Electronic Structure and Conductivity of a Disordered $A_{1-x}B_x$ Binary Alloy in the Cluster Approach for the Hubbard Model

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Abstract—We propose a method for calculating the electronic band structure of disordered systems with strong electron correlations. Various approaches to the description of electrical conductivity of disordered systems are considered. Calculations are based on determining the one-particle Green function of the system, which is averaged over different configurations of a cluster, on the Boltzmann formalism, and the Kubo linear response theory. As the basic model, we use the Hubbard model for an $A_{1-x}B_x$ binary alloy.

1. INTRODUCTION

Advances in the study of various properties of disordered systems (alloys, solid solutions, amorphous metals, semiconductors, and so on) are due to the development of their electronic theory. A large number of publications are devoted to analysis of spectral characteristics of disordered systems [1−3]. Various methods have been worked out for calculating the configuration-averaged Green function of the system. Considerable efforts have been made to generalize the coherent potential approximation, which is the best single-site approximation for describing the properties of various alloys. However, in this method, statistical interatomic correlations cannot be taken into account. To account for correlations determined by multiple scattering of electrons from different lattice sites or the existence of a short-range order in the arrangement of atoms, it is necessary to exceed the limits of the single-site approximation. A large number of publications are devoted to this problem (for example, cluster generalizations of the coherent potential approximation, which are based on analysis of a single cluster in an effective medium [1] and "traveling-cluster" approximation [4]). In [5−7], a method was developed for accounting for statistical correlations based on the cluster expansion for one- and two-particle Green's functions that determine the electron energy spectrum and electrical conductivity of alloys. The topicality of such a problem is dictated, for example, by the need in study of the rearrangement of the electron spectrum during ordering of alloy, which has been predicted earlier [8, 9], when a gap in the electron spectrum appears at energies corresponding to the Brillouin zone boundary of an ordered alloy. In this case, the behavior of the alloy conductivity for long-range ordering substantially depends on the position of the Fermi level relative to the gap being formed. It was proposed in [8, 9] that a metal−insulator transition can occur in the case when the Fermi level gets into the region of such a gap.

Kinetic characteristics of disordered systems have been studied intensely in recent years (among other things, in connection with analysis of the Anderson transition [10]). The most consistent theory used in these studies is the "weak localization" theory [11, 12], which makes it possible to consider small effects preceding localization and emerging in the conducting state with the help of perturbation theory. We are speaking of the Kubo theory of linear reaction for electrons interacting with impurities, which is constructed in terms of one-particle Green's functions calculated in the self-consistent Born approximation. In the case of a degenerate electron gas (which is mainly considered in the literature), the small parameter of the theory is quantity $\lambda = \hbar/E_F\tau$ (E_F is the Fermi energy and τ is the electron relaxation time associated with elastic scattering by impurities). Therefore, for $\lambda \ll 1$, scattering is weak and does not lead to strong changes in one-particle properties (electron density of states), although the inclusion of quantum corrections in λ to the conductivity is sufficient for the emergence of weak localization effects [13]. It is necessary to develop a consistent theory, which would be valid for
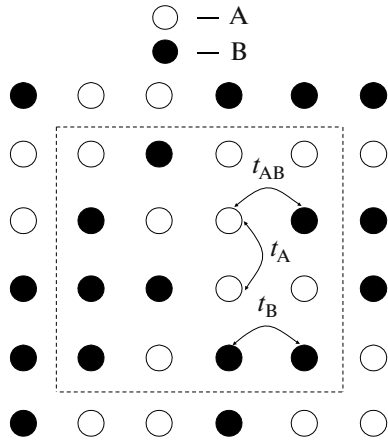
Fig. 1. Fragment of a crystal lattice with fully disordered (random) distribution of ions A and B. Dashed rectangle marks the cluster boundaries.

strong scattering also, when one-particle properties of the system may change significantly.

The theory of electrical conduction of disordered system with strong electron correlations is at the stage of development. New approaches to the description of the conductivity of systems with strong electron correlations have become especially topical after the discovery of spin-dependent transport, which has wide prospect of application in microelectronics [14–16].

In this study, we propose a method for calculating the electronic band structure of disordered systems with strong electron correlations using the cluster approach that has become very popular in recent years [17, 18]. The advantage of this approach is direct accounting for electron correlations as well as short-range magnetic and structural orderings that play a significant role in the description of low-dimensional magnetic systems and various alloys. The structure of the cluster theory has two main stages of constructing the solution: (i) the choice of the cluster and the determination of its multielectron eigenstates by the exact diagonalization method and (ii) the calculation of thermodynamics quantities and their averaging over disorder, viz., cluster configurations with different arrangements of ions. As the basic model, we use the Hubbard model for a binary $A_{1-x}B_x$ alloy. We consider various approaches to the description of the electrical conductivity of disordered systems, which are based on the calculation of the one-particle Green function of the system, averaged over various configurations, the Boltzmann formalism, and the Kubo theory of linear response.

2. MINIMAL MODEL AND METHOD

In this study, we confine our analysis to a simple 2D square lattice of binary alloy $A_{1-x}B_x$. The results of calculation of the electronic structure will be given for

$x = 0.5$; however, the approach considered here can be used for any concentration x ($0 \leq x \leq 1$). Let us first consider the completely disordered case when A and B ions are distributed at random among crystal lattice sites and then consider the possibility of accounting for the short-range order and the arrangement of A and B species of ions. The model Hamiltonian in the general form can be written as

$$\hat{H} = \sum_{i,\sigma} \varepsilon_i a_{i,\sigma}^\dagger a_{i,\sigma} - \sum_{\langle i,j \rangle \sigma} t_{ij} a_{i,\sigma}^\dagger a_{j,\sigma} + \sum_{i,\sigma} \frac{U_i}{2} n_{i,\sigma} n_{i,\bar{\sigma}}, \quad (1)$$

where $a_{i,\sigma}^\dagger$ and $a_{i,\sigma}$ are the creation and annihilation operators for the electron with spin projection $\sigma = \uparrow$, $\downarrow$ at the ith crystal lattice site and $n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma}$ is the operator of the number of electrons with spin projection σ ($\bar{\sigma} = -\sigma$). In accordance with the Pauli principle, one site can accommodate not more than two electrons with opposite projection of spin σ. In Hamiltonian (1), ε_i is the energy of the electron at the ith site. Energy ε_i assumes the value of ε_A with a probability of $1 - x$ and $\varepsilon_i = \varepsilon_A + \Delta$ with probability x. In other words, $\varepsilon_i = \varepsilon_A$ if site i is occupied by an ion of species A and $\varepsilon_i = \varepsilon_A + \Delta$ if site i belongs to a type-B ion. For convenience, we will henceforth assume that energy ε_A equals zero. Quantity t_{ij} is the integral of hopping from site j to site i ($t_{ij} = t_A$ if $i, j \in$ A; $t_{ij} = t_B$ if $i, j \in$ B, and $t_{ij} = t_{AB}$ is $i \in$ A, $j \in$ B, and vice versa). Quantity U_i is the Coulomb interaction parameter at site i ($U_i = U_A$ if $i \in$ A and $U_i = U_B$ if $i \in$ B). Hamiltonian (1) does not possess translation invariance; therefore, correlation functions $K(\omega, \mathbf{r}_1, \mathbf{r}_2)$ depend on the arrangement of atoms and, hence, on both coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ and not only on their difference. However, the system is translation-invariant overall; therefore, the correlator averaged over disorder must depend on difference $\mathbf{r}_1 - \mathbf{r}_2$:

$$K(\omega, \mathbf{r}_1 - \mathbf{r}_2) = \langle K(\omega, \mathbf{r}_1, \mathbf{r}_2) \rangle_{\text{disord}}.$$

Figure 1 shows a fragment of the crystal lattice with fully disordered (random) distribution of atoms. In the lattice, we choose a cluster of size $N_c \times N_c$ (dashed rectangle in Fig. 1) so that approximate ratio $N_A/N_B \approx (1 - x)/x$ holds, where N_A and N_B is the numbers of A and B ions in the cluster. Forming a superlattice from such clusters, one can simulate disorder in the system; in this case, averaging over disorder corresponds to averaging over an ensemble of such superlattices with different configurations of ions in a cluster. However, mean value of ions $\langle N_A \rangle = 1 - x$ and $\langle N_B \rangle = x$ remains unchanged.

