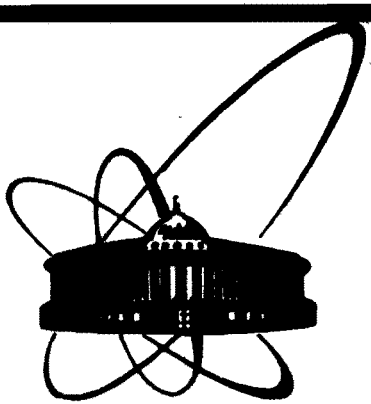

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ON THE THEORY OF DISORDERED SYSTEMS. SPECTRA OF QUASI-PARTICLES

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1. INTRODUCTION

Quite a number of works are devoted to the investigation of the spectral characteristics of disordered systems (for example, alloys)[1-3]. The various methods to calculate the averaged over all the configurations alloy Green function of the system were developed. At the same time the efforts were made to generalize the coherent potential approximation. However available generalizations on the clusters of two or more impurities are not quite satisfactory[1,2]. It should be noted also, that the most of results are obtained in not very realistic tight-bond model[2,3].

A new approach for the investigation of the disordered system spectra based on using projection operator technique (see,e.g.,[4]) is developed in this work. Advantages of this approach involve the fact that the projected (averaged) Green function of the system contains explicitly the self energy (mass operator) expressed through the Hamiltonian of the system.

The explicit expansion into a power series of interaction for the self energy, in which multiple occupancy corrections[1] are taken into account automatically, is obtained. The structure of the series obtained distincts from the cumulant expansion and does not result in false poles when this series is summed up partially. To avoid these false poles the complicated self-consistent procedure is usually used[5]. For the tight-bond model the series obtained is easily summed up in single site, pair, etc., approximations.

The electrons interacting by means of arbitrary potential with the chaotically distributed scattering centres are also considered with the aid of the obtained explicit expansion for the mass operator. In this case the closed systems of equations for the determination of the spectra are obtained taking into account the single-center and pair scatterings in both the unrenormalized and renormalized representations.

2. PROJECTION FORMALISM

We shall consider the system described by the Hamiltonian H, in which excitations are not interacting. Let us introduce the Green function for such a system

$$G(\lambda) = \frac{1}{\lambda - H},$$

which determines both the spectrum and density of state of the excitations.

If H has the random variables, as it is in the disordered system, then the quantities observed are determined by the Green function averaged over various realizations of the random variables

$$\langle G(\lambda)\rangle = PG(\lambda)P = P\frac{1}{\lambda - H}P, \qquad (1)$$

where P is the corresponding averaging operator, and $P^2 = P$, i.e., the operator P is assumed to be projection one. It is easy to show /6/, that

$$PG(\lambda)P = [\lambda - PHP - M(\lambda)]^{-1}P;$$

$$M(\lambda) = PHQ\frac{1}{\lambda - QHQ}QHP; \quad Q = 1 - P.$$

We shall write the Hamiltonian H as

$$H = H_0 + V,$$

i.e., we split it into the translationally inveraint part H_0 and the part V, describing the disorder. Taking into account that $PH_0Q = QH_0P = 0$, we obtain

$$\langle G(\lambda)\rangle = \frac{1}{\lambda - H_0 - \langle V\rangle - M(\lambda)}; \quad M(\lambda) = PV\frac{1}{\lambda - H_0 - QV}QVP. \qquad (2)$$

It is convenient to split the Hamiltonian into H_0 and V by the introduced projection operator

$$H = (P + Q)H = \langle H\rangle + H - \langle H\rangle.$$

Then

$$H_0 = \langle H\rangle; \quad V = H - \langle H\rangle \qquad \langle V\rangle = 0. \qquad (3)$$

Neglecting the self energy (mass operator) $M(\lambda)$ in (2) and using (3), we obtain the virtual crystal approximation

$$\langle G(\lambda)\rangle \approx G^0 = \frac{1}{\lambda - \langle H\rangle}.$$

The matrix elements of the operator $\langle G(\lambda)\rangle$ may be obtained from the system of equations

$$\sum_{n_1}[\lambda - \langle H\rangle - M(\lambda)]_{nn_1}[\langle G(\lambda)\rangle]_{n_1n'} = \delta_{nn'}, \qquad (4)$$

where, the indexes n determine the quantum numbers of selected representation. For example, all averaged values in quasimomentum representation are diagonal and Eq.(4) is reduced to

$$G(\lambda, \vec{g}) = \frac{1}{\lambda - \lambda(\vec{g}) - M(\lambda, \vec{g})}, \qquad (5)$$

where, $G(\lambda, \vec{g}) = [\langle G(\lambda)\rangle]_{\vec{g}\vec{g}}$, $M(\lambda, \vec{g}) = [M(\lambda)]_{\vec{g}\vec{g}}$, $\lambda(\vec{g})$ is the excitation spectrum in virtual crystal. We emphasize, that Eq.(2) determines the explicit expansion of the mass operator, which may be used to calculate $M(\lambda)$ in any approximation. In this technique there are no problems as to consideration of kinematic corrections associated with constrains on the summation indexes, as it takes place when the series in V for the Green function (1) is partially summing up /1/. By using the expansion (2) in V the multiple occupancy corrections are taken into account automatically. It will be seen subsequently. The expansion (2) in V is of the form

$$M(\lambda) = \sum_{n=1}^{\infty} PV\left[\frac{1}{\lambda - \langle H\rangle}QV\right]^n P, \qquad (6)$$

where Eqs.(3) are used and, therefore, $QVP = VP$. It should be noted, that the expansion (6) is of different structure as compared with cumulant one, which is unconvenient, as it has been emphasized already.

3. DIAGONAL DISORDER IN THE TIGHT-BOND MODEL

We shall consider a conventional problem of the tight-bond method, when the Hamiltonian for the site representation is of the form

$$H_{\vec{\ell}\vec{\ell}'} = \epsilon_{\vec{\ell}}\,\delta_{\vec{\ell}\vec{\ell}'} + W_{\vec{\ell}\vec{\ell}'},$$

where, $\epsilon_{\vec{\ell}}$ is the energy in the lattice site $\vec{\ell}$, $W_{\vec{\ell}\vec{\ell}'}$ are the overlap integrals between the various cells of crystal each being the random function of the lattice site. Taking the Hamiltonian of virtual crystal

$$H_{0\,\vec{\ell}\vec{\ell}'} = \langle H_{\vec{\ell}\vec{\ell}'}\rangle = \langle\epsilon_{\vec{\ell}}\rangle\,\delta_{\vec{\ell}\vec{\ell}'} + \langle W_{\vec{\ell}\vec{\ell}'}\rangle$$

depending upon the difference $\vec{\ell} - \vec{\ell}'$ only, we obtain for perturbation

$$V_{\vec{\ell}\vec{\ell}'} = (\epsilon_{\vec{\ell}} - \langle\epsilon_{\vec{\ell}}\rangle)\,\delta_{\vec{\ell}\vec{\ell}'} + W_{\vec{\ell}\vec{\ell}'} - \langle W_{\vec{\ell}\vec{\ell}'}\rangle.$$

We shall consider now the diagonal disorder and take as perturbation

$$V_{\vec{\ell}\vec{\ell}'} = (\epsilon_{\vec{\ell}} - \langle \epsilon_{\vec{\ell}} \rangle)\,\delta_{\vec{\ell}\vec{\ell}'} = v_{\vec{\ell}}\,\delta_{\vec{\ell}\vec{\ell}'}$$

