Effect of external electric field on the energy spectrum of an electron in a two-dimensional crystal lattice

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The spectrum of the states of an electron in the combined field of immobile scattering centers that make up a periodic two-dimensional structure is determined in the presence of a constant external force (electric field). A dispersion equation that is accurate with respect to all the energy parameters of the system and takes into account the Stark effect and the field emission of the electrons is derived. The results are of interest for field-emission spectroscopy of submonolayer films on surfaces of solids.

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1. INTRODUCTION

The properties of periodic structures having fewer spatial dimensions (two-dimensional and one-dimensional crystals) are being intensively investigated at present in connection with searches for methods of producing high-temperature superconductivity,[1] as well as in connection with the solution of various problems of physics of submonolayer films on surfaces of solids (see, e.g., the review Bol'shov *et al.*[2]). The present paper contains a solution of the Schrödinger equation that describes the three-dimensional motion of an electron in the combined field of immobile interaction centers that make up a regular two-dimensional lattice, in the presence of a constant external field normal to the plane. The solution obtained generalizes the results of Demkov and Subramanyan[3,4] to include the case when an external field acts on the electron, and the results of Demkov and Drukarev[5] and of Slonim and the present author[6] to include the case of an infinite number of ordered scattering centers. In the long-wave approximation (the model of zero-radius potentials[7]) a dispersion equation is derived [see (13) below], which is accurate with respect to all the energy parameters of the problem. It describes the motion of the electron with account taken of all the significant interactions–exchange, and autoionization (the tunnel effect responsible for the finite lifetime of the electron relative to escape to the vacuum).

Besides being of general interest, the solution of the problem posed in this article is stimulated also by the practical needs of the rapidly developing field-emission spectroscopy of solid surfaces (see in this connection the reviews[8,9]). Present-day experiments make it possible to measure with high accuracy not only the integral but also the differential currents of field-emission electrons. The energy distribution of the electrons released by the tunnel mechanism is presently an important source of information on the character of the motion of the electrons near the surface–the level density, the dispersion law, the configuration of the wave functions, etc. The modern theory of the energy distribution of field-emission electrons was developed by Gadzuk,[10,11] Plummer,[12,13] Modinos,[14,15] and a number of others (see the reviews[8,9,16]). Their studies were devoted mainly to the spectra of clean surfaces.

The influence of single adsorbed atoms was taken into account by Duke and Alferieff,[17] and also by Brodskiĭ and Urbach.[18–20] The corresponding results are applicable at small degrees of coating, when the interaction of the adsorbed particles can be neglected. At higher degrees of coatings, when a two-dimensional crystal lattice is formed on the surface,[2] the character of the influence of the adsorbed particles on the spectrum of the released electrons will undergo qualitative changes. Actually, as follows from the exact solution, the probability of detachment of the electron from the two-dimensional (or one-dimensional) crystal has a qualitatively new energy dependence—it is weak for all values of the quasimomentum vector, with the exception of a small vicinity of the symmetry point Γ. At $q=0$ the electron energy is as a rule minimal, but the rate of disintegration of these states turns out to be maximal and in sufficiently weak fields it can exceed by several orders of magnitude the rate of disintegration of single-center systems, which was first determined by Demkov and Drukarev.[5]

The probability of the departure of the electrons from the volume bands, on the contrary, increases rapidly with increasing energy (see Refs. 8, 9, 16). The competition of two tunneling channels (from the surface of the solid and from the two-dimensional film) can result in a great variety of energy dependences of the field-emission electron currents. An analysis of all the possible situations is of independent and special interest, and we confine ourselves here to a solution of the fundamental problem of the dispersion law of the band states of the electron in a two-dimensional crystal lattice in the presence of a constant electric field. We shall not assume beforehand that the field is weak, and obtain a dispersion equation that is valid in the general case.