Let us consider a disordered binary alloy in the absence of the electron–electron interaction ($U_i = 0$). The calculation procedure includes the calculation of the complete set of eigenvalues and eigenstates of Hamiltonian $\hat{H}_c$ of the cluster in the grand canonical ensemble by the exact diagonalization method ($\hat{H}_c \rightarrow$

(a)

(b)
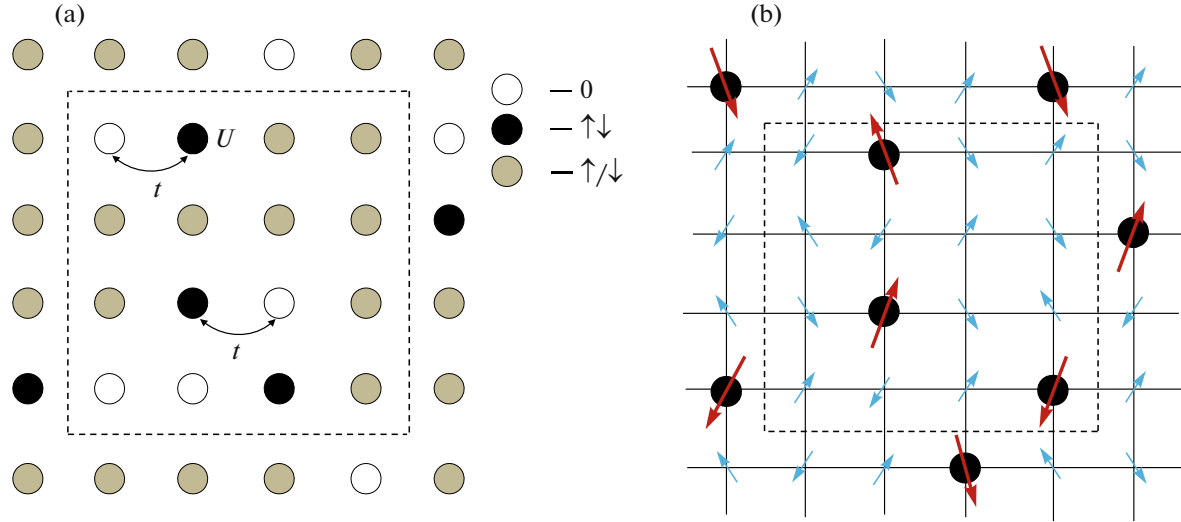
Fig. 2. Fragments of a crystal lattice with a random distribution of (a) electrons with spin projection $\sigma = \uparrow, \downarrow$, "zeros" and "twos" for the single-band Hubbard model and (b) magnetic impurities in Kondo alloys. Dashed rectangles mark the cluster boundaries.

$\hat{K} = \hat{H}_c - \mu \hat{N}$) with average number of electrons $\langle \hat{N} \rangle = N_e$, where $\hat{N}$ is the number-of-particle operator, and the evaluation of quantum-statistical mean values averaged over disorder corresponds to different configurations of the cluster. It is convenient to perform calculations using the approach described by Dagotto [19, 20]. Here, we only briefly describe the main ideas as applied to our problem, referring the reader to original publications [19, 20] for additional explanation and details. The main idea is that for the matrix representation of operator $\hat{K}$, the following basis of one-electron states is used:

$$a_{1,\uparrow}^\dagger |0\rangle, a_{2,\uparrow}^\dagger |0\rangle, ..., a_{L,\uparrow}^\dagger |0\rangle,$$
$$a_{1,\downarrow}^\dagger |0\rangle, a_{2,\downarrow}^\dagger |0\rangle, ..., a_{L,\downarrow}^\dagger |0\rangle,$$

where $L = N_c \times N_c$. In this case, various random configurations of the cluster with mean number of electrons $\langle \hat{N} \rangle = N_e$ satisfying condition $N_A/N_B \approx (1-x)/x$ are generated (see above).

We can generalize the proposed method to the general case of systems with strong electron correlations and take into account, instead of the random distribution of A and B ions, the random distribution of electrons with spin projection $\sigma = \uparrow, \downarrow$, "zeros," and "twos" (so-called states with zero and two electrons per crystal lattice sites). By way of example, Fig. 2a shows one of possible configurations of distribution of electrons with spin projection $\sigma = \uparrow, \downarrow$ in the cluster for the single-band Hubbard model in the absence of ionic disorder. The approach considered here can also be generalized and used for describing the Kondo lattices (Fig. 2b) with magnetic impurities (or in the Shubin–Vonsovsky s–d exchange model in which perturbation theory is known to be inapplicable to

analysis of a weak interaction of conduction electrons with the localized moment of the impurity) as well as system with the strong electron–phonon interaction.

Using unitary transformation U, we can reduce the matrix of operator $\hat{K}$ to diagonal form:

$$U^\dagger KU = \begin{pmatrix} E_1 & 0 & ... & 0 \\ 0 & E_2 & ... & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & ... & E_{2L} \end{pmatrix},$$

where $E_1, E_2, ..., E_{2L}$ are the eigenvalues of operator $\hat{K}$. The proper basis of operator $\hat{K}$ can be written as

$$u_1^\dagger |0\rangle, u_2^\dagger |0\rangle, ..., u_{2L}^\dagger |0\rangle.$$

Here,

$$u_m = \sum_j \sum_\sigma U_{m,j_\sigma}^\dagger a_{j,\sigma},$$

$j_\sigma = (j, \sigma)$, and m runs through values from 1 to $2L$. The quantum-statistical mean of operator $\hat{O}$ for the given electron and ion configurations of a cluster can be written in form

$$\langle \hat{O} \rangle = \text{Tr}(\hat{O} e^{-\beta \hat{K}})/Z_c,$$

where

$$Z_c = \prod_{\lambda=1}^{2L} (1 + \exp(-\beta E_\lambda))$$

is the partition function for the given cluster and $\beta = 1/k_B T$. For $\hat{O} = a_{i,\sigma} a_{j,\sigma'}^\dagger$, static Green function $G_{i,j,\sigma,\sigma'} = \langle a_{i,\sigma} a_{j,\sigma'}^\dagger \rangle$ has form

$$G_{i,j,\sigma,\sigma'} = \mathrm{Tr}(a_{i,\sigma}a_{j,\sigma'}^{\dagger}\exp(-\beta\hat{K}))/Z_c.$$

Since

$$a_{i\sigma}^{\dagger} = \sum_{\nu=1}^{2L}u_{\nu}^{\dagger}U_{\nu,i_{\sigma}}^{\dagger}, \quad a_{i\sigma} = \sum_{\nu=1}^{2L}U_{i_{\sigma},\nu}u_{\nu},$$

we obtain

$$G_{i,j,\sigma,\sigma'} = \sum_{\lambda=1}^{2L}U_{i_{\sigma},\lambda}\frac{1}{1+\exp(-\beta E_{\lambda})}U_{\lambda,j_{\sigma'}}^{\dagger}.$$

Using the Wick theorem, more complex two-particle correlators can be expressed in terms of one-particle Green's functions:

$$\langle a_{j_1,\sigma}a_{j_2,\sigma}^{\dagger}a_{j_3,\sigma}a_{j_4,\sigma}^{\dagger}\rangle = \langle a_{j_1,\sigma}a_{j_2,\sigma}^{\dagger}\rangle\langle a_{j_3,\sigma}a_{j_4,\sigma}^{\dagger}\rangle$$
$$+ \langle a_{j_1,\sigma}a_{j_4,\sigma}^{\dagger}\rangle\langle a_{j_2,\sigma}^{\dagger}a_{j_3,\sigma}\rangle.$$

Time-dependent observable quantities can be calculated using two-time Green's functions

$$G_{i,j,\sigma,\sigma}^{>}(t) = \langle a_{i,\sigma}(t)a_{j,\sigma}^{\dagger}(0)\rangle,$$

$$G_{i,j,\sigma,\sigma}^{<}(t) = \langle a_{i,\sigma}^{\dagger}(0)a_{j,\sigma}(t)\rangle,$$

where

$$a_{i,\sigma}(t) = \exp(i\hat{H}_c t)a_{i,\sigma}\exp(-i\hat{H}_c t).$$

It should be noted that operator $\hat{H}_c$ has a diagonal form in the same basis $\{u_m^{\dagger}|0\rangle\}$ as operator $\hat{K}$; therefore, we can show that

$$a_{i,\sigma}(t) = \sum_{\nu}\left[\sum_{\lambda=1}^{2L}U_{i_{\sigma},\lambda}\exp(-it\rho_{\lambda})U_{\lambda,\nu}^{\dagger}\right]a_{\nu},$$

where $a_{\nu} = a_{\nu,\uparrow}$ if $\nu \le L$ and $a_{\nu} = a_{\nu-L,\downarrow}$ if $\nu > L$; ρ_{λ} are the eigenvalues of operator $\hat{H}_c$, and $E_{\lambda} = \rho_{\lambda} - \mu$. Substituting this expression into the definition of time-dependent Green's functions, we obtain

$$G_{i,j,\sigma,\sigma}^{>}(t) = \sum_{\lambda=1}^{2L}U_{i_{\sigma},\lambda}\frac{\exp(-it\rho_{\lambda})}{1+\exp(-\beta(\rho_{\lambda}-\mu))}U_{\lambda,j_{\sigma}}^{\dagger}.$$

The retarded Green function can be defined as

$$G_{i,j,\sigma}^{R}(\omega) = \int_{-\infty}^{\infty}G_{i,j,\sigma}^{R}(t)e^{i\omega t}dt,$$

where

$$G_{i,j,\sigma,\sigma}^{R}(t) = -i\theta(t)(G_{i,j,\sigma,\sigma}^{>}(t) + G_{j,i,\sigma,\sigma}^{<}(t)).$$

Using the expressions for $G_{i,j,\sigma,\sigma}^{>}(t)$ and $G_{j,i,\sigma,\sigma}^{<}(t)$, we can finally obtain the cluster retarded Green function in terms of the eigenvalues and eigenvectors of operator $\hat{H}_c$:

$$G_{i,j,\sigma}^{R}(\omega) = \sum_{\lambda=1}^{2L}U_{j_{\sigma},\lambda}U_{\lambda,i_{\sigma}}^{\dagger}\frac{1}{\omega-\rho_{\lambda}+i\delta}\bigg|_{\delta\to+0}$$

$$= P\sum_{\lambda=1}^{2L}U_{j_{\sigma},\lambda}U_{\lambda,i_{\sigma}}^{\dagger}\frac{1}{(\omega-\rho_{\lambda})} \qquad (2)$$

$$- i\pi\sum_{\lambda=1}^{2L}U_{j_{\sigma},\lambda}U_{\lambda,i_{\sigma}}^{\dagger}\delta(\omega-\rho_{\lambda}).$$

Here, letter P in front of the first sum indicates calculation in the sense of the principal value.

