traveling thermal grating and δn is the change in contrast due to interference of the standing and traveling thermal gratings.

A correlation was noted between the period and depth of modulation of the Stokes wave. The depth increases with increase in the period. In the case of constant time of switching on, this can be explained by the change in the pump spectrum. Of course, additional experimental investigations are needed to verify this explanation. This includes studies of the spectra of the incident and scattered radiation. Nevertheless, in the case of STS of sufficiently short pump pulses, it is possible in principle to distinguish STS-I from STS-II from the shape of the Stokes pulses and to draw conclusions on the width of the pump spectrum. The presence of a characteristic modulation of the intensity of the scattered radiation, and the correlation of the period with the modulation depth in the present experiment, conform to the mechanism described above.

The STS mirror can find application in those cases in which the required shift of frequency in the reflection with reversal of the wave front is minimal. For example, in the scheme of reversal of the wave front in resonant four-photon interaction,[8] the STS mirror can replace the ordinary mirror which requires careful alignment, and the SMBS mirror can also find application in well known systems for decoupling amplifying stages in laser systems with a narrow amplification band, where the frequency shift of the SMBS leads the radiation out of the amplification band.

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Autoionizing band of electron–exciton complexes and their role in reflection of slow electrons from the surface of a solid

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The model of multichannel small-radius interactions is used to obtain an analytical solution of the problem of electron reflection from the surface of a two-dimensional ordered lattice of two-level atoms. The positions of singularities of the reflection coefficient on a complex energy plane are used to reconstruct the energy spectrum of electron–exciton states. The conditions for the existence of autoionizing bands of electron–exciton complexes are determined and it is shown that in the presence of such bands the energy and angular dependences of the elastic reflection coefficient have characteristics Fano-Feshbach singularities. Numerical calculations are carried out for a monolayer of Xe atoms adsorbed physically on the surface of niobium.

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1. INTRODUCTION

In the last 10–15 years the experiments on low-energy electron diffraction have provided direct confirmation that monolayers of adsorbed atomic particles form regular structures (two- and one-dimensional crystals) at sufficiently low temperatures.[1,2] The properties of periodic low-dimensional structures are not identical with the properties of bulk crystals composed of the same atoms. Investigations of the geometry and spectra of ordered adsorbed monolayers are among the most interesting current topics in the physics of surface phenomena. Systems of this kind may exhibit, in particular, collective states of basically new type in the form of autoionizing bands, i.e., slowly decaying band states located against the background of the vacuum continuum.[3-6]

The dispersion law of such states should be a complex function of the real quasimomentum $\mathbf{q}$:

$$E(\mathbf{q})=E_0(\mathbf{q})-i\Gamma(\mathbf{q}). \tag{1}$$

The imaginary part of the dispersion law—the function $\Gamma(\mathbf{q})$—represents the time spent by an electron in a periodic structure. If the continuum of the vacuum states has a lower limit (usually taken to be zero), the average lifetime of a band state is found to a nonanalytic function of the quasimomentum.[4-6]

Autoionizing bands are a natural analog of one-center decaying states, i.e., of autoionizing levels of negative ions first discovered in the early sixties in experimental studies of the scattering of slow monochromatic electrons on gas targets (see, for example, the reviews in Refs. 7 and 8). Such bands may be exhibited by periodic low-dimensional structures in the case of a strong exchange interaction between one-center resonance levels.[1)] They are most likely in the case of monolayers of atomic particles with a quasistationary level of a long-lived negative ion in the range of energies under consideration. It must be stressed that autoionizing bands differ greatly from the familiar "surface resonances," which are formed from the Tamm bands because of the possibility of energy exchange between the normal and longitudinal (relative to the surface) degrees of freedom of an electron.[11]

An electron may leave a periodic structure for a number of reasons, for example, because of a change in the conditions of motion over long distances (which happens when an external field is applied[3]) or because of the finite permeability of potential (centrifugal) barriers surrounding individual interaction centers,[4,5] or because of possible exchange of energy with the internal degrees of freedom of the atomic cores.[6]

The "field"[3] and "potential"[4,5] autoionizing bands are of the one-particle type. Two-particle collective autoionizing states may form as a result of an exchange interaction between one-center Feshbach resonances.[6] Such resonances are exhibited by practically all the atomic particles, which should make it possible to detect experimentally the autoionizing bands of electron-exciton complexes predicted by us in Ref. 6. In experiments on reflection of slow monochromatic electrons from the surface of a solid covered by a monolayer of adsorbed atomic particles the existence of such states should be manifested by characteristic resonance and threshold dependences of all the measured quantities. These dependences will be derived and investigated below within the framework of a rigorously solvable model of multichannel zero-radius potentials,[12] supplemented by an allowance for the direct interactions of the cores[13] (in the present case, this will be done by allowing for the exciton degree of freedom of the system under discussion).

2. FORMULATION OF THE PROBLEM. GENERAL SOLUTION

We shall consider the problem of electron scattering by a system of fixed interaction centers (atomic cores) located at points $\mathbf{R}_s$ ($s=1,\ldots,N$). The Hamiltonian of the system is

$$H(\mathbf{r},\{\xi\})=-\Delta/2+H_A(\{\xi\})+\sum_{s=1}^{N}U_s(\mathbf{r}_s,\xi_s). \tag{2}$$

Here, $\mathbf{r}$ is the coordinate of an electron; $\mathbf{r}_s=\mathbf{r}-\mathbf{R}_s$; ξ_s is a set of internal variables of the s-th core; U_s is the interaction of an electron with the s-th center; H_A is the Hamiltonian of the system of interacting atomic cores:

$$H_A=\sum_{s=1}^{N}H_0(\xi_s)+\sum_{s,s'}{}' V_{ss'}(\xi_s,\xi_{s'}); \tag{3}$$

where H_0 is the Hamiltonian of an isolated center; $V_{ss'}$ is the direct (i.e., not related to repeated scattering of an electron) interaction between the cores.

