} \mathcal{G}_\sigma(\mathbf{k}| - i\omega_n) &= -\mathcal{G}_\sigma(\mathbf{k}|i\omega_n), \\ \Lambda_\sigma(\mathbf{k}| - i\omega_n) &= -\Lambda_\sigma(\mathbf{k}|i\omega_n) \end{aligned} \tag{21}$$

of Green's function exists. This last property permits us to simplify considerably our equations (18) and (19). In the normal state, in this special case of half-filling, the $\Lambda_\sigma(i\omega)$ equation has the form $(\mu = U/2)$:

$$\Lambda_\sigma(i\omega_n) = -\frac{i\omega_n}{\omega_n^2 + \mu^2} + \frac{3\mu^2}{(\omega_n^2 + \mu^2)^2}\ \phi_\sigma(i\omega_n), \tag{22}$$

where

$$\phi_\sigma(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon^2(\mathbf{k})\, \Lambda_\sigma(i\omega_n)}{1 - \varepsilon(\mathbf{k})\, \Lambda_\sigma(i\omega_n)}. \tag{23}$$

These equations have the same form as the analogous equations of [12] and differ from them by the factor 3 in the second term of the right-hand side of (22). The nature of this factor is explained by the fact that the contribution to $Z(i\omega_n)$ of the irreducible Green's function $\widetilde{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; \sigma_1, i\omega_1|\sigma_1, i\omega_1; \sigma, i\omega)$ with opposite spins $(\sigma_1 = -\sigma)$ is twice that of the function with parallel spins $(\sigma_1 = \sigma)$. Allowance for only the latter would give a factor unity. The sum in equation (23) can be evaluated by using the relation:

$$\frac{1}{N} \sum_{\mathbf{k}} f(\varepsilon(\mathbf{k})) = \int_{-W/2}^{W/2} \rho_0(\varepsilon)\ d\varepsilon\ f(\varepsilon),$$

where for the bare density of electron states of energy band $\rho_0(\varepsilon)$ we used the Hubbard [8] form

$$\rho_0(\varepsilon) = \frac{4}{\pi W} \sqrt{1 - \frac{4\varepsilon^2}{W^2}} \ \theta\left(\frac{W}{2} - |\varepsilon|\right).$$

Here W is the band width and θ is the step function. By using the result of such summation [12] we obtain:

$$\begin{aligned} \phi(i\omega_n) &= \frac{W}{2} \frac{\lambda(i\omega_n)}{\left[1 + \sqrt{1 - \lambda^2(i\omega_n)}\right]^2}, \\ \lambda(i\omega_n) &= \frac{W}{2} \Lambda(i\omega_n). \end{aligned} \tag{24}$$

Now we can find the renormalized density of electron states $\rho(E)$ which is equal to

$$\begin{aligned} \rho_0(E) &= -\frac{1}{\pi N} \ Im \sum_{\mathbf{k}} \mathcal{G}_\sigma(\mathbf{k}|E + i\delta) = \\ &= -\frac{4}{\pi W} \ Im \frac{1 - \sqrt{1 - \lambda^2(E + i\delta)}}{\lambda(E + i\delta)}. \end{aligned} \tag{25}$$

From (25) and previous equations we can see that the quantity $\rho(E = 0)$ is not zero if Coulomb interaction is less than the value $\sqrt{3}W/2$ and is zero when U is more than this value. There is critical value of Coulomb repulsion $U_c = \sqrt{3}W/2$ which determines the metal-insulator phase transition.

The influence of the strong coupling electron-phonon interactions on this criterion has been investigated by us in paper [24]. We have examined this influence by investigating the Hubbard–Holstein model. The interactions of electron and phonons are assumed to be localized at the lattice sites arising from the interactions of fluctuations of electron density with optical phonons with bare frequency ω_0. The electron-phonon interactions constant g is considered by us as a large quantity. After applying the Lang–Firsov canonical transformation [25] we derive the polaron Hamiltonian of Hubbard type [24]. Now the polarons, i.e., the electrons dressed with displacements of the ions take part in the hopping process of delocalization. The number of phonons in phonon clouds is proportional to the square of interaction constant g and is considered as another large parameter of the theory. It was proved by us [24,26] that the phonon cloud surrounding the polaron has a collective mode of oscillation with frequency ω_c:

$$\omega_c = \alpha\omega_0, \qquad \alpha = \frac{1}{2} \left(\frac{g}{\omega_0}\right)^2.$$

The chemical potential of polarons $\widetilde{\mu}$ and their on-site interactions $\widetilde{U}$ are considerably renormalized by electron-phonon interaction in comparison with their initial values:

$$\widetilde{\mu} = \mu + \alpha\hbar\omega_0, \qquad \widetilde{U} = U - 2\alpha\hbar\omega_0.$$

Thanks the presence of phonon clouds and their oscillation the electron quantum transitions between ion energy levels are accompanied by emission and absorption of the energy of collective mode $\hbar\omega_c$ and as the consequence the essential renormalization of local one-particle and irreducible two-particle Green's functions takes place.

It has turned out that in the presence of strong electron-phonon interaction which preserve the repulsion character of the renormalized quantity $\widetilde{U} > 0$ the phase transition between metal and insulator takes place at the same critical value U_c as for electron system. In this case the superconducting state is not realized.

But in the case when the attraction between electrons mediated by phonons surpass their Coulomb repulsion and $\widetilde{U}$ is negative ($\widetilde{U} < 0$), the superconducting phase is admitted and the condition of realization of the phase transitions between normal and superconducting metal and between insulator and superconducting state have been established.

4. CONCLUSIONS

1. A new diagrammatic approach has been elaborated for strongly correlated electron systems the main elements of which are the many-particle on-site irreducible Green's functions, which contain the main charge and spin fluctuations of the system.

2. The new correlation function $Z(\mathbf{x}, \mathbf{x}')$ which is a sum of strong coupled irreducible diagrams has been introduced and the Dyson equation for renormalized one-particle Green's function established.

3. The summing of a special class of diagrams permits us to take into account the most essential charge and spin correlations and as a consequence to obtain the close equation for determining the Z-correlation function.

4. The generalization of this diagram approach for electron-phonon system with strong interaction between them has been realized. The existence of collective mode of phonon clouds surrounding polarons has been proved and the influence of the absorption and emission of that frequency during the polaron quantum transition has been investigated.

5. The Mott–Hubbard phase transition has been investigated and was proved that critical value of Coulomb repulsion at which this transition takes place is equal to

$$U_c = \frac{\sqrt{3}}{2}\, W.$$

This result remains true when instead of the electrons the polarons take part in the delocalization process but the renormalized interaction $\widetilde{U}$ remains repulsive.

6. In the case when the attraction of electrons mediate by phonon surpass on-site repulsion, the system can be in three states insulator, normal metal and superconductor.

7. The diagrammatic method permits its generalization to discuss the models with several electron subsystems as three-band Hubbard model [8] and periodic Anderson model.

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