2. DISPERSION LAW OF AN ELECTRON IN THE FIELD OF A TWO-DIMENSIONAL CRYSTAL LATTICE IN THE PRESENCE OF A CONSTANT EXTERNAL FORCE

We consider the spectrum of the eigenvalues of the Hamiltonian:

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$$H(\mathbf{r})=-\frac{\Delta}{2}+\sum_s u_s(\mathbf{r}_s)-fz, \quad \mathbf{r}_s=\mathbf{r}-\mathbf{R}_s. \tag{1}$$

Here $\mathbf{r}$ is the coordinate of the electron; u_s is the potential of the interaction with the s-th atomic core, which will henceforth be regarded for simplicity as short-range and spherically symmetrical; $\mathbf{R}_s=(as_x, as_y, 0)$, $s_{x,y}=0, \pm 1, \ldots$. The Oz axis is directed along the field intensity vector F, the lattice plane is normal to the vector $\mathbf{f}(\mathbf{R}_s\cdot\mathbf{f}=0)$. We use the atomic system of units throughout.

We confine ourselves to the solution of the problem for a simple rectangular lattice, although analogous results can be obtained also in a more general case.

Since autoionization is possible, the eigenvalue spectrum of the Hamiltonian (1) is certainly continuous, but if the rate of disintegration is low enough, then we can, as usual, confine ourselves to finding solutions of a stationary Schrodinger equation with a wave going off to infinity ($\psi\sim e^{ip(\varepsilon)z}$ as $z\to\infty$), corresponding to the solution of the homogeneous Lippmann–Schwinger equation. In the long-wave approximation (zero-radius interaction model[7]) the system of exact algebraic equations describing the motion of the electron in the combined field of the immobile scattering centers, in the presence of an external constant force, takes the form [see Eqs. (3) and (11) of Ref. 6]

$$[\varkappa-(-2E)^{1/2}-2\pi G_f^p(E,\mathbf{R}_s,\mathbf{R}_s)]\tau_s=2\pi\sum_{s'\neq s}G_f^{(+)}(E,\mathbf{R}_s,\mathbf{R}_{s'})\tau_{s'},$$
$$\psi(r)=\text{const}\sum_s G_f^{(+)}(E,\mathbf{r},\mathbf{R}_s)\tau_s. \tag{2}$$

Here E is the energy of the considered state, reckoned from the potential of the electric field on the plane $z=0$, $\varkappa=(-2\varepsilon_0)^{1/2}$, $|\varepsilon_0|$ is the binding energy of the electron in the field of the isolated scattering center, $G_f^{(+)}(E,\mathbf{R},\mathbf{R}')$ is the Green's function of the electron in a homogeneous electric field, $G_f^p(E,\mathbf{R},\mathbf{R})$ is the regularized Green's function taken at equal values of the argument;

$$G_f^p=G_f^{(+)}-G_0^{(+)}, \quad G_0^{(+)}=-\frac{1}{2\pi|\mathbf{R}-\mathbf{R}'|}\exp(i(2E)^{1/2}|\mathbf{R}-\mathbf{R}'|)$$

is the Green's function of the free motion.

With account taken of the translational symmetry of the interactions, we seek solutions of the system (2) in the quasimomentum representation:

$$\tau_s=A(\mathbf{q})\exp(i\mathbf{q}\mathbf{R}_s) \tag{3}$$

($\mathbf{q}$ is the two-dimensional quasimomentum vector in the plane of the lattice). For the eigenvalues of the Hamiltonain (1) [the complex function of the real quasimomentum $E(\mathbf{q})$] we obtain the following dispersion equation

$$\varkappa-(-2E)^{1/2}=D(E,\mathbf{q}). \tag{4}$$

The function $D(E,\mathbf{q})$ is determined here by the double series over the centers

$$D(E,\mathbf{q})=2\pi\left\{\sum_s G_f^{(+)}(E,\rho,\mathbf{R}_s)e^{i\mathbf{q}\mathbf{R}_s}-G_0^{(+)}(E,\rho,0)\right\}_{\rho\to 0}. \tag{5}$$