We shall assume that before the scattering event the system of atomic cores is in the ground state whose energy will be regarded as zero. We shall denote the corresponding wave function by the ket vector $|0\rangle$. In addition to the ground state of the system of cores, we shall allow for the presence of N excited states which correspond, in the site representation, to the localization of an excitation at one of the centers. In the zeroth (in respect of $V_{ss'}$) approximation the wave functions of these states have clearly the form

$$|s\rangle=\varphi^{(1)}(\xi_s)\prod_{s'\neq s}\varphi^{(0)}(\xi_{s'}); \tag{4}$$

here, $\varphi_s^{(0)}$ and $\varphi_s^{(1)}$ are the wave functions of the s-th isolated center which is in the ground ($\varphi_s^{(0)}$) or excited ($\varphi_s^{(1)}$) states:

$$H_0\varphi^{(1)}(\xi_s)=\omega_0\varphi^{(1)}(\xi_s). \tag{5}$$

In the $|0\rangle$, $|s\rangle$ representation the Hamiltonian of a system of cores is an $(N+1)$-row nondiagonal matrix whose elements are

$$(\hat{H}_A)_{mm'}=(1-\delta_{m0})(1-\delta_{m'0})[\omega\delta_{mm'}+(1-\delta_{mm'})V_{mm'}];\quad m,\ m'=0,\ s;\ \ s=1,\ldots,N. \tag{6}$$

Here, $\omega=\omega_0+\Delta\omega$ is the excitation energy of an atomic core which is in a lattice and $V_{mm'}$ includes the interaction between cores responsible for the transfer of excitation along the lattice.

The stationary problem of the scattering of an electron on a system of interacting atomic centers should clearly be formulated on the basis of a representation which diagonalizes the Hamiltonian $\hat{H}_A$. We shall introduce the matrix of the corresponding unitary transformation $\hat{R}$:

$$(\hat{R}\hat{H}_A\hat{R}^{-1})_{nn'}=(1-\delta_{n0})\delta_{nn'}\varepsilon(n),\quad |n\rangle=\hat{R}|s\rangle \tag{7}$$

and we shall write down the multichannel Lippmann–Schwinger equation:

$$\Psi=\Psi_0+\Big(\hat{E}-\hat{\hat{H}}+\sum_s\hat{u}_s+i\eta\Big)^{-1}\sum_s\hat{u}_s\Psi,\qquad \Psi_0=e^{i\mathbf{kr}}|0\rangle. \tag{8}$$

Here, Ψ is the $(N+1)$-dimensional vector of the states in the whole system whose components correspond to the trajections along the unit vectors $|0\rangle$ and $|n\rangle$, i.e., to the motion of an electron in the field of atomic cores which are in stationary states;

$$\hat{u}_s=\hat{R}\hat{U}_s\hat{R}^{-1},\quad \hat{\tilde{H}}=\hat{R}\hat{H}\hat{R}^{-1},\quad \hat{\tilde{H}}_A=\hat{R}\hat{H}_A\hat{R}^{-1},$$

$$\Big(\hat{E}-\hat{\tilde{H}}+\sum_s\hat{u}_s+i\eta\Big)^{-1}\equiv G_0=-(2\pi|\mathbf{r}-\mathbf{r}'|)^{-1}\times\exp\big(i\,(2\,(\hat{E}-\hat{\tilde{H}}_A))^{1/2}|\mathbf{r}-\mathbf{r}'|\big),\tag{9}$$

$\hat{E}=E\hat{1}$ is the diagonal matrix of free Green functions ($\hat{1}$ is a unit matrix).

We shall now determine the total operator for the scattering of an electron by a system of interacting centers:

$$\hat{T}=\sum_{s=1}^{N}\hat{u}_s+\sum_{s=1}^{N}\hat{u}_s\hat{G}_0\hat{T}.\tag{10}$$

The operator $\hat{T}$ is an integral with respect to the electron coordinate and a matrix in the channel indices. We shall seek the solution of the problem by the method of equations describing multiple interactions. We shall introduce one-center scattering operators:

$$\hat{t}_s=\hat{u}_s+\hat{u}_s\Big(\hat{E}-\hat{\tilde{H}}+\sum_{s'\neq s}\hat{u}_s+i\eta\Big)^{-1}\hat{u}_s\tag{11}$$

and we shall assume that

$$\hat{T}=\sum_{s=1}^{N}\hat{T}^{(s)}.$$

Then, $\hat{T}^{(s)}$ is described by equations (see a similar derivation in Ref. 14)

$$\hat{T}^{(s)}=\hat{t}_s+\hat{t}_s\sum_{s'\neq s}\hat{G}_0\hat{T}^{(s')}.\tag{12}$$

We shall now assume that the electron–atom interactions do not overlap in space, i.e., when $s\neq s'$, we have

$$\hat{u}_s\hat{u}_{s'}=0.\tag{13}$$

It is then easily shown (see, for example, Refs. 9, 13, and 16) that the exact solution of a system of integral equations (12) is expressed in terms of solutions of a system of algebraic equations defining the projections of the vectors $\mathbf{T}^{(s)}=\hat{T}^{(s)}|\mathbf{k},0\rangle$ onto the states

$$|l_sm_sn\rangle=Y_{l_sm_s}(\mathbf{r}_s/r_s)j_{l_s}(k(n)r_s)\,|n\rangle.$$

Here, $Y_{lm}(\mathbf{r}/r)$ is a spherical function; $j_l(x)$ is a spherical Bessel function; $k(n)=[2(E-\varepsilon(n)]^{1/2}$. The system is

$$T^{(s)}_{l_sm_s}(n)=\langle l_sm_sn|\hat{t}_s|\mathbf{k},0\rangle+\sum_{s'\neq s}\sum_{n'}\sum_{l_s'm_s'}\sum_{l_s,m_s,}\langle l_sm_sn|\hat{t}_s|l_s'm_s'n'\rangle F^{l_s'm_s'}_{l_sm_s}(k(n),\mathbf{R}_s,\mathbf{R}_{s'})T^{(s')}_{l_sm_s}(n'),\tag{14}$$

where $T^{(s)}_{l_sm_s}(n)=\langle l_sm_sn|\mathbf{T}^{(s)}\rangle$ and the propagation matrix $F^{l_s,m_s'}_{l_sm_s}$ is identical with the expression (23) in Ref. 9.