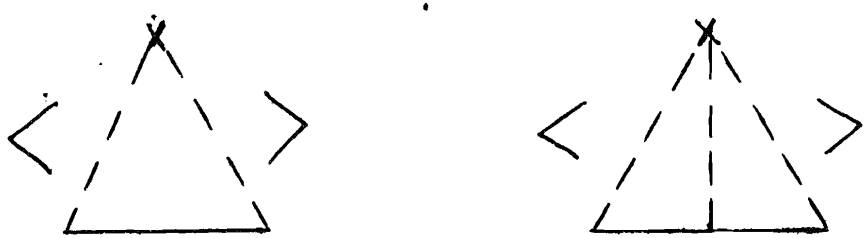
We assume for simplicity that the values of $v_{\vec{\ell}}$ are not correlated on the various sites, i.e.,

$$\langle v_{\vec{\ell}}\, v_{\vec{\ell}'} \rangle = \langle v_{\vec{\ell}} \rangle \langle v_{\vec{\ell}'} \rangle = 0 \qquad (\vec{\ell} \neq \vec{\ell}') \tag{7}$$

We shall describe expansion (6) for the mass operator in the site representation by the usual diagram technique. Then for the second order of the perturbation theory we have the diagram (a), shown in Fig. 1, where the propagator of virtual crystal $G^0(\vec{\ell}-\vec{\ell}') = \left(\frac{1}{\lambda - \langle H \rangle}\right)_{\vec{\ell}\vec{\ell}'}$ is designated by a solid line but single site scattering being a cross with one dotted line (it correcponds to $v_{\vec{\ell}}$). Due to conditions (7) and $\langle V \rangle = 0$ the dotted lines for the various sites are closed. The analytical expression corresponding to this diagram is as follows

$$M^{(2)}_{\vec{\ell}\vec{\ell}'}(\lambda) = \langle v^2_{\vec{\ell}} \rangle\, G^0(0)\, \delta_{\vec{\ell}\vec{\ell}'} .$$

For the third order of the perturbation theory there is also one term, which is described by the diagram (b) in Fig. 1.



(a) (b)

Fig. 1.

The appropriate analytical expression is of the form

$$M^{(3)}_{\vec{\ell}\vec{\ell}'}(\lambda) = \langle v^3_{\vec{\ell}} \rangle\, [G^0(0)]^2\, \delta_{\vec{\ell}\vec{\ell}'} .$$

For the third term of expansion (6) (the fourth order of the perturbation theory) we have the diagrams, shown in Fig. 2. The first two diagrams are the skeleton ones, the third diagram may be included in the bare Green function as renormalization and the fourth diagram describes a multiple occupancy correction (the line above connects the diagram parts, which correspond the same site). The last diagram, shown in Fig. 2,

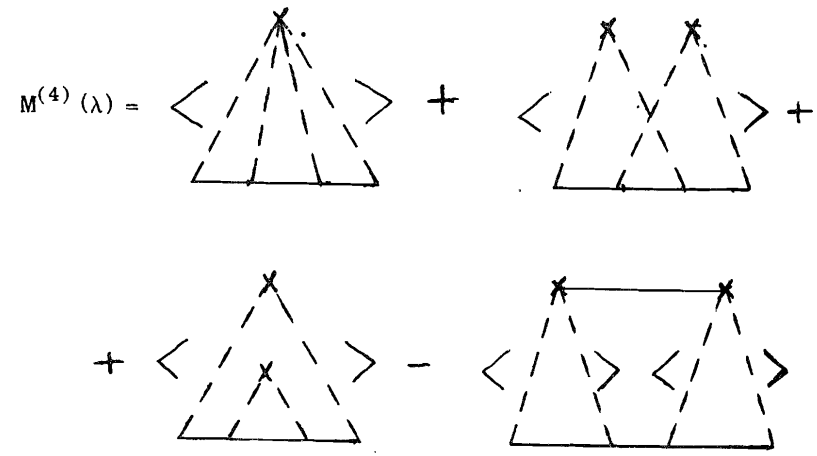


Fig. 2.

is described by the expression

$$\langle v^2_{\vec{\ell}} \rangle\, [G^0(0)]^3 \langle v^2_{\vec{\ell}} \rangle .$$

We should note, that all the presented diagrams are irreducible (the reducible diagrams are canceled).

It may be shown, that the structure of the term of expansion for the mass operator (6) in the n-th order perturbation theory is of the following symbolic form

$$\begin{aligned} M^{(n)}_{\vec{\ell}\vec{\ell}'}(\lambda) = [\,\langle n \rangle &- \sum_{i+j=n} \overline{\langle i \rangle \langle j \rangle} - \sum_{i+j+k=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle} - \\ &- \sum_{i+j+k+m=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle} - \ldots + \sum_{i+j+k=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle} + \\ &+ \sum_{i+j+k+m=n} \left(\overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle} + \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle} \right) + \ldots \\ &+ \sum_{i+j+k+m=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle} + \sum_{i+j+k+m+p=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle \langle p \rangle} + \ldots \\ &- \sum_{i+j+k+m=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle} - \sum_{i+j+k+m+p=n} \overline{\langle i \rangle \langle j \rangle \langle k \rangle \langle m \rangle \langle p \rangle} - \ldots \\ &+ \ldots\,]_{\vec{\ell}\vec{\ell}'} ; \quad \langle 0 \rangle = 0; \quad \langle 1 \rangle = 0. \end{aligned} \tag{8}$$

Here $\langle n \rangle$ denotes a sum of the all averaged irreducible diagrams without coupling lines on top in the n-th order perturbation theory (for example, the first three diagrams, shown in

Fig. 2, corresponding to the fourth order). For diagrams with more than two crosses (the various sites) a summation over indexes of the sites, not coinciding with $\vec{\ell}$, $\vec{\ell}'$, is implied. The remaining terms in (8) describe the multiple occupancy correction diagrams (as the last diagram, shown in Fig. 2). These diagrams are irreducible also. The coupling line ⌐¬ connects any two crosses of various irreducible diagrams $\langle i \rangle$ and $\langle j \rangle$, making these crosses corresponding to the same site. The remaining (uncoupling) sites in $\langle i \rangle$ and $\langle j \rangle$ distinct from coupling ones. The symbol $\langle i \rangle\langle j \rangle$ denotes a sum of all the possible couplings of two crosses. The lines ⌐¬⌐¬, ⌐⌐¬¬,... denote the coupling of three, four crosses, etc. for various $\langle i \rangle$. The solid lines below denote the bare Green function $G^0(\vec{\ell}_1 - \vec{\ell}_2)$ binding diagrams $\langle i \rangle$. The lines, coupling the even number of crosses, attach negative sign for the diagram, but the lines, coupling the odd number of crosses, attach positive one. The definite sign of the diagram is determined by all the coupling lines appearing in this diagram. The correction diagrams do not involve the $\langle i \rangle\langle j \rangle\langle k \rangle\langle m \rangle$ - type diagrams, in which the inner propagator is renormalized by the diagrams being absent in V-expansion for the averaged Green function $[\langle G(\lambda) \rangle]_{\vec{\ell}\vec{\ell}'}$. Taking into account the above V-mentioned we describe $M^{(n)}_{\vec{\ell}\vec{\ell}'}(\lambda)$ as follows

$$M^{(n)}_{\vec{\ell}\vec{\ell}'}(\lambda) = \{ \langle n \rangle + \sum_{\substack{i,j,\ldots,k=2 \\ (i+j+\ldots+k=n)}}^{n-2} [\langle i \rangle\langle j \rangle \ldots \langle k \rangle]_c \}_{\vec{\ell}\vec{\ell}'} . \qquad (9)$$

Here, $[\langle i \rangle\langle j \rangle \ldots \langle k \rangle]_c$ denotes any couplings in the diagram $\langle i \rangle\langle j \rangle \ldots \langle k \rangle$ (accounting a sign). For these diagrams the number of the factors and the number of the correction diagrams in the n-th order as well is determined by a condition i+j+...+k=n (for example, at n=4 i=j=2 we have one correction diagram - $\langle 2 \rangle\langle 2 \rangle$, i.e., the last diagram shown in Fig. 2).