The electronic structure is calculated using the cluster perturbation theory [17, 18]. There exist many modifications of this theory (for example, the cluster perturbation theory in the representation of the Hubbard operators [21, 22]), but the main idea of this cluster approach is the same. It involves the division of the lattice into clusters of a certain size, exact diagonalization in an individual cluster, and inclusion of the interaction between clusters using perturbation theory.

The hopping matrix can be written in form

$$t_{fi,gj} = t_{ij}^{c}\delta_{fg} + T_{fi,gj},$$

where t_{ij}^{c} is the hopping matrix within a cluster and $T_{fi,gj}$ is the residue responsible for intercluster hopping. Here, i and j are the intracluster indices of sites and f and g are cluster indices. In this cluster approximation, the full Green function is evaluated using the following matrix equation:

$$\hat{D}^{-1} = \hat{G}^{c-1} - \hat{T},$$

where Green function $\hat{G}^c$ describes the motion of electrons in an individual cluster. This equation can also be written in a different equivalent form

$$\hat{D}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}^c,$$

where $\hat{G}_0^{-1} = \omega - \hat{t}^c - \hat{T}$. Here, $\hat{G}_0$ is the Green function of the system without the interaction and $\hat{\Sigma}^c$ is the cluster self-energy part.

If we now consider a superlattice (i.e., a lattice composed of individual clusters), we can perform the Fourier transformation and pass from cluster indices to the corresponding wavevector in the reciprocal space. The Brillouin zone determined in this way is reduced as compared to the initial Brillouin zone corresponding to the initial lattice. Then we can write

$$T_{ij}(\tilde{\mathbf{k}}) = \sum_{f}t_{0i,fj}\exp(i\tilde{\mathbf{k}}\cdot\mathbf{r}_f), \qquad (3)$$

where $\mathbf{r}_f$ is the radius vector of cluster $f \ne 0$ relative to the main cluster with index "0" and $\tilde{\mathbf{k}}$ is the wavevector in the reduced first Brillouin zone. We can now write the equation for the full Green function as

$$\hat{D}^{-1}(\tilde{\mathbf{k}},\omega) = \hat{G}^{c-1}(\omega) - \hat{T}(\tilde{\mathbf{k}}). \qquad (4)$$

The artificial division of the lattice into clusters and the account for intracluster hopping separately from intercluster hopping breaks translation invariance. For its restoration within the cluster perturbation theory, the following procedure is used:

$$G(\mathbf{k}, \omega) = \frac{1}{L} \sum_{i,j=1}^{L} D_{ij}(\mathbf{k}, \omega) \exp[-i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)], \qquad (5)$$

where $\mathbf{r}_i$ is the radius vector of sites in a cluster and $\mathbf{k}$ is the wavevector in the initial first Brillouin zone. In this relation, we assume that $T_{ij}(\tilde{\mathbf{k}}) = T_{ij}(\mathbf{k})$.

Full Green function $\hat{D}$ can be calculated directly from Eq. (4); however, we must first determine cluster Green's function $\hat{G}_c$, which is usually done using the Lanczos algorithm, and perform the procedure for finding the inverse matrix. The entire procedure take considerable computer time. However, this calculation can be accelerated on account of the fact that cluster Green's function $\hat{G}_c$ is independent of the wavevector. Let us write Eq. (4) as

$$\hat{D}^{-1}(\tilde{\mathbf{k}}, \omega) = \omega - \hat{t}^c - \hat{\Sigma}^c - \hat{T}(\tilde{\mathbf{k}}).$$

It can clearly be seen that the poles of the full Green function at each point of the reduced first Brillouin zone are determined by the Hamiltonian of an individual cluster, but with additional terms depending on the wavevector. If we recollect the structure of these terms (3), we can note that periodic boundary conditions with a certain phase determined by the wavevector and the lattice period are imposed on an isolated cluster. With account of this analysis, we can write the Hamiltonian of an individual cluster in form

$$\hat{H}_c(\tilde{\mathbf{k}}) = \hat{H}_c + \hat{T}(\tilde{\mathbf{k}}). \qquad (6)$$

If we now use expression (2), we obtain full Green's function $\hat{D}$ by solving the eigenvalue problem for Hamiltonian (6) at each point of the reduced first Brillouin zone. We obtain the one-particle Green function from Eq. (5). This procedure is equivalent to the algorithm of expansion of the reduced zone, which is based on the Bloch theorem [23].

To consider a disordered binary alloy, we must determine the procedure of Green's function averaging over disorder (over configurations of the cluster with different distributions of ions). The calculation procedure includes the specification of a certain configuration of the cluster with random distributions of ions of different species. In the numerical algorithm, all sites of the cluster are sampled at random and assume state A with probability $1 - x$ or state B with probability x. Therefore, the average number of ions of species A and of species B remains constant:

$$\langle N_A \rangle = 1 - x, \qquad \langle N_B \rangle = x.$$

In the case of a disordered system, Hamiltonian (1) contains terms that are inhomogeneous in space;

therefore, the Fourier transform of these terms contains two wavevectors $\mathbf{k}$ and $\mathbf{k}'$. For large clusters, the nondiagonal component for $\mathbf{k} \neq \mathbf{k}'$ are proportional to $\sqrt{1/L}$ because of the random distribution of the potential, where L is the number of sites in the cluster. An analogous decrease in the contribution from nondiagonal components is observed when averaging is performed over a large number of cluster configurations with a random distribution of ions. Therefore, Green's function for a heterogeneous system also depends on two wavevectors $G_{\mathbf{k}\mathbf{k}'}(\omega)$; for large clusters or after averaging over random cluster configurations, the nondiagonal elements of Green's function for $\mathbf{k} \neq \mathbf{k}'$ are proportional to $\sqrt{1/L}$. Thus, in the limit of a large cluster or after averaging over a large number of random configurations of the cluster, Green's function becomes diagonal in the wavevector, $\bar{G}_\mathbf{k}(\omega) = \langle G_{\mathbf{k}\mathbf{k}'}(\omega) \rangle_{\mathrm{conf}}$ [23].

For each cluster configuration, Green's function (5) is calculated based on the cluster perturbation theory. Having performed an analogous calculation for N_{conf} different configurations of clusters, we carry out the averaging procedure:

$$\bar{G}(\mathbf{k}, \omega) = \langle G(\mathbf{k}, \omega) \rangle_{\mathrm{conf}}. \qquad (7)$$

The Green function obtained in this way is used for calculating the spectral density of one-particle excitations,

$$A_\sigma(\mathbf{k}, \omega) = -\frac{1}{\pi} \lim_{\delta \to +0} \mathrm{Im}\, \bar{G}_\sigma(\mathbf{k}, \omega + i\delta),$$

and the density of one-particle states for the given spin projection,

$$N_\sigma(\omega) = \frac{1}{N_k} \sum_\mathbf{k} A_\sigma(\mathbf{k}, \omega),$$

where N_k is the number of points in the first Brillouin zone. As a consequence of the anticommutation relation $[a_{i,\sigma}, a_{i,\sigma}^\dagger]_+ = 1$ for fermions, the total spectral weight is conserved for any wavevector $\mathbf{k}$:

$$\sum_\sigma \int A_\sigma(\mathbf{k}, \omega) d\omega = 2.$$

We will now consider the results of calculations of the electronic band structure and the electrical conductivity for a binary alloy with Hamiltonian (1) in the absence of the electron—electron interaction ($U_i = 0$) for the following values of model parameters:

$$t_A = 1.0 \text{ eV}, \quad t_B = 0.85 \text{ eV}, \quad t_{AB} = 0.8 \text{ eV},$$
$$\Delta = 0.5 \text{ eV}.$$

In the absence of the electron—electron interaction, the band structure is independent of temperature and the number of electrons in the system; i.e., the "rigid band" approximation holds. Figure 3 shows the results of calculation of the electronic band structure
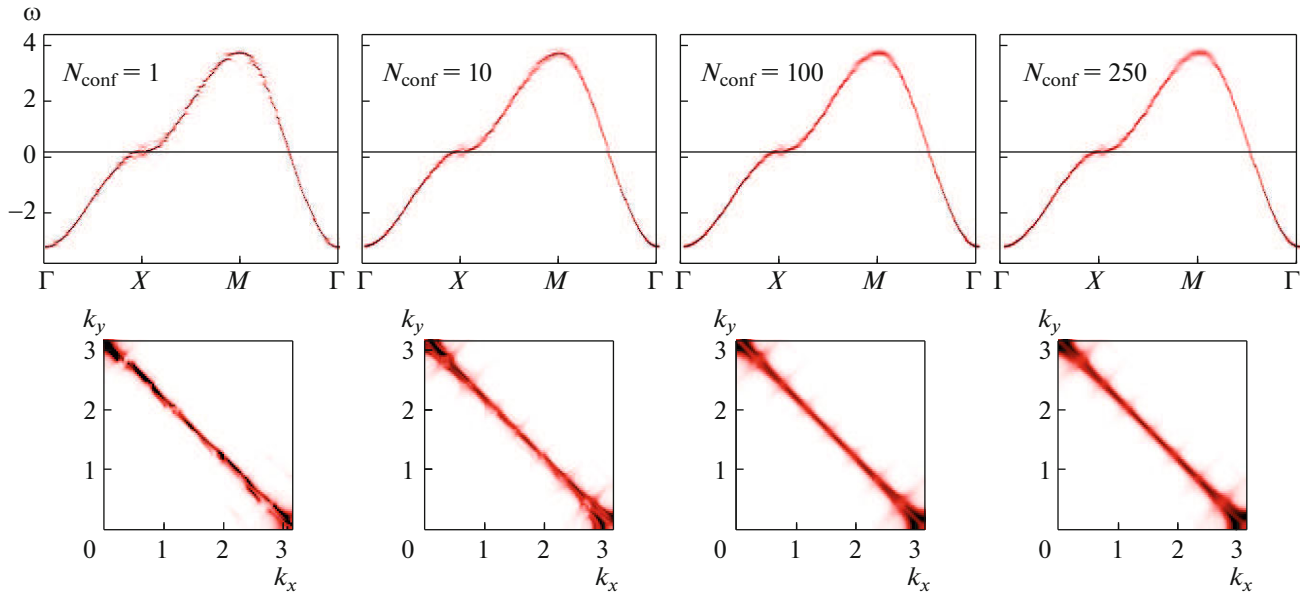
Fig. 3. Electronic band structure of a binary alloy in the absence of the electron–electron interaction in the cluster approximation. Upper panels show the dispersion of Fermi quasiparticle excitations along the symmetric directions of the Brillouin zone, which was obtained for a 8×8 cluster using different numbers of random configurations $N_{\text{conf}} = 1-250$ for averaging over disorder. The lower panels show the corresponding Fermi surfaces in the first quarter of the first Brillouin zone in the case of half-filling.