The operators $\hat{t}_s$ introduced by Eq. (11) describe [in the $\hat{R}$ representation, see Eq. (7)] $(N+1)$-channel scattering by the s-th atomic core interacting ($\hat{V}\neq 0$) with all the other centers in the system. The operators $\hat{t}_s$ can be expressed in terms of the matrix $\hat{R}$ and in terms of the operators of the one-center $(N+1)$-channel scattering in the site representation:

$$\hat{t}_s=\hat{R}\hat{t}^{(s)}_{sr}(\hat{E}-\hat{H}_A)\hat{R}^{-1}.\tag{15}$$

For $\hat{V}=0$ the elements of the matrix $\hat{t}^{(s)}_{sr}$ describing the scattering of an electron by the s-th core, can be expressed in a self-evident manner in terms of the operators for the scattering of an electron by an isolated (two-level) atom:

$$[\hat{t}^{(s)}_{sr}(E-\hat{H}_0)]_{nm}=\hat{t}_{00}\delta_{n0}\delta_{m0}+\hat{t}_{11}\delta_{ns}\delta_{ms}+\hat{t}_{01}\delta_{n0}\delta_{ms}+\hat{t}_{10}\delta_{ns}\delta_{m0}\tag{16}$$

(for $n, m=0, s$; site representation) or

$$[\hat{t}^{(s)}_{sr}(E-\hat{H}_0)]_{nm}=\hat{t}_{00}\delta_{nm}\quad(\text{for }\ n,m\neq 0,s).\tag{17}$$

Here, $\hat{t}_{00,11}$ are the integral (with respect to r and r′) operators of the elastic scattering of an electron by an isolated atom which is in the ground (or excited) state; $\hat{t}_{01}$ are the integral operators of the inelastic scattering.

If $V\neq 0$, the analytic dependence of $\hat{t}$ on $\hat{E}-\hat{H}_A$ is not affected (because $\hat{V}$ does not act on r). In the case of the interactions described by $\hat{u}_s$, which decrease sufficiently rapidly with distance, this dependence has the usual form[14-15]

$$\hat{t}_{sr}(\hat{E}-\hat{H}_A)=\hat{K}_{sr}(\hat{1}+i(2(\hat{E}-\hat{H}_A))^{1/2}\hat{K}_{sr})^{-1}\tag{18}$$

(here, $\hat{K}_{sr}$ is the Hermitian scattering operator). The formulas (16)–(18) make it possible to relate the matrix elements for the two-channel one-center scattering $\langle l_sm_s|\hat{t}_s|l_s'm_s'\rangle$ with the one-center matrix elements of the $(N+1)$-channel scattering.

In the problem of the scattering of an electron by a periodic lattice, which we shall solve below, the above approach makes it possible to avoid introduction of indeterminate phenomenological parameters and to express all the constants of the electron–exciton interaction in terms of physical quantities known from experiments on the gaseous phase.

For the sake of simplicity, we shall ignore a possible change in the electron momentum because of the scattering by a single atom[2)] and we shall consider only the waves[3)] with $l=0$. Then, the system of equations (14) can be represented as follows:

$$\sum_m(K^{-1}_{(s)})_{nm}T^{(s)}(m)+i(2(E-\varepsilon(n)))^{1/2}T^{(s)}(n)-2\pi\sum_{s'\neq s}G_0^{(+)}(k(n),\mathbf{R}_s,\mathbf{R}_{s'})T^{(s')}(n)=\delta_{n0}\exp(i\mathbf{k}\mathbf{R}_s),\tag{19}$$

where

$$(K_s^{-1})_{nm}=\langle 0,0,n|\hat{K}_s^{-1}|0,0,m\rangle,$$

$$G_0^{(+)}(k(n),\mathbf{R}_s,\mathbf{R}_{s'})=-(2\pi|\mathbf{R}_s-\mathbf{R}_{s'}|)^{-1}\exp(i(2(E-\varepsilon(n)))^{1/2}|\mathbf{R}_s-\mathbf{R}_{s'}|).\tag{20}$$

The quantities $T^{(s)}(n)$ defined by the system (19) represent amplitudes of spherical waves traveling in the various channels away from the individual scattering centers. The differential cross sections for the elastic ($n=0$) and inelastic ($n\neq 0$) scattering are

$$\frac{d\sigma(n)}{d\Omega}=\frac{k(n)}{k}\Big|\sum_s T^{(s)}(n)\exp(-i\mathbf{k}_f(n)\mathbf{R}_s)\Big|^2,\tag{21}$$

$$k=(2E)^{1/2},\quad \mathbf{k}_f(n)=\mathbf{r}k(n)/r.$$

We shall now specify the model of interactions between the cores assuming for the matrix $\hat{V}$ in Eq. (6) a translation-invariant dependence on the indices: $\hat{V}_{nn'}=V(|n-n'|)$; $n, n'=1,\ldots,N$. We shall first consider one-dimensional systems. Generalization to the more complex case of a two-dimensional crystal will be clear from the nature of the equations given below. The nature of the matrix $\hat{R}$ responsible for a transition from the site to the exciton representation is well known:

$$(\hat{R})_{ns}=N^{-1/2}\exp\left(i\frac{2\pi}{N}(n-1)(s-1)\right),$$
$$(\hat{R})_{00}=1,\quad (\hat{R})_{0n}=(\hat{R})_{n0}=0,\quad \mathbf{R}_s=(as,0,0). \tag{22}$$

The functions (19) occurring in the system $K^{-1}_{nm}(E)$ are assumed to be known from the one-center calculations (if $E>0$, they can be, in principle, reconstructed from the data on the electron–atom scattering). We shall assume them to be constant, which corresponds to the model of zero-radius potentials.[12,13] We shall assume that

$$K_{00}^{-1}(E)=\varkappa_0,\quad K_{11}^{-1}(E)=\varkappa_1,\quad K_{01}^{-1}(E)=\varkappa_{01}.$$

In the limit $N\to\infty$ we shall go over from discrete indices n to the exciton quasimomentum $\mathbf{p}=(p,0,0)$, where $p=2\pi(n-1)/aN$, and a is a lattice constant, and we shall replace summation with integration in accordance with the rule

$$N^{-1}\sum_{n=1}^{N}\to\frac{a}{2\pi}\int_0^{2\pi/a}dp.$$

The system (19) then becomes

$$(\varkappa_0+ik)T^{(s)}(0)-2\pi\sum_{s'\neq s}G_0^{(+)}(E,\mathbf{R}_s,\mathbf{R}_{s'})T^{(s')}(0)$$
$$+\frac{a\varkappa_{01}}{2\pi}\int_0^{2\pi/a}dp\exp(ip\mathbf{R}_s)T^{(s)}(p)=\exp(ik\mathbf{R}_s), \tag{23a}$$

$$(\varkappa_0+ik(p))T^{(s)}(p)-2\pi\sum_{s'\neq s}G_0^{(+)}(E-\varepsilon(p),\mathbf{R}_s,\mathbf{R}_{s'})T^{(s')}(p)$$
$$+\frac{\varkappa_1-\varkappa_0}{2\pi}\int_0^{2\pi/a}\exp(i(\mathbf{p}'-\mathbf{p})\mathbf{R}_s)T^{(s)}(p')dp'+\varkappa_{01}\exp(-ip\mathbf{R}_s)T^{(s)}(0)=0. \tag{23b}$$

Here, $\varepsilon(p)$ is the dispersion law of an exciton [for example, in the tight-binding approximation the interaction between the cores corresponds to $\varepsilon(p)=\omega+2\beta\cos ap$].

