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# Tight-binding model in the theory of disordered crystals

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This paper presents a new method of describing electronic spectrum, thermodynamic potential, and electrical conductivity of disordered crystals based on the Hamiltonian of multi-electron system and diagram method for Green's functions finding. Electronic states of a system were described by multi-band tight-binding model. The Hamiltonian of a system is defined on the basis of the wave functions of electron in the atom nucleus field. Electrons scattering on the oscillations of the crystal lattice are taken into account. The proposed method includes long-range Coulomb interaction of electrons at different sites of the lattice. Precise expressions for Green's functions, thermodynamic potential and conductivity tensor are derived using diagram method. Cluster expansion is obtained for density of states, free energy, and electrical conductivity of disordered systems. We show that contribution of the electron scattering processes to clusters is decreasing along with increasing number of sites in the cluster, which depends on small parameter. The computation accuracy is determined by renormalization precision of the vertex parts of the mass operators of electron-electron and electron-phonon interactions. This accuracy also can be determined by small parameter of cluster expansion for Green's functions of electrons and phonons.

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## 1. Introduction

Progress in describing of disordered systems is strongly connected with development of electron theory. Substitution alloys are best described among disordered systems. Traditional knowledge about physical properties of alloys is based on Born approximation of the scattering theory. But this approach obviously cannot be applied in case of a large scattering potential difference of components that holds for the description of alloys with simple, transition, and rare-earth elements. The same difficulty relates the pseudopotential method.[1] Because of non-local nature of pseudopotential, the problem of pseudopotential transferability exists. It is impossible to use nuclear potentials determined by the properties of some systems to describe other systems. Because of using theory of Vanderbilt ultra-soft potentials[2,3] and method of projector-augmented waves proposed by Blochl,[3,4] in investigations of electronic structure and properties of the system have been achieved fundamental progress. Significant success in the study of electronic structure and properties of the systems achieved recently because of the use of ultra-soft pseudopotential Vanderbilt[2,3] and the method of projector-augmented waves in density functional theory proposed by Blochl.[3,4] This approach was developed further because of use of the generalized gradient approximation in density functional theory of multi-electron systems, developed at Perdew works.[5−9] In projector-augmented waves approach, the wave function of valence states of electron (all-electron orbital) is expressed by using the conversion through the pseudo orbital. Pseudo orbital expands to pseudo partial waves in the augment area. Even so all-electron orbital in the same area is expanded with the same coefficients via partial waves, described by Kohn–Sham equation. Expression for pseudo Hamiltonian which we have in equation for pseudo wave function is derived by minimizing the full energy functional. Using this equation and expanding pseudo orbital by plane waves, we can derive set of equations for expansion coefficients. From this system it is possible to get electron energetic spectrum, wave functions, and value of the full energy functional. It is shown in Ref. 9 the way to use this method for describing the electron structure of crystals, using VASP program package. Using cluster methods of calculation and GAUSSIAN program package, this approach could be used for description molecule electronic structure.

It should be noted, recently in Refs. 9–16 simple effective calculation method of electronic structure and properties for big molecules had been proposed. This method is based upon tight-binding model and functional density theory, which includes long-range Coulomb interaction of electrons on different sites of crystal lattice. Long-range Coulomb interaction of electrons on different sites is described in the local density approximation.

But mentioned methods[5−16] are used only for description of ideal ordered crystals and molecules.

In disordered crystals, effects associated with localized electronic states and lattice vibrations occur. They cannot be described in a model of an ideal crystal. In this regard, other approaches are developing too.

Essential achievement in description of properties of disordered systems is connected with application of tight binding model in the multi-electron scattering, including approximation of coherent potential. Starting from Slater's and Koster's work,[17,18] there was wide use of the tight binding model in electronic structure calculations and in description of ideal crystals properties. Later it was generalized for the case of disordered systems.

In Refs. 19 and 20, method of describing magnetic alloys, electronic structure based on functional density theory is proposed. The effective potential in Kohn–Sham equation[21,22] consists of atomic potential and Pauli addition, which is expressed through magnetic field induction. Atomic potential and induction of magnetic field are expressed through variational derivative of exchange-correlation energy by electronic density and magnetization, respectively. Calculations of electronic structure of magnetic alloy are based on already mentioned effective mass potentials using the self-consistent Korringa–Kohn–Rostoker coherent potential approximation, but more developed in Refs. 23–25. In Ref. 19 proposed a method of calculating the parameters of interatomic pair correlations due to the pair mixing potential, which is expressed through the second derivative of the thermodynamic potential of the alloy concentration.[26] This thermodynamic potential is calculated in one site coherent potential approximation. It should be noted that the methods developed in Refs. 17–19, 23–25, do not include long-range Coulomb interaction of electrons at different lattice sites.

For calculations of energetic spectrum, free energy and electroconductivity of disordered crystals in our work developed multi scattering theory based on Green's functions. Electronic correlations in crystal are described in multiband tight-binding model. It includes wave functions and atomic potentials recalculation with taking into account electronic density redistribution as a result of atomic interaction. The model includes long-range Coulomb interaction of electrons on different sites of crystal lattice. The wave functions of noninteracting atoms are calculated based on Kohn–Sham equation using Perdew potentials.[5–9] Electron scattering processes on the ionic core potentials of different sorts and on oscillations of crystal lattice are taken into account. Calculations of two-time Green's functions based on temperature Green's functions.[27]

This uses a known relation between spectral representation for two-time and temperature Green's function.[28]

Calculation of two-time Green's function of disordered crystal is based on diagram technics, analogous to diagram technic for homogeneous system.[28] Set of equations for temperature Green's function, expressions for free energy and electoconductivity of solids are derived. Accuracy of the energetic spectrum calculation, free energy, and crystal conductivity calculations is based on renormalization of vertex parts of the electron-electron and electron-phonon mass operators.

## 2. Hamiltonian of Electrons and Phonons System for Disordered Crystals

Hamiltonian of disordered system (alloy, disordered semiconductor) consists of Hamiltonian of electrons in the external nucleus field, the Hamiltonian of electron-electron interaction, the Hamilton of nucleus, and the Hamiltonian of electron-nucleus interaction. Motion of ion subsystem reduces to nucleus oscillations near equilibrium position under the influence of nucleus interaction force and their indirect interaction through electrons. In the Wannier representation, the system Hamiltonian is:[27]

$$H = H_0 + H_{\text{int}}, \tag{1}$$

where zero-order Hamiltonian

$$H_0 = H_e^{(0)} + H_{ph}^{(0)}, \tag{2}$$

consists of the Hamiltonian of the electrons in the field of cores of atoms ideal ordered crystal.

$$H_e^{(0)} = \sum_{\substack{ni\gamma \\ n'i'\gamma'}} h_{ni\gamma,n'i'\gamma'}^{(0)} a_{ni\gamma}^+ a_{n'i'\gamma'}, \tag{3}$$

and the harmonic phonon Hamiltonian for the motion of the cores of atoms ideal ordered crystal

$$H_{ph}^{(0)} = \sum_{ni\alpha} \frac{P_{ni\alpha}^2}{2M_i} + \frac{1}{2} \sum_{\substack{ni\alpha \\ n'i'\alpha'}} \Phi_{ni\alpha,n'i'\alpha'}^{(0)} u_{ni\alpha} u_{n'i'\alpha'}. \tag{4}$$

Here, the cores of atoms are located on a periodic lattice (i.e., the unperturbed system is periodically ordered and has no disorder). The symbol $n$ denotes the unit cell, $i$ denotes $i$th basis vector in the $n$th unit cell, and $\gamma$ denotes all of the other quantum numbers for the orbital, including spin. Disorder will enter for the species of core at a particular lattice site, which need not be periodic via a perturbed Hamiltonian term (see below). The symbol $h^{(0)}$ denotes the "hopping integral" that connects the respective orbitals. For the phonon Hamiltonian, $n$ and $i$ are the same as before, namely the unit cell and basis site within the unit cell, while $\alpha$ is a spatial direction ($x, y,$ or $z$). $P_{ni\alpha}$ is the core momentum, $M_i$ is the mass of the core, $u_{ni\alpha}$ is the deviation of the core from the equilibrium position of the lattice site, and $\Phi_{ni\alpha,n'i'\alpha'}^{(0)}$ is the corresponding spring-constant matrix.

The interaction Hamiltonian in Eq. (1) is the perturbation of the system due to all of the effects we will be including. It is composed of six pieces:

$$H_{\text{int}} = \delta\Phi + H_{ec} + H_{eph} + H_{ee} + H_{phc} + H_{phph}, \tag{5}$$

$\delta\Phi$ is the modification of the core-core Coulomb interaction due to the disordered atoms added to the system; it is the difference between the original core-core repulsion Hamiltonian and the new one. The electronic Hamiltonian is modified by

the term

$$H_{ec} = \sum_{\substack{ni\gamma \\ n'i'\gamma'}} w_{ni\gamma,n'i'\gamma'} a^{+}_{ni\gamma} a_{n'i'\gamma'} \tag{6}$$

which is the difference between the new hopping Hamiltonian and the original periodic one. The electron-phonon interaction is given by

$$H_{eph} = \sum_{\substack{ni\gamma \\ n'i'\gamma'}} v'_{ni\gamma,n'i'\gamma'} a^{+}_{ni\gamma} a_{n'i'\gamma'} \tag{7}$$

It is described in more detail below. The Hamiltonian of the Coulomb interaction between electrons is given by the term

$$H_{ee} = \frac{1}{2} \sum_{\substack{n_1,n_2 \\ n_3,n_4}} v^{(2)n_1,n_2}_{n_3,n_4} a^{+}_{n_1} a^{+}_{n_2} a_{n_3} a_{n_4} \, , \tag{8}$$

$$n = (ni\gamma) \, .$$

The modification of the interaction of the phonons with the cores caused of the disordering of the atoms is given by

$$H_{phc} = \frac{1}{2} \sum_{\substack{ni\alpha \\ n'i'\alpha'}} \Delta M^{-1}_{ni\alpha,n'i'\alpha'} P_{ni\alpha} P_{n'i'\alpha'}$$

$$+ \frac{1}{2} \sum_{\substack{ni\alpha \\ n'i'\alpha'}} \Delta\Phi_{ni\alpha,n'i'\alpha'} u_{ni\alpha} u_{n'i'\alpha'} \, , \tag{9}$$

where

$$\Delta M^{-1}_{ni\alpha,n'i'\alpha'} = \left( \frac{1}{M_{ni'}} - \frac{1}{M_i} \right) \delta_{nn'} \delta_{ii'} \delta_{\alpha\alpha'} \, , \tag{10}$$

$\Delta\Phi_{ni\alpha,n'i'\alpha'} = \Phi_{ni\alpha,n'i'\alpha'} - \Phi^{(0)}_{ni\alpha,n'i'\alpha'}$, and $M_{ni}$, $M_i$ are the masses of the atoms at site $(ni)$ for disordered and ordered alloy, respectively.