So, the self energy involves the correction terms describing the multiple occupancy corrections besides the irreducible diagrams $\langle n \rangle$ (the first term in Eq(9)). These kinematic corrections are obtained here by means of direct calculation automatically and they have the structure being appropriate for the partial summation of the series (6) as will be seen below. Let us sum, for example, all the single site nonrenormalized graphs. It is easily seen from (9), that in this approximation the mass operator

$$M_{\vec{\ell}\vec{\ell}'}(\lambda) = \sum_{n=2}^{\infty} M^{(n)}_{\vec{\ell}\vec{\ell}'}(\lambda) \qquad (10)$$

has a form as shown in Fig. 3.

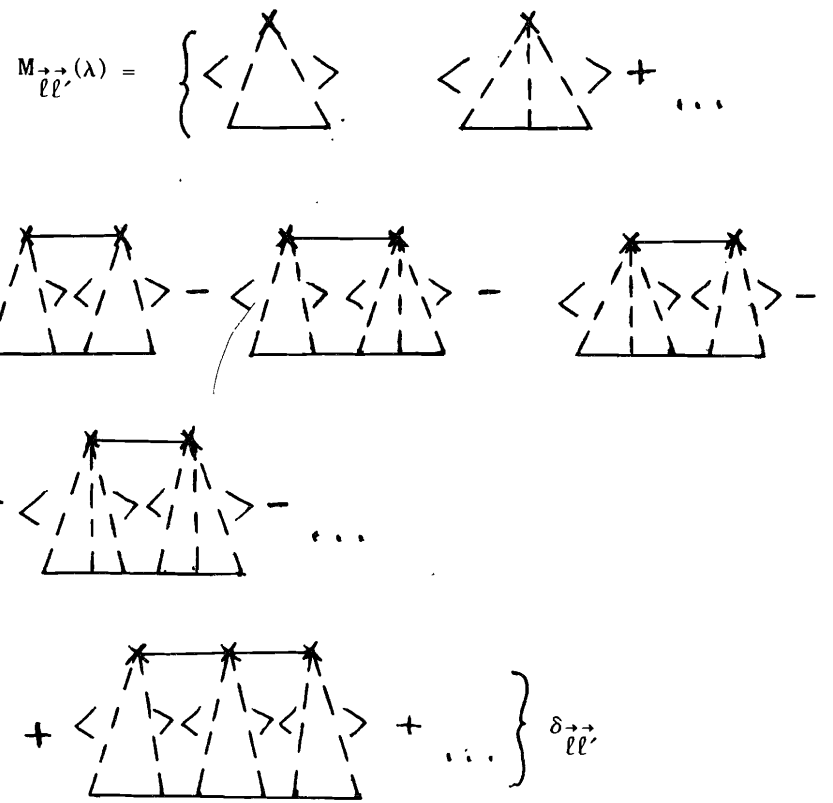


Fig. 3.

Summing these graphs we obtain

$$M_{\vec{\ell}\vec{\ell}'}(\lambda) = \{ \langle t_1 \rangle - \langle t_1 \rangle G^0(0) \langle t_1 \rangle + \langle t_1 \rangle G^0(0) \langle t_1 \rangle G^0(0) \langle t_1 \rangle - \ldots \}\delta_{\vec{\ell}\vec{\ell}'} = \frac{\langle t_1 \rangle}{1 + G^0(0) \langle t_1 \rangle} \delta_{\vec{\ell}\vec{\ell}'} . \qquad (11)$$

Here, $\langle t_1 \rangle$ is averaged t_1-matrix, describing single site scattering (Fig. 4).

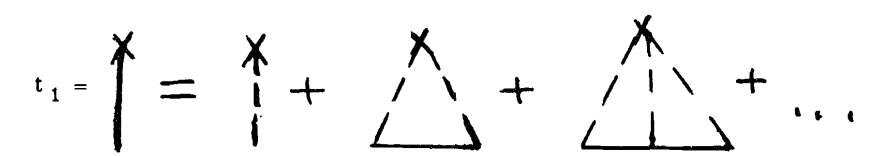


Fig. 4.

The result, given by Eq.(11), is the known averaged t-matrix approximation for the mass operator [1,2]. For two-component disordered alloy A-B with the concentration of the component A being equal to c

$$\langle t_1 \rangle = \frac{c v_A}{1 - v_A G^0(0)} + \frac{(1-c) v_B}{1 - v_B G^0(0)}; \quad v_i = \epsilon_i - \langle \epsilon \rangle; \quad \langle \epsilon \rangle \equiv \langle \epsilon_\ell \rangle \qquad i = A, B.$$

Substituting this expression for $\langle t_1 \rangle$ in (11) we obtain the averaged t-matrix approximation for the mass operator in the case of disordered alloy.

It is easy to sum all the single site graphs in Eq.(10) (see (8)) taking into account the graphs renormalizing the inner propagators $G^0(0)$. In this single site approximation in Eqs.(9) and (10) the graphs, given in Fig. 5, are summed. The corresponding analytic expression is of the form

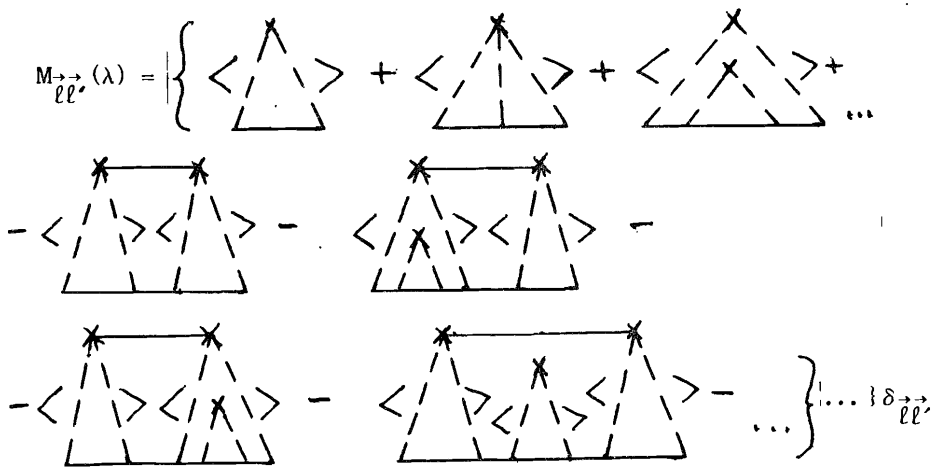


Fig. 5.

$$M_{\vec{\ell}\vec{\ell}'}(\lambda) = \{ \langle \tilde{t}_1 \rangle - \langle \tilde{t}_1 \rangle G'(0) \langle \tilde{t}_1 \rangle + \ldots \} \delta_{\vec{\ell}\vec{\ell}'} = \frac{\langle \tilde{t}_1 \rangle}{1 + G'(0) \langle \tilde{t}_1 \rangle} \delta_{\vec{\ell}\vec{\ell}'} \quad (12)$$

Here, $\langle \tilde{t}_1 \rangle$ is determined by a sum of the graphs given in Fig.6, where the double line $=$ denotes the function $G'(0)$, i.e., the Green function of the system $[\langle \frac{1}{\lambda - H} \rangle]_{\vec{\ell}\vec{\ell}}$, in which all the scattering processes are taken into account besides the scattering on the fixed site $\vec{\ell}$.