The equations obtained have an obvious physical meaning. The first two terms in Eq. (23a) describe the elastic scattering of an electron by a system of unexcited atomic cores and the term proportional to the coupling parameter of the channels $\varkappa_{01}$ allows for the possibility of exciton excitation. Similarly, the first two terms in Eq. (23b) describe the scattering of an electron by a system of centers which contains one free exciton. The electron–exciton interaction, which is diagonal in respect of the number of excitons, is allowed for by the term with $(\varkappa_1-\varkappa_0)$. This interaction describes the electron–exciton scattering and it is responsible for the formation of bound electron–exciton pairs (see below). The last term in Eq. (23b) allows for the possibility of absorption of an exciton by an electron, i.e., for the autoionization of an electron–exciton complex.

It is now appropriate to consider all those corrections to the system (23) which are needed to allow for the influence of various physical factors ignored above. First of all, we shall note the generalization to the case of a two-dimensional lattice involves the simple replacement of single sums and one-dimensional integrations with double sums over the indices of the centers $[s=(s_x,s_y,0)]$ and two-dimensional integration with respect to the projections of the exciton quasimomentum vector $[\mathbf{p}=(p_x,p_y,0)]$. Integration is carried out over the first Brillouin zone with a normalization factor $\Omega_0/(2\pi)^\nu$, where Ω_0 is the area of a unit cell in a two-dimensional lattice (or the length in a one-dimensional lattice) and $\nu=1,2$ indicate one- and two-dimensional cases, respectively.

The presence of any external field $U(z)$ (including the presence of a crystal surface) can be allowed for by the simple replacement of the free Green function $[\hat{G}_0\to(\hat{E}-H-U(z)\hat{1}+i\eta)^{-1}]$; at the same time it is obviously necessary to replace the incident wave $e^{i\mathbf{k}\cdot\mathbf{r}}$ with the corresponding solution of the distorted plane wave type. Weak damping of an exciton (radiative or due to its interaction with the surface of a crystal) is allowed for most simply by introducing a small imaginary part in the dispersion law $\varepsilon(\mathbf{p})$. In terms of the system (23), dropping of the model of nonoverlapping interactions of Eq. (13) is equivalent to introduction of dependences of the functions $(\varkappa_1-\varkappa_0)$ and $\varkappa_{01}$ on the exciton quasimomentum $\mathbf{p}$.

An analysis of the influence of all these factors should be the next stage in the development of the theory of autoionizing bands of electron–exciton complexes. We shall confine ourselves to the solution of the problem in terms of the simplest possible representations, which nevertheless retain all the qualitatively important features of the general case.

We shall seek the solution of the system (23) in the form

$$T^{(s)}(0)=\exp(i\mathbf{k}\mathbf{R}_s)T(0),\quad T^{(s)}(\mathbf{p})=\exp(i(\mathbf{k}-\mathbf{p})\mathbf{R}_s)T(\mathbf{p}). \tag{24}$$

Then, the quantities $d\sigma(n)/d\Omega$ are given by

$$\frac{d\sigma(0)}{d\Omega}=\frac{1}{4\pi^2}|T(0)|^2S(E,\mathbf{k},\mathbf{k}_f),$$
$$\frac{d\sigma(\mathbf{p})}{d\Omega}=\frac{1}{4\pi^2}|T(\mathbf{p})|^2\frac{k(\mathbf{p})}{k}S(E,\mathbf{k},\mathbf{k}_f,\mathbf{p}); \tag{25}$$

here,

$$S(E,\mathbf{k},\mathbf{k}_f,\mathbf{p})=\left|\sum_s\exp(i(\mathbf{k}-\mathbf{k}_f-\mathbf{p})\mathbf{R}_s)\right|^2$$
$$=\frac{(2\pi)^{2\nu}}{\Omega_0}\left|\sum_b\delta(\mathbf{k}-\mathbf{k}_f-\mathbf{p}-\mathbf{b})\right|^2 \tag{26}$$

are structure factors[18] depending only on the lattice geometry (**b** is the reciprocal lattice vector). The factor S in $d\sigma/d\Omega$ determines the positions of the diffraction maxima and the relevant functions are well known.[18,19] The main task of the theory is thus to calculate the dynamic factors $T(0)$ and $T(\mathbf{p})$, which can be found exactly for the adopted interaction model.

Substituting the expressions in Eq. (24) into the system (23) and taking $T(0)$ from Eq. (23a), we find that $T(\mathbf{p})$ is described by the following integral equation:

$$Z(\mathbf{p},\mathbf{k})T(\mathbf{p})-(\varkappa_1-\varkappa_0-\varkappa_{01}^2Z_0^{-1}(E,\mathbf{k}))\frac{\Omega_0}{(2\pi)^\nu}\int d\mathbf{p}'\,T(\mathbf{p}')=\varkappa_{01}Z_0^{-1}(E,\mathbf{k}); \tag{27}$$

here

$$Z_0(E,\mathbf{k})=\varkappa_0+ik-2\pi\sum_{\mathbf{R}_s\neq\mathbf{R}_{s'}}G_0^{(+)}(E,\mathbf{R}_s,\mathbf{R}_{s'})\exp(i\mathbf{k}\mathbf{R}_{ss'}), \tag{28a}$$

$$Z(\mathbf{p},\mathbf{k})=\varkappa_0+ik(\mathbf{p})-2\pi\sum_{\mathbf{R}_s\neq\mathbf{R}_{s'}}G_0^{(+)}(E-\varepsilon(\mathbf{p}),\mathbf{R}_s,\mathbf{R}_{s'})\exp(i(\mathbf{k}-\mathbf{p})\mathbf{R}_{ss'}). \tag{28b}$$