for a 8×8 cluster using various numbers of random configurations $N_{\text{conf}} = 10-250$ for averaging over disorder. Here and below, color shows the distribution of the total spectral weight

$$A(\mathbf{k}, \omega) = \sum_{\sigma} A_{\sigma}(\mathbf{k}, \omega),$$

and the initial spectral line broadening is $\delta = 0.01$ eV.

Figure 4 shows the results of calculation for clusters of different sizes from 8×8 to 32×32 with $N_{\text{conf}} = 10$. It can be seen that with increasing cluster size and the number of configurations N_{conf}, over which the averaging is performed, the fictitious discontinuities in the electron dispersion, which appear due to artificial increase in the period of translation of the crystal lattice during the formation of a cluster superlattice, are blurred.

Hamiltonian (1) can be written in the $\mathbf{k}$ representation in the form of the sum of two contributions:

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$$

$$= \sum_{\sigma,\mathbf{k}} \varepsilon_{\mathbf{k}} a^{\dagger}_{\sigma,\mathbf{k}} a_{\sigma,\mathbf{k}} + \sum_{\sigma,\mathbf{k},\mathbf{k'}} V_{\mathbf{k},\mathbf{k'}} a^{\dagger}_{\sigma,\mathbf{k}} a_{\sigma,\mathbf{k'}}.$$

If $1 - x > x$, i.e., more than half of the lattice is filled with ions of species A, it is convenient to choose for $\hat{H}^{(0)}$ the Hamiltonian of the lattice with only A ions at its sites and with a hopping t_{A} between them, while $\hat{H}^{(1)}$ will describe perturbation (scattering) due to the

addition of ions of species B, and vice versa. Full Green's function

$$G_{\sigma}(\mathbf{k}, \mathbf{k'}, \omega) = \lim_{\delta \to +0} \left\langle 0 \left| a_{\sigma,\mathbf{k'}} \frac{1}{\omega - \hat{H} + i\delta/2} a^{\dagger}_{\sigma,\mathbf{k}} \right| 0 \right\rangle$$

can be represented with the help of the Dyson equation in form

$$G_{\sigma}(\mathbf{k}, \mathbf{k'}, \omega) = G_{\sigma}^{(0)}(\mathbf{k}, \omega)$$

$$+ \sum_{\mathbf{k''}} G_{\sigma}^{(0)}(\mathbf{k}, \omega) H^{(1)}_{\mathbf{k},\mathbf{k''}} G_{\sigma}(\mathbf{k''}, \mathbf{k'}, \omega),$$

where $G_{\sigma}^{(0)}(\mathbf{k}, \omega)$ is the initial Green function corresponding to $\hat{H}^{(0)}$. Or

$$G_{\sigma}(\mathbf{k}, \omega) = \left[\frac{1}{G_{\sigma}^{(0)}(\mathbf{k}, \omega)} - \Sigma'_{\sigma}(\mathbf{k}, \omega) - i\Sigma''_{\sigma}(\mathbf{k}, \omega) \right]^{-1},$$

where $G_{\sigma}(\mathbf{k}, \omega) = \langle G_{\sigma}(\mathbf{k}, \mathbf{k'}, \omega) \rangle_{\text{disord}}$ is the Green function averaged over disorder, and

$$\Sigma_{\sigma}(\mathbf{k}, \omega) = \Sigma'_{\sigma}(\mathbf{k}, \omega) + i\Sigma''_{\sigma}(\mathbf{k}, \omega)$$

is the mass operator containing the imaginary and real parts. If the short-range structural order exists in the distribution of atoms, it is convenient to choose for $G_{\sigma}^{(0)}(\mathbf{k}, \omega)$ the Green function corresponding to the fully ordered lattice, and $\hat{H}^{(1)}$ will then describe the perturbation caused by disorder in the distribution of atoms. The imaginary part of mass operator $\Sigma''_{\sigma}(\mathbf{k}, \omega)$
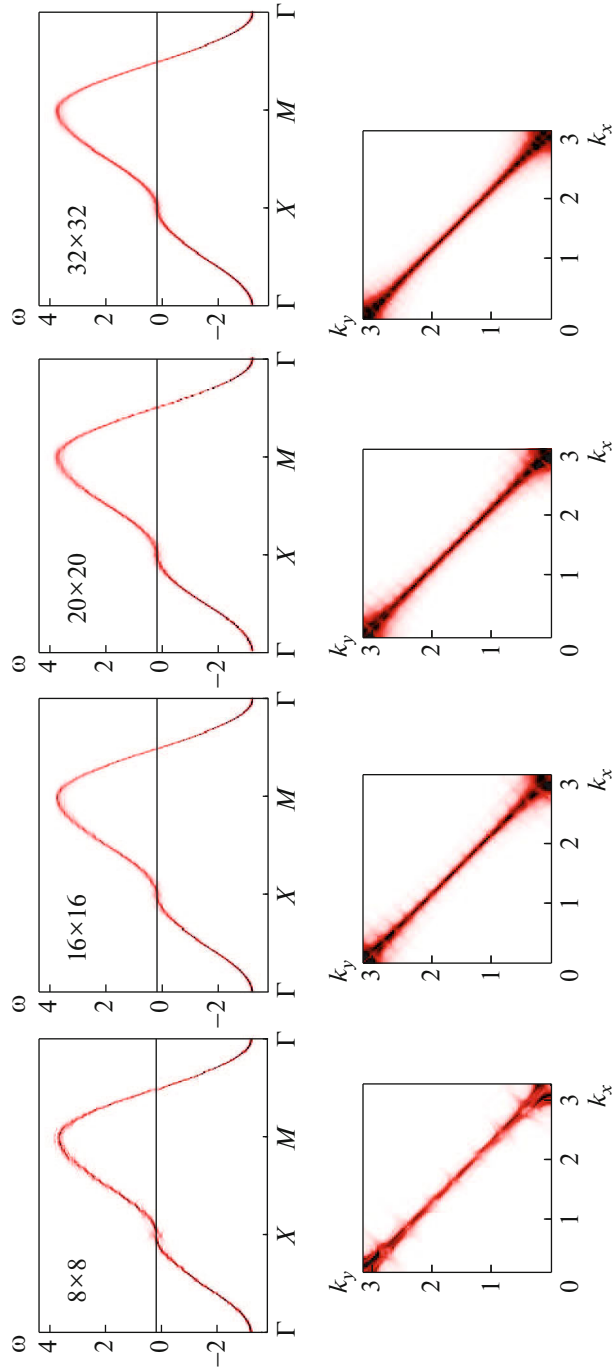
Fig. 4. Electronic band structure of a binary alloy in the absence of the electron—electron interaction in the cluster approximation. Upper panels show the dispersion of Fermi quasiparticle excitations along the symmetric directions of the Brillouin zone, which was obtained for 8×8–32×32 clusters using a fixed number of random configurations $N_{conf} = 10$ for averaging over disorder. The lower panels show the corresponding Fermi surfaces in the first quarter of the first Brillouin zone in the case of half-filling.

determines lifetime $\tau_\sigma(\mathbf{k}) \sim 1/\Sigma_\sigma''(\omega(\mathbf{k}))$ or the decay of quasiparticle excitations with spin projection σ and dispersion broadening (see Figs. 3 and 4). In Figs. 3 and 4, we can observe nonuniform broadening of dispersion; i.e., lifetime $\tau(\mathbf{k})$ determined by scattering processes is not the same for different $\mathbf{k}$ in the first Brillouin zone. It should be noted that this broadening is much larger than the initial broadening δ used in the numerical algorithm. Therefore, the method used here makes it possible to find lifetime $\tau(\mathbf{k})$ required for calculating the conductivity.