The three-dimensional Green's functions $G_f^{(+)}(E,\mathbf{R},\mathbf{R}')$ can be expressed in terms of derivatives of a bilinear combination of two linearly independent solutions of the Airy equation.[6] This representation, however, is difficult to use when calculating the sum over s in (5). We therefore use for $G_f^{(+)}(E,\mathbf{R},\mathbf{R}')$ the spectral representation given, for example, in Ref. 21:

$$G_f^{(+)}(E,\mathbf{R},\mathbf{R}')=\int d\mathbf{k}\,dE_z\frac{\varphi_{k,E_z}(\mathbf{R})\varphi^*_{k,E_z}(\mathbf{R}')}{E-E_z-k^2/2+i\eta}. \tag{6}$$

Here

$$\varphi_{\mathbf{k},E_z}(\mathbf{r})=(2\pi^3(2f)^{1/3})^{-1/2}e^{i\mathbf{k}\mathbf{r}}V\left(-\frac{2(E_z+fz)}{(2f)^{2/3}}\right)$$

are the wave functions of the free motion in a homogeneous electric field

$$\langle\mathbf{k},E_z|\mathbf{k}',E_z'\rangle=\delta(\mathbf{k}-\mathbf{k}')\delta(E_z-E_z'),$$

$V(x)$ is an Airy function of the first kind,[22] E_z is the energy of the longitudinal motion, and $\mathbf{k}$ is the transverse momentum [$\mathbf{k}=(k_x, k_y, 0)$].

We now interchange in (5) the order of integration and summation. Then, using the well known equality

$$\sum_s\exp[i(\mathbf{k}-\mathbf{q})\mathbf{R}_s]=\frac{(2\pi)^2}{\Omega_0}\sum_{\mathbf{b}}\delta(\mathbf{k}-\mathbf{q}-\mathbf{b}) \tag{7}$$

(see, e.g., Ref. 23, p. 311), where $\mathbf{b}$ is the reciprocal-lattice vector and Ω_0 is the area of the unit cell, we obtain for the function $D(E,\mathbf{q})$ the representation

$$D(E,\mathbf{q})=2\pi\left\{N\sum_{\mathbf{b}}\int_{-\infty}^{\infty}dE_z\frac{V^2(-2E_z/(2f)^{2/3})}{E-(\mathbf{q}+\mathbf{b})^2/2-E_z+i\eta}-(2\pi)^{-3}\int\frac{d\mathbf{p}\,e^{i\mathbf{p}\rho}}{E-p^2/2+i\eta}\right\}_{\rho\to 0},$$
$$N=\frac{(2\pi)^2}{\Omega_0}((2\pi^3)(2f)^{1/3})^{-1}. \tag{8}$$

At $\rho=0$ the curly bracket in (8) contains the difference between a sum that diverges at large $\mathbf{b}$ and an integral that diverges at large momenta. The integral under the summation sign is equal, apart from a normalization factor, to the one-dimensional Green's function in a homogeneous electric field f at a longitudinal energy $\tilde{E}=E-(\mathbf{q}+\mathbf{b})^2/2$.

The regular method of constructing the Green's function of any one-dimensional Schrödinger equation is well known (see, e.g., Ref. 24, p. 136). We have accordingly

$$D(E,\mathbf{q})=2\pi\left\{N\sum_{\mathbf{b}}V(x)[U(x)+iV(x)]-(2\pi)^{-3}\int\frac{d\mathbf{p}\,e^{i\mathbf{p}\rho}}{E-p^2/2+i\eta}\right\}_{\rho\to 0},$$
$$x=\frac{2E-(\mathbf{q}+\mathbf{b})^2}{(2f)^{2/3}}. \tag{9}$$

Here $U(x)$ is the second linearly independent solution of the Airy equation.[22]

The obtained representation makes it possible to separate immediataly the imaginary part of the function $D(E,\mathbf{q})$ (we have in mind the imaginary part of the complex function at real values of the argument):

$$\operatorname{Im}D(E,\mathbf{q})=\frac{(2\pi)^3}{\Omega_0}N\sum_{\mathbf{b}}V^2\left(\frac{2|E|+(\mathbf{q}+\mathbf{b})^2}{(2f)^{2/3}}\right). \tag{10}$$

At $f<\Omega_0^{-3/2}$ the series in powers of $\mathbf{b}$ in (10) converges very rapidly and we can confine ourselves to the first term with $\mathbf{b}=0$.