The solution of Eq. (27) are

$$T(0)=[1+(\varkappa_1-\varkappa_0)D(E,\mathbf{k})]/Z_0(E,\mathbf{k})\left[1+\left(\varkappa_1-\varkappa_0-\frac{\varkappa_{01}^2}{Z_0(E,\mathbf{k})}\right)D(E,\mathbf{k})\right], \tag{29}$$

$$T(\mathbf{p})=\frac{\varkappa_{01}}{Z_0(E,\mathbf{k})Z(\mathbf{p},\mathbf{k})[1+(\varkappa_1-\varkappa_0-\varkappa_{01}^2/Z_0(E,\mathbf{k}))D(E,\mathbf{k})]}, \tag{30}$$

$$D(E,\mathbf{k})=\frac{\Omega_0}{(2\pi)^\nu}\int\frac{d\mathbf{p}}{Z(\mathbf{p},\mathbf{k})}. \tag{31}$$

In the framework of the multichannel model of zero-radius potential[12,13] the solutions (29) and (30) are exact. This makes it possible to consider the spectrum of eigenvalues of the Hamiltonian (2) without the usual assumption that the electron–exciton interaction constant is small and, in particular, to investigate the role of formation and dissociation of bound electron–exciton pairs in the process of electron reflection from periodic structures.4)

3. SPECTRUM OF ELECTRON–EXCITON STATES IN TWO- AND ONE-DIMENSIONAL CRYSTALS

The spectrum of electron and electron–exciton states can be found by investigating singularities of the functions $T(0)$ and $T(\mathbf{p})$ on a complex plane of energies E. For a fixed value of $\mathbf{k}_\parallel$ ($\mathbf{k}_\parallel$ is the projection of the electron momentum $\mathbf{k}=(\mathbf{k}_\parallel,\mathbf{k}_\perp)$ onto the plane of a grating in the one-dimensional case or on the axis of a linear chain in the one-dimensional case) these singularities may include poles of $E(\mathbf{k}_\parallel)$, corresponding to one-particle band states of an electron and an electron–exciton pair bound to form a complex, and also branching points which are the boundaries of the one-particle (vacuum) and two-particle (electron–exciton) continua.

We shall consider first the important case of sufficiently small values of the parameter $\varkappa_{01}$ which corresponds to, for example, the assumption of the existence of a long-lived autoionizing state of the Feshbach resonance type in the case of an isolated atom. In the zeroth approximation the spectrum of the lattice and electron eigenvalues is given by the roots of the equations

$$Z_0(E,\mathbf{k}_\parallel)=0, \tag{32}$$

$$1+(\varkappa_1-\varkappa_0)D(E,\mathbf{k}_\parallel)=0,\quad \operatorname{Im}D(E,\mathbf{k}_\parallel)=0. \tag{33}$$

The solution of the first of these equations gives a band of free electrons whose dispersion law is $E_1(\mathbf{k}_\parallel)$ in the field of nonexcited interaction centers. This band has been investigated in, for example, Refs. 12 and 21. The real solutions of Eq. (33) describe a band of states of an electron–exciton complex.[6] These solutions lie below the boundary of the continuum states of a free exciton and a bound electron, whose energies are

$$E(\mathbf{p},\mathbf{q})=\varepsilon(\mathbf{p})+E_1(\mathbf{q}),\quad \mathbf{k}_\parallel=\mathbf{q}+\mathbf{p}. \tag{34}$$

For arbitrary values of the parameters the solutions of Eq. (33) can be found only numerically but in the tight-binding approximation we can also solve the problem analytically. Let us assume that

$$\alpha a\gg1,\quad a\Delta\ll\alpha,\quad \alpha=(2(\omega-E))^{1/2},$$
$$\varepsilon(\mathbf{p})=\omega+2\beta\cos\mathbf{ap}, \tag{35}$$

where $\Delta=4\beta$ is the width of an exciton band. Then, for example, in the case of a one-dimensional chain of atoms, Eq. (33) becomes

$$(\varkappa_1-\varkappa_0)a=\left\{(\varkappa_0-\alpha)^2a^2-4\left(e^{-2\alpha a}+\frac{\beta^2a^2}{\alpha^2}+\frac{2\beta a}{\alpha}e^{-\alpha a}\cos qa\right)\right\}^{1/2}. \tag{36}$$

Hence, we can see that in the case of a one-dimensional crystal the formation of electron–exciton complexes is possible if

$$\varkappa_1>\varkappa_0. \tag{37}$$

The condition (37) has a simple physical meaning. If $\varkappa_1>\varkappa_0>0$, it means that the energy binding an electron to an excited atom should be greater than the binding energy in the case of an electron and a nonexcited atom. (It is intuitively clear that only then an exciton moving in a structure can drag an electron behind.) The real solutions of Eq. (33) can then be interpreted as states of a one-center Feshbach resonance, which is collective over the centers because of the translational symmetry. However, one should point out that the branch of bound states of an electron–exciton pair exists also when $\varkappa_0<0$, $\varkappa_0<\varkappa_1$. This case (for $\varkappa_1<0$) corresponds to the conditions when the repulsion of an electron by a nonexcited atom is stronger than by an excited one.

Solving Eq. (36), we find the dispersion law of an electron–exciton complex near the bottom of a band of a one-dimensional crystal:

$$E_0(q)=\omega-\varkappa_1^2/2+\frac{4\varkappa_1(e^{-\varkappa_1a}-\beta a/\varkappa_1)^2}{a^2(\varkappa_1-\varkappa_0)}+\frac{q^2}{2m^*},$$
$$m^*=\frac{(\varkappa_1-\varkappa_0)}{8\beta a}e^{\varkappa_1a} \tag{38}$$

(here, q is the quasimomentum of an electron–exciton complex and m^* is its effective mass). In general, Eq. (33) can be solved numerically.

Among known autoionizing states of atomic particles those of negative rare gas ions are among the most thoroughly investigated (see, for example, Ref. 23). The parameters of ordered adsorbed monolayers, formed at low temperatures on metal or graphite surfaces, are also known for these gases[24] and this makes it possible to make the most definite predictions in such cases.