To account for the existence of a short-range order in the distribution of atoms, we can specify various ordered regions of smaller size in averaging the Green function over disorder within the cluster. The middle panels in Fig. 5 show the results of calculations of the electronic band structure and density of states, which were obtained by averaging the Green function over different configurations of a 16 × 16 cluster containing ordered regions with a size from 2 × 2 to 12 × 12; we used the configurations in which ordered regions were distributed at random within the cluster. The upper and lower panels in Fig. 5 show for comparison the results of calculation for the same parameters in the cases of fully disordered and ordered alloys, respectively. For convenience of comparison, the band structure of the fully ordered alloy (lower panels in Fig. 5) is given for the unreduced Brillouin zone. It can be seen from Fig. 5 (middle panels) that in the presence of such ordered regions, a gap (pseudogap) appears in the spectrum for energies corresponding to the Brillouin zone boundary for a fully ordered alloy. An analogous situation associated with the emergence of a pseudogap in strongly correlated systems with a short-range antiferromagnetic order was considered, for example, in [24]. If the chemical potential lies in the true dielectric gap (Fig. 5, lower panels), an insulator–poor metal–metal transition is observed upon enhancement of disorder (see Fig. 5).

3. ELECTRICAL CONDUCTIVITY

Let us consider the Hamiltonian of the 2D Hubbard model in an external ac electromagnetic field described by vector potential $\mathbf{A}(\mathbf{r}, t)$:

$$\hat{H} = \hat{T}_A + \hat{U}$$

$$= -t\sum_{\mathbf{r},\mathbf{l},\sigma}[a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r}+\mathbf{l},\sigma}\exp[ieA_\mathbf{l}(\mathbf{r},t)] + a_{\mathbf{r}+\mathbf{l},\sigma}^\dagger a_{\mathbf{r},\sigma}$$

$$+ \exp[-ieA_\mathbf{l}(\mathbf{r},t)]] + U\sum_r n_{\mathbf{r}\uparrow}n_{\mathbf{r}\downarrow},$$

where $\mathbf{r}$ is the radius vector of a crystal lattice site, $\mathbf{l}$ is the unit vector along the coordinate (crystallographic) axes, $A_\mathbf{l}(\mathbf{r}, t)$ is the component of vector $\mathbf{A}(\mathbf{r}, t)$ along

direction $\mathbf{l}$, and $\hbar = c = a = 1$. Operator $\hat{T}_A$ can be expanded into a power series in electric charge e:

$$\hat{T}_A = \hat{T} - e\sum_{\mathbf{r},\mathbf{l}}\hat{j}_\mathbf{l}(\mathbf{r})A_\mathbf{l}(\mathbf{r},t) - \frac{e^2}{2}\sum_{\mathbf{r},\mathbf{l}}\hat{K}_\mathbf{l}(\mathbf{r})A_\mathbf{l}^2(\mathbf{r},t) + ...,$$

where

$$\hat{T} = -t\sum_{\mathbf{r},\mathbf{l},\sigma}[a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r}+\mathbf{l},\sigma} + a_{\mathbf{r}+\mathbf{l},\sigma}^\dagger a_{\mathbf{r},\sigma}]$$

is the kinetic energy operator in zero electromagnetic field,

$$\hat{j}_\mathbf{l}(\mathbf{r}) = it\sum_\sigma(a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r}+\mathbf{l},\sigma} - a_{\mathbf{r}+\mathbf{l},\sigma}^\dagger a_{\mathbf{r},\sigma})$$

is the operator of the "paramagnetic" current density in direction $\mathbf{l}$, and

$$\hat{K}_\mathbf{l}(\mathbf{r}) = -t\sum_\sigma(a_{\mathbf{r},\sigma}^\dagger a_{\mathbf{r}+\mathbf{l},\sigma} + a_{\mathbf{r}+\mathbf{l},\sigma}^\dagger a_{\mathbf{r},\sigma})$$

is the operator of the "diamagnetic" current density in direction $\mathbf{l}$. Therefore, the Hamiltonian can be written as $\hat{H} = \hat{H}_0 + \hat{V}$. Here, the first term $\hat{H}_0$ defines the Hamiltonian of the Hubbard model with account for the Coulomb interaction of electrons in the absence of the vector potential, while second term $\hat{V}$ describes the interaction with the field and vanishes for $\mathbf{A}(\mathbf{r}, t) = 0$.

In the linear response theory, the expression for the total current has form

$$\hat{J}_\mathbf{l}(\mathbf{r},t) = -\frac{\partial\hat{H}}{\partial A_\mathbf{l}(\mathbf{r},t)} = e\hat{j}_\mathbf{l}(\mathbf{r}) + e^2\hat{K}_\mathbf{l}(\mathbf{r})A_\mathbf{l}^2(\mathbf{r},t) + ...,$$
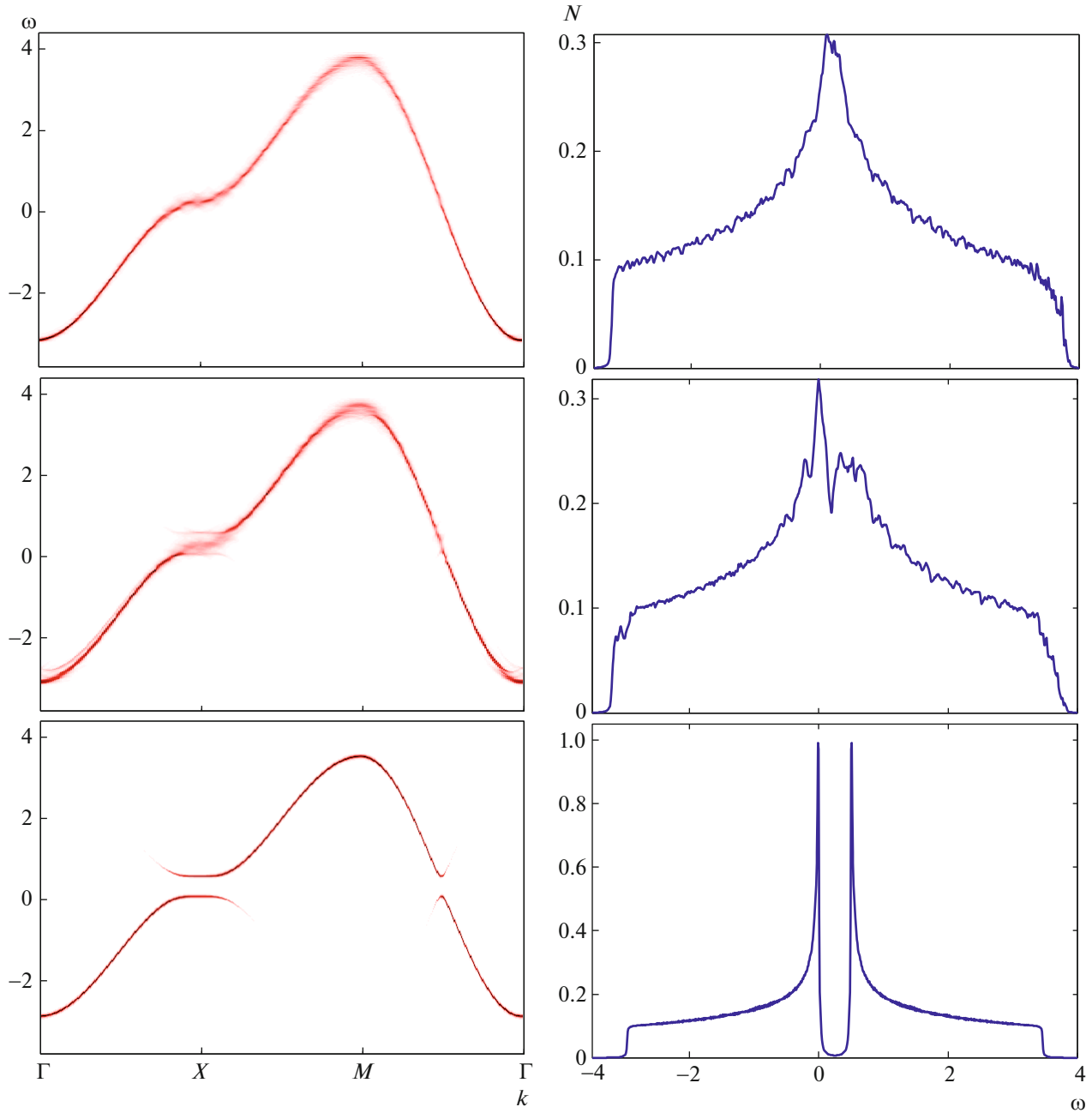
where the first and second terms correspond to the paramagnetic and diamagnetic contributions, respectively. Using the nonstationary perturbation theory, we can show that for $A_\mathbf{l}(\mathbf{r}, t) = \delta_{\mathbf{l}, x}A_x(\mathbf{r}, t)$, we obtain

$$\langle\hat{J}_x(\mathbf{q},\omega)\rangle = e^2\langle\hat{K}_x\rangle A_x(\mathbf{q},\omega)$$

$$+ e^2\left[\frac{1}{N}\left\langle\phi_0\left|\hat{j}_x(-\mathbf{q})\frac{1}{\hat{H}_0 - E_0 + \omega + i\delta}\hat{j}_x(\mathbf{q})\right|\phi_0\right\rangle\right.$$

$$\left.+ \frac{1}{N}\left\langle\phi_0\left|\hat{j}_x(\mathbf{q})\frac{1}{\hat{H}_0 - E_0 - \omega - i\delta}\hat{j}_x(-\mathbf{q})\right|\phi_0\right\rangle\right]A_x(\mathbf{q},\omega),$$

where angle brackets indicate quantum-mechanical averaging over the ground state $|\phi_0\rangle$ of the system with energy E_0. Here, we consider the situation at zero temperature. Then the expression for the frequency dependence of the real part of conductivity $\sigma_1(\omega)$ for $\mathbf{q} = 0$ has form

$$\sigma_1(\omega) = \mathrm{Re}\,\sigma_{xx}(\omega) = D\delta(\omega)$$

$$+ \frac{e^2\pi}{N}\sum_{n\neq 0}\frac{|\langle\phi_0|\hat{j}_x|\phi_n\rangle|^2}{E_n - E_0}\delta(\omega - (E_n - E_0)), \quad (8)$$