The expression (12) for $M(\lambda)$ corresponds to coherent potential approximation [1-3]. In the case of two-component disordered

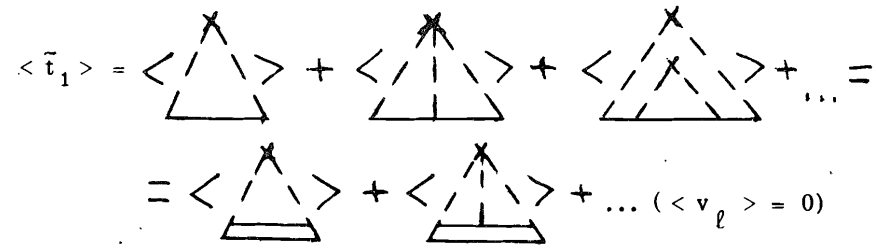


Fig. 6.

alloys A-B considered above this expression may be written more usual as

$$M(\lambda) = \frac{c\Delta}{1 - (\Delta - M(\lambda)) G(0)}; \quad \Delta = \epsilon_A - \epsilon_B; \quad G(0) = [\langle G(\lambda) \rangle]_{\vec{\ell}\vec{\ell}}.$$

We shall consider now pair diagrams (which describe pair-defects scattering) as well as single ones for all the orders of expansion in V. Firstly, we take into account the unrenormalized diagrams only, i.e., the diagrams involving the functions $G^0(\vec{\ell}_1 - \vec{\ell}_2)$ as the inner propagator. Then in order to take into account all the single and pair diagrams in (10), the unrenormalized single and pair graphs are to sum in all $\langle n \rangle, \langle i \rangle, \langle j \rangle \ldots$ from (8). It is easily seen, that the sum of these graphs involving in $\langle n \rangle$, for all the orders of expansion (6) gives the result

$$\sum_{n=2}^{\infty}{}^{(1,2)} \langle n \rangle_{\vec{\ell}\vec{\ell}'} = \langle t_1 \rangle \delta_{\vec{\ell}\vec{\ell}'} + \langle \bar{t}_2 \rangle_{\vec{\ell}\vec{\ell}'}. \quad (13)$$

Here, $\Sigma^{(1,2)}$ denotes the summation over the unrenormalized single and pair graphs, t_1 is the single site scattering matrix (Fig. 4), t_2 is the irreducible part of the two site scattering matrix t_2 (Fig. 7), which is obtained by substracting of the

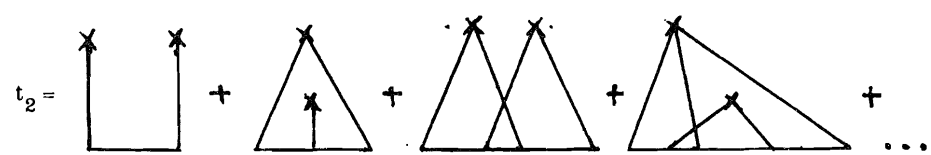


Fig. 7.

first term from t_2 (the first diagram on Fig. 7). For the part (i,j) sites, being at a distance $\vec{R} = \vec{i} - \vec{j}$, t_2 may be described as follows

$$t_2^{ij} = t_1^i G^o(R) t_1^j + t_1^j G^o(R) t_1^i + \\ + t_1^i G^o(R) t_1^j G^o(R) t_1^i + t_1^j G^o(R) t_1^i G^o(R) t_1^j + \ldots \quad (14)$$

where, t_1^i is the scattering t_1-matrix for the site i. So, for the part (i,j) t_2 may be written as the matrix

$$t_2 = \begin{pmatrix} t_2^{ii} & t_2^{ij} \\ t_2^{ji} & t_2^{jj} \end{pmatrix}, \quad (15)$$

in which the diagonal terms are determined by even in $G^o(\vec{R})$ terms of analytic expression (14), but the off-diagonal ones being odd in $G^o(\vec{R})$ terms of (14).

The reducible part of $<t_2>$ provides no contribution into (13), as it is canceled with the appropriate diagrams due to the operator Q in expression (6), that results in the diagrams given in expression (8) (see, for example, Fig.2). As to the correction (coupled) diagrams (8) (arising also due to projection operator Q in (6)) those diagrams having one or two coupling lines are to sum over all the orders of perturbation theory. In considered unrenormalized representation all $<n>$ (having no more than 2 crosses) are coupled.

In order to obtain, for example, the averaged t-matrix approximation for impurity pair scattering /1,2/ corresponding to independent scattering by each pair those diagrams for the mass operator from mentioned above are to take into account, in which the number of sites (crosses) are fixed by the values of pair sites for which the matrix element $M_{ij}(\lambda)$ is calculated. It is easily seen, that the sum of such diagrams gives the following result

$$M_{ij}(\lambda) = M(\vec{R}) = \sum_n^{(1,2)} \bar{M}_{ij}^{(n)} = <t_1 + t_2> - <t_1 + t_2>(G^o(0) + P_2(\vec{R}))\times -$$

$$\times <t_1 + t_2> + <t_1 + t_2>(G^o(0) + P_2(\vec{R}))<t_1 + t_2>(G^o(0) + P_2(\vec{R})) \times \quad (16)$$

$$\times <t_1 + t_2> - \ldots = \frac{<t_1 + t_2>}{1 + (G^o(0) + P_2(\vec{R}))<t_1 + t_2>}.$$

Here, $\bar{M}_{ij}^{(n)}$ denotes the diagrams with fixed site numbers (i,j), t_2 is the matrix (15), $P_2(\vec{R})$ denotes the matrix

$$P_2(\vec{R}) = \begin{pmatrix} 0 & G^o(\vec{R}) \\ G^o(\vec{R}) & 0 \end{pmatrix}.$$

So, expression (16) for M is the matrix (2x2) with diagonal matrix elements (even in $P_2(\vec{R})$) and with off-diagonal ones (odd

in $P_2(\vec{R})$). Expression (16) follows from (8), taking of the mentioned fact, that reducible diagrams in t_2 are canceled. For disordered binary alloy expression (16) is transformed into the known form

$$M(\vec{R}) = \frac{c t_1 + c^2 t_2}{1 + [G^o(0) + P_2(\vec{R})](c t_1 + c^2 t_2)}.$$

Here, t_2 (15) may be described as

$$t_2 = \frac{t_1^2 P_2(\vec{R})}{1 - t_1 P_2(\vec{R})},$$

being in the same agreement with respect to both the diagonal and off-diagonal matrix elements, as in (16).

In the case of pair defects we shall generalize now the coherent potential approximation (12). For this purpose the inner propagators involved in the graphs summed in (16) are to be renormalized by adding the same graphs from (8) (having the same fixed outer sites) but with $<n>$ stringed on the inner propagators. It results in the fact, that the diagrams describing pair scattering are renormalized by using instead of the propagator G^o the full propagator, in which the scattering by considered pair is excluded. In the matrix representation the result for disordered alloy may be described as follows /5/

$$M(\vec{R}) = \frac{r_2(\Gamma')}{1 + \Gamma' r_2(\Gamma')};$$

$$r_2(\Gamma') = c r(\Gamma_d') + \frac{c^2 r^2(\Gamma_d')\Gamma_n'}{1 - r(\Gamma_d')\Gamma_n'};$$

$$r(\Gamma_d') = \frac{\Delta}{1 - \Gamma_d' \Delta}.$$

The second-order matrix Γ' is determined analogously to the expression for $G'(0)$ in the single site self-consistent approximation /1,5/

$$\Gamma' = \frac{<G(\lambda)>}{1 + M(\lambda)<G(\lambda)>}, \qquad \Gamma' = \Gamma_d' + \Gamma_n',$$

where, $<G(\lambda)>$, $M(\lambda)$ are the second-order matrix too, Γ_d', Γ_n' are the diagonal and off-diagonal parts of Γ', respectively,

The consideration carried out is easily generalized on the clusters comprising the arbitrary numbers of the impurity centers.