We also include the cubic anharmonic potential terms for the phonons (under the assumption that they remain small and can be treated perturbatively) via

$$H_{phph} = \frac{1}{3!} \sum_{\substack{ni\alpha \\ n'i'\alpha' \\ n''i''\alpha''}} \Phi_{ni\alpha,n'i'\alpha',n''i''\alpha''} u_{ni\alpha} \times u_{n'i'\alpha'} u_{n''i''\alpha''} \, . \tag{11}$$

The operators $a^{+}_{ni\gamma}$, $a_{ni\gamma}$ create and destroy electrons in the state described by Vane's function $\phi_{ni\gamma}(\xi) = \langle \xi | ni\gamma \rangle$, where $\xi = (\mathbf{r}, \sigma')$ are the spatial and $z$-component of spin coordinates of the wave function.

To construct Wannier functions, we use analytical expressions for the wave functions $\psi_{ni\delta}(\mathbf{r} - \mathbf{r}_{ni})$ of an electron in the field of nuclei of atoms of type $\lambda$ localized at the lattice sites $(ni)$ of a perfectly ordered crystal. Here $\delta = \tilde{\varepsilon}lm$ is a superindex

which incorporates the quantum numbers for the principle energy eigenvalue $\tilde{\varepsilon}$, the standard angular momentum quantum numbers $l$ and $m$, $\mathbf{r}$ is the electron position vector, $\mathbf{r}_{ni}$ is the position vector for the atom at site $(ni)$ in equilibrium.

$$\mathbf{r}_{ni} = \mathbf{r}_n + \boldsymbol{\rho}_i \,,$$

$$\mathbf{r}_n = \sum_{\nu} l_{\nu} \mathbf{a}_{\nu} \,, \tag{12}$$

$\mathbf{r}_n$ is the position vector of the node n of the crystal lattice, $\boldsymbol{\rho}_i$ is the vector of the relative position of the node of the sublattice i in the unit cell $n$. Vectors $\boldsymbol{\rho}_i$ are called basic translation vectors of the crystal lattice, the number of which is determined by the dimension of the crystal. The coordinates $l_{\nu}$ of the radius vector of the crystal lattice $\mathbf{r}_n$ node are integers.

Basis orthogonalization performed with Lowdin method:[29]

$$\left| \tilde{\psi}_{ni\delta} \right\rangle = S^{-1/2} \left| \psi_{ni\delta} \right\rangle, \ S_{ni\delta,n'i'\delta'} = \langle \psi_{ni\delta} \psi_{n'i'\delta'} \rangle \,, \tag{13}$$

where $S_{ni\delta,n'i'\delta'}$ are overlapping matrix.

Vane's functions $\phi_{ni\gamma}(\mathbf{r}, \sigma')$, on which Hamiltonian of the system is represented as in Eq. (1), are defined from equation:

$$\phi_{ni\gamma}(\mathbf{r}, \sigma') = \tilde{\psi}_{ni\delta}(\mathbf{r} - \mathbf{r}_{ni})\chi_{\sigma}(\sigma') \,, \tag{14}$$

where $\chi_{\sigma}(\sigma')$-spin part of wave function, $\gamma = \delta\sigma$.

The orthogonized wave function can be represented as:

$$\tilde{\psi}_{ni\delta}(\mathbf{r} - \mathbf{r}_{ni}) = \tilde{R}_{i\delta}(|\mathbf{r} - \mathbf{r}_{ni}|)Y_{lm}(\widehat{\mathbf{r} - \mathbf{r}_{ni}}) \,,$$

$$Y_{lm}(\widehat{\mathbf{r} - \mathbf{r}_{ni}}) = Y_{lm}(\theta, \varphi) \,, \tag{15}$$

where $\theta, \varphi$ are the angular spherical coordinates of the vector $r - r_{ni}$.

The radial part of the wave function is given by the equation

$$\tilde{R}_{i\delta}(|\mathbf{r} - \mathbf{r}_{ni}|)Y_{lm}(\theta = 0, \varphi = 0) = \sum_{l_1^{(1)}, l_2^{(1)}, l_3^{(1)}, \delta_1} S_{n_1 i_1 \delta_1, ni\delta}^{-1/2} R_{\tilde{\varepsilon}_1 l_1}(r_1) Y_{l_1 m_1}(\theta_1, \varphi_1) \,. \tag{16}$$

In expression (16),

$$\mathbf{r}_1 = \mathbf{r} - \mathbf{r}_{n_1 i_1} = \mathbf{r} - \mathbf{r}_{ni} - \mathbf{r}_{n_1 i_1 i} \,, \tag{17}$$

$$\mathbf{r}_{n_1 i_1 i} = \mathbf{r}_{n_1 i_1} - \mathbf{r}_{ni} = (x_{n_1 i_1 i}^1, x_{n_1 i_1 i}^2, x_{n_1 i_1 i}^3) \,, \tag{18}$$

$$x_{n_1 i_1 i}^{\alpha} = \sum_{\nu} l_{\nu}^{(1)} a_{\nu}^{\alpha} + \rho_{i_1}^{\alpha} - \rho_i^{\alpha} \,, \tag{19}$$

$$r_1 = \left( r_{n_1 i_1 i}^2 + |\mathbf{r} - \mathbf{r}_{ni}|^2 - 2|\mathbf{r} - \mathbf{r}_{ni}| \, x_{n_1 i_1 i}^3 \right)^{1/2} \,, \tag{20}$$

$$\theta_1 = \pi - \arccos \frac{r_{n_1 i_1 i}^2 - r^2 - r_1^2}{2rr_1} \,, \tag{21}$$

$$\varphi_1 = \pi - arctg \frac{x_{n_1 i_1 i}^2}{x_{n_1 i_1 i}^1} \,, \tag{22}$$

Here it is taken into account that the coordinates of the radius vector of the crystal lattice site $\mathbf{r}_n$ are equal $l_\nu = 0$. In expression (18), $x^1_{n_1 i_1 i}/r_{n_1 i_1 i}, x^2_{n_1 i_1 i}/r_{n_1 i_1 i}$, $x^3_{n_1 i_1 i}/r_{n_1 i_1 i}$ there are projections of a unit vector directed along the vector $\mathbf{r}_{n_1 i_1} - \mathbf{r}_{ni}$, which are called directing cosines $l_{n_1 i_1 i}, m_{n_1 i_1 i}, n_{n_1 i_1 i}$. The overlap matrix $S_{ni\delta, n'i'\delta'}$ is found from the equation:

$$S_{n_1 i_1 \delta_1, n_2 i_2 \delta_2} = \iiint R_{\bar{\varepsilon}_1 l_1}(r_1) Y^*_{l_1 m_1}(\theta_1, \varphi_1) R_{\bar{\varepsilon}_2 l_2}(r_2) Y_{l_2 m_2}(\theta_2, \varphi_2) r_1^2$$
$$\times \sin\theta_1 dr_1 d\theta_1 d\varphi_1 . \tag{23}$$

In expression (23),

$$\mathbf{r}_1 = \mathbf{r} - \mathbf{r}_{n_1 i_1}, \mathbf{r}_2 = \mathbf{r} - \mathbf{r}_{n_2 i_2} = \mathbf{r}_1 - \mathbf{r}_{n_2 i_2 i_1} ,$$

$$r_2 = \left( \left( x_1^1 - x^1_{n_2 i_2 i_1} \right)^2 + \left( x_1^2 - x^2_{n_2 i_2 i_1} \right)^2 + \left( x_1^3 - x^3_{n_2 i_2 i_1} \right)^2 \right)^{1/2} ,$$

$$x_1^1 = r_1 \sin\theta_1 \cos\varphi_1, x_1^2 = r_1 \sin\theta_1 \sin\varphi_1, x_1^3 = r_1 \cos\theta_1 ,$$

$$x^\alpha_{n_2 i_2 i_1} = \sum_\nu l^{(2)}_\nu a^\alpha_\nu + \rho^\alpha_{i_2} - \rho^\alpha_{i_1} , \tag{24}$$

$$\cos\theta_2 = \frac{r_1 \cos\theta_1 - x^3_{n_2 i_2 i_1}}{r_2} , \tag{25}$$

$$\varphi_2 = \arccos \frac{r_1 \sin\theta_1 \cos\varphi_1 - x^1_{n_2 i_2 i_1}}{r_2 (1 - \cos^2\theta_2)^{1/2}} . \tag{26}$$

To find the matrix $S^{-1/2}_{n_1 i_1 \delta_1, ni\delta}$ in expression (16), we find the Fourier transform of the matrix

$$S_{i\delta, i'\delta'}(\mathbf{k}) = \sum_{n'} S_{ni\delta, n'i'\delta'} e^{i\mathbf{k}(\mathbf{r}_{n'i'} - \mathbf{r}_{ni})} . \tag{27}$$

The vector $\mathbf{k}$ is defined by the expression

$$\mathbf{k} = \sum_\nu k_\nu \mathbf{b}_\nu , \tag{28}$$

$$(\mathbf{a}_\nu \mathbf{b}_{\nu'}) = 2\pi \delta_{\nu\nu'} ,$$

$\mathbf{b}_\nu$-basis vectors of translations of the reciprocal lattice.