Fig. 5. Electronic band structure of a binary alloy in the absence of the electron–electron interaction in the cluster approximation. Left middle panel shows the dispersion of Fermi quasiparticle excitations along the symmetric directions of the Brillouin zone and the density of states, which were obtained for a 16×16 cluster containing ordered regions of different sizes. The upper and lower panels show the results of calculations for the same parameters in the cases of fully disordered and ordered alloys, respectively.

where

$$D = \pi e^2 \langle -\hat{K}_x \rangle - 2\frac{\pi e^2}{N} \sum_{n \neq 0} \frac{|\langle \phi_0 | \hat{j}_x | \phi_n \rangle|^2}{E_n - E_0}$$

is the Drude weight. In deriving expression (8), we used completeness condition for

$$I = \sum_n |\phi_n\rangle\langle\phi_n|,$$

$\hat{H}_0|\phi_n\rangle = E_n|\phi_n\rangle$. A more detailed derivation of Eq. (8) can be found in [25]. It is known that $\sigma_1(\omega)$ and $\langle \hat{K}_x \rangle$ are connected by the sum rule:

$$\int_0^\infty \sigma_1(\omega)d\omega = \frac{\pi e^2}{2}\langle -\hat{K}_x \rangle.$$

The Drude weight D can be used as the order parameter for a metal–insulator transition [25]. Vanishing of D indicates the dielectric ground state of the system. For noninteracting fermions, we can obtain from Eq. (8) the well-known expression for the Drude conductivity:

$$\sigma_1(\omega) = \frac{n_e e^2 \pi}{m_e} \delta(\omega),$$

where $n_e = N_e/N$ is the concentration of carriers (free electrons) and m_e is the electron mass.

At finite temperatures, the second term in Eq. (8) for the grand canonical ensemble has form

$$\frac{1}{\omega}\frac{\pi e^2}{N}(1 - e^{-\beta\omega})e^{\beta\Omega}\sum_{nm}e^{-\beta E_n}\langle\phi_n|\hat{j}_\alpha^\dagger|\phi_m\rangle$$
$$\times\langle\phi_m|\hat{j}_\beta|\phi_n\rangle\delta(\omega + E_n - E_m),$$

where Ω is the thermodynamic potential and $-\partial\Omega/\partial\mu = \langle N_e\rangle$, $e^{-\beta\Omega} = \mathrm{Tr}(e^{-\beta(\hat{H}_0 - \mu\hat{N})})$ [26]. Since the eigenvalue problem

$$(\hat{H}_0 - \mu\hat{N})|\phi_n\rangle = E_n|\phi_n\rangle$$

cannot be solved exactly, we have to use various approximations.

Let us apply the cluster approach for analyzing the conductivity of a disordered binary alloy with the help of the Kubo formalism. We choose a large enough cluster and calculate exactly the dynamic conductivity at a finite temperature. We consider the case of noninteracting fermions ($U_i = 0$), but with account for disordered distribution of ions (energy of electrons at a site) and the corresponding integrals of hopping (1) between the nearest sites. To account for the random nature of the ion distribution in the lattice, we must perform the procedure of averaging over different cluster configurations.

In the framework of the Kubo formalism, the dynamic conductivity in the long-wave limit ($\mathbf{q} = 0$) has form [27]

$$\sigma_{xx}(\omega) = -e^2\frac{\langle -K_x\rangle - \Lambda_{xx}(0,\omega)}{i(\omega + i\delta)}\bigg|_{\delta\to +0}, \qquad (9)$$

where

$$\Lambda_{xx}(\mathbf{q},\omega) = i\frac{1}{L}\int_0^\infty e^{i(\omega+i\varepsilon)t} \qquad (10)$$
$$\times\langle[j_x(\mathbf{q},t), j_x(-\mathbf{q},0)]\rangle dt, \qquad \varepsilon\to +0,$$

$$\langle -K_x\rangle = \frac{1}{L}\sum_l\langle -K_x(l)\rangle,$$

$$j_x(\mathbf{q},t) = \sum_l e^{-i\mathbf{q}\mathbf{r}_l}j_x(l,t).$$

Here, $\langle...\rangle$ is the quantum-statistical average, $j_x(l, t)$ is the operator of the paramagnetic part of the x component of the current density at point l in the Heisenberg representation,

$$j_x(l,t) = \exp(i\hat{H}_c t)j_x(l)\exp(-i\hat{H}_c t),$$

and $K_x(l)$ is the operator of the kinetic energy density for motion along the x axis. In the case of a disordered system, these operators can be written as

$$j_x(l) = i\sum_\sigma t_{l+l_x,l}(a_{l+l_x,\sigma}^\dagger a_{l,\sigma} - a_{l,\sigma}^\dagger a_{l+l_x,\sigma}),$$

$$K_x(l) = -\sum_\sigma t_{l+l_x,l}(a_{l+l_x,\sigma}^\dagger a_{l,\sigma} + a_{l,\sigma}^\dagger a_{l+l_x,\sigma}).$$

Considering that $\Lambda_{xx}(\mathbf{q}, \omega)$ is a complex-valued function, we obtain from Eq. (9)

$$\sigma_1(\omega) = \mathrm{Re}\,\sigma_{xx}(\omega) = 2\pi e^2 D\delta(\omega) + \frac{e^2}{\omega}\mathrm{Im}\,\Lambda_{xx}(0,\omega),$$

where

$$D = \frac{\langle -K_x\rangle}{2} - \frac{1}{2}\mathrm{Re}\,\Lambda_{xx}(0, \omega\to 0)$$

is the Drude weight.

In the calculation of conductivity, the main problem is the determination of the quantum-statistical mean of the commutator in expression (10). We can show that for determining $\Lambda_{xx}(\mathbf{q}, \omega)$, it is sufficient to calculate only the following mean value:

$$\langle j_x(l,t)j_x(l',0)\rangle$$
$$= -\bigg\langle\sum_\sigma t_{l+l_x,l}(a_{l+l_x,\sigma}^\dagger(t)a_{l,\sigma}(t) - a_{l,\sigma}^\dagger(t)a_{l+l_x,\sigma}(t))$$
$$\times\sum_{\sigma'} t_{l'+l_x',l'}(a_{l'+l_x',\sigma'}^\dagger(0)a_{l',\sigma'}(0) - a_{l',\sigma'}^\dagger(0)a_{l'+l_x',\sigma'}(0))\bigg\rangle.$$

Here, $a_{l,\sigma}(t)$ and $a_{l,\sigma}^\dagger(t)$ are the operators in the Heisenberg representation. After removing the parentheses, we obtain four terms with an analogous structure, which contain mean values of the four Fermi operators. In the cluster approach, these terms can be expressed in terms of the eigenvalues and eigenvectors of Hamiltonian $\hat{H}_c$ of an individual cluster (see Section 2). In particular, we write the general structure of the mean values considered here, omitting spin index σ for convenience:

$$\langle a_i^\dagger(t)a_j(t)a_{i'}^\dagger(0)a_{j'}(0)\rangle = \sum_{\eta\lambda'}U_{\eta\lambda'}\exp(it\rho_{\lambda'})U_{\lambda'i}^\dagger$$
$$\times\sum_{\nu\lambda}U_{j\lambda}\exp(-it\rho_\lambda)U_{\lambda\nu}^\dagger\langle a_\eta^\dagger a_\nu a_{i'}^\dagger a_{j'}\rangle.$$

Using the Wick theorem, we can write

$$\langle a_\eta^\dagger a_\nu a_i^\dagger a_{j'}\rangle = (\delta_{\eta\nu} - \langle a_\nu a_\eta^\dagger\rangle)(\delta_{i'j'} - \langle a_{j'} a_{i'}^\dagger\rangle)$$
$$+ (\delta_{\eta j'} - \langle a_{j'} a_\eta^\dagger\rangle)\langle a_\nu a_{i'}^\dagger\rangle,$$

where

$$\langle a_\nu a_\eta^\dagger\rangle = \sum_\lambda U_{\nu\lambda} \frac{1}{1 + \exp[-\beta(\rho_\lambda - \mu)]} U_{\lambda\eta}^\dagger.$$

Here, ρ_λ are the eigenvalues of cluster Hamiltonian $\hat{H}_c$, U is the matrix of the unitary transformation of $\hat{H}_c$ to the diagonal form, μ is the chemical potential, and $\beta = 1/k_B T$ is the reciprocal temperature.