We now obtain an expansion of the real part of the dispersion function $D(E,\mathbf{q})$ in even powers of the field intensity. To this end we use the Feynman integral representation

$$G_f^{(1)}(E,z,z')=\frac{-i}{(2\pi i)^{1/2}}\int_0^\infty \frac{dt}{t^{1/2}} \times\exp\left\{i\left(\frac{(z-z')^2}{2t}+\left(Et+\frac{f}{2}(z+z')t-\frac{f^2t^3}{24}\right)\right)\right\}, \tag{11}$$

$G_f^{(1)}(E,z,z')$ is the one-dimensional Green's function of the electron in the field f. We deform in (11) the integration contour in such a way that it goes off to infinity along the imaginary negative semiaxis.[6] We now expand the exponential $\exp(-if^2t^3/24)$ in a series and integrate term by term. As a result we obtain the representation

$$\operatorname{Re} D(E,\mathbf{q})=-2\pi\left\{\frac{1}{2\Omega_0(2\pi)^{1/2}}\sum_{n=0}^{\infty}\left(\frac{f^2}{24}\right)^n (2)^{3n+1/2}\frac{\Gamma(3n+1/2)}{\Gamma(n+1)} \times\sum_{\mathbf{b}}(2|E|+(\mathbf{q}+\mathbf{b})^2)^{-3n-1/2}-(2\pi)^{-3}\int\frac{dp}{E-p^2/2+i\eta}\right\}. \tag{12}$$

At $E\Omega_0<1$ the series (12) also converges rapidly and, accurate to terms $\sim(E\Omega_0)^3$, we confine ourselves in it to terms with $\mathbf{b}=0$.

The dispersion equation that determines the complex function acquires ultimately the form

$$\varkappa-(-2E)^{1/2}=\sum_{s\neq 0}R_s^{-1}\exp(-(-2E)^{1/2}R_s+i\mathbf{q}\mathbf{R}_s) -\frac{1}{\Omega_0}\left(\frac{\pi}{2}\right)^{1/2}\sum_{n=1}^{\infty}\left(\frac{f^2}{24}\right)^n\frac{2^{3n+1/2}\Gamma(3n+1/2)}{\Gamma(n+1)}\sum_{\mathbf{b}}(2|E|+(\mathbf{q}+\mathbf{b})^2)^{-3n-1/2} -\frac{4i}{\Omega_0(2f)^{1/2}}\sum_{\mathbf{b}}V^2\left(\frac{2|E|+(\mathbf{q}+\mathbf{b})^2}{(2f)^{1/2}}\right),\quad E=E(\mathbf{q})<0. \tag{13}$$

(The divergences in the term that does not contain the field intensity cancel each other, after which the term can be easily transformed to the known form. See the analogous situation described in Ch. VI, Sec. 3 of the monograph of Demkov and Ostrovskiĭ.[7])

The terms separated in the dispersion function have a clear physical meaning—they take into account respectively the exchange interaction, the polarization of the electron cloud, and the possibility of tunnel autoionization. When all the interactions are "turned off," Eq. (13) determines one infinitely degenerate energy level of an isolated atom

$$E(\mathbf{q})=-\tfrac{1}{2}\varkappa^2. \tag{14}$$

exchange interaction: the term

$$\sim\sum_{s\neq 0}R_s^{-1}\exp[-(-2E)^{1/2}R_s+i\mathbf{q}\mathbf{R}_s],$$

lifting the degeneracy, forms band states that are collectivized over the centers and are classified by the quasimomentum vector $\mathbf{q}$. The dispersion law for these states is determined by the Subramanyan equation[4,7]

$$\varkappa-(-2E)^{1/2}=\sum_{s\neq 0}R_s^{-1}\exp(-(-2E)^{1/2}R_s+i\mathbf{q}\mathbf{R}_s). \tag{15}$$