Summing over $n'$ on the right-hand side of formula (27) is easy to do if we replace it according to (12) by summing over and use

$$\mathbf{k}(\mathbf{r}_{n'i'} - \mathbf{r}_{ni}) = \sum_{\alpha=1}^3 \sum_v k_v b_v^\alpha \left( \sum_{v'} l'_{v'} a^\alpha_{v'} + \rho^\alpha_{i'} - \rho^\alpha_i \right) . \tag{29}$$

The matrix $S_{ni\delta, n'i'\delta'}$ has an infinite rank. The rank of the matrix $S_{i\delta, i'\delta'}(\mathbf{k})$ is finite, which allows you to find the matrix $S^{-1/2}_{i\delta, i'\delta'}(\mathbf{k})$. The matrix $S^{-1/2}_{n_1 i_1 \delta_1, ni\delta}$ in expression (16) is found from the equation:

$$S^{-1/2}_{ni\delta, n'i'\delta'} = \frac{1}{N} \sum_{\mathbf{k}} S^{-1/2}_{i\delta, i'\delta'}(\mathbf{k}) e^{-i\mathbf{k}(\mathbf{r}_{n'i'} - \mathbf{r}_{ni})} . \tag{30}$$

Values $h^{(0)}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}$ in Eq. (3) are the matrix elements of the kinetic and potential energy $\sum_{ni} v^{\lambda i} (\mathbf{r} - \mathbf{r}_{ni})$ of electron in the field of cores of atoms ideal ordered crystal Values $h^{(0)}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}$ defined by expression:

$$h^{(0)}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2} = \varepsilon_{i_1 \tilde{\varepsilon}} \delta_{n_1 i_1 \delta_1, n_2 i_2 \delta_2} \delta_{\sigma_1, \sigma_2} + \sum_{l_1^{(3)}, l_2^{(3)}, l_3^{(3)}, i_3 \neq 0,0,0,i_1} v^{n_3 i_3}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}, \gamma = \delta \sigma \,, \tag{31}$$

$$v^{n_3 i_3}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2} = \iiint \tilde{R}_{i_1 \delta_1} (r_1) Y^*_{l_1 m_1} (\theta_1, \varphi_1) v^{i_3} (r_3) \tilde{R}_{i_2 \delta_2} (r_2) Y_{l_2 m_2}$$
$$\times (\theta_2, \varphi_2) r_1^2 \sin \theta_1 dr_1 d\theta_1 d\varphi_1 \delta_{\sigma_1, \sigma_2} \,, \tag{32}$$

$$\varepsilon_{i_1 \tilde{\varepsilon}} = -\frac{me^4 (Z_{i_1})^2}{2\hbar^2 \tilde{\varepsilon}^2}, \tilde{\varepsilon} = 1, 2, 3, \ldots, v^{i_3} (r_3) = -\frac{Z_{i_3} e^2}{r_3} \,. \tag{33}$$

In the formula (33), $m$, $e$ — the mass and charge of the electron, respectively, $Z_i$ are the ordinal number of an atom of the sort $\lambda$ located in the site $ni$ of an ideally ordered crystal $\hbar$-Planck's constant. The expression for $r_3$ are obtained from expression (24) for $r_2$ replacement $x^\alpha_{n_2 i_2 i_1}$ by $x^\alpha_{n_3 i_3 i_1}$.

The matrix element of the electron-ion interaction Hamiltonian in Eq. (6) is given by

$$w_{ni\gamma, n'i'\gamma'} = \sum_{n''i''} w^{n''i''}_{ni\gamma, n'i'\gamma'} \,, \tag{34}$$

where

$$w^{n''i''}_{ni\gamma, n'i'\gamma'} = \sum_\lambda c^\lambda_{n''i''} \, w^{\lambda n''i''}_{ni\gamma, n'i'\gamma'} \,, \tag{35}$$

$$w^{\lambda n''i''}_{ni\gamma, n'i'\gamma'} = v^{\lambda n''i''}_{ni\gamma, n'i'\gamma'} + \Delta v^{\lambda n''i''}_{ni\gamma, n'i'\gamma'} - v^{i''}_{ni\gamma, n'i'\gamma'} \,. \tag{36}$$

The symbol $v^{\lambda n''i''}_{ni\gamma, n'i'\gamma'}$ is a matrix element of the potential of the core of the atom $v^{\lambda i} (\mathbf{r} - \mathbf{r}_{ni})$.

Expression for $v^{\lambda n_3 i_3}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}$ obtained from formula (32) $v^{i_3} (r_3)$ by $v^{\lambda n''i''} (r_3)$ replacing. In Eq. (35), $c^\lambda_{ni}$ is a discrete binary random number taking the values of 1 or 0 depending on whether an atom of type $\lambda$ is at site $(ni)$ or not, respectively. The symbol $\Delta v^{\lambda n''i''}_{ni\gamma, n'i'\gamma'}$ will be defined next.

The expression for the electron-phonon interaction in Eq. (7) is found through derivatives of the potential energy of the electrons in the ion core field due to a displacement of the atom by the vector $\mathbf{u}_{ni}$. In Eq. (7), the value of $v'_{ni\gamma, n'i'\gamma'}$ is given by

$$v'_{ni\gamma, n'i'\gamma'} = \sum_{n''i''\alpha} v'^{n''i''\alpha}_{ni\gamma, n'i'\gamma'} u_{n''i''\alpha} \,, \tag{37}$$

where

$$v'^{n''i''\alpha}_{ni\gamma, n'i'\gamma'} = \sum_\lambda c^\lambda_{n''i''} v'^{\lambda n''i''\alpha}_{ni\gamma, n'i'\gamma'} \tag{38}$$

with $v'^{\lambda n'' i'' \alpha}_{n i \gamma, n' i' \gamma'}$ the matrix elements of the following operator

$$-\mathrm{e}_{n'' i'' \alpha} \frac{d}{d \left| \mathbf{r} - \mathbf{r}_{n'' i''} \right|} v^{\lambda i''} \left( \left| \mathbf{r} - \mathbf{r}_{n'' i''} \right| \right) ,$$

$$\mathrm{e}_{n'' i''} = \frac{\mathbf{r} - \mathbf{r}_{n'' i''}}{\left| \mathbf{r} - \mathbf{r}_{n'' i''} \right|} . \tag{39}$$

Expression for $v'^{\lambda n_3 i_3 \alpha}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}$ obtained from formula (32) replacing $v^{i_3} \left( r_3 \right)$ by

$$- \frac{\left( x_1^\alpha - x^\alpha_{n_3 i_3 i_1} \right)}{r_3} \frac{d}{d r_3} v^{\lambda n_3 i_3} \left( r_3 \right) . \tag{40}$$

The term $\Delta v^{\lambda n'' i''}_{n i \gamma, n' i' \gamma'}$ in Eq. (36) describes electron scattering on the static displacement of the atoms and is defined by the equation

$$\Delta v^{\lambda n'' i''}_{n i \gamma, n' i' \gamma'} = \sum_\alpha v'^{\lambda n'' i'' \alpha}_{n i \gamma, n' i' \gamma'} u^{s, \lambda}_{n'' i'' \alpha} , \tag{41}$$

where $u^{s, \lambda}_{n'' i'' \alpha}$ is the $\alpha$-projection of the static displacement of the atom of type $\lambda$ in the site $n'' i''$ caused by the difference in the atomic radii of the components of the disordered crystal.

Upon receipt of expressions (34)–(41), it was taken into account that potential energy operator of electron in the field of atoms core can be expressed: $v^{ni} \left( \mathrm{r} - \mathrm{r}'_{ni} \right)$, $\mathbf{r}'_{ni} = \mathbf{r}_{ni} + \mathbf{u}^s_{ni} + \mathbf{u}_{ni}$, where $\mathbf{r}$ — electron's radius vector, $\mathbf{r}_{ni}$ — radius-vector of atom's equilibrium position in site of crystal lattice $(ni)$, $\mathbf{u}^s_{ni}$ — vector of atom's static displacement from equilibrium position in site $(ni)$, $\mathbf{u}_{ni}$ — atoms displacement operator in site $(ni)$. Expanding $v^{ni} \left( \mathrm{r} - \mathrm{r}'_{ni} \right)$ the series in powers $u_{ni\alpha}$ and restricting ourselves to linear terms, we arrive at expressions (34)–(41).

