Single-electron density matrix and the metal-insulator criterion for crystalline solids

S. V. Vonsovskiĭ and M. I. Katsnel'son

Institute of Metal Physics, Ural Branch of the Academy of Sciences of the USSR, Sverdlovsk

Usp. Fiz. Nauk **158**, 723–728 (August 1989)

Already in 1935 S. P. Shubin[1] suggested a very elegant formulation of the foundations of band theory in terms of the single-electron density matrix $\hat{\rho}$. The subsequent development of this formulation intended to incorporate the electron-electron interaction and formulate a rigorous metal-insulator criterion (MIC) for many-electron systems. However, the research carried out by S. P. Shubin together with one of the present authors (S. V.) remained unfinished because of Shubin's arrest in 1937 and his tragic death. In addition to Shubin's original paper,[1] his ideas were developed by M. I. Sergeev[2] and several others,[3,4] but the general development of the many-particle theory of solids followed a different path. Yet even today, some fifty years later, we find that the results obtained in the intervening decades have not rendered Shubin's approach obsolete. Furthermore, we believe that his ideas continue to hold significant interest, especially with regard to methodology. In this report we shall attempt to reinterpret Shubin's ideas in the language of contemporary band theory.

In a crystal the density matrix $\hat{\rho}$ is periodic in the coordinate representation:

$$\rho(\mathbf{r}', \mathbf{r}) = \sum_{\sigma} \langle \psi_{\sigma}^{+}(\mathbf{r})\, \psi_{\sigma}(\mathbf{r}') \rangle, \tag{1}$$

$$\rho(\mathbf{r}'+\mathbf{R}_n,\ \mathbf{r}+\mathbf{R}_n) = \rho(\mathbf{r}',\ \mathbf{r}), \tag{2}$$

where $\Psi_{\sigma}^{+}(\mathbf{r})$, $\Psi_{\sigma}(\mathbf{r})$ are the creation and annihilation operators for an electron at point $\mathbf{r}$ with spin projection σ; $\mathbf{R}_n$ is the lattice translation vector. Consider the properties of the eigenfunctions $\varphi_i(\mathbf{r})$ of the single-particle density matrix

$$\int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}')\, \varphi_i(\mathbf{r}') = \rho_i \varphi_i(\mathbf{r}). \tag{3}$$

Acting with the translation operator $\hat{T}_n$ on the vector $\mathbf{R}_n$ on the left-hand side of expression (3) we obtain:

$$\begin{aligned} \hat{T}_n \hat{\rho} \varphi_i &= \int d\mathbf{r}' \rho(\mathbf{r}+\mathbf{R}_n, \mathbf{r}')\, \varphi_i(\mathbf{r}') \\ &= \int d\mathbf{r}' \rho(\mathbf{r}+\mathbf{R}_n, \mathbf{r}'+\mathbf{R}_n)\, \varphi_i(\mathbf{r}'+\mathbf{R}_n) \\ &= \int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}')\, \varphi_i(\mathbf{r}'+\mathbf{R}_n) = \hat{\rho} \hat{T}_n \varphi_i. \end{aligned} \tag{4}$$

Then, following the standard proof of the Bloch theorem,[5] it is easy to demonstrate that the functions $\varphi_i(\mathbf{r})$ can be represented in the Bloch-functional form:

$$\varphi_{\mathbf{k}}(\mathbf{k}, \mathbf{r}) = \exp(i\mathbf{k}\mathbf{r})\, u_{\mathbf{k}}(\mathbf{k}, \mathbf{r}), \tag{5}$$

where $i \equiv (\mathbf{k}, \zeta)$ is the crystal momentum that falls in the first Brillouin zone and ζ is the "zone number index",

$$u_{\mathbf{k}}(\mathbf{k}, \mathbf{r}+\mathbf{R}_n) = u_{\mathbf{k}}(\mathbf{k}, \mathbf{r}). \tag{6}$$

Neglecting the electron-electron interaction we obtain $\hat{\rho} = f(\hat{H}_0)$ and $\rho_{\zeta}(\mathbf{k}) = f(E_{\zeta}(\mathbf{k}))$, where $\hat{H}_0$ is the single-particle Hamiltonian; $E_{\zeta}(\mathbf{k})$ is the band dispersion; $f(E)$ is the Fermi distribution function. Then the Bloch functions (5) become solutions of the Schrödinger equation also. Generally, in a many-particle system $[\hat{\rho}, \hat{H}_0] \neq 0$ and the functions (5) as well as the eigenfunctions $\rho_{\zeta}(\mathbf{k})$ are not directly related to the energy spectrum. We emphasize, nonetheless, that these functions can be introduced quite rigorously and play a crucial role in the foundations of band theory, as we shall demonstrate below.