Turning on the electric field distorts the corresponding wave functins, and the corrections to the spectrum in a weak field can be obtained from an equation that takes into account the polarizability of the considered states but ignores the decay:

$$\varkappa-(-2E)^{1/2}=\sum_{s\neq 0}R_s^{-1}\exp(-(-2E)^{1/2}R_s+i\mathbf{q}\mathbf{R}_s) -\frac{2^{7/2}\Gamma(7/2)f^2}{12\Omega_0(2\pi)^{1/2}}\sum_{\mathbf{b}}(2|E|+(\mathbf{q}+\mathbf{b})^2)^{-1/2}. \tag{16}$$

Allowance, in the dispersion equation, for the imaginary part of the function $D(E,\mathbf{q})$ leads to damping of the considered states. At $f<|E|^{3/2}$ the imaginary part is exponentially small, corresponding to the quasiclassical conditions of electron tunneling through a field barrier. In the highest-order approximation in the small parameter $f|E|^{-3/2}$ we have for the imaginary part of the complex dispersion law $E(\mathbf{q})$

$$\operatorname{Im}E(\mathbf{q})=2^{1/2}|E_0(\mathbf{q})|^{1/2}\exp(-2/3f^{-1}(2|E_0(\mathbf{q})|+q^2)^{3/2}) \times\left\{\Omega_0\left[1+\sum_{s\neq 0}\exp(-2^{1/2}|E_0(\mathbf{q})|^{1/2}R_s+i\mathbf{q}\mathbf{R}_s)\right]\right\}^{-1}(2|E_0(\mathbf{q})|+q^2)^{-1/2}. \tag{17}$$

Here $E_0(\mathbf{q})$ are real solutions of the Subramanyan equation (15).

Comparison of the obtained expressions with the Demkov–Drukarev solution for one isolated center[5]

$$E=-E_0-\frac{f^2}{32E_0^2}-\frac{if}{2^{7/2}|E_0|^{1/2}}\exp\left(-\frac{2}{3f}(2|E_0|)^{3/2}\right), \tag{18}$$

shows that at $|E_0|\Omega_0\ll 1$ the strong exchange interaction between the ordered identical centers greatly increases the polarizability of the electron cloud (by approximately $(\lambda/a)^2$ times, where $\lambda^2=(2|E_0|)^{-1}$), and alters qualitatively the energy dependence of the disintegration rate. In fact, the energy of the band states at the symmetry points Γ, X and W has extrema (see, e.g., Ref. 25, p. 74) corresponding to quasimomentum values $q=0$, $q=\pi/\Omega_0^{1/2}$ and $q=\pi(2/\Omega_0)^{1/2}$. At $|E|\Omega_0\ll 1$ the inequality $q^2>(2|E(\mathbf{q})|)$ is satisfied in a large part of the first Brillouin zone, i.e., the decay is strongly suppressed for practically all the band states, including those adjacent to the boundary of the continuous spectrum.[1)] Only in a small vicinity of the minimal energy $E(\Gamma)(\delta q\sim f^{1/3}(1+E_q''(\Gamma))^{-1})$ does the decay have a higher (compared with the case of isolated center) probability:

$$\Gamma(\mathbf{q})\sim(|E|\Omega_0)^{-1}\frac{|E|^{3/2}}{f}\Gamma_0,\quad \Gamma_0=\frac{f}{2^{3/2}|E|^{1/2}}\exp\left(-\frac{2}{3f}(2|E|)^{3/2}\right). \tag{19}$$

It is easy to understand the origin of the large factors in (19) for $\Gamma(\mathbf{q})$. The first of them takes into account the coherence of the interactions over the scales of the damping length of the wave function of the single-center state. The second large factor, $|E|^{3/2}/f$, takes into account the quasi-one-dimensional character of the autoionization of the states of the flat lattice. The kinematic suppression of the field emission of the electrons from the surface of a two-dimensional crystal takes place also at $|E|\Omega_0\sim 1$. By way of illustration we have calculated the imaginary part of the function $E(\mathbf{q})$ for several characteristic values of the parameters $\varkappa a$ and $\varkappa^3/f$. The results of the calculations by means of formulas (15)–(17) are shown in Figs. 1 and 2.