The matrix of the force constants arising from the direct Coulomb interaction of the ionic cores has the form:

$$\Phi_{n i \alpha, n' i' \alpha'} = - \frac{Z_{ni} Z_{n' i'} e^2}{4 \pi \varepsilon_0 \left| \mathbf{r}_n + \boldsymbol{\rho}_i - \mathbf{r}_{n'} - \boldsymbol{\rho}_{i'} \right|^5}$$

$$\times \left[ 3 \left( r_{n\alpha} + \rho_{i\alpha} - r_{n'\alpha} - \rho_{i'\alpha} \right) \left( r_{n\alpha'} + \rho_{i\alpha} - r_{n'\alpha'} - \rho_{i'\alpha'} \right) \right. \tag{42}$$

$$\left. - \left| \mathbf{r}_n + \boldsymbol{\rho}_i - \mathbf{r}_{n'} - \boldsymbol{\rho}_{i'} \right|^2 \delta_{\alpha\alpha'} \right] , n i \neq n' i' .$$

where $Z_{ni}$ is the serial number of the atom located in the lattice site $ni$ of the disordered crystal, is given by the expression

$$Z_{ni} = \sum_\lambda c^\lambda_{ni} Z_i . \tag{43}$$

This matrix $\Phi_{n i \alpha, n' i' \alpha'}$ satisfies the following constraint:

$$\sum_{n' i'} \Phi_{n i \alpha, n' i' \alpha'} = 0 . \tag{44}$$

Matrix $\Phi_{ni\alpha,n'i'\alpha'}^{(0)}$ derived from expression for matrix $\Phi_{ni\alpha,n'i'\alpha'}$ in which $Z_{ni} = Z_i$. To calculate multicenter integrals $v_{n_3,n_4}^{(2)n_1,n_2}$, $n = (ni\gamma)$ in formula (8), we approximate atomic orbitals by Gaussian functions in accordance with the formula:

$$\tilde{R}_{i\delta}\left(|\mathbf{r} - \mathbf{r}_{ni}|\right) = \sum_{p} A_{i\delta}^{p} e^{-b_{pi\delta}\left((x^1 - x_{ni}^1)^2 + (x^2 - x_{ni}^2)^2 + (x^3 - x_{ni}^3)^2\right)}. \tag{45}$$

The product of two Gaussian functions centered on different sites can easily be reduced to one Gaussian function, the center of which in the general case does not coincide with the lattice site.[30] As a result, for multicenter integrals, we obtain the expression:

$$v_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}^{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2} = e^2 \delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3} \sum_{p_1, p_2, p_3, p_4} A_{i_1 \delta_1}^{p_1} A_{i_2 \delta_2}^{p_2} A_{i_3 \delta_3}^{p_3} A_{i_4 \delta_4}^{p_4}$$

$$\times \iint \frac{1}{|\mathbf{r}' - \mathbf{r}''|} R_{p_1 n_1 i_1 \delta_1, p_4 n_4 i_4 \delta_4}\left(|\mathbf{r}' - \mathbf{r}_{n_1 i_1, n_4 i_4}^c|\right) R_{p_2 n_2 i_2 \delta_2, p_3 n_3 i_3 \delta_3}$$

$$\times \left(|\mathbf{r}'' - \mathbf{r}_{n_2 i_2, n_3 i_3}^c|\right) Y_{l_1 m_1}^*\left(\mathbf{r}' - \mathbf{r}_{n_1 i_1}\right) Y_{l_2 m_2}^*\left(\mathbf{r}'' - \mathbf{r}_{n_2 i_2}\right)$$

$$\times Y_{l_3 m_3}\left(\mathbf{r}'' - \mathbf{r}_{n_3 i_3}\right) Y_{l_4 m_4}\left(\mathbf{r}' - \mathbf{r}_{n_4 i_4}\right) d^3 r'_1 d^3 r''_1. \tag{46}$$

In expression (46),

$$R_{p_1 n_1 i_1 \delta_1, p_4 n_4 i_4 \delta_4}\left(|r' - r_{n_1 i_1, n_4 i_4}^c|\right)$$

$$= \exp\left(-(b_{p_1 i_1 \delta_1} + b_{p_4 i_4 \delta_4})\left|r' - r_{p_1 n_1 i_1 \delta_1, p_4 n_4 i_4 \delta_4}^c\right|^2 + d_{p_1 n_1 i_1 \delta_1, p_4 n_4 i_4 \delta_4}\right), \tag{47}$$

$$R_{p_2 n_2 i_2 \delta_2, p_3 n_3 i_3 \delta_3}\left(|r'' - r_{n_2 i_2, n_3 i_3}^c|\right)$$

$$= \exp\left(-(b_{p_2 i_2 \delta_2} + b_{p_3 i_3 \delta_3})\left|r'' - r_{p_2 n_2 i_2 \delta_2, p_3 n_3 i_3 \delta_3}^c\right|^2 + d_{p_2 n_2 i_2 \delta_2, p_3 n_3 i_3 \delta_3}\right), \tag{48}$$

$$x_{p_1 n_1 i_1 \delta_1, p_2 n_2 i_2 \delta_2}^{\alpha c} = \frac{b_{p_1 i_1 \delta_1} x_{n_1 i_1}^{\alpha} + b_{p_2 i_2 \delta_2} x_{n_2 i_2}^{\alpha}}{b_{p_1 i_1 \delta_1} + b_{p_2 i_2 \delta_2}}, \tag{49}$$

$$d_{p_1 n_1 i_1 \delta_1, p_2 n_2 i_2 \delta_2} = (b_{p_1 i_1 \delta_1} + b_{p_2 i_2 \delta_2}) \sum_{\alpha} \left(x_{p_1 n_1 i_1 \delta_1, p_2 n_2 i_2 \delta_2}^{\alpha c}\right)^2$$

$$- b_{p_1 i_1 \delta_1} \sum_{\alpha} \left(x_{n_1 i_1}^{\alpha}\right)^2 - b_{p_2 i_2 \delta_2} \sum_{\alpha} \left(x_{n_2 i_2}^{\alpha}\right)^2, \tag{50}$$

$$x_{n_1 i_1}^{\alpha} = \sum_{\nu} l_{\nu}^{(1)} a_{\nu}^{\alpha} + \rho_{i_1}^{\alpha}, \quad x_{n_2 i_2}^{\alpha} = \sum_{\nu} l_{\nu}^{(2)} a_{\nu}^{\alpha} + \rho_{i_2}^{\alpha}. \tag{51}$$

In expression (49), $x_{p_1 n_1 i_1 \delta_1, p_2 n_2 i_2 \delta_2}^{\alpha c}$ are the coordinates of the center of the Gaussian orbital, to which the product of two Gaussian orbitals, centered on different sites $n_1 i_1$, $n_2 i_2$ is reduced.

Spherical harmonics in expression (46) are calculated by the formula:

$$Y_{l_1 m_1}^*\left(r' - r_{n_1 i_1}\right) = Y_{l_1 m_1}^*\left(\theta'_1, \varphi'_1\right), \tag{52}$$

$$Y_{l_4 m_4}\left(\mathbf{r}' - \mathbf{r}_{n_4 i_4}\right) = Y_{l_4 m_4}\left(\theta'_4, \varphi'_4\right), \tag{53}$$

$$Y^*_{l_2 m_2}\left(\mathbf{r}'' - \mathbf{r}_{n_2 i_2}\right) = Y^*_{l_2 m_2}\left(\theta''_2, \varphi''_2\right), \tag{54}$$

$$Y_{l_3 m_3}\left(\mathbf{r}'' - \mathbf{r}_{n_3 i_3}\right) = Y_{l_3 m_3}\left(\theta''_3, \varphi''_3\right). \tag{55}$$

In the formula (46),

$$\left|\mathbf{r}' - \mathbf{r}''\right| = \left(\sum_\alpha \left(x'^\alpha_1 - x''_1\alpha\right)^2\right)^{1/2}, \tag{56}$$

$$d^3 r'_1 = r'^2_1 \sin\theta'_1 dr'_1 d\theta'_1 d\varphi'_1, \tag{57}$$

$$d^3 r''_1 = r''^2_1 \sin\theta''_1 dr''_1 d\theta''_1 d\varphi''_1. \tag{58}$$

Using formulas (24)–(26), (32), integration in expression (46) can be performed numerically.

So, formulas (24)–(26), (32) describe the procedure for calculating matrix elements $h^{(0)}_{n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}$, $v^{(2)n_1 i_1 \gamma_1, n_2 i_2 \gamma_2}_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}$ Hamiltonian (1), containing one-electron and two-electron integrals.

The matrix elements $v^{(2)ni\gamma, n_2 i_2 \gamma_2}_{n_1 i_1 \gamma_1, n'i'\gamma'}$ in Eq. (46) for identical sites $(ni)$ are calculated by integrating over the corresponding angular variables. Integrals of the product of three spherical functions (a so-called Gaunt integral) are found by using Clebsch-Gordan coefficients.[31] This yields

$$v^{(2)ni\gamma, ni\gamma_2}_{ni\gamma_1, ni\gamma'}$$

$$= e^2 \delta_{\sigma\sigma'} \delta_{\sigma_2 \sigma_1} \sum_{\substack{|l-l'| \le l_3 \le l+l' \\ |l_2-l_1| \le l_3 \le l_2+l_1 \\ l+l'+l_3 = 2k, k_1 \in \mathbb{N} \\ l_2+l_1+l_3 = 2k_1, k_1 \in \mathbb{N}}} \frac{1}{2l_3 + 1} \left[\frac{(2l_3+1)(2l'+1)(2l_3+1)(2l_1+1)}{(2l+1)(2l_2+1)}\right]^{1/2}$$

$$\times c(l_3 l' l; 0, 0) c(l_3 l' l; m' - m, m') c(l_3 l_1 l_2; 0, 0) c(l_3 l_1 l_2; m_2 - m_1, m_1)$$

$$\times \sum_{p,p',p_1,p_2} A^p_{i\delta} A^{p'}_{i\delta'} A^{p_1}_{i\delta_1} A^{p_2}_{i\delta_2} \int_0^\infty dr_1 r_1^2 \exp - \left((b_{pi\delta} + b_{p'i\delta'}) r_1^2\right)$$

$$\times \int_0^{r_1} dr_2 r_2^2 \frac{r_2^{l_3}}{r_1^{l_3+1}} \exp - \left((b_{p_1 i\delta_1} + b_{p_2 i\delta_2}) r_2^2\right)$$

$$+ \int_0^\infty dr_2 r_2^2 \exp - \left((b_{p_1 i\delta_1} + b_{p_2 i\delta_2}) r_2^2\right)$$

$$\times \int_0^{r_2} dr_1 r_1^2 \frac{r_1^{l_3}}{r_2^{l_3+1}} \exp - \left((b_{pi\delta} + b_{p'i\delta'}) r_1^2\right), \tag{59}$$

where $l$ and $m$ are the standard angular momentum quantum numbers, $c(l''l'l; m'', m')$ are the standard Clebsch-Gordan coefficients.[31] Integration in formula (59) can be performed analytically.