As in Ref. 5, the matrix element of the coordinate $\hat{x}_{\alpha}$ in the $i \equiv (\mathbf{k}, \zeta)$ representation can be derived directly from expressions (5) and (6):

$$\langle \mathbf{k}\zeta | x_{\alpha} | \mathbf{k}'\zeta' \rangle = \langle \mathbf{k}\zeta | x_{\alpha}^{(1)} | \mathbf{k}'\zeta' \rangle + \langle \mathbf{k}\zeta | x_{\alpha}^{(2)} | \mathbf{k}'\zeta' \rangle, \tag{7a}$$

$$\langle \mathbf{k}\zeta | x_{\alpha}^{(1)} | \mathbf{k}'\zeta' \rangle = i \frac{\partial}{\partial k_{\alpha}} \delta(\mathbf{k}-\mathbf{k}')\, \delta_{\zeta\zeta'}, \tag{7b}$$

$$\langle \mathbf{k}\zeta | x_{\alpha}^{(2)} | \mathbf{k}'\zeta' \rangle = (2\pi)^3 \delta(\mathbf{k}-\mathbf{k}') \int d\mathbf{r}\, u_{\zeta}^{*}(\mathbf{k}, \mathbf{r}) \frac{\partial}{\partial k_{\alpha}} u_{\zeta'}(\mathbf{k}, \mathbf{r}), \tag{7c}$$

The same derivations applies for the mean value of the velocity operator $\hat{v}_{\alpha} = \dot{\hat{x}}_{\alpha}$ for the states given by Eq. (5):

$$v_{\alpha}(\mathbf{k}, \zeta) = \left\langle \mathbf{k}\zeta \left| \frac{i}{\hbar} [\hat{H}_0, \hat{x}_{\alpha}] \right| \mathbf{k}\zeta \right\rangle = \frac{1}{\hbar} \frac{\partial}{\partial k_{\alpha}} \langle \mathbf{k}\zeta | H_0 | \mathbf{k}\zeta \rangle. \tag{8}$$

Now let us proceed to examine the problem of the accelerating influence of a constant homogeneous electric field $\mathbf{F}$ on the electronic system of the crystal. As S. P. Shubin emphasized,[1] this is the problem that determines the MIC, which is so central to band theory. In an electronic field the Hamiltonian has the form

$$\begin{aligned} \hat{\mathscr{H}}_{\mathrm{F}} &= \sum_j \hat{H}_0(j) - eF_{\alpha} \sum_j \hat{x}_{\alpha}(j) \\ &\quad + \frac{1}{2} \sum_{j,j'} \hat{W}(j, j') \equiv \hat{\mathscr{H}} - eF_{\alpha}\hat{x}_{\alpha}, \end{aligned} \tag{9}$$

where j is the index which labels the electrons, $\hat{W}(j, j')$ is the electron-electron interaction Hamiltonian. We can write the equation of motion for the density matrix of the total many-electron system U[6]:

$$i\hbar \frac{\partial \hat{U}}{\partial t} = [\hat{\mathscr{H}} - eF_{\alpha}\hat{x}_{\alpha},\ \hat{U}], \tag{10}$$

and proceed to the "interaction representation," where

 0038-5670/89/080720-03$01.80 © 1990 American Institute of Physics

$$\widetilde{U}(t) = \left(\exp\frac{i\widehat{\mathcal{H}}t}{\hbar}\right)\hat{U}(t)\exp\left(-\frac{i\widehat{\mathcal{H}}t}{\hbar}\right),$$
$$\hat{x}_\alpha(t) = \left(\exp\frac{i\widehat{\mathcal{H}}t}{\hbar}\right)\hat{x}_\alpha\exp\left(-\frac{i\widehat{\mathcal{H}}t}{\hbar}\right) \tag{11}$$

and so forth. We note here, that the interaction representation was also originally proposed by S. P. Shubin. It was employed in his unpublished calculations as well as in a paper[7] written by one of us at his suggestion.