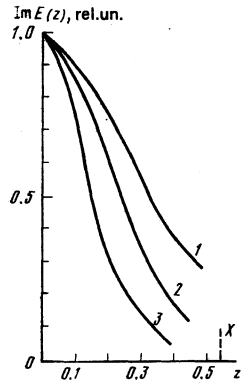

FIG. 1. Energy dependence of the autoionization probability at different values of the parameter $\nu=\varkappa^3/f$: curve 1—for $\nu=1$, curve 2—for $\nu=2$, curve 3—for $\nu=5$. The abscissas represent the change of the energies of the band states along the symmetry axes $\mathbf{q}=(q_x, 0, 0)$. In the calculation it was assumed that $\varkappa a=2$, $E(\mathbf{q})=-\varepsilon_0(1+\delta(\cos q_x a+\cos q_y a))$, $\delta=4e^{-\varkappa a}/\varkappa a$, $\varepsilon_0=\frac{1}{2}\varkappa^2$; $z=[E_0-E_0(\Gamma)]/|E_0(X)|$, $E_0=\mathrm{Re}E(\mathbf{q})$.

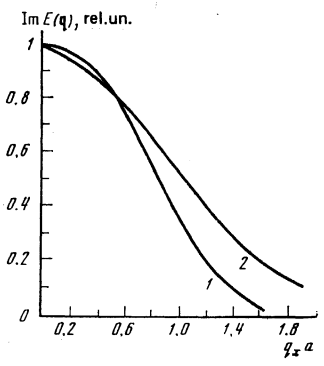

FIG. 2. Dependence of the autoionization probability on the quasimomentum $\mathbf{q}=(q_x, 0, 0)$ at various values of the parameter $\varkappa a$. Curve 1—for $\varkappa a=1.5$; curve 2—for $\varkappa a=2.5$. The ratio m/m^* is respectively 0.67 and 0.40.

The results show that in weak electric fields the energy spectra of the electrons released from states of two-dimensional (adsorbed) crystal films should take the form of a narrow peak at minimal, and not maximal as usual,[8] energies.[2)] This indicates also that, in principle, effective depletion of the low-lying band states is possible by specially selecting the amplitude and duration of the external electric-field pulses.

3. CONCLUSION

We dwell in conclusion on some general questions of the theory of interaction of quasistationary states in the presence of translational symmetry. The question of the character of electron motion in weakly decaying states that are collectivized over the centers is, in our opinion, of great interest for solid state physics, and has apparently not been discussed so far in the literature. Examples of single-center quasistationary states are well known in atomic physics, and together with the "field" resonances considered in the present paper they include numerous cases of potential (centrifugal or shape) and Feshbach resonances (see, e.g., the review by Schulz[26]). The possibility of formation, in periodic structures, of weakly decaying autoionization bands of single-center shape resonances was demonstrated elsewhere.[27] Of fundamental interest is the question of the character of the interaction in a periodic structure of resonance states of the Feshbach type. An analysis of the corresponding two-center model[28] shows that if no account is taken of the exciton effect (i.e., without allowance for the possibility of direct exchange of interaction between the cores) the need for a double inealstic transition greatly hinders the transition of the electron from one center to another. In periodic structures, such resonances can yield only weakly collectivized and in this sense rapidly decaying states.