## 3. Green's Functions of Electrons and Phonons System

We employ a Green's function based formalism to perform the calculations. Ultimately, we need the real-time retarded $G_r^{AB}(t, t')$ and advanced $G_\alpha^{AB}(t, t')$ Green's functions, which are each defined as follows:[32]

$$G_r^{AB}(t, t') = -\frac{i}{\hbar}\theta(t - t')\langle[\tilde{A}(t), \tilde{B}(t')]\rangle,$$

$$G_a^{AB}(t, t') = \frac{i}{\hbar}\theta(t' - t)\langle[\tilde{A}(t), \tilde{B}(t')]\rangle. \tag{60}$$

Here, the operators are expressed in the Heisenberg representation

$$\tilde{A}(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar}, \tag{61}$$

where $\hbar$ is Planck's constant, $H = H - \mu_e N_e$, $\mu_e$ is chemical potential of the electronic subsystem and $N_e$ is the electron number operator given by

$$N_e = \sum_{ni\gamma} a_{ni\gamma}^+ a_{ni\gamma}. \tag{62}$$

In addition, the commutator or anticommutator is defined via

$$[A, B] = AB \mp BA, \tag{63}$$

where the commutator is used for Bose operators $(-)$ and the anticommutator is used for Fermi operators $(+)$. The symbol $\theta(t)$ is Heaviside's unit step function. The angle brackets $\langle\ldots\rangle$ denote the thermal averaging with respect to the density matrix $\rho$

$$\langle A\rangle = \text{Tr}(\rho A), \quad \rho = e^{(\Omega - H)/\Theta}, \tag{64}$$

where $\Omega$ is thermodynamic potential of the system given by $\exp(\Omega/\Theta) = \text{Tr}\exp(-H/\Theta)$ and $\Theta = k_b T$, with $k_b$ Boltzmann's constant and $T$ the temperature. Note that even though the real-time Green's functions appear to depend on two different times, because of time-translational invariance for equilibrium systems, they actually depend only on the time difference $t - t'$.

Our procedure for calculating the real-time Green's functions follows the standard one—we first determine the thermal Green's functions (defined below) and then analytically continue them to real time using the conventional spectral relations.

The thermal Green's function are defined by

$$G^{AB}(\tau, \tau') = -\langle T_\tau \tilde{A}(\tau)\tilde{B}(\tau')\rangle, \tag{65}$$

where the imaginary-time operator $\tilde{A}(\tau)$ is derived from the real-time Heisenberg representation and the substitution $t = -i\hbar\tau$. Hence,

$$\tilde{A}(\tau) = e^{H\tau}Ae^{-H\tau}. \tag{66}$$

In addition, the time-ordering operator satisfies

$$T_r\tilde{A}(\tau)\tilde{B}(\tau') = \theta(\tau - \tau)\tilde{A}(\tau)\tilde{B}(\tau') + \pm\theta(\tau' - \tau)\tilde{B}(\tau')\tilde{A}(\tau), \tag{67}$$

where the plus sign is used for Bose operators and the minus sign for Fermi operators.

We next go to the interaction representation by introducing the operator

$$\sigma(\tau) = e^{H_0 \tau} e^{-H\tau} \,, \tag{68}$$

with $H = H_0 + H_{\text{int}}$ and $H_0 = H_0 - \mu_e N_e$.

Differentiating the expression for $\sigma(\tau)$ in Eq. (68) with respect to $\tau$ and then integrating from 0 with the boundary condition $\sigma(0) = 1$, we obtain:

$$\sigma(\tau) = T_\tau \exp\left[ -\int_0^\tau H_{\text{int}}(\tau') d\tau' \right] \,, \tag{69}$$

where $H_{\text{int}}(\tau) = e^{H_0 \tau} H_{\text{int}} e^{-H_0 \tau}$. Employing this result yields

$$\tilde{A}(\tau) = \sigma^{-1}(\tau) A(\tau) \sigma(\tau) \,, \tag{70}$$

with $A(\tau)$ in the Heisenberg representation with respect to the noninteracting Hamiltonian. Substituting these results into the definition of the thermal Green's function creates the alternate interaction-representation form for the Green's function, given by

$$G^{AB}(\tau, \tau') = -\frac{\langle T_\tau A(\tau) B(\tau') \sigma(1/\Theta) \rangle_0}{\langle \sigma(1/\Theta) \rangle_0} \,, \tag{71}$$

where all time dependence is with respect to the noninteracting Hamiltonian and the trace over all states is with respect to the noninteracting states

$$\langle A \rangle_0 = \text{Tr}(\rho_0 A), \quad \rho_0 = e^{(\Omega_0 - H_0)/\Theta} \,. \tag{72}$$

This last result forms the starting point for the perturbative expansion employed here.

The diagrammatic method is generated by expanding $\sigma(\tau)$ in a power series in terms of $H_{\text{int}}(\tau)$ and then using Wick's theorem to evaluate the resulting operator averages (since the noninteracting Hamiltonian is quadratic[28]). This technique then generalizes the approach used for the homogeneous system.[28] The denominator in Eq. (71) cancels all disconnected diagrams in the expansion, as usual. So the thermal Green's function are expanded in terms of connected diagrams. Using the standard relations between the spectral representations of thermal and real-time Green's functions,[30] we obtain the following Dyson equation for the electronic Green's function in the real frequency domain (hereinafter the dependence on $r$ is suppressed):[28]

$$G^{aa^+}(\varepsilon) = G_0^{aa^+}(\varepsilon) + G_0^{aa^+}(\varepsilon)\left(w + \Sigma_{eph}(\varepsilon) + \Sigma_{ee}(\varepsilon)\right) G^{aa^+}(\varepsilon)$$

$$G^{uu}(\varepsilon) = G_0^{uu}(\varepsilon) + G_0^{uu}(\varepsilon)\left(\Delta\Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon)\right)$$
$$\times G^{uu}(\varepsilon) + G_0^{uP}(\varepsilon)\Delta M^{-1} G^{Pu}(\varepsilon) \,,$$

$$G^{PP}(\varepsilon) = G_0^{PP}(\varepsilon) + G_0^{PP}(\varepsilon)\Delta M^{-1} G^{PP}(\varepsilon) + G_0^{Pu}(\varepsilon)$$
$$\times \left(\Delta\Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon)\right) G^{uP}(\varepsilon) \,,$$

$$G^{uP}(\varepsilon) = G_0^{uP}(\varepsilon) + G_0^{uP}(\varepsilon)\Delta M^{-1}G^{PP}(\varepsilon) + G_0^{uu}(\varepsilon)$$
$$\times \left(\Delta\Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon)\right)G^{uP}(\varepsilon),$$
$$G^{Pu}(\varepsilon) = G_0^{Pu}(\varepsilon) + G_0^{Pu}(\varepsilon)\left(\Delta\Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon)\right)$$
$$\times G^{uu}(\varepsilon) + G_0^{PP}(\varepsilon)\Delta M^{-1}G^{Pu}(\varepsilon), \tag{73}$$

where $\varepsilon = \hbar\omega$. Here $G^{aa^+}(\varepsilon)$, $G^{uu}(\varepsilon)$, $G^{PP}(\varepsilon)$, $G^{uP}(\varepsilon)$, $G^{Pu}(\varepsilon)$ are the real-frequency representation of the single-particle Green's function of the electrons, the coordinate-coordinate, momentum-momentum, coordinate-momentum, and momentum-coordinate Green's functions of the phonons, respectively; and $\Sigma_{eph}(\varepsilon)$, $\Sigma_{phe}(\varepsilon)$, $\Sigma_{ee}(\varepsilon)$, $\Sigma_{phph}(\varepsilon)$ are the corresponding self-energies (mass operators) for the electron-phonon, phonon-electron, electron-electron and phonon-phonon interactions.

The real-time and real-frequency Green's functions are related by standard Fourier transform relations given by,

$$G_{r,a}^{AB}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_{r,a}^{AB}(\omega)\ e^{-i\omega t}d\omega \tag{74}$$

and

$$G_{r,a}^{AB}(\omega) = \int_{-\infty}^{\infty} G_{r,a}^{AB}(t)\ e^{i\omega t}dt. \tag{75}$$

The thermal Green's functions are periodic (bosons) or antiperiodic (fermions) on the interval $-1/\Theta \leq \tau < 1/\Theta$, and hence have a Fourier series representation in terms of their Matsubara frequencies, as follows:

$$G^{AB}(\tau) = \Theta\sum_{\omega_n} G^{AB}(\omega_n)e^{-i\omega_n\tau} \tag{76}$$

and

$$G^{AB}(\omega_n) = \frac{1}{2}\int_{-1/\Theta}^{1/\Theta} G^{AB}(\tau)\ e^{i\omega_n\tau}d\tau, \tag{77}$$

where the Matsubara frequencies satisfy

$$\omega_n = \begin{cases} 2n\pi\Theta & \text{for Bose particles}, \\ (2n+1)\pi\Theta & \text{for Fermi particles}, \end{cases} \tag{78}$$
$$n = 0,\ \pm 1,\ \pm 2,\dots$$

Note that the thermal Green's functions are equal to the retarded Green's functions evaluated at the Matsubara frequencies for positive Matusbara frequencies and are equal to the advanced Green's functions evaluated at the Matsubara frequencies for negative Matsubara frequencies.