We calculated the dispersion law of an electron–exciton complex for the parameters $\varkappa_0=-0.17$, $\varkappa_1=0.20$, $\omega=0.30$ (a.u.) (Ref. 23), $\Delta=0.5$ eV, $a=8.5$ a.u. (Ref. 25), which correspond to a two-dimensional crystal lattice of xenon (Xe) atoms on the surface of niobium.[24] A unit cell of the adsorption structure is hexagonal close-packed. The first Brillouin zone for a lattice with this geometry is shown in Fig. 1. Figure 2 gives the dispersion law of an electron–exciton complex in a two-dimensional crystal of Xe atoms. It follows from these results that in the case of monolayers of rare gas atoms adsorbed physically on the surface of a solid there should be a branch of collective states of elec-

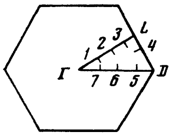

FIG. 1. First Brillouin zone and points at which calculations were carried out.

tron–exciton complexes with a binding energy of an electron–exciton pair amounting to ~0.2–0.3 eV. The width of a band of states of such complexes is ~0.2 eV. The predicted states are effectively a new quasiparticle: an "electroexciton" which carries a unit charge, has a relatively large effective mass (~$6m_e$–$7m_e$), and a large internal excitation energy (~8 eV).

Since at the limit of states of free electrons and excitons the integral (31) diverges as a square root in the one-dimensional case and logarithmically in the two-dimensional case (see, for example, Ref. 26), the condition (37) is sufficient for the existence of electron–exciton complexes only in periodic low-dimensional structures. The condition should be more stringent in the three-dimensional case because a three-dimensional integral of the (31) type assumes finite values at the boundary. However, we may expect that crystals of rare gas elements may also exhibit states of electron–exciton complexes because of the large value of the electron–exciton interaction constant $a(\varkappa_1-\varkappa_0)$ ~4.

For $E>0$ the states of such complexes lie above the boundary of the vacuum continuum. Allowance for the possibility of energy exchange between electrons and the exciton degree of freedom ($\varkappa_{01}\neq 0$) results in this case in autoionization, which is represented by the imaginary part of the solution of the equation

$$1+(\varkappa_1-\varkappa_0-\varkappa_{01}^2/Z_0(E,\mathbf{q}))D(E,\mathbf{q})=0,\qquad (\mathbf{q}=k\mathbf{R}_s/R_s). \tag{39}$$

For small values of $\varkappa_{01}$ the solutions of Eq. (39) can be found by iteration over the terms with an imaginary component. We find that

$$E(\mathbf{q})=E_0(\mathbf{q})+\Phi(\mathbf{q})-i\Gamma(\mathbf{q}),$$

$$\Gamma(\mathbf{q})=-\frac{\varkappa_{01}^2}{(\varkappa_1-\varkappa_0)^2}\left(\frac{dD(E,\mathbf{q})}{dE}\right)^{-1}_{E=E_0}\frac{\operatorname{Im}Z_0(\mathbf{q})}{|Z_0(E,\mathbf{q})|^2}, \tag{40}$$

$$\Phi(\mathbf{q})=-\Gamma(\mathbf{q})\frac{\operatorname{Re}Z_0(\mathbf{q})}{\operatorname{Im}Z_0(\mathbf{q})}. \tag{41}$$

In the most important (from the practical point of view) case of a two-dimensional crystal lattice (see, for example, Refs. 12 and 22), we have

$$\operatorname{Im}Z_0(E,\mathbf{q})=\frac{2\pi}{\Omega_0}\sum_{\mathbf{b}}\frac{\eta(k^2-(\mathbf{q}+\mathbf{b})^2)}{[k^2-(\mathbf{q}+\mathbf{b})^2]^{1/2}}, \tag{42}$$

where η is the Heaviside function. [The expression for $\Gamma(\mathbf{q})$ applicable to one-dimensional crystals is given in our earlier paper.[6]] The autoionization width of electron–exciton complexes is thus a nonanalytic function of the quasimomentum [we should bear in mind that the values of $E_0(\mathbf{q})$ and $\mathbf{q}$ occurring in Eq. (42) are related by the dispersion law found by solving Eq. (33)]. At the points governed by the condition

$$2E_0(\mathbf{q})=k^2=(\mathbf{q}+\mathbf{b})^2, \tag{43}$$

the imaginary part of the complex dispersion law of electron–exciton complexes has a discontinuity associated with opening up of a new decay channel accompanied by the umklapp process ($\mathbf{k}_{\parallel}=\mathbf{q}+\mathbf{b}$).

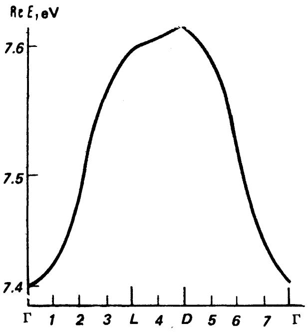

FIG. 2. Dispersion law of an electron–exciton complex in a two-dimensional crystal of Xe atoms. The parameters of the model used in the calculations are given in the text.

The results of calculations of $\Gamma(\mathbf{q})$ are:

Im E:	Γ	1	2	L	4	5
$\Gamma(q)$, 10^{-2} eV:	0.37	2.6	0.35	0.52	1.6	1.0

The parameter $\varkappa_{01}^2$ was reconstructed from the experimental data on the width of the autoionizing state $(\mathrm{Xe}^-)^{ai}$, reported as ~9×10^{-3} eV in Ref. 7, and was selected to be 1.36×10^{-2} eV. A calculation of the values of Re Z_0 was made using the modified (for the case of a two-dimensional lattice) Ewald method.[12]

We shall now discuss the changes which are sufficient to modify Eq. (41) in order to allow for the way that the decay is influenced by an external electric field or by the surface of a crystal with which an electron interacts in accordance with the one-dimensional potential $U(z)$. This can be done simply by modifying Eq. (41) as a result of the following substitution (see a similar conclusion in Ref. 3):

$$\operatorname{Im}Z_0(\mathbf{q})\to\sum_{\mathbf{b}}\chi_U^2(E-(\mathbf{q}+\mathbf{b})^2/2,0)\,\rho(E-(\mathbf{q}+\mathbf{b})^2/2), \tag{44}$$

where $\rho(\varepsilon)$ is the density of states and χ_U is the regular solution of the one-dimensional Schrödinger equation:

$$-\frac{1}{2}\frac{d^2\chi_U}{dz^2}+U(z)\chi_U=\left(E-\frac{1}{2}(\mathbf{q}+\mathbf{b})^2\right)\chi_U. \tag{45}$$