The mean value of any operator $\hat{A}$ becomes[6]

$$\langle A(t)\rangle = \mathrm{Sp}(\hat{A}\hat{U}(t)) = \mathrm{Sp}(\tilde{A}(t)\,\widetilde{U}(t)), \tag{12}$$

while the equation of motion takes the form

$$\frac{\partial\widetilde{U}(t)}{\partial t} = \frac{ieF_\alpha}{\hbar}[\hat{x}_\alpha(t),\ \widetilde{U}(t)]. \tag{13}$$

Let us decompose $x_\alpha(t)$ as

$$\hat{x}_\alpha(t) = \hat{x}_\alpha + \int_0^t \mathrm{d}\tau\hat{v}_\alpha(\tau) \equiv \hat{x}_\alpha^{(1)} + \hat{x}_\alpha^{(2)} + \int_0^t \mathrm{d}\tau\hat{v}_\alpha(\tau). \tag{14}$$

In the $|\mathbf{k}\zeta>$ representation only the first term contains a singularity of the same order as the derivative of a δ-function. The other two terms, $\hat{x}_\alpha{}^2$ and $\hat{v}_\alpha(t)$, are less singular. They can lead to interband transitions and to Zener breakdown, but can be ignored in calculating the system response to a weak, homogeneous constant field, i.e. in the derivation of the MIC.[5] Consequently, we can perform the $\hat{x}_\alpha(t)\to\hat{x}_\alpha{}^1$ substitution in Eq. (13). Let us write the density matrix of the total N-electron system U in terms of the Bloch functions (5):

$$\langle\mathbf{k}_1\zeta_1,\ \ldots,\ \mathbf{k}_N\zeta_N|\widetilde{U}|\mathbf{k}_1'\zeta_1',\ \ldots,\ \mathbf{k}_N'\zeta_N'\rangle.$$

It follows from (7b) that for a single-particle operator $\hat{f}$

$$\begin{aligned}\langle\mathbf{k}\zeta|[\hat{x}_\alpha^{(1)},\ \hat{f}]|\mathbf{k}'\zeta'\rangle &= \sum_{\mathbf{k}'',\zeta''}[\langle\mathbf{k}\zeta|x_\alpha^{(1)}|\mathbf{k}''\zeta''\rangle\langle\mathbf{k}''\zeta''|f|\mathbf{k}'\zeta'\rangle\\ &\quad-\langle\mathbf{k}\zeta|f|\mathbf{k}''\zeta''\rangle\langle\mathbf{k}''\zeta''|x_\alpha^{(1)}|\mathbf{k}'\zeta'\rangle]\\ &= i\left(\frac{\partial}{\partial k_\alpha}+\frac{\partial}{\partial k_\alpha'}\right)\langle\mathbf{k}\zeta|f|\mathbf{k}'\zeta'\rangle.\end{aligned} \tag{15}$$

Equation (13) then takes the form

$$\begin{aligned}&\frac{\partial}{\partial t}\langle\mathbf{k}_1\zeta_1,\ \ldots,\ \mathbf{k}_N\zeta_N|\widetilde{U}(t)|\mathbf{k}_1'\zeta_1',\ \ldots,\ \mathbf{k}_N'\zeta_N'\rangle\\ &= -\frac{eF_\alpha}{\hbar}\sum_{j=1}^N\left(\frac{\partial}{\partial k_{j\alpha}}+\frac{\partial}{\partial k_{j\alpha}'}\right)\\ &\times\ \langle\mathbf{k}_1\zeta_1,\ \ldots,\ \mathbf{k}_N\zeta_N|\widetilde{U}(t)|\mathbf{k}_1'\zeta_1',\ \ldots,\ \mathbf{k}_N'\zeta_N'\rangle.\end{aligned} \tag{16}$$

One can easily verify by direct substitution that the solution of the Cauchy problem for Eq. (6) can be written as

$$\begin{aligned}&\langle\mathbf{k}_1\zeta_1,\ \ldots|\widetilde{U}(t)|\mathbf{k}_1'\zeta_1',\ \ldots\rangle\\ &= \langle\tilde{\mathbf{k}}_1(t)\zeta_1,\ \ldots|\widetilde{U}(0)|\tilde{\mathbf{k}}_1'(t)\zeta_1',\ \ldots\rangle,\end{aligned} \tag{17}$$

where $\tilde{\mathbf{k}}_i(t) = \mathbf{k}_i - (e\mathbf{F}t/h)$. Furthermore, the time dependence of the single-particle density matrix $\hat{\rho}$, which is obtained from $\widehat{U}$ by integrating over the coordinates of all electrons save one, follows the law