After calculating all mean values, we obtain the following expression for the Fourier transform in the long-wave limit ($\mathbf{q} = 0$):

$$\langle j_x(0,t) j_x(0,0)\rangle$$
$$= \sum_{\lambda\neq\lambda'} \frac{\exp[it(\rho_\lambda - \rho_{\lambda'})]}{(1 + \exp[\beta(\rho_\lambda - \mu)])(1 + \exp[-\beta(\rho_{\lambda'} - \mu)])}$$
$$\times \left|\sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda})\right|^2.$$

Using this expression, we find

$$\Lambda_{xx}(q=0,\omega) = \mathrm{Re}\,\Lambda_{xx}(0,\omega) + i\,\mathrm{Im}\,\Lambda_{xx}(0,\omega),$$

where

$$\mathrm{Re}\,\Lambda_{xx}(0,\omega)$$
$$= \frac{2}{L}\sum_{\lambda\neq\lambda'} \frac{\left|\sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda})\right|^2}{(1 + \exp[\beta(\rho_\lambda - \mu)])(1 + \exp[-\beta(\rho_{\lambda'} - \mu)])}$$
$$\times \frac{(\rho_{\lambda'} - \rho_\lambda)}{(\rho_{\lambda'} - \rho_\lambda)^2 - \omega^2},$$

$$\mathrm{Im}\,\Lambda_{xx}(0,\omega) = \frac{\pi}{L}(1 - e^{-\beta\omega})$$
$$\times \sum_{\lambda\neq\lambda'} \frac{\left|\sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda})\right|^2}{(1 + \exp[\beta(\rho_\lambda - \mu)])(1 + \exp[-\beta(\rho_{\lambda'} - \mu)])}$$
$$\times \delta(\omega - (\rho_{\lambda'} - \rho_\lambda)).$$

Therefore, the real part of the conductivity has form

$$\sigma_1(\omega) = 2\pi e^2 D\delta(\omega) + \frac{e^2\pi(1 - e^{-\beta\omega})}{\omega L}$$
$$\times \sum_{\lambda\neq\lambda'} \frac{\left|\sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda})\right|^2}{(1 + \exp[\beta(\rho_\lambda - \mu)])(1 + \exp[-\beta(\rho_{\lambda'} - \mu)])} \quad (11)$$
$$\times \delta(\omega - (\rho_{\lambda'} - \rho_\lambda)),$$

where

$$D = \frac{\langle -K_x\rangle}{2} - \frac{1}{L}$$
$$\times \sum_{\lambda\neq\lambda'} \frac{\left|\sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda})\right|^2}{(1 + \exp[\beta(\rho_\lambda - \mu)])(1 + \exp[-\beta(\rho_{\lambda'} - \mu)])} \quad (12)$$
$$\times \frac{1}{(\rho_{\lambda'} - \rho_\lambda)}.$$

This expression is in full agreement with the definition of the real part of conductivity (8) at zero temperature. We can note that to within the temperature factors, the role of matrix element $\langle\phi_0|j_x|\phi_n\rangle$ in expressions (11) and (12) is played by the sum

$$\langle\lambda|j_x|\lambda'\rangle = \sum_l t_{l+l_x,l}(U_{\lambda',l}^\dagger U_{l+l_x,\lambda} - U_{\lambda',l+l_x}^\dagger U_{l\lambda}). \quad (13)$$

Using the cluster approach, we can also calculate the mean kinetic energy

$$\langle K_x\rangle = \frac{1}{L}\sum_\lambda \frac{1}{1 + \exp[-\beta(\rho_\lambda - \mu)]}$$
$$\times \sum_l t_{l+l_x,l}(U_{\lambda l}^\dagger U_{l+l_x,\lambda} + U_{\lambda,l+l_x}^\dagger U_{l\lambda}). \quad (14)$$

In the case of a finite temperature, we can formulate the following sum rule:

$$\int_{-\infty}^{\infty} \sigma_1(\omega)d\omega = e^2\pi\langle -K_x\rangle.$$

We can easily verify that conductivity $\sigma_1(\omega)$ obtained above satisfies this rule by integrating expression (11) with respect to frequency.

For calculating the conductivity of a disordered alloy, we must also perform averaging over different random cluster configurations. A certain cluster configuration can be obtained analogously to the procedure described in Section 2. Further, we evaluate sum (13) for each cluster configuration and perform averaging over all such configurations:

$$\overline{\langle\lambda|j_x|\lambda'\rangle} = \langle\langle\lambda|j_x|\lambda'\rangle\rangle_{\mathrm{conf}}.$$

An analogous averaging must also be carried out for mean kinetic energy $\langle K_x\rangle$. In this case, the sum appearing in expression (14) is averaged over random configurations of the cluster; namely,

$$\overline{\langle\lambda|K_x|\lambda\rangle} = \langle\langle\lambda|K_x|\lambda\rangle\rangle_{\mathrm{conf}},$$

where

$$\langle\lambda|K_x|\lambda\rangle = \sum_l t_{l+l_x,l}(U_{\lambda l}^\dagger U_{l+l_x,\lambda} + U_{\lambda,l+l_x}^\dagger U_{l\lambda}).$$

In this case, we form the full spectrum of all random cluster configurations $\{\bar{\rho}_\lambda\}$. The procedure of averaging over disorder proposed here can be treated as averaging of a certain supercluster consisting of noninteracting smaller clusters with a random distribution of ions of different species. This effectively increases the size of the region over which the averaging is performed and provides a better approximation in the case of a disordered alloy.

Thus, we obtain the mean values of the matrix element of current and of the kinetic energy of motion in direction x, which are substituted in expressions (11) and (12). Finally, for a disordered alloy, we get

$$
\sigma_1(\omega) = 2\pi e^2 D\delta(\omega) + \frac{e^2\pi(1 - e^{-\beta\omega})}{\omega L}
$$
$$
\times\sum_{\lambda\neq\lambda'}\frac{\overline{|\langle\lambda|j_x|\lambda'\rangle|^2}}{(1 + \exp[\beta(\bar{\rho}_\lambda - \mu)])(1 + \exp[-\beta(\bar{\rho}_{\lambda'} - \mu)])} \quad (15)
$$
$$
\times\delta(\omega - (\bar{\rho}_{\lambda'} - \bar{\rho}_\lambda)),
$$

where

$$
D = \frac{\langle -K_x \rangle}{2} - \frac{1}{L}
$$
$$
\times\sum_{\lambda\neq\lambda'}\frac{\overline{|\langle\lambda|j_x|\lambda'\rangle|^2}}{(1 + \exp[\beta(\bar{\rho}_\lambda - \mu)])(1 + \exp[-\beta(\bar{\rho}_{\lambda'} - \mu)])} \quad (16)
$$
$$
\times\frac{1}{(\bar{\rho}_{\lambda'} - \bar{\rho}_\lambda)},
$$

$$
\langle K_x \rangle = \frac{1}{L}\sum_\lambda\frac{\overline{\langle\lambda|K_x|\lambda\rangle}}{(1 + \exp[-\beta(\bar{\rho}_\lambda - \mu)])}. \quad (17)
$$

In the cluster approach, we calculate the conductivity of a disordered binary alloy in the Kubo formalism using expressions (15)−(17). The results of such a calculation of conductivity for a 50×50 cluster as a function of the number of particles in the system or the position of the chemical potential are shown in Fig. 6 in the limit $\omega \to 0$ at $T = 50$ K for $\Delta = -0.5, 0, 0.5$ eV. Figure 6l shows for comparison the results of the same calculation for a system with one species of ions ($x = 0$). These curves were obtained after approximation of data according to Gauss, which had to be done for eliminating the effects associated with the finiteness of the cluster. In all figures, the conductivity is given in the units of $\sigma_0 = e^2/\hbar$.

In the Boltzmann formalism (τ approximation), the dynamic conductivity has form

$$
\sigma_{ij}(\omega, \mu, T) = e^2\sum_\lambda\int\frac{d\mathbf{k}}{4\pi^3}
$$
$$
\times\frac{v_{\lambda i}(\mathbf{k})v_{\lambda j}(\mathbf{k})\left(-\frac{\partial n_F(\varepsilon, \mu, T)}{\partial\varepsilon}\right)_{\varepsilon=\varepsilon_\lambda(\mathbf{k})}}{1/\tau_\lambda(\mathbf{k}) - i\omega}, \quad (18)
$$

where $v_{\lambda i}(\mathbf{k}) = \hbar^{-1}\partial\varepsilon_\lambda(\mathbf{k})/\partial k_i$ is the group velocity of electrons (quasiparticles), $\tau_\lambda(\mathbf{k}) \sim 1/\Sigma''(\varepsilon_\lambda(\mathbf{k}))$ is the mean free time, λ is the band index, and n_F is the Fermi−Dirac distribution function. Expression (18) is the corollary of the more general quantum-kinetic Boltzmann equation for electrical conductivity [26]:

$$
\sigma_{\mu\nu} = e^2\int\frac{d^3p}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}v_{\mathbf{p}\mu}v_{\mathbf{p}\nu}
$$
$$
\times\left(-\frac{dn_F(\omega)}{d\omega}\right)A(\mathbf{p}, \omega)\Lambda(\mathbf{p}, \omega),
$$
$$
\mathbf{v_k}\Lambda(\mathbf{k}, \omega) = \frac{1}{2}A(\mathbf{k}, \omega)\mathbf{v_k} + \frac{n_i}{2\Gamma(\mathbf{k}, \omega)} \quad (19)
$$
$$
\times\int\frac{d^3p}{(2\pi)^3}|T_{\mathbf{kp}}|^2 A(\mathbf{p}, \omega)\mathbf{v_p}\Lambda(\mathbf{p}, \omega),
$$

where $T_{\mathbf{kp}}$ is the matrix of charge carriers scattering from impurities,

$$
2\Gamma(\mathbf{k}, \omega) = n_i\int\frac{d^3p}{(2\pi)^3}|T_{\mathbf{pk}}|^2 A(\mathbf{p}, \omega),
$$

n_i is the impurity concentration, and $A(\mathbf{p}, \omega)$ is the spectral weight of quasiparticles. The scattering matrix is connected with the self-energy part by relation $\Sigma(\mathbf{p}, \omega_\mathbf{p}) = n_i T_{\mathbf{pp}}$. These expressions show that the evaluation of mass operator Σ in the cluster approximation (see Section 2) makes it possible to use expression (18) and more general expression (19) for determining conductivity.