We shall now consider in greater detail the influence of an external electric field $U(z)=-fz$ on the autoionization of an electron–exciton complex. We then have

$$\chi_U=V(-x),\qquad x=\frac{2E-(\mathbf{q}+\mathbf{b})^2}{(2f)^{2/3}},$$

and Im Z_0 is given by

$$\operatorname{Im}Z_0(E,\mathbf{q})=\frac{2\pi}{\Omega_0(2f)^{1/3}}\sum_{b}V^2\left(\frac{(\mathbf{q}+\mathbf{b})^2-2E}{(2f)^{2/3}}\right) \tag{46}$$

(V is the Airy function). We shall now discuss the case of a sufficiently weak field **f**, when the direct ionization of an electron–exciton pair can be ignored [$E_0\gg(2f)^{2/3}$]. We can then see from Eq. (46) that a weak external electric field is sufficient to alter greatly the lifetime of an electron–exciton complex. In fact, when the conditions

$$\min(k^2-2E_0(\mathbf{q}),\,k^2)\gg k^2-(\mathbf{q}+\mathbf{b})^2\sim f^{2/3},$$
$$\operatorname{Im}Z_0(\mathbf{q},\mathbf{f})/\operatorname{Im}Z_0(q,0)\approx x^{1/2}V^2(-x) \tag{47}$$

are satisfied Eq. (47) tends to zero for positive values $x \to 0$, i.e., the lifetime of an electron–exciton complex proportional to $(\mathrm{Im}\, Z_0)^{-1}$ rises steeply.

A similar result has been obtained earlier[10] for an isolated Feshbach resonance.

We shall conclude by discussing some special cases of the asymptotically exact equation (39). We shall assume that the width of an exciton band is negligible ($\Delta = 0$). Then, as expected, Eq. (33) reduces to the well-known equation in the theory of impurity states (see, for example, Ref. 27):

$$(\varkappa_1 - \varkappa_0)^{-1} = \frac{\Omega_0}{(2\pi)^\nu} \int d\mathbf{p} \left\{ \varkappa_0 - \alpha + \sum_{s \neq 0} \frac{\exp(-\alpha R_s + i\mathbf{p}\mathbf{R}_s)}{R_s} \right\}^{-1}, \tag{48}$$

$$\alpha = (2(\omega - E))^{1/2}.$$

The formula (41) governs in this case the average lifetime of an autoionizing impurity level with a two-dimensional crystal lattice (in this case, an excited atom of the crystal can be regarded as an impurity). A similar result is also obtained in the other limiting case which corresponds to the formation of an impurity exciton level in the field of a localized negative ion ($\varkappa_0 > 0$, $e^{-\alpha R} \ll 0$).

Several interesting cases can be investigated by assuming that $\varkappa_0 = \varkappa_1$. If $E < 0$, we find that, for example, the dispersion equation (39) is identical, apart from the dimensions of integration, with Eq. (2.2) in the review by Levinson and Rashba,[33] where the theory of bound states formed by an electron and a nonconserved quasiparticle is presented for the case of a strong nondiagonal interaction. However, it should be pointed out that in addition to the cases considered earlier, this limit of Eq. (39) allows for the usually neglected effects of the dispersion of quasiparticle states [$\varepsilon(\mathbf{p}) \neq \mathrm{const}$].

4. RESONANCE AND THRESHOLD SINGULARITIES OF THE CROSS SECTION FOR THE SCATTERING OF ELECTRONS BY ONE- AND TWO-DIMENSIONAL CRYSTAL

We shall now use Eqs. (25), (29), and (30) to consider the problem of the angular and energy dependences of the cross section for the elastic scattering of an electron by ordered structures. Let $\varkappa_{01}$ be sufficiently small and then

$$|E - E_0(\mathbf{q})| \gg \Gamma(\mathbf{q}) \tag{49}$$

the role of exciton states is unimportant and we have $T(0) \approx Z_0^{-1}$. The scattering is of the potential type and the elastic reflection coefficient $\sim |T(0)|^2 \equiv F(E, \theta)$ can only have Bragg singularities. A calculation of $F(E, \theta)$ in the case when the condition (49) is satisfied is the subject of the kinematic theory of low-energy electron diffraction (see, for example, the review in Ref. 17) and a detailed analysis of the potential scattering by a one-dimensional chain has been made using the zero-radius potential model.[28] It should be pointed out that when the conditions (43) are satisfied, the function Z_0 diverges (in accordance with a square-root law in the two-dimensional case) and $F(E, \theta)$ vanishes.

In the range of energies satisfying the condition $|E - E_0(\mathbf{q})| \lesssim \Gamma(\mathbf{q})$, the scattering process becomes resonant because of the capture of an electron in an autoionizing band of electron–exciton complexes. Substituting Eq. (40) in the elastic scattering amplitude $T(0)$, we find that near a resonance

$$T(0) = \frac{1}{Z_0(E, \mathbf{k}_\parallel)} \frac{E - E_0(\mathbf{k}_\parallel)}{E - E_0(\mathbf{k}_\parallel) - \Phi(\mathbf{k}_\parallel) + i\Gamma(\mathbf{k}_\parallel)}. \tag{50}$$

We shall now give the expression for the reflection coefficient F in the Fano formula[29]:

$$F(E, \theta) = F_0 \frac{(\gamma + \varepsilon)^2}{1 + \varepsilon^2}; \tag{51}$$

here

$$\gamma = \frac{\mathrm{Re}\, Z_0}{\mathrm{Im}\, Z_0}, \quad F_0 = |Z_0(E, \mathbf{k}_\parallel)|^{-2}, \quad \varepsilon = \frac{E - E_0 - \Phi}{\Gamma}.$$

The expressions obtained make it possible to predict the characteristic form of resonance singularities of the energy and angular dependences of the coefficients of reflection of electrons by a monolayer of adsorbed atoms. It follows[5)] from Eq. (51) that for a fixed angle of incidence θ the function $F(E, \theta)$ has a minimum at $\varepsilon = -\gamma$ [$F(\varepsilon + \gamma = 0) = 0$] which changes to a resonance peak at $\varepsilon = \gamma^{-1}$. The amplitude of the peak and the energy interval occupied by the resonance singularity are governed by the value of the "profile index" γ. The structure appears most clearly for small values of γ. The characteristic parameters E_0, Φ, and Γ are different for different angles of incidence and are mainly governed by the dispersion law of electron–exciton complexes. This is illustrated in Fig. 3, which gives the results of our calculations of the coefficient of elastic reflection of monochromatic electrons by a monolayer of adsorbed Xe atoms. The orientation of the electron beam relative to the crystallographic axes is shown in Fig. 4. (The parameters of the model used have been listed above.)