$$\rho_\zeta(\mathbf{k},t) = \rho_\zeta(\tilde{\mathbf{k}}(t),0) \tag{18}$$

[recall that $\hat{\rho}$ is diagonal in the Bloch-functional representation (5)]. The time dependence of the mean value of any single-particle operator $\hat{A}$ is thus

$$\begin{aligned}\langle A(t)\rangle &= \sum_{\mathbf{k},\zeta}\langle\mathbf{k}\zeta|A|\mathbf{k}\zeta\rangle\rho_\zeta(\tilde{\mathbf{k}}(t),0)\\ &= \sum_{\mathbf{k},\zeta}\left\langle\mathbf{k}+\frac{e\mathbf{F}t}{\hbar},\zeta\right|A\left|\mathbf{k}+\frac{e\mathbf{F}t}{\hbar},\zeta\right\rangle\rho_\zeta(\mathbf{k}).\end{aligned} \tag{19}$$

Formally equation (19) appears identical to its analog in single-particle theory,[1] but we have also shown that it remains valid for many-particle systems as long as interband transitions are neglected (we emphasize that the band index ζ was introduced in Eqs. (3), (5) and is not directly related to the energy spectrum).

Substituting the current density operator $\hat{j}_\alpha = e\hat{v}_\alpha$ for $\hat{A}$, we can calculate its time derivative at $t=0$, which is the standard practice in the derivation of the MIC.[5] We obtain ($j_\alpha = \langle j_\alpha(t)\rangle$):

$$\frac{\mathrm{d}j_\alpha}{\mathrm{d}t} = e^2F_\beta\sum_{\mathbf{k},\zeta}m_{\alpha\beta}^{-1}(\mathbf{k},\zeta)\rho_\zeta(\mathbf{k}), \tag{20}$$

where

$$m_{\alpha\beta}^{-1}(\mathbf{k},\zeta) = \hbar^{-1}\frac{\partial}{\partial k_\alpha}v_\beta(\mathbf{k},\zeta) = \hbar^{-2}\frac{\partial^2}{\partial k_\alpha\partial k_\beta}\langle\mathbf{k}\zeta|H_0|\mathbf{k}\zeta\rangle \tag{21}$$

plays the role of the inverse effective mass tensor. As in usual band theory, this quantity is periodic in $\mathbf{k}$ in the inverse lattice. Consequently, if $\rho\zeta(\mathbf{k}) = \rho\zeta$ is independent of $\mathbf{k}$, the contribution of the appropriate band to $\mathrm{d}j_\alpha/\mathrm{d}t$ is zero. This is usually proven[5] by transforming the volume integral (20) into the surface integral of $v_\alpha(\mathbf{k},\zeta)$ over the Brillouin zone boundary, with the opposite faces of the zone canceling each other. In the usual band theory one can have $\rho_\zeta = 0$ (empty band) and $\rho_\zeta = 1$ (full band), and the well-known Wilson MIC[5] can be formulated in the following manner: if at temperature $T=0$ all bands are either empty or full, the crystal is not a metal. As we have shown, generalizing this criterion to the many-electron case involves two modifications: first, the band classification is performed using the eigenfunctions of the single-particle density matrix, rather than the single-particle Hamiltonian; second, one should take into account the possibility of the system remaining nonmetallic even with $\rho_\zeta\neq 0,1$. Thus we have proven that the system cannot be metallic if the bands are uniformly occupied at $T=0$. The converse is not necessarily true: in general, one can construct a distribution $\rho_\zeta(\mathbf{k})$ which differs from a constant and yet turns the integral (20) into zero.

Now we shall cite a number of concrete cases in which this MIC is applied to many-particle systems. As a first example, consider the approximation employed by Gutzwiller[8] to describe a strongly correlated electron gas. In this approximation the distribution function $\rho(\mathbf{k}) = \Sigma_\sigma\langle c_{\mathbf{k}\sigma}+c_{\mathbf{k}\sigma}\rangle$ takes on a very simple form

$$\begin{aligned}p(\mathbf{k}) &= a_1,\quad E_\mathbf{k}<E_\mathrm{F},\\ &= a_2,\quad E_\mathbf{k}>E_\mathrm{F},\end{aligned} \tag{22}$$

where $0<a_2<a_1<1$; $z = a_1 - a_2$ is the discontinuity in the distribution function at the Fermi surface $E_\mathbf{k} = E_\mathrm{F}$. Substituting (22) into (20) and integrating by parts we obtain