4. ELECTRON SPECTRUM IN ARBITRARY STOCHASTIC POTENTIAL

We consider the model in which electrons, interacting with the random field of N_i impurity centres, are described by the Hamiltonian

$$H = H^0 + H'; \quad H^0 = \frac{\vec{p}^{\,2}}{2m}; \quad H' = \sum_{\ell=1}^{N_i} \phi_\ell = \sum_{\ell=1}^{N_i} \phi(\vec{r} - \vec{r}_\ell). \tag{17}$$

Here, $\vec{p}$ and m are the momentum and mass of the electron, respectively, $\phi(\vec{r} - \vec{r}_\ell)$ is the interaction energy of the electron being in $\vec{r}$-point with the impurity center ℓ ($\vec{r}_\ell$ is the radius-vector of impurity center ℓ). The self energy for electrons we shall calculate in self representation of H^0. The eigenvalues and eigenfunctions of H^0 are

$$\epsilon^0_{\vec{k}} = \frac{\vec{k}^{\,2}}{2m}, \quad |\vec{k}> = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{\Omega}}, \quad (h = 1),$$

where, Ω is the volume of the system under consideration. In this representation the matrix element of interaction is of the form

$$H'_{\vec{k}\vec{k}'} = \sum_\ell (\phi_\ell)_{\vec{k}\vec{k}'}; \quad (\phi_\ell)_{\vec{k}\vec{k}'} = \frac{1}{\Omega} e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell} \phi_{\vec{k}\vec{k}'}; \quad \phi_{\vec{k}\vec{k}'} = \int e^{-i(\vec{k}-\vec{k}')\vec{r}} \phi(\vec{r})\, d\vec{r}. \tag{18}$$

Here, $\phi_{\vec{k}\vec{k}'}$ is the matrix element of the scattering center potential being in the origin of coordinates. Integration in $\vec{r}$ is carried out over the whole space, as it is assumed for simplicity, that the potential ϕ has a finite range of action.

In this case we determine impurity centers configuration averaging P of the quantity A, which depends on the impurity coordinates, as follows

$$PA = <A> = \int_\Omega \cdots \int_\Omega \frac{d\vec{r}_1}{\Omega} \cdots \frac{d\vec{r}_{N_i}}{\Omega} A(\vec{r}_1, \ldots, \vec{r}_{N_i}). \tag{19}$$

i.e., the correlation in the scattering centers positions is simply neglected.

It is easy to obtain the average value of the interaction Hamiltonian

$$<H'> = H'_{\vec{k}\vec{k}} = c'\phi_{\vec{k}\vec{k}}; \qquad c' = \frac{N_i}{\Omega}.$$

As is seen from Eq.(18) $\phi_{\vec{k}\vec{k}} = \int \phi(\vec{r})\, d\vec{r}$ does not depend on $\vec{k}$. Splitting as before the Hamiltonian of the system (17) on $H_0 = <H>$ and $V = H - <H>$ we see, that $<H'>$ shifts the energy levels of the electron $\epsilon^0_{\vec{k}}$ by $c'\phi_{\vec{k}\vec{k}}$ which is finite at finite impurity centers concentration and does not depend on $\vec{k}$. It is convenient for us to exclude this constant shift by changing zero energy, level and assuming, that $H'_{\vec{k}\vec{k}} = 0$.

Taking into account that $<H'_{\vec{k}\vec{k}'}> = 0$ now, we consider the expansion for $M(\lambda, \vec{k})$ in $H'_{\vec{k}\vec{k}_1}$. It is easily shown by means of Eqs.(6), (18), (19), that the first term of the expansion of $M(\lambda, \vec{k})$ is equal to

$$\sum_{\vec{k}_1} <H'_{\vec{k}\vec{k}_1} \frac{1}{\lambda - \epsilon^0_{\vec{k}_1}} H'_{\vec{k}_1\vec{k}}> = \frac{1}{\Omega^2} \sum_{\vec{k}_1} <\sum_{\ell\ell_1} \exp[-i(\vec{k}-\vec{k}_1)(\vec{r}_\ell - \vec{r}_{\ell_1})]> \times$$

$$\times \phi_{\vec{k}\vec{k}_1} \frac{1}{\lambda - \epsilon^0_{\vec{k}_1}} \phi_{\vec{k}_1\vec{k}} = \frac{N_i}{\Omega^2} \sum_{\vec{k}_1} \phi_{\vec{k}\vec{k}_1} \frac{1}{\lambda - \epsilon^0_{\vec{k}_1}} \phi_{\vec{k}_1\vec{k}}. \tag{20}$$

It is seen, that this term of the expansion for $M(\lambda, \vec{k})$ is nonvanishing only, if $\vec{r}_\ell = \vec{r}_{\ell_1}$ (as $\phi_{\vec{k}\vec{k}} = 0$), i.e., it describes electron scattering by each impurity center independently. Eq.(20) may be compared with the diagram (a), shown in Fig. 8 which ver-

(a) (b)

Fig. 8.

tex corresponds to $\frac{1}{\Omega}\phi_{\vec{k}\vec{k}_1}$ (the momentum $\vec{k}$ passes to $\vec{k}_1$). The bare propagator $\frac{1}{\lambda - \epsilon^0_{\vec{k}_1}}$ is shown by a solid line with the vector $\vec{k}_1$ and single impurity scattering being a dotted line with a cross. To obtain the analytic expression by means of such a diagram we should make also the summation with respect to all the inner momenta ($\vec{k}_1 \neq \vec{k}$) and impurity centers positions as well.

The different terms of expansion (6) for $M(\lambda, \vec{k})$ will be also nonzero provided that no less than 2 impurity coordinates

coincide. So, the third-order term in H′ is proportional to c′ and shown in Fig. 8 as the diagram (b). The fourth-order term is shown in Fig. 9. These diagrams correspond to the following analytic expression

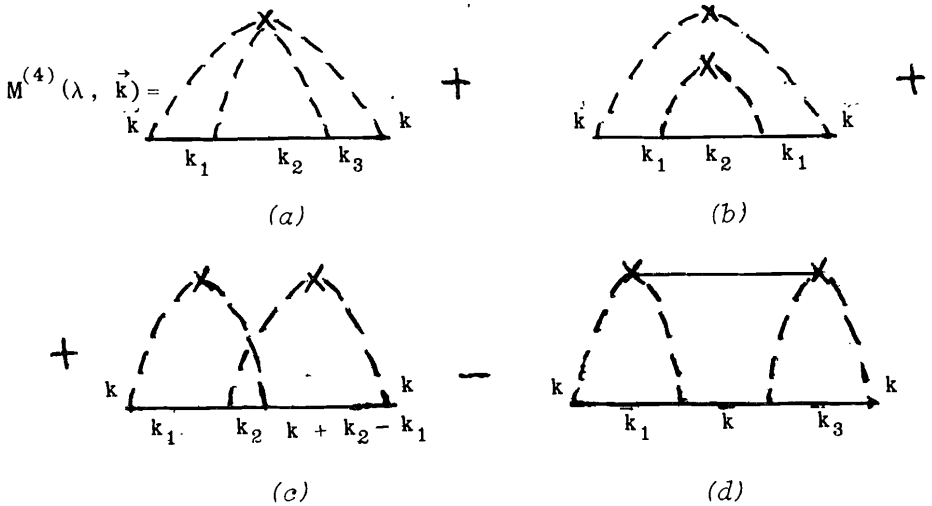


Fig. 9.