The situation should be different if the exciton effect is taken into account. A multichannel model of zero-radius potentials, which includes the possibility of direct interaction of the cores, was proposed in Ref. 29. An analysis of the band states within the framework of this exactly solvable model shows that in periodic structures having a channel through which the electron is free to go off to infinity (semi-bounded crystals, two-dimensional and one-dimensional structures), the dispersion law of the electron–exciton complexes undergoes qualitative changes in comparison with those known presently for unbounded three-dimensional crystals.[30] In particular, the imaginary part of the complex dispersion law, which describes the probability of detachment of an electron from the structure when the electron adsorbs the exciton energy, turns out to be a non-analytic function of the quasimomentum even within the limits of the first Brillouin zone. A similar result takes place also for the case of potential resonances.[27] The predicted anomalies of the rate of disintegration of the electron autoionization states in periodic structures might be observable in a great variety of electronic transitions such as the photoeffect, field emission, as well as in elastic reflection of monochromatic electrons from the surface of a solid coated by a monolayer film of adsorbed particles.

[1)] At sufficiently low values of the parameter $\varkappa a$, the upper edges of the energy band can be located above the vacuum energy level ($E=0$).

[2)] When the condition $m/m_{\mathrm{eff}}<1$ is satisfied (m_{eff} is the effective mass of the electron near the bottom of the $E(\Gamma)$ band.

[1]V. L. Ginzburg, Usp. Fiz. Nauk **113**, 335 (1974) [Sov. Phys. Usp. **17**, 446 (1974)].
[2]L. A. Bol'shov, A. P. Napartovich, A. G. Naumovets, and A. G. Fedorus, Usp. Fiz. Nauk **122**, 125 (1977) [Sov. Phys. Usp. **20**, 432 (1977)].
[3]Yu. N. Demkov and R. Subramanyan, Zh. Eksp. Teor. Fiz. **57**, 698 (1969) [Sov. Phys. JETP **30**, 381 (1969)].
[4]R. Subramanyan, Candidate's Dissertation, LGU, 1968.
[5]Yu. N. Demkov and G. F. Drukarev, Zh. Eksp. Teor. Fiz. **47**, 918 (1964) [Sov. Phys. JETP **20**, 614 (1964)].
[6]F. I. Dalidchik and V. Z. Slonim, Zh. Eksp. Teor. Fiz. **70**, 47

(1976) [Sov. Phys. JETP 43, 25 (1976)].
[7]Yu. N. Demkov and V. N. Ostrovskiĭ, Metod potentsialov nulevogo radiusa v atomnoĭ fizike (The Method of Zero-Radius Potentials in Atomic Physics), Izd. LGU, 1975.
[8]E. M. Plummer and J. M. Gadzuk, Rev. Mod. Phys. 45, 487 (1973).
[9]A. M. Brodskii and Yu. M. Gurevich, Teoriya élektronnoĭ emissii iz metallov (Theory of Electron Emission from Metals), Nauka, Moscow, 1973.
[10]J. M. Gadzuk, Phys. Rev. B 1, 2088 (1970).
[11]J. M. Gadzuk, Phys. Rev. B 3, 1772 (1971).
[12]E. M. Plummer and A. E. Bell, J. Vac. Sci. Tech. 9, 583 (1972).
[13]A. R. Penn and E. M. Plummer, Phys. Rev. B 9, 1216 (1974).
[14]A. Modinos and N. Nicolaou, J. Phys. C4, 338, 2859, 2875 (1971).
[15]A. Modinos, Phys. Rev. B 11, 3686 (1975).
[16]R. Fischer and H. Neumann, Electron Field Emission from Semiconductors (Russ. transl.), Nauka, 1971.
[17]C. B. Duke and M. E. Alferieff, J. Chem. Phys. 46, 923 (1967).
[18]A. M. Brodskii and M. I. Urbakh, Phys. Status Solidi B 76, 93 (1976).
[19]M. I. Urbakh, Izv. Akad. Nauk SSSR Ser. Fiz. 40, 1605 (1976).
[20]M. I. Urbakh, Candidate's dissertation, Electrochemistry Inst., USSR Acad. Sci., Moscow, 1976.
[21]V. Z. Slonim and F. I. Dalidchik, Zh. Eksp. Teor. Fiz. 71, 2057 (1976) [Sov. Phys. JETP 44, 1081 (1976)].
[22]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika, nerelyativistskaya teoriya (Quantum Mechanics, Nonrelativistic Theory), Nauka, Moscow, 1974 [Pergamon].
[23]J. Callaway, Energy Band Theory, Academic, 1964.
[24]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, Rasseyanie, reaktsii i raspady v nerelyativistskoi kvantovoi mekhanike (Scattering, Reactions, and Decays in Nonrelativistic Quantum Mechanics), Nauka, 1969.
[25]W. A. Harrison, Solid State Theory, McGraw, 1970.
[26]George J. Schulz, Rev. Mod. Phys. 45, 378 (1973).
[27]G. V. Golubkov, F. I. Dalidchik, and G. K. Ivanov, Surface Sci., 1980, in press.
[28]F. I. Dalidchik, Yad. Fiz. 21, 51 (1975) [Sov. Nucl. Phys. 21, 26 (1975)].
[29]F. I. Dalidchik, Teor. Eksp. Khim. 10, 579 (1974).
[30]I. B. Levinson and E. I. Rashba, Usp. Fiz. Nauk 111, 683 (1973) [Sov. Phys. Usp. 16, 892 (1974)].