$$\frac{dj_\alpha}{dt} = \frac{e^2 F_\beta}{\hbar} \sum_{\mathbf{k}} \frac{\partial v_\beta(\mathbf{k})}{\partial k_\alpha} \rho(\mathbf{k}) = -\frac{e^2 F_\beta}{\hbar} \sum_{\mathbf{k}} v_\beta(\mathbf{k}) \frac{\partial \rho(\mathbf{k})}{\partial k_\alpha}$$
$$= \frac{Ze^2 F_\beta}{\hbar} \sum_{\mathbf{k}} v_\beta(\mathbf{k}) \frac{\partial E_{\mathbf{k}}}{\partial k_\alpha} \delta(E_{\mathbf{k}} - E_F). \quad (23)$$

This result indicates, in particular, that $dj_\alpha/dt \sim Z$ and tends to zero as $Z \to 0$. Consequently, in the Gutzwiller approximation Z plays the role of the "effective number of carriers," which was deduced in Refs. 9, 10 from other considerations.

The second interesting example is furnished by the case of an antiferromagnetic dielectric. This situation corresponds to the ground state of the narrow-band Hubbard model with the number of electrons equal to the number of sites. The antiferromagnetic dielectric was originally examined by Slater[11]; a more detailed discussion is available in Ref. 12. In this system the non-zero single-particle mean values are

$$\langle c^+_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} \rangle = u^2_{\mathbf{k}}, \quad \langle c^+_{\mathbf{k}\uparrow} c_{\mathbf{k}+\varkappa\downarrow} \rangle = u_{\mathbf{k}} v_{\mathbf{k}},$$
$$\langle c^+_{(\mathbf{k}+\varkappa)\downarrow} c_{\mathbf{k}\uparrow} \rangle = u_{\mathbf{k}} v_{\mathbf{k}}, \quad \langle c^+_{\mathbf{k}+\varkappa\downarrow} c_{\mathbf{k}+\varkappa\downarrow} \rangle = v^2_{\mathbf{k}}, \quad (24)$$

where $\varkappa$ is the antiferromagnet vector; $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ are the parameters of the u–v Bogolyubov transformation, expressed in terms of the trial electron spectrum.[12] We are only concerned with the condition

$$u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1. \quad (25)$$

In order to obtain $\rho_{\mathbf{k}}$ we must diagonalize the matrix of elements (24)

$$\det \begin{vmatrix} u^2_{\mathbf{k}} - \rho_{\mathbf{k}} & u_{\mathbf{k}} v_{\mathbf{k}} \\ u_{\mathbf{k}} v_{\mathbf{k}} & v^2_{\mathbf{k}} - \rho_{\mathbf{k}} \end{vmatrix} = 0. \quad (26)$$

Taking into account (25) we find that equation (26) has two solutions: $\rho_{\mathbf{k}} = 0$ and $\rho_{\mathbf{k}} = 1$. Accordingly, a state with mean values as in expression (24) is nonmetallic in view of our MIC criterion (in Ref. 12 this result was obtained by direct calculation of the frequency-dependent conductivity).

A third nontrivial example is furnished by the narrow-band Hubbard model in the limit of a nearly half-full band (see Ref. 13). As the authors of Ref. 13 demonstrated, in this model carriers with the "incorrect" spin projection in the ferromagnetic phase can be described by the Green's function

$$G_+(\mathbf{k}, E) = \sum_{\mathbf{q}}](f_{\mathbf{q}} + N_{\mathbf{k}+\mathbf{q}})(E - t_{\mathbf{q}} + \hbar\omega_{\mathbf{k}+\mathbf{q}})^{-1}], \quad (27)$$

where $t_{\mathbf{q}}$ is the trial electron spectrum; $f_{\mathbf{q}} = f(t_{\mathbf{q}})$; $\omega_{\mathbf{q}}$ is the magnon frequency; $N_{\mathbf{q}} = N(\hbar\omega_{\mathbf{q}})$ is the Bose distribution function. Neglecting the magnon energy $\hbar\omega_{\mathbf{q}}$, we find that $G_+(\mathbf{k}, E)$ does not depend on $\mathbf{k}$. Consequently the distribution function

$$\rho_+(\mathbf{k}) = -\frac{1}{\pi} \int_{-\infty}^{\infty} dE f(E) \operatorname{Im} G_+(\mathbf{k}, E). \quad (28)$$

also does not depend on $\mathbf{k}$ and hence in this model the current carried by the states with the "incorrect" spin projection is zero within limits set by the ratio of the electron to magnon masses. In Ref. 13 this result was obtained via a fairly cumbersome computation of conductivity.