The electronic Green's functions are infinite matrices with indices given by the lattice site $n$, the basis site $i$, and the other quantum numbers $\gamma$. Similarly, the

phonon Green's functions also are infinite matrices with the same lattice and basis site dependence plus a dependence on the spatial coordinate direction $\alpha$. This produces some simple equations for the noninteracting Green's functions, namely.[28]

$$G_0^{aa^+}(\varepsilon) = [\varepsilon - H_0^{(1)}]^{-1} , \tag{79}$$

with

$$H_0^{(1)} = \left\| h_{n'/r,n'i\gamma'}^{(0)} \right\| , \tag{80}$$

$$G_0^{uu}(\varepsilon) = \left[ \omega^2 M^{(0)} - \Phi^{(0)} \right]^{-1} , \tag{81}$$

with

$$\Phi^{(0)} = \left\| \Phi_{ni\alpha,n'i'\alpha'}^{(0)} \right\| \tag{82}$$

and

$$M^{(0)} = \| M_i \delta_{nn'} \delta_{ii'} \delta_{\alpha\alpha'} \| . \tag{83}$$

Here, the double lines denote a matrix.

When the perturbations are small, given by

$$\frac{\left( \frac{\varepsilon^2}{\hbar^2} \Delta M + \Delta \Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon) \right)_{ni\alpha,n'i'\alpha'}}{\Phi_{ni\alpha,n'i'\alpha'}^{(0)}} \ll 1 , \tag{84}$$

then the solution of the system of equations in Eq. (73) becomes

$$G^{aa^+}(\varepsilon) = \left[ \varepsilon - H_0^{(1)} - (w + \Sigma_{eph}(\varepsilon) + \Sigma_{ee}(\varepsilon)) \right]^{-1} ,$$

$$G^{uu}(\varepsilon) = \left[ \omega^2 M^{(0)} - \Phi^{(0)} - \left( \frac{\varepsilon^2}{\hbar^2} \Delta M + \Delta \Phi + \Sigma_{phe}(\varepsilon) + \Sigma_{phph}(\varepsilon) \right) \right]^{-1} , \quad (85)$$

$$G^{PP}(\varepsilon) = \frac{\varepsilon^2}{\hbar^2} \left( M^{(0)} \right)^2 G^{uu}(\varepsilon) ,$$

where

$$\Delta M = \| (M_i - M_{ni}) \delta_{nn'} \delta_{ii'} \delta_{\alpha\alpha'} \| , \varepsilon = \hbar\omega . \tag{86}$$

The vertex correction $\Gamma_{ni\gamma,n_1 i_1 \gamma_1}^{n_2 i_2 \alpha_2}(\tau_2, \tau, \tau_1)$ of the electronic self-energy due to the electron-phonon interaction $\Sigma_{eph\ ni\gamma,n'i'\gamma'}(\tau, \tau')$ is described by the diagram in Fig. 1. The solid lines correspond to electronic propagators $G_{ni\gamma,n'i'\gamma'}^{aa^+}(\tau, \tau')$ and the dashed lines correspond to phonon propagators $G_{ni\gamma,n'i'\gamma'}^{aa^+}(\tau, \tau')$.

Note that the unshaded triangle in Fig. 1 corresponds to the equation

$$\Gamma_{nij,n_1 i_1 \gamma_2}^{(0)n_2 i_2 \alpha_2}(\tau_2, \tau, \tau_1) = v_{ni\gamma,n_1 i_1 \gamma_1}^{(n_2 i_2 \alpha_2)} \delta(\tau - \tau_2) \delta(\tau - \tau_1) . \tag{87}$$

In Fig. 1, the internal summations for $\tilde{n}\gamma$ imply both a summation over $ni\gamma$ and an integration over the internal time $\tau$.
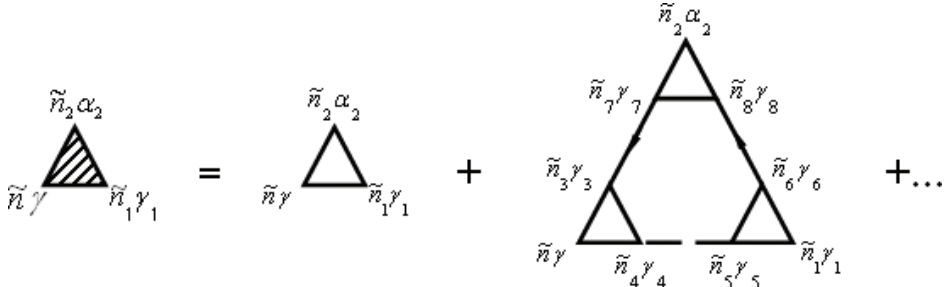
Fig. 1.   Diagrams for the vertex corrections $\Gamma^{n_2 i_2 \alpha_2}_{ni\gamma,n_1 i_1 \gamma_1}(\tau_2, \tau, \tau_1) = \Gamma^{\tilde{n}_2 \alpha_2}_{\tilde{n}\gamma,\tilde{n}_1 \gamma_1}$. Here $\tilde{n} = (ni\tau)$.

Explicitly, the electron-phonon self-energy become

$$\Sigma_{\text{e}ph\ ni\gamma,n'i'\gamma'}(\varepsilon) = -\frac{1}{4\pi i} \int_{-\infty}^{\infty} d\varepsilon' \coth\left(\frac{\varepsilon'}{2\Theta}\right)\ \Gamma^{(0)n_1 i_1 \alpha_1}_{ni\gamma,\ n_3 i_3 \gamma_3}$$

$$\times \left[ G^{uu}_{n_1 i_1 \alpha_1, n_2 i_2 \alpha_2}(\varepsilon') - G^{uu\ *}_{n_1 i_1 \alpha_1, n_2 i_2 \alpha_2}(\varepsilon') \right]\ G^{aa^+}_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}$$

$$\times (\varepsilon - \varepsilon') \Gamma^{n_2 i_2 \alpha_2}_{n_4 i_4 \gamma_4, n'i'\gamma'},\ \Gamma^{(0)n_1 i_1 \alpha_1}_{ni\gamma,n_3 i_3 \gamma_3} = v'^{n_1 i_1 \alpha_1}_{ni\gamma,n_3 i_3 \gamma_3}, \tag{88}$$

where repeated indices are summed over.

The self-energy of the phonon due to the phonon-electron interaction is given by

$$\Sigma_{\text{phe}\ ni\alpha,n'i'\alpha'}(\varepsilon) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon' f(\varepsilon') \Gamma^{(0),ni\alpha}_{n_2 i_2 \gamma_2, n_1, i_1 \gamma_1}$$

$$\times \left\{ \left[ G^{aa^+}_{n_1 i_1 \gamma_1, n_3 i_3 \gamma_3}(\varepsilon + \varepsilon') - G^{aa^+\ *}_{n_1 i_1 \gamma_1, n_3 i_3 \gamma_3}(\varepsilon + \varepsilon') \right] \right.$$

$$\times G^{aa^+\ *}_{n_4 i_4 \gamma_4, n_2 i_2 \gamma_2}(\varepsilon') + G^{aa^+}_{n_1 i_1 \gamma_1, n_3, i_3 \gamma_3}(\varepsilon + \varepsilon')$$

$$\left. \times \left[ G^{aa^+}_{n_4 i_4 \gamma_4, n_2 i_2 \gamma_2}(\varepsilon') - G^{aa^+\ *}_{n_4 i_4 \gamma_4, n_2 i_2 \gamma_2}(\varepsilon') \right] \right\} \Gamma^{n'i'\alpha'}_{n_3 i_3 \gamma^3, n_4 i_4 \gamma_4}, \tag{89}$$

$f(\varepsilon)$ — the so-called Fermi-Dirac distribution function. The vertex part $\Gamma^{n_2 i_2 \gamma_2, n_1 i_1 \gamma_1}_{ni\gamma,n'i'\gamma'}(\tau_2, \tau_1 \tau, \tau')$ of the electronic self-energy $\Sigma_{ee\ ni\gamma,n'i'\gamma'}(\tau, \tau')$ is given in Fig. 2.