$$M^{(4)}(\lambda, \vec{k}) = \frac{1}{\Omega^4} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3} [N_i + N_i (N_i - 1)\delta_{\vec{k}_1 \vec{k}_3} +$$

$$+ N_i (N_i - 1)\delta_{\vec{k}+\vec{k}_2, \vec{k}_1+\vec{k}_3} - N_i \delta_{\vec{k}\vec{k}_2}] \phi_{\vec{k}\vec{k}_1} \frac{1}{\lambda - \epsilon^0_{\vec{k}_1}} \times \qquad (21)$$

$$\times \phi_{\vec{k}_1\vec{k}_2} \frac{1}{\lambda - \epsilon^0_{\vec{k}_2}} \phi_{\vec{k}_2\vec{k}_3} \frac{1}{\lambda - \epsilon^0_{\vec{k}_3}} \phi_{\vec{k}_3\vec{k}} .$$

The first term of this expression (corresponding to the diagram (a) in Fig. 9) describes independent single site scatterings and is proportional to the impurity centers concentration c′. The second and the third terms (21) (the diagrams (b) and (c) in Fig.9) correspond to pair-impurity scattering being proportional to c′. The last term in (21) (the diagram (d)), as easily seen, is proportional to c'/Ω and is vanishing at thermodynamics transition

$$\lim_{\substack{\Omega \to \infty \\ N_i \to \infty}} \frac{N_i}{\Omega} = c', \qquad (22)$$

Subsequently (22) will be assumed to be realized. We should note, that the reducible diagram, occuring in the fourth order, is canceled. It may be realized similarly, that for all the orders of expansion in H′ the mass operator is of the form

$$M^{(n)}(\lambda, \vec{k}) = \langle n \rangle_{\vec{k}\vec{k}} . \qquad (23)$$

Here, as in Eq.(9), $\langle n \rangle_{\vec{k}\vec{k}}$ denotes a sum of all the irreducible diagrams with the other momenta $\vec{k}$ in the n-th order perturbation theory. These diagrams may be presented in the same form as the diagrams of section 3 (for example, as the graphs, shown in Fig. 2). But in this case the value $(\phi)_{\vec{k}\vec{k}_1}$ corresponds to one crossed dotted line, the value $\frac{1}{\lambda - \epsilon^0_{\vec{k}_1}}$ corresponds to the solid line and a summation is performed over all the inner momenta and all the scatterers as well (see (20)). After averaging these diagrams acquire a form of the diagrams shown in Figs. 8, 9. Averaging results in closing of the dotted lines which correspond to the different sites and in the definite relations between the inner momenta (see Fig. 9). At the transition (22) the diagrams being analogous to the correction ones in (8) (with coupled crosses) provide no contribution now, as it was elucidated for the diagram (d) in Fig. 9.

Therefore, calculating the mass operator

$$M(\lambda, \vec{k}) = \sum_{n=2}^{\infty} \langle n \rangle_{\vec{k}\vec{k}} , \qquad (24)$$

we may classify diagrams into single-, two-impurity ones, etc., as in section 3. Summing all the single-impurity diagrams, then two-impurity ones, etc., we may obtain expansion for $M(\lambda, \vec{k})$ over the impurity concentration c′.

Let us sum, for example, single-impurity diagrams (with one cross) over all the orders of the perturbation theory. It is easily seen, that the result will be as follows

$$G(\lambda, \vec{k}) = \frac{1}{\lambda - \epsilon^0_{\vec{k}} - M(\lambda, \vec{k})}; \quad M(\lambda, \vec{k}) = c' t_{\vec{k}\vec{k}} = \sum_{\ell} \langle (T_\ell)_{\vec{k}\vec{k}} \rangle ;$$

$$t_{\vec{k}\vec{k}'} = \phi_{\vec{k}\vec{k}'} + \frac{1}{\Omega} \sum_{\vec{k}_1} \frac{\phi_{\vec{k}\vec{k}_1} \phi_{\vec{k}_1\vec{k}'}}{\lambda - \epsilon^0_{\vec{k}_1}} + \qquad (25)$$

$$+ \frac{1}{\Omega^2} \sum_{\vec{k}_1 \vec{k}_2} \frac{\phi_{\vec{k}\vec{k}_1} \phi_{\vec{k}_1\vec{k}_2} \phi_{\vec{k}_2\vec{k}'}}{(\lambda - \epsilon^0_{\vec{k}_1})(\lambda - \epsilon^0_{\vec{k}_2})} + \ldots$$

Here, t is the scattering operator for single center situated in the origin of coordinates. It is assosiated with the scattering operator T_ℓ for the centre situated in the point $\vec{r}_\ell$ by the relation [7]

$$(T_\ell)_{\vec{k}\vec{k}'} = \frac{1}{\Omega} e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell} t_{\vec{k}\vec{k}'} . \qquad (26)$$

The operator T_ℓ satisfies the equation /7/

$$T_\ell = \phi_\ell(1 + \frac{1}{d^o} T_\ell); \quad \frac{1}{d^o} = \frac{1}{\lambda - H_o} . \tag{27}$$

As it is seen from Eqs.(26), (27) the operator t is determined by the following integral equation

$$t_{\vec{k}\vec{k}'} = \phi_{\vec{k}\vec{k}'} + \frac{1}{\Omega} \sum_{\vec{k}_1} \phi_{\vec{k}\vec{k}_1} \frac{1}{d^o_{\vec{k}_1}} t_{\vec{k}_1\vec{k}'}; \tag{28}$$

$$\frac{1}{d^o_{\vec{k}}} = (\frac{1}{\lambda - H_o})_{\vec{k}\vec{k}} = \frac{1}{\lambda - \epsilon^o_{\vec{k}}} .$$

If the potential ϕ is local, as in section 3 for the diagonal disorder, then for disordered alloy it is of the form

$$\phi(\vec{r}) = \Delta v \delta(\vec{r}); \quad \phi_{\vec{k}\vec{k}'} = \Delta v, \tag{29}$$

where, v is the volume of the crystal unit cell. For such a case it is easily seen from Eqs.(25), (28), that

$$c' t_{\vec{k}\vec{k}'} = \langle t_1 \rangle = \frac{c\Delta}{1 - G^o(0)}; \quad G^o(\vec{r}_\ell - \vec{r}_{\ell'}) = \frac{1}{N} \sum_{\vec{k}} \frac{e^{-i\vec{k}(\vec{r}_\ell - \vec{r}_{\ell'})}}{\lambda - \epsilon^o_{\vec{k}}} . \tag{30}$$

It agrees with the result of section 3 of this work (N is the number of crystal sites).