The above examples demonstrate the utility of Shubin's MIC in the analysis of concrete many-particle models. The metal–insulator criterion also permits us to discuss an important general question: whether the metal–insulator transition (MIT) can be related to the changes in the symmetry of the system.[14] It turns out that this is possible, and that the metallic phase plays the role of the lower-symmetry (ordered) phase. The point is that if the density matrix $\hat{\rho}$ is proportional to the unity matrix (considering only a single band for simplicity), then its eigenfunctions form an arbitrary orthonormal set of linear combinations of the Bloch functions (5). In other words, the full band can not only be described by a Slater determinant of Bloch functions, but also of Wannier functions, as well as an infinite number of other functions. In a partially filled band the Bloch-functional representation is unqiue. Apparently this is the symmetry of the nonmetallic phase that is broken by MIT. The continuity of the metallic energy spectrum in the vicinity of the ground state can then be treated as a manifestation of Goldstone's theorem, while the single-particle density matrix

$$\sum_\sigma \langle \psi^+_\sigma(\mathbf{r}) \psi_\sigma(\mathbf{r}') \rangle = \sum_{\mathbf{k}} \rho(\mathbf{k}) \exp[i\mathbf{k}(\mathbf{r} - \mathbf{r}')] \quad (29)$$

becomes the correlation function of the order parameter: it falls off exponentially as $|\mathbf{r} - \mathbf{r}'| \to \infty$ in the nonmetallic phase (and is generally proportional to $\delta(\mathbf{r} - \mathbf{r}')$ if $\rho(\mathbf{k}) = \text{const}$), and falls off according to a power law in the metallic phase (because of the discontinuity in $\rho(\mathbf{k})$ at the Fermi surface). Thus, even though an MIT order parameter may be difficult or even impossible to define, the notions of long-range order and symmetry-breaking can still be applied to this type of phase transition.

The techniques involving the exact single-particle density matrix could be fruitfully applied to other problems in solid state physics, particularly to the problem of the electron-phonon interaction. We believe that the above-discussed examples suffice to demonstrate the fecundity of an idea proposed by S. P. Shubin fifty years ago and subsequently bypassed in the development of band theory because of the tragic events in our history.

[1]S. P. Shubin, Dokl. Akad. Nauk SSSR **8**, 15 (1935).
[2]M. I. Sergeev, Zh. Eksp. Teor. Fiz. **8**, 948 (1938).
[3]S. V. Vonsovskiĭ, Izv. Akad. Nauk SSSR, Ser. Fiz. **12**, 337 (1948).
[4]S. V. Vonsovskiĭ, Izv. Akad. Nauk SSSR, Ser. Fiz. **16**, 387 (1952).
[5]S. V. Vonsovskiĭ and M. I. Katsnel'son, *Quantum Solid State Physics* (in Russian), Nauka, M., 1983.
[6]L. D. Landau and E. M. Lifshits, *Quantum Mechanics: Nonrelativistic Theory*, *3rd. ed.*, Pergamon Press, Oxford, 1977 [Russ. original, Nauka, M., 1947].
[7]S. V. Vonsovsky (Vonsovskiĭ), J. Phys. USSR **10**, 367 (1946).
[8]M. C. Gutzwiller, Phys. Rev. **137**, 1726 (1965).
[9]W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[10]N. H. March, M. Suzuki, and M. Parinello, Phys. Rev. B **19**, 2027 (1979).
[11]J. C. Slater, Phys. Rev. **82**, 538 (1951).
[12]M. I. Katsnelson (Katsnel'son) and V. Yu. Irkhin, J. Phys. C **17**, 4291 (1984).
[13]V. Yu. Irkhin and M. I. Katsnel'son, Fiz. Tverd. Tela (Leningrad) **25**, 3383 (1983) [Sov. Phys. Solid State **25**, 1947 (1983)]; J. Phys. C **18**, 4173 (1985).
[14]S. V. Vonsovskiĭ and M. I. Katsnel'son, in *Electronic Structure and Properties of Solids* (in Russian) (ed. Yu. A. Izyumov), Izd. UNTs, Sverdlovsk, 1982, p. 3.

Translated by A. Zaslavsky