Note that the unshaded square in Fig. 2 corresponds to the equation

$$\tilde{v}^{(2)ni\gamma,n_2 i_2 \gamma_2}_{n_1 i_1 \gamma_1, n'i'\gamma'} = v^{(2)ni\gamma,n_2 i_2 \gamma_2}_{n_1 i_1 \gamma_1, n'i'\gamma'} - v^{(2)ni\gamma,n_2 i_2 \gamma_2}_{n'i'\gamma',n_1 i_1 \gamma_1}. \tag{90}$$

Using this vertex function, then yields the contribution to the electron self-energy from the electron-electron interaction:

$$\Sigma_{eeniy,n'i'\gamma'}(\varepsilon) = \Sigma^{(1)}_{eenty,n'i'\gamma'} + \Sigma^{(2)}_{eeniy,n'i'\gamma'}(\varepsilon), \tag{91}$$

$$\Sigma^{(1)}_{\text{ee}\ n,n'} = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon' f(\varepsilon') \Gamma^{(0)n_2,n_1}_{n,n'} \left[ G^{aa^+}_{n_1,n_2}(\varepsilon') - G^{aa^+}_{n_1,n_2}(\varepsilon') \right]$$
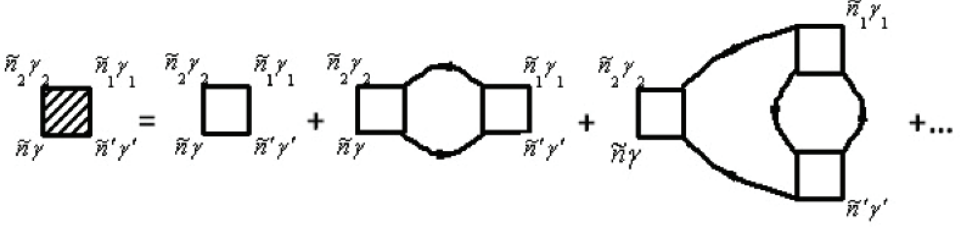
Fig. 2. Diagrams for vertex part $\Gamma^{n_2 i_2 \gamma_2, n_1 i_1 \gamma_1}_{ni\gamma, n'i'\gamma'}(\tau_2, \tau_1 \tau, \tau') = \Gamma^{\tilde{n}_2 \gamma_2, \tilde{n}_1 \gamma_1}_{\tilde{n}\gamma, \tilde{n}'\gamma'}$. Here $\tilde{n} = (ni\tau)$.

$$
\Sigma^{(2)}_{ee\ n,n'}(\varepsilon) = \left(\frac{1}{2\pi i}\right)^2 \int_{-\infty}^{\infty} d\varepsilon_1 \int_{-\infty}^{\infty} d\varepsilon_2 f(\varepsilon_1) f(\varepsilon_2) \Gamma^{(0)n,n_3}_{n_2,n_1}
$$

$$
\times \left[ G^{aa^+}_{n_2,n_5}(\varepsilon - \varepsilon_1 - \varepsilon_2) G^{aa^+\,*}_{n_1,n_4}(\varepsilon_1) - \right.
$$

$$
\left. - G^{aa^+\,*}_{n_2,n_5}(\varepsilon - \varepsilon_1 - \varepsilon_2) G^{aa^+}_{n_1,n_4}(\varepsilon_1) \right]
$$

$$
\times \left[ G^{aa^+}_{n_6,n_3}(\varepsilon_2) - G^{aa^+\,*}_{n_6,n_3}(\varepsilon_2) \right]
$$

$$
- \left[ G^{aa^+}_{n_2,n_5}(\varepsilon - \varepsilon_1 - \varepsilon_2) - G^{aa^+\,*}_{n_2,n_5}(\varepsilon - \varepsilon_1 - \varepsilon_2) \right]
$$

$$
\times \left[ G^{aa^+}_{n_1,n_4}(\varepsilon_1) G^{aa^+}_{n_6,n_3}(\varepsilon_2) \right.
$$

$$
\left. \left. - G^{aa^+\,*}_{n_1,n_4}(\varepsilon_1) G^{aa^+\,*}_{n_6,n_3}(\varepsilon_2) \right] \right\} \Gamma^{n_5,n_6}_{n_4,n'}, \tag{92}
$$

$$
\Gamma^{(0)n,n_3}_{n_2,n_1} = \tilde{v}^{(2)n,n_3}_{n_2,n_1} = v^{(2)n,n_3}_{n_2,n_1} - v^{(2)n,n_3}_{n_1,n_2} \quad n = ni\gamma \tag{93}
$$

A similar result for the contribution to the phonon self-energy $\Sigma_{phph}(\varepsilon)$ from phonon-phonon coupling, is given in Refs. 30–33

In deriving the expressions in Eqs. (88), (90), and (92), we employed the standard resummation techniques for any function $\phi(z)$ that is analytic in the region covered by the contour C, which encloses all of the Matsubara frequencies. Namely, we have

$$
\Theta \sum_{\mathfrak{c}_n} \phi(i\omega_n) = \frac{1}{4\pi i} \oint_C dz \coth\left(\frac{z}{2\Theta}\right) \phi(z) \tag{94}
$$

$$
(\omega_n = 2n\pi\Theta)
$$

for the Bosonic case, and

$$
\Theta \sum_{\omega_n} \phi(i\omega_n) = -\frac{1}{2\pi i} \oint_C dz \tilde{f}\left(\frac{z}{\Theta}\right) \phi(z) \tag{95}
$$

$$
(\omega_n = (2n+1)\pi\Theta)
$$

for the Fermionic case, with

$$
\tilde{f}\left(\frac{z}{\Theta}\right) = \frac{1}{\exp\left(\frac{z}{\Theta}\right) + 1}. \tag{96}
$$

We comment that for the many-body Green's functions described here, it is customary to have the chemical potential situated at zero frequency, as we do here.

In general, the renormalization of the vertex of the functions in the expressions (88), (90), and (92) for mass operators can be performed using Figs. 1 and 2. The diagrams in Figs. 1 and 2 corresponds to the equation

$$\Gamma_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}^{n' i' \alpha'} = \Gamma_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}^{(0)n' i' \alpha'} - \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \Gamma_{n_5 i_5 \gamma_5, n_6 i_6 \gamma_6}^{(0)n' i' \alpha'} \left[ G_{n_6 i_6 \gamma_6, n_7 i_7 \gamma_7}^{aa^+}(\varepsilon) \right.$$

$$\left. \times G_{n_8 i_8 \gamma_8, n_5 i_5 \gamma_5}^{aa^+}(\varepsilon) - G_{n_6 i_6 \gamma_6, n_7 i_7 \gamma_7}^{aa^+ *}(\varepsilon) G_{n_8 i_8 \gamma_8, n_5 i_5 \gamma_5}^{aa^+ *}(\varepsilon) \right]$$

$$\times \Gamma_{n_7 i_7 \gamma_7, n_8 i_8 \gamma_8}^{(0)n_9 i_9 \alpha_9} G_{n_9 i_9 \alpha_9, n_{10} i_{10} \alpha_{10}}^{uu}(0) \Gamma_{n_3 i_3 \gamma_3, n_4 i_4 \gamma_4}^{n_{10} i_{10} \alpha_{10}} \tag{97}$$

and

$$\Gamma_{n_4, n'}^{n_5, n_6} = \Gamma_{n_4, n'}^{(0)n_5, n_6} - \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \Gamma_{n_4, n_8}^{(0)n_5, n_7}$$

$$\times \left[ G_{n_7, n_9}^{aa^+}(\varepsilon) G_{n_8, n_{10}}^{aa^+ *}(\varepsilon) - G_{n_7, n_9}^{aa^+ *}(\varepsilon) G_{n_8, n_{10}}^{aa^+}(\varepsilon) \right]$$

$$\times \Gamma_{n_{10}, n'}^{n_9, n_6}, n = ni\gamma. \tag{98}$$

By repeated indices in expressions (97) and (98), summation is implied. The Fermi level $\varepsilon_F \equiv \mu_e$ of the system is determined by the equation:

$$\langle Z \rangle = \int_{-\infty}^{\infty} f(\varepsilon) g_e(\varepsilon) d\varepsilon,$$

$$f(\varepsilon) = \frac{1}{\exp(\frac{\varepsilon - \varepsilon_F}{\Theta}) + 1}, \tag{99}$$

where $\langle Z \rangle$ is the average number of electrons per atom and $g_e(\varepsilon)$ is the many-body electronic density of states, which satisfies

$$g_e(\varepsilon) = -\frac{1}{\pi \nu N} \operatorname{Im} \operatorname{Tr} \left\langle G^{aa^+}(\varepsilon) \right\rangle_c. \tag{100}$$

Here, $\langle \ldots \rangle_c$ denotes configurational averaging over the disorder, $N$ is the number of primitive lattice cells and $\nu$ is the number of atoms per primitive cell. We drop the letter $c$ on the configurational averaging for simplicity. In Eq. (99), we have $\langle Z \rangle$ is the average number of electrons per atom.

It should be noted that the first term in the electron self-energy due to electron-electron interactions, $\Sigma_{ee\,ni\gamma, n' i' \gamma'}^{(1)}$ in Eq. (91), describes the Coulomb and exchange electron-electron interactions in the Hartree-Fock approximation. The second term, $\Sigma_{ee\,ni\gamma, n' i' \gamma'}^{(2)}(\varepsilon)$, which is caused by corrections beyond Hartree-Fock, describes the effects of electron correlations. The expression for the Green's function in Eq. (85) differs from the corresponding expressions for the Green's function of a single-particle Hamiltonian of a disordered system only from the different self-energy contributions. Hence, we solve for the Green's function using the well-known methods of disordered systems theory.[33]

Performing averaging over the distribution of atoms of different sort and localized magnetic moments projection at the sites of the crystal lattice and neglecting the contribution of processes of electron scattering in clusters consisting of three or more atoms that are small by the above parameter[35] for the density of electronic states we obtain:

$$g_e\left(\varepsilon\right) = \frac{1}{v} \sum_{i,\delta,\sigma,\lambda,m_{\lambda i}} P_{0i}^{\lambda m_{\lambda i}} g_{0\,i\delta\,\sigma}^{\lambda m_{\lambda i}}\left(\varepsilon\right)\,, \tag{101}$$

$$g_{0\,i\delta\,\sigma}^{\lambda m_{\lambda i}}(\varepsilon) = -\frac{1}{\pi}\ \mathrm{Im}\ \left\{ \tilde{G} + \tilde{G}t_{0i}^{\lambda m_{\lambda i}}\ \tilde{G} + \sum_{(lj)\neq(0i)\lambda',m_{\lambda' j}} P_{lj\ 0\,i}^{\lambda'\,m_{\lambda' j}/\lambda\,m_{\lambda i}} \right.$$

$$\left. \times \tilde{G}\left[ t_{lj}^{\lambda'\,m_{\lambda' j}} + T^{(2)\lambda m_{\lambda i}\,0i,\lambda'm_{\lambda' j}lj} \right] \tilde{G} \right\}^{0i\delta\sigma,0i\delta\sigma}\,,$$

$$T^{(2)\lambda m_{\lambda i}0i,\lambda'm_{\lambda' j}lj} = \left[ I - t^{\lambda m_{\lambda i}0i}\tilde{G}t^{\lambda'm_{\lambda' j}lj}\tilde{G} \right]^{-1} t^{\lambda m_{\lambda i}0i}\tilde{G}t^{\lambda'm_{\lambda' j}lj}\left[ I + \tilde{G}t^{\lambda m_{\lambda i}0i} \right] \tag{102}$$

where $\tilde{G} = \tilde{G}^{aa^+}(\varepsilon)$.