The diagram technique allows one to obtain also the renormalized single-impurity approximation, if to sum also the diagrams of the type (b) on Fig. 9 besides diagrams with one cross (their sum is $c' t_{\vec{k}\vec{k}}$). Summing the mentioned diagrams over all the orders, we obtain

$$M(\lambda, \vec{k}) = c' \tilde{t}_{\vec{k}\vec{k}} = \sum_\ell \langle (\tilde{T}_\ell)_{\vec{k}\vec{k}} \rangle ;$$

$$\tilde{t}_{\vec{k}\vec{k}'} = \phi_{\vec{k}\vec{k}'} + \frac{1}{\Omega} \sum_{\vec{k}_1} \frac{\phi_{\vec{k}\vec{k}_1} \phi_{\vec{k}_1\vec{k}'}}{\lambda - \epsilon^o_{\vec{k}_1} - c' \tilde{t}_{\vec{k}_1\vec{k}_1}} + \tag{31}$$

$$+ \frac{1}{\Omega^2} \sum_{\vec{k}_1\vec{k}_2} \frac{\phi_{\vec{k}\vec{k}_1} \phi_{\vec{k}_1\vec{k}_2} \phi_{\vec{k}_2\vec{k}'}}{(\lambda - \epsilon^o_{\vec{k}_1} - c' \tilde{t}_{\vec{k}_1\vec{k}_1})(\lambda - \epsilon^o_{\vec{k}_2} - c' \tilde{t}_{\vec{k}_2\vec{k}_2})} + \ldots ;$$

$$(\tilde{T}_\ell)_{\vec{k}\vec{k}'} = \frac{1}{\Omega} e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell} \tilde{t}_{\vec{k}\vec{k}'} .$$

So, we have the closed system of equations

$$G(\lambda, \vec{k}) = \frac{1}{\lambda - \epsilon^o_{\vec{k}} - c' \tilde{t}_{\vec{k}\vec{k}}}; \tag{32}$$

$$\tilde{t}_{\vec{k}\vec{k}'} = \phi_{\vec{k}\vec{k}'} + \frac{1}{\Omega} \sum_{\vec{k}_1} \phi_{\vec{k}\vec{k}_1} G(\lambda, \vec{k}_1) \tilde{t}_{\vec{k}_1\vec{k}'} .$$

allowing to calculate the electron spectrum for the arbitrary potential $\phi(\vec{r})$ in renormalized single-impurity approximation. If to take approximation (29) for the potential, we obtain from Eqs.(31), (32)

$$M(\lambda, \vec{k}) = \frac{c\Delta}{1 - \Delta G(0)}; \quad G(\vec{r}_\ell - \vec{r}_{\ell'}) = \frac{1}{N} \sum_{\vec{k}} \frac{e^{-i\vec{k}(\vec{r}_\ell - \vec{r}_{\ell'})}}{\lambda - \epsilon^o_{\vec{k}} - M(\lambda, \vec{k})} . \tag{33}$$

This is the so-called approximation of the modified propagator for diagonal disorder /3/.

Let us consider now the mass operator $M(\lambda, \vec{k})$, accounting the quadratic with respect to impurity concentration terms. In this case single- and two-crossed graphs are to be taken into account (two-crossed diagrams (b) and (c) are shown in Fig. 9). As is easily seen from Eqs.(20), (21), (23), (24) and (8) the mass operator in this approximation may be described in the form

$$M(\lambda, \vec{k}) = \langle \sum_\ell (T_\ell)_{\vec{k}\vec{k}} \rangle + \frac{1}{2!} \langle \sum_{\ell \neq m} [T_{\ell m} - \tag{34}$$

$$- T_\ell - T_m - T_\ell \frac{1}{d^o} T_m - T_m \frac{1}{d^o} T_\ell]_{\vec{k}\vec{k}} \rangle .$$

Here, $T_{\ell m}$ is the two-center scattering operator for the points $\vec{r}_\ell$ and $\vec{r}_m$. It may be expressed by means of the operator T_ℓ as follows /7/

$$T_{\ell m} = T_\ell + T_m + T_\ell \frac{1}{d^o} T_m + T_m \frac{1}{d^o} T_\ell + T_\ell \frac{1}{d^o} T_m \frac{1}{d^o} T_\ell + T_m \frac{1}{d^o} T_\ell \frac{1}{d^o} T_m + \ldots \tag{35}$$

The diagram representation of $T_{\ell m} - T_\ell - T_m$ is shown in Fig. 7. As the mass operator involves only the irreducible part of the pair-defect T-matrix (as it follows from the diagram analysis given above), we subtracted out of $T_{\ell m}$ the terms describing single-impurity scattering (T_ℓ and T_m) and the reducible part of (35) as well corresponding to the first diagram in Fig. 7. The opeartor $T_{\ell m}$ satisfies the equation /7/

$$T_{\ell m} = (\phi_\ell + \phi_m)(1 + \frac{1}{d^o} T_{\ell m}) . \tag{36}$$

The matrix element $(T_{\ell m})_{\vec{k}\vec{k}'}$ may be given in the form

$$(T_{\ell m})_{\vec{k}\vec{k}'} = \frac{1}{\Omega} T_{\vec{k}\vec{k}'}(r) e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell} , \tag{37}$$

where, $\vec{r} = \vec{r}_m - \vec{r}_\ell$ is the distance between two scattering centers, $T_{\vec{k}\vec{k}'}(\vec{r})$ is the scattering operator on two centers one of which is in the origin of coordinates and the second one being in point $\vec{r}$. According to (36), $T_{\vec{k}\vec{k}'}(\vec{r})$ satisfies the equation

$$T_{\vec{k}\vec{k}'}(\vec{r}) = \Phi_{\vec{k}\vec{k}'}(\vec{r}) + \frac{1}{\Omega}\sum_{\vec{k}_1}\Phi_{\vec{k}\vec{k}_1}(\vec{r})\frac{1}{d^o_{\vec{k}_1}}T_{\vec{k}_1\vec{k}'}(\vec{r});$$

$$\Phi_{\vec{k}\vec{k}'}(\vec{r}) = (1 + e^{-i(\vec{k}-\vec{k}')\vec{r}})\phi_{\vec{k}\vec{k}'}. \qquad (38)$$

Substituting Eqs.(26), (37) into (34) and taking into account, that for any pair of impurities (ℓ, m) the ensemble averaging gives the equal results, we obtain

$$M(\lambda, \vec{k}) = \frac{N_i}{\Omega}t_{\vec{k}\vec{k}} + \frac{N_i(N_i-1)}{2!\,\Omega^2}\int d\vec{r}\, T_{\vec{k}\vec{k}}(\vec{r}) -$$

$$- \frac{N_i(N_i-1)}{\Omega}t_{\vec{k}\vec{k}} - \frac{N_i(N_i-1)}{\Omega^2}t_{\vec{k}\vec{k}}\frac{1}{d^o_{\vec{k}}}t_{\vec{k}\vec{k}}\,; \qquad (39)$$

The integral over $\vec{r}$ in (39) comes from $< T_{\vec{k}\vec{k}}(\vec{r}) >$, which is calculated with the aid of procedure (19). It should be noted that the singularity occurring in the second term of (39) at the thermodynamic limiting transition (22) is canceled with the third term of (39). So, Eq.(39) gives the mass operator up to the terms being proportional to c'^2 and scattering operators involved are determined by Eqs.(28) and (38).

For the local potential (29) Eq.(34) may be described in the form (taking into account (30))

$$M(\lambda, \vec{k}) = c\frac{\Delta}{1-\Delta G^o_o} + Q_{\vec{k}} - c^2\left(\frac{\Delta}{1-\Delta G^o_o}\right)^2\frac{1}{\lambda - \epsilon^o_{\vec{k}}}\,;$$

$$G^o_\ell = \frac{1}{N}\sum_{\vec{k}}\frac{e^{i\vec{k}\vec{r}_\ell}}{\lambda - \epsilon^o_{\vec{k}}}\,. \qquad (40)$$

Here, the quantity

$$Q_{\vec{k}} = \frac{N_i(N_i-1)}{2!} < [T_{\ell m} - T_\ell - T_m]_{\vec{k}\vec{k}} >,$$

for the local potential is of the known form, which corresponds to the "two-body problem" /3/

$$Q_{\vec{k}} = c^2\frac{\Delta}{1-\Delta G^o_o}\sum_{\ell\neq o}\frac{A^o_\ell e^{i\vec{k}\vec{r}_\ell} + (A^o_\ell)^2}{1-(A^o_\ell)^2}\,, \qquad (41)$$

$$A^o_\ell = \frac{\Delta}{1-\Delta G^o_o}G^o_\ell\,,$$

where, the summation is performed over all the lattice sites. Substituting Eq.(41) into (40) and taking into account that

$$\frac{\Delta}{1-\Delta G^o_o}\times\frac{1}{\lambda - \epsilon^o_{\vec{k}}} = \sum_{\ell\neq o}A^o_\ell e^{i\vec{k}\vec{r}_\ell} + A^o_o\,,$$

we rewrite expression for $M(\lambda, \vec{k})$ in the case of local potential as follows /3,8/

$$M(\lambda, \vec{k}) = \frac{c\Delta}{1-\Delta G^o_o}\left[1 - cA^o_o + c\sum_{\ell\neq o}\frac{(A^o_\ell)^3 e^{i\vec{k}\vec{r}_\ell} + (A^o_\ell)^2}{1-(A^o_\ell)^2}\right].$$

Here, the first term describes isolated-impurity scattering and the rest ones give the pair scattering.