An experimental detection of such a structure would provide a reliable confirmation of the existence of autoionizing bands of bound electron–exciton pairs in monolayers of physically adsorbed atoms. However, one can suggest a somewhat different variant of an experiment involving determination of the angular dependence of the reflection coefficient for a fixed energy of the incident electrons (corresponding to a band of

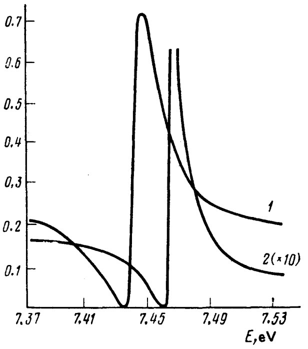

FIG. 3. Energy dependences of the coefficient of electron reflection from monolayer of Xe atoms plotted for different angles θ of the incidence of electrons: 1) $\theta = 0°$; 2) $\theta = 8°30'$.

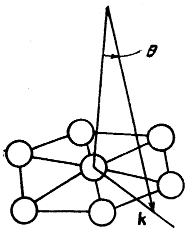

FIG. 4. Orientation of an electron beam relative to the crystallographic axes of a two-dimensional lattice of Xe atoms.

states of electron–exciton complexes). The results of calculations illustrating this possibility are given in Fig. 5.

We shall now analyze the threshold singularities of the function $F(E, \theta)$ which are associated with the opening up of inelastic scattering channels accompanied by the creation of a free exciton. We shall begin by noting that in the presence of a band of bound $[E_1(\mathbf{p}_e) < 0]$ states (within the framework of the adopted model this case corresponds to the values $\varkappa_0 > 0$) the process of exciton creation is also possible for $E < \varepsilon_{\min}(\mathbf{p})$. We then clearly have to satisfy the conditions

$$E=\varepsilon(\mathbf{p})+E_1(\mathbf{p}_e), \qquad \mathbf{k}_\parallel=\mathbf{p}+\mathbf{p}_e+\mathbf{b}n, \quad n=0, \pm1, \dots \tag{52}$$

(here, $\mathbf{p}$ and $\mathbf{p}_e$ are, respectively, the exciton and electron quasimomenta). Near the electron "trapping" threshold the energy dependence of the elastic reflection coefficient is given by

$$F=F_0-\frac{2F_0^{1/2}\varkappa_{01}^2|D|^{-1}}{(\varkappa_1-\varkappa_0)^2}\cos(\delta_0-\delta_1); \tag{53}$$

here,

$$F_0=\left|Z_0(E,\mathbf{k}_\parallel)-\frac{\varkappa_{01}^2}{\varkappa_1-\varkappa_0}\right|^2, \quad \delta_1=\operatorname{arctg}\frac{\operatorname{Im}D(E,\mathbf{k}_\parallel)}{\operatorname{Re}D(E,\mathbf{k}_\parallel)},$$
$$\delta_0=\operatorname{arctg}\frac{\operatorname{Im}Z_0(E,\mathbf{k}_\parallel)}{\operatorname{Re}Z_0(E,\mathbf{k}_\parallel)-\varkappa_{01}^2(\varkappa_1-\varkappa_0)^{-1}} \tag{54}$$

[we must bear in mind that if $E=E_{\text{th}}(\mathbf{k}_\parallel)$, the function D^{-1} vanishes and δ_1 has a nonanalytic singularity].

The threshold discussed above corresponds to the situation in which an electron that excites first an exciton cannot leave a structure (a crystal) without reabsorption of the exciton excitation energy. However, at sufficiently high energies the process of reflection of an electron accompanied by simultaneous creation of a free exciton becomes possible if $[E > \varepsilon_{\min}(\mathbf{p})]$. We shall consider the nature of the threshold singularity of the function $F(E, \theta)$ in this case.

For simplicity, we shall consider only the one-dimensional model for which the analytic form of the function $Z_0(E, \mathbf{k}_\parallel)$ is known (see, for example, Ref. 22). According to Eq. (29), at low values of $\delta E=|E-E_{\text{th}}|$, we have

$$T(0)\approx\Phi_1+\Phi_2\delta E+\Phi_3(\delta E)^{1/2}(a\varkappa_0-\ln a^2\delta E)^{-1}, \tag{55}$$

where Φ_1, Φ_2, and Φ_3 are slowly varying functions of the energy and quasimomentum. The singularities $F(E, \theta)$ predicted by Eq. (55) are fully analogous to those which are known to occur in the case of the scattering amplitude of two particles near the threshold of a three-body reaction (see, for example, Ref. 30).

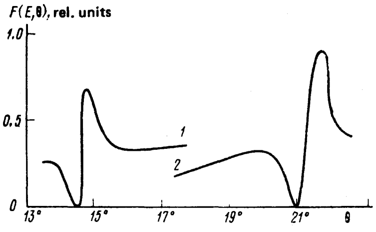

FIG. 5. Angular dependences of the coefficient of electron reflection from a monolayer of Xe atoms at a fixed electron energy: 1) $E=7.5$ eV; 2) $E=7.55$ eV.

CONCLUSIONS

We have considered only one possible experimental arrangement designed to detect a branch of autoionizing states of electron–exciton complexes. In this arrangement one should look for singularities of the angular and energy dependences of the coefficient of elastic reflection of slow monochromatic electrons from the surface of a solid covered with a layer of physically adsorbed atomic particles. However, one can expect the resonance mechanism to appear similarly also in certain photoprocesses, for example, in the photodetachment of an inner electron from an atom of a physically adsorbed monolayer. There is also a considerable interest in the nature of the appearance of states of electron–exciton complexes in experiments involving "transmission" through thin insulating films. The first experiment of this type, characterized by a high resolution and indicating the presence of bound electron-exciton states in three-dimensional organic crystals, was carried out recently by Sanche (Ref. 31).[6] We shall conclude by noting that bands of electron–exciton complexes can be expected also on the surfaces of molecular crystals, particularly on crystals formed from rare gas atoms.

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[1] The exchange interaction of decaying states in two-center systems was considered by us earlier in Refs. 9 and 10.

[2] The system of equations (14) makes it possible to allow consistently for the selection rules governing the momenta of the incident (l_s) and scattered (l_s') electron inter acting with