Similarly averaging of the phonon Green's function $G^{uu}(\varepsilon)$ yields the phononic density of states:

$$g_{ph}\left(\varepsilon\right) = \frac{1}{\nu} \sum_{i,\alpha,\lambda} P_{0i}^{\lambda} g_{0i\alpha}^{\lambda}\left(\varepsilon\right)\,,$$

$$g_{0i\alpha}^{\lambda}(\varepsilon) = -\frac{1}{\pi}2\frac{\varepsilon}{\hbar^2} M_i \mathrm{Im}\left\{ \tilde{G} + \tilde{G}\ t^{\lambda\,0i}\ \tilde{G} + \sum_{\substack{(lj)\neq(0i)\\\lambda'}} P_{lj\ 0i}^{\lambda'/\lambda} \right.$$

$$\left. \times \tilde{G}\left[ t^{\lambda'\,lj} + T^{(2)\lambda 0i,\lambda'lj} \right] \tilde{G} \right\}^{0i\alpha,0i\alpha}\,, \tag{103}$$

where $\tilde{G} = \tilde{G}^{uu}(\varepsilon)$.

The free energy per atom, can be presented by[35,36]

$$F = \langle\delta\Phi\rangle - \Theta\ S_c + \Omega_e + \Omega_{ph} + \mu_e\langle Z\rangle\,, \tag{104}$$

where $\Omega_e$, $\Omega_{ph}$ are given by

$$\Omega_e = -\Theta \int_{-\infty}^{\infty} \ln\left(1 + e^{(\mu_e-\varepsilon)/\Theta}\right)\ g_e(\varepsilon)d\varepsilon\,, \tag{105}$$

$$\Omega_{ph} = \Theta \int_{-\infty}^{\infty} \ln\left(1 - e^{-\varepsilon/\Theta}\right)g_{ph}(\varepsilon)\ d\varepsilon\,. \tag{106}$$

Here, $S_c$ is the configurational entropy.

Employing the diagram technique outlined above and in Refs. 35 and 36, and neglecting contributions to electron scattering on clusters of three or more sites, yields the following for the DC conductivity ($\omega \to 0$):

$$
\sigma_{\alpha\beta} = \frac{e^2\hbar}{4\pi V_1} \left\{ \int_{-\infty}^{\infty} d\varepsilon_1 \frac{\partial f}{\partial \varepsilon_1} \sum_{s,s'=+,-} (2\delta_{ss'} - 1) \sum_{i,\gamma} \left\{ [v_\beta \tilde{K}\left(\varepsilon_1^s, v_\alpha, \varepsilon_1^{s'}\right)] \right. \right.
$$

$$
+ \sum_{\lambda,m_{\lambda i}} P_{0i}^{\lambda m_{\lambda i}} \tilde{K}(\varepsilon_1{}^{s'}, v_\beta, \varepsilon_1{}^s)(t_{0i}^{\lambda m_{\lambda i}}(\varepsilon_1{}^s)\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})t_{0i}^{\lambda m_{\lambda i}}(\varepsilon_1{}^{s'})
$$

$$
+ \sum_{\lambda,m_{\lambda i}} P_{0i}^{\lambda m_{\lambda i}} \sum_{\substack{lj \neq 0i, \\ \lambda',m_{\lambda'j}}} P_{lj\ 0i}^{\lambda'm_{\lambda'j}/\lambda m_{\lambda i}} \left[ [\tilde{K}(\varepsilon_1{}^{s'}, v_\beta, \varepsilon_1{}^s)v_\alpha \tilde{G}(\varepsilon_1{}^{s'})] \right.
$$

$$
\times T^{(2)\lambda m_{\lambda i}0i,\lambda'm_{\lambda'j}lj}(\varepsilon_1{}^{s'})[\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})v_\beta \tilde{G}(\varepsilon_1{}^s)]T^{(2)\lambda\ m_{\lambda i}0i,\lambda'm_{\lambda'j}lj}(\varepsilon_1{}^s)
$$

$$
+ \tilde{K}(\varepsilon_1{}^{s'}, v_\beta, \varepsilon_1{}^s) \left[ (t_{lj}^{\lambda'm_{\lambda'j}}(\varepsilon_1{}^s)\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})t_{0i}^{\lambda m_{\lambda i}}(\varepsilon_1{}^{s'}) \right.
$$

$$
+ \left( t_{0i}^{\lambda m_{\lambda i}}(\varepsilon_1{}^s) + t_{lj}^{\lambda'm_{\lambda'j}}(\varepsilon_1{}^s) \right) \tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})T^{(2)\lambda\ m_{\lambda i}0i,\lambda'm_{\lambda'j}lj}(\varepsilon_1{}^{s'})
$$

$$
+ T^{(2)\lambda'm_{\lambda'j}lj,\lambda m_{\lambda i}0i}(\varepsilon_1{}^s)\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})t_{0i}^{\lambda m_{\lambda i}}(\varepsilon_1{}^{s'})
$$

$$
+ T^{(2)\lambda'm_{\lambda'j}lj,\lambda m_{\lambda i}0i}(\varepsilon_1{}^s)\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})T^{(2)\lambda m_{\lambda i}0i,\lambda'm_{\lambda'j}lj}(\varepsilon_1{}^{s'})
$$

$$
+ \left. \left. \left. T^{(2)\lambda'm_{\lambda'j}lj,\lambda m_{\lambda i}0i}(\varepsilon_1{}^s)\tilde{K}(\varepsilon_1{}^s, v_\alpha, \varepsilon_1{}^{s'})T^{(2)\lambda'm_{\lambda'j}lj,\lambda m_{\lambda i}0i}(\varepsilon_1{}^s) \right] \right] \right\}^{0i\gamma,0i\gamma}
$$

$$
+ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\varepsilon_1 d\varepsilon_2 f(\varepsilon_1) f(\varepsilon_2) \left\langle \Delta G_{\alpha\beta}^{II}(\varepsilon_1, \varepsilon_2) \right\rangle \right\} , \tag{107}
$$

where

$$
\tilde{K}\left(\varepsilon_1^s, v_\alpha, \varepsilon_1^{s'}\right) = \tilde{G}^{aa^+}\left(\varepsilon_1^s\right) v_\alpha \tilde{G}^{aa^+}\left(\varepsilon_1^{s'}\right) ,
$$

$$
\tilde{G}^{aa^+}\left(\varepsilon_1^+\right) = \tilde{G}_r^{aa^+}(\varepsilon_1) \tag{108}
$$

$$
\tilde{G}^{aa^+}\left(\varepsilon_1^-\right) = \tilde{G}_a^{aa^+}(\varepsilon_1) = \left(\tilde{G}_r^{aa^+}\right)^*(\varepsilon_1) .
$$

The electron velocity satisfies the conventional definition

$$
v_\alpha(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial H_0^{(1)}(\mathbf{k})}{\partial k_\alpha} . \tag{109}
$$

Note that, the computation accuracy is determined by renormalization precision of the vertex parts of the mass operators of electron-electron and electron-phonon interactions. This accuracy also can be determined by small parameter of cluster expansion for Green's functions of electrons and phonons.

## 4. Conclusions

This work presents a new method of describing electronic spectrum, thermodynamic potential and electrical conductivity of disordered crystals based on the Hamiltonian of multi-electron system and diagram method for Green's functions finding. Precise expressions for Green's functions, thermodynamic potential and conductivity tensor are derived using diagram method. The computation accuracy is determined by renormalization precision of the vertex parts of the mass operators of electron-electron and electron-phonon interactions. This accuracy also can be determined by small parameter of cluster expansion for Green's functions of electrons and phonons.

The microelectronics phenomena in different submicrostructures, high level parameter integrations and packing, are very important from many aspects of fundamental research. From one side, it is important to fulfill many goals on the way to miniaturization, but for such scientific question there are many open problems very creative for advance investigations. Anyhow, the scientific perspectives in classic semiconductor technologies are not with an open vision to give new fundamental results. There are strong technological limitations to make thinner and thinner layers for microelectronics demands. Our research try to open new frontiers and in the fields of electronics parameter integrations instead of different microdevices technological integration (Fig. 1). But, this scientific and research problem is not easy to understand, because of many open questions and not enough investigated problems and appropriate answers. One of these aspects is much more deeply and precisely controls of the particles motion and their trajectories phenomena changes.

Therefore, we have developed the research results on the field of Brownian particles motion. Also, here we applied fractal nature in Brownian motion chaotically structures. On that way, we practically developed the mathematical-physics methods to control chaotically motion and transform to control structures on the way to real particles order. From these points of view, we are coming to the point to explain and understand some processes in the nature of material sciences, especially ceramic structures. For these problems, we have open frontiers to use some ideas of similarities in the motion of particles from phenomena in the live systems and to compare with particles motion in inorganic world. All of these are specific ideas of biomimetic similarities. This Brownian particles motion effects have a great importance for advanced miniaturization and packaging presented on Fig. 1.

Some of our experimental results with sub-microorganisms of size between 0.5 $\mu$m and 3 $\mu$m are inspiration for Brownian motion fractal nature analysis, which could be applicable for particles such as electrons. For better understanding of these processes, we provide some necessary tools for further research.

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