To obtain renormalized representation for the mass operator, allowing for both the single- and two-defect scatterings, we sum in (24) besides two-crossed diagrams, summed in (39), also all diagrams, resulting in the renormalization of the inner propagators G^o. It is easily seen that as a result of such a procedure we obtain

$$M(\lambda, \vec{k}) = c'\tilde{t}_{\vec{k}\vec{k}} + \frac{N_i(N_i-1)}{2!} < [\tilde{Q}_{\ell m} - \tilde{T}_\ell\frac{1}{d}\tilde{T}_m -$$

$$- \tilde{T}_m\frac{1}{d}\tilde{T}_\ell - \tilde{T}_\ell\frac{1}{d}\tilde{T}_m\frac{1}{d}\tilde{T}_\ell - \tilde{T}_m\frac{1}{d}\tilde{T}_\ell\frac{1}{d}\tilde{T}_m]_{\vec{k}\vec{k}} >. \qquad (42)$$

Here,

$$(\tilde{T})_{\vec{k}\vec{k}'} = \frac{1}{\Omega}e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell}\tilde{t}_{\vec{k}\vec{k}'}\,; \quad \tilde{Q}_{\ell m} = \tilde{T}_{\ell m} - \tilde{T}_\ell - \tilde{T}_m\,;$$

$$(\tilde{T}_{\ell m})_{\vec{k}\vec{k}'} = \frac{1}{\Omega}e^{-i(\vec{k}-\vec{k}')\vec{r}_\ell}\tilde{T}_{\vec{k}\vec{k}'}(\vec{r}), \quad (\vec{r} = \vec{r}_m - \vec{r}_\ell); \quad \frac{1}{d} = \frac{1}{\lambda - H}\,, \qquad (43)$$

where, $\tilde{T}_{\vec{k}\vec{k}'}(\vec{r})$ is determined by Eq.(38), in which a substitution is needed

$$T_{\vec{k}\vec{k}'}(\vec{r}) \rightarrow \tilde{T}_{\vec{k}\vec{k}'}(\vec{r}); \quad \frac{1}{d^{o}_{\vec{k}}} \rightarrow \frac{1}{d_{\vec{k}}} = G(\lambda, \vec{k}). \tag{44}$$

The last two terms in (42) are due to the fact, that $\tilde{T}_{\ell}$ involves now the second diagram of Fig. 7 and therefore it is to be extracted from $Q_{\ell m}$. Taking into account Eq.(43) we may rewrite expression (42) as

$$M(\lambda, \vec{k}) = c'\tilde{t}_{\vec{k}\vec{k}} + \frac{N_i(N_i-1)}{2!\,\Omega^2}\int d\vec{r}\,\tilde{T}_{\vec{k}\vec{k}}(\vec{r}) - \frac{N_i(N_i-1)}{\Omega}\tilde{t}_{\vec{k}\vec{k}} - \frac{N_i(N_i-1)}{\Omega^2}\tilde{t}_{\vec{k}\vec{k}}\,G(\lambda, \vec{k})\,\tilde{t}_{\vec{k}\vec{k}} - \frac{N_i(N_i-1)}{\Omega^3}\sum_{\vec{k}'}\tilde{t}_{\vec{k}\vec{k}'}\,G(\lambda, \vec{k}')\,\tilde{t}_{\vec{k}'\vec{k}'}\,G(\lambda, \vec{k}')\,\tilde{t}_{\vec{k}'\vec{k}}\,. \tag{45}$$

So, to determine the electron spectrum we have the closed system comprising the equation

$$G(\lambda, \vec{k}) = \frac{1}{\lambda - \epsilon^{o}_{\vec{k}} - M(\lambda, \vec{k})}; \tag{46}$$

Eq.(45), Eq.(32), where $G(\lambda, \vec{k}_1)$ is determined by Eq.(46), and Eq.(38) with the substitution (44).

For the local potential (29) (disordered alloy)

$$\tilde{Q}_{\vec{k}} = \frac{N_i(N_i-1)}{2!}\langle[\tilde{Q}_{\ell m}]_{\vec{k}\vec{k}}\rangle = c^2\frac{\Delta}{1-\Delta G_o}\sum_{\ell\neq o}\frac{A_\ell e^{i\vec{k}\vec{r}_\ell} + A_\ell^2}{1 - A_\ell^2};$$

$$G_\ell = \frac{1}{N}\sum_{\vec{k}} e^{i\vec{k}\vec{r}_\ell}\,G(\lambda, \vec{k}); \quad A_\ell = \frac{\Delta}{1-\Delta G_o}G_\ell,$$

$c'\tilde{t}_{\vec{k}\vec{k}}$ is determined by Eq.(33) and

$$\frac{\Delta}{1-\Delta G_o}G(\lambda, \vec{k}) = \sum_{\ell} A_\ell e^{i\vec{k}\vec{r}_\ell},$$

where, $\sum_{\ell}$ involves the term with $\vec{r}_\ell = 0$. Substituting these expressions into (42) we obtain for the local potential /3,8/.

$$M(\lambda, \vec{k}) = \frac{c\Delta}{1-\Delta G_o}\left(1 - cA_o - cA_o^2 + c\sum_{\ell\neq o}\frac{A_\ell^3 e^{i\vec{k}\vec{r}_\ell} + A_\ell^4}{1 - A_\ell^2}\right).$$

The consideration carried out in this section is directly generalized to the impurity complexes consisting from the greater number of impurities.

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Лось В.Ф.
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К теории неупорядоченных систем. Спектры квазичастиц

Развит новый метод вычисления спектров неупорядоченных систем,основанный на формализме проекционного оператора, в котором автоматически учитываются поправки на многократное заполнение узлов. Получен явный вид ряда по взаимодействию для массового оператора усредненной по конфигурациям функции Грина. Показано, что этот ряд /отличный от кумулянтного/ легко суммируется в кластерном приближении. Получены замкнутые системы уравнений для определения спектра электронов, взаимодействующих посредством произвольного потенциала с хаотически распределенными примесными центрами, с учетом рассеяния на изолированных центрах и на парах примесей.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Los' V.F.
E17-86-845

On the Theory of Disordered Systems. Spectra of Quasi-Particles

New method for the disordered systems spectra calculation based on the projection operator technique, in which multiple-occupancy corrections are taken into account automatically, is developed. The explicit expansion in power of interaction for the self-energy of the configurationally averaged Green function is obtained. It is shown that this expansion (distinct from cumulant one) can be easily summed up in the cluster approximation. For the electrons which interact by means of arbitrary potential with the chaotically distributed scattering centres the closed systems of equations for the electron spectrum are obtained for the single centres and pairs of impurities scattering.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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