Figure 6 shows the results of calculation of the dispersion (Figs. 6a−6c), density of states (Figs. 6e−6g) and conductivity (Figs. 6i−6k) of a disordered binary alloy using the cluster approach for $\Delta = -0.5, 0, 0.5$ eV. Figs. 6d, 6h, and 6l show for comparison the results of calculation for a system with a single species of ions ($x = 0$). In this case, mean free time τ is independent of wavevector $\mathbf{k}$ since there is no disorder in the system. The conductivity as a function of the position of chemical potential μ (number of particles in the system) was calculated in the limit $\omega \to 0$ at $T = 50$ K. Blue circles in Figs. 6i−6l are the results of calculation of conductivity in the cluster perturbation theory for a 16×16 cluster in Boltzmann formalism (18), while red triangles are the results of calculation in the Kubo formalism (15)−(17) for a 50×50 cluster. All curves in Figs. 6 are the result of averaging over 20 random cluster configurations.

It can clearly be seen from Figs. 6a−6d that the existence of disorder in the system leads to dispersion broadening, which is nonuniform in wavevector $\mathbf{k}$ and depends on parameter Δ. For $\Delta = -0.5$ eV, the strongest broadening occurs near point $(0, 0)$ and gradually decreases towards point (π, π). For $\Delta = 0.5$ eV, an analogous behavior is observed in the opposite direction (from point (π, π) to point $(0, 0)$). At $\Delta = 0$, slight dispersion broadening is also observed, but now it is sym-
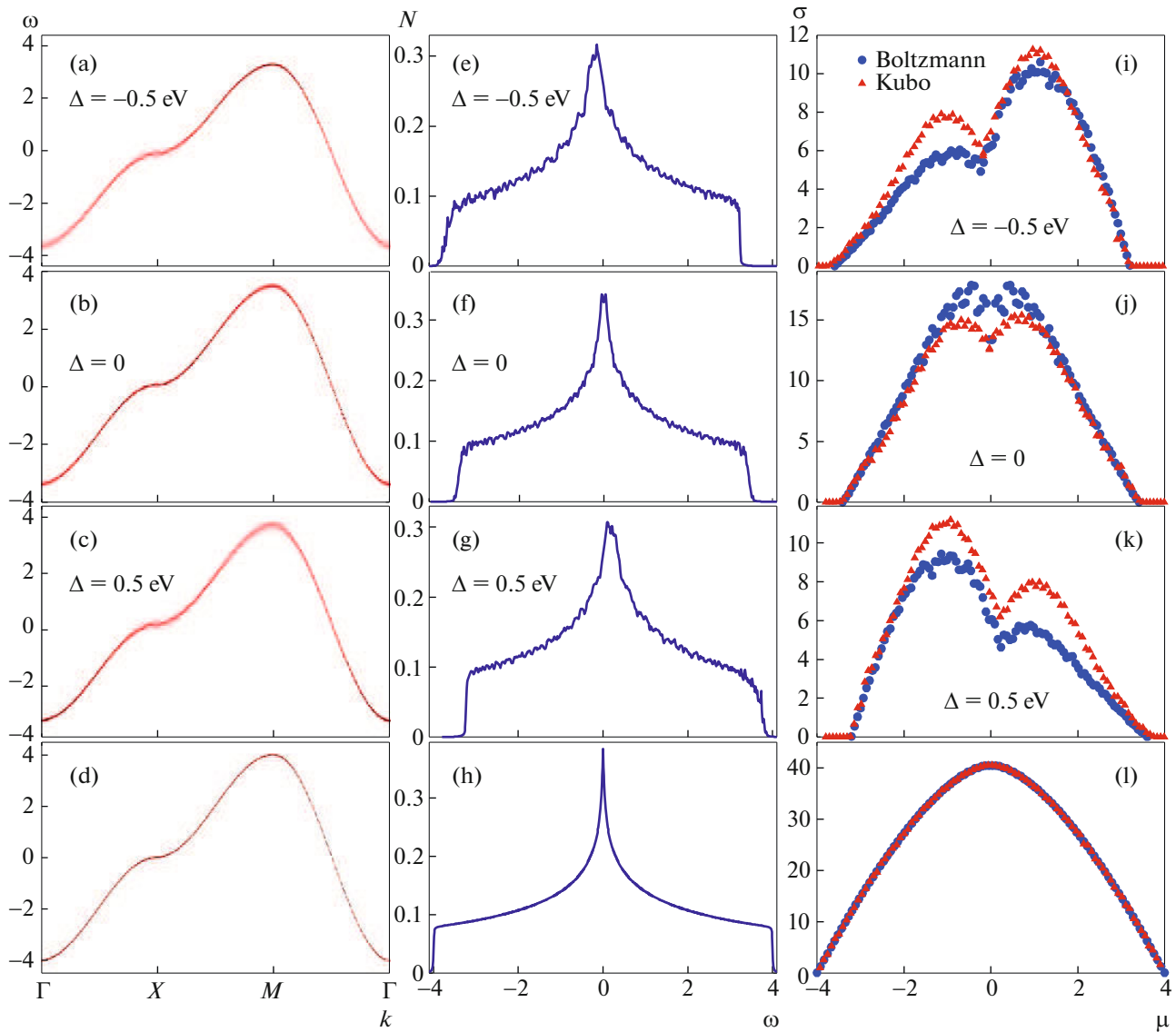
Fig. 6. Dispersion, density of states, and conductivity of a disordered binary alloy in the cluster approach for $\Delta = -0.5, 0, 0.5$ eV. Lower panels show for comparison the results of calculation for a system with one species of ions ($x = 0$). The conductivity depending on the position of chemical potential μ (number of particles in the system) was obtained in the limit $\omega \to 0$ at $T = 50$ K in the Boltzmann formalism for a 16×16 cluster (blue circles) and in the Kubo formalism for a 50×50 cluster (red triangles). Averaging was performed over 20 random cluster configurations.

metric relative to $\omega = 0$ (the broadening near points $(0, 0)$ and (π, π) is the same). Our calculations show that asymmetry in dispersion broadening (and, hence, in the mean free time) is determined by parameter Δ, and the value of broadening depends not only on the value of random potential, but also on the nonuniformity of the hopping parameter. In this case, a logarithmic singularity is observed in the density of states for any value of Δ (see Figs. 6e–6g).

Comparison of the curves in Figs. 6i–6k shows that the calculations based on the cluster approach in the two different formalisms lead to the qualitatively the same behavior of conductivity. Quantitative differ-

ences are due to a small size of the cluster (50×50) used in calculations in the Kubo formalism as compared to the number of points in the first Brillouin zone (600×600) used in the calculations based on the Boltzmann formalism. In the case of a homogeneous system without disorder, the results coincide quantitatively (Fig. 6l). The effect of parameter Δ on the dispersion broadening is clearly manifested in the $\sigma(\mu)$ dependences of the conductivity. For $\Delta = 0$, the curve is symmetric about the middle of the zone, while for $\Delta \neq 0$, there appears asymmetry.

The important result of our calculations is that in the presence of disorder (impurities) in the system, the

logarithmic singularity in the density of states is preserved (see Fig. 6), but conductivity $\sigma(\mu)$ has a dip (even for $\Delta = 0$) associated with scattering of carriers.

4. DISCUSSION AND CONCLUSIONS

Generalizing our results, we can indicate the main advantages and disadvantages of the proposed method. The disadvantages obviously include (i) computational limitations determining the maximal possible size of the cluster and (ii) limitations associated with the use of the tight binding method. The advantages include the possibility of implementation of the main idea of the proposed method in the algorithm of the DFT calculations for actual compounds. In addition, this method makes it possible to analyze diversified systems such as disordered and ordering alloys, systems with strong electron correlations and the electron−phonon interaction, magnetic alloys, and various systems with a short-range order, which experience phase separation (spatially inhomogeneous systems). For the latter systems, the limitations associated with the cluster size are most important.

In this study, we have reported on the results of calculations of the electronic band structure and conductivity of a binary alloy in the absence of the electron−electron interaction, when the band structure is independent of temperature and the number of electrons in the system (i.e., the "rigid band" approximation holds). The cluster approach used in this study has made it possible to perform calculations for quite large clusters, which is essential in analysis of disordered systems. In particular, the simulation of the ordered phase in a disordered surrounding has revealed the emergence of a pseudogap in the spectrum for energies corresponding to the boundary of the Brillouin zone for a fully ordered alloy. Therefore, in the case of half-filling, an insulator−poor metal−metal transition will be observed upon an increase of disorder.

Comparison of the results of calculation of conductivity using the cluster perturbation theory in the Boltzmann formalism and in the Kubo formalism for quite large clusters shows good agreement. Since the calculations based on the Kubo formalism were exact (but for a finite cluster), we can state that the application of the mean-free-time approximation in the Boltzmann formalism (i.e., representation of relaxation time $\tau(\mathbf{k})$ in terms of the reciprocal imaginary part of the mass operator obtained using the cluster approach) is a quite good approximation for analyzing disordered systems. It should be noted that such an approximation is not obvious because the relaxation time in the Boltzmann equation is a more complex quantity [26].

It is found that in the presence of disorder (impurities) in the system, the $\sigma(\mu)$ dependence of the static conductivity has a dip in the low-temperature limit, which is associated with charge carrier scattering;

however, the logarithmic singularity in the density of states is preserved in this case. In our opinion, such a behavior of the conductivity can be treated as a manifestation of localization appearing in the system.

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