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Fokker-Planck equation in the absence of detailed balance

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It is shown that the usual Fokker-Planck (FP) equation is not suitable for describing kinetic effects that are caused by breakdown of detailed balance. For the case of elastic scattering, a modified FP equation is obtained, containing third-order derivatives with respect to the momentum. Its properties are investigated. The problem of describing the photogalvanic effect and the anomalous Hall effect on the basis of the FP equation is considered.

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1. It is customary to suppose that one of the basic principles of kinetics is the principle of detailed balancing (PDB).[1,2] In the simplest case of elastic scattering of particles by immovable centers, the PDB states that

$$W_{\mathbf{kk}'}=W_{\mathbf{k}'\mathbf{k}}, \tag{1}$$

where $W_{\mathbf{kk}'}$ is the differential probability of a transition from a state with momentum $\mathbf{k}'$ to a state $\mathbf{k}$. It is well known that the PDB does not reflect any fundamental symmetry relation in either a quantum or a classical description of scattering.[3-5] The fundamental symmetry relations for $W_{\mathbf{kk}'}$, reflecting the invariance of the equations of motion to space and time reflections (P and T transformations), have the form[3,5]

$$W_{\mathbf{kk}'}=W_{-\mathbf{k},-\mathbf{k}'}, \quad W_{\mathbf{kk}'}=W_{-\mathbf{k}',-\mathbf{k}}. \tag{2}$$

If one of these relations is violated, the PDB is invalid. In particular, P invariance is absent if the scattering potential is deprived of a center of symmetry (Fig. 1), and T invariance is violated in the presence of a magnetic field (Fig. 2).

Until recently, no kinetic phenomena connected in principle with absence of detailed balance were known; but in recent years, the situation has changed. At present a number of such phenomena are known. These are the anomalous Hall effect,[6] the kinetics of gases with rotational degrees of freedom,[7] and the photogalvanic effect in media without a center of symmetry.[8] Investigation of these effects has been carried out essentially on the basis of the Boltzmann equation

$$\frac{\partial f_{\mathbf{k}}}{\partial t}=\int (W_{\mathbf{kk}'}f_{\mathbf{k}'}-W_{\mathbf{k}'\mathbf{k}}f_{\mathbf{k}})\,d\mathbf{k}'. \tag{3}$$

The peculiarities of kinetics in the absence of detailed balance are due to the fact that the balance of arrivals and departures is accomplished not according to the scheme $\mathbf{k}\rightleftarrows\mathbf{k}'$, but by means of the cycles $\mathbf{k}\to\mathbf{k}'\to\mathbf{k}''\to\ldots\to\mathbf{k}$.[1)]

2. In many physical situations,[2,10,11] the basic equation of kinetics is the Fokker–Planck (FP) equation

$$\partial f_{\mathbf{k}}/\partial t+\operatorname{div} j_{\mathbf{k}}(f_{\mathbf{k}})=0. \tag{4}$$

The current $\mathbf{j}_{\mathbf{k}}$ is connected locally with the distribution function. We pose the following question: how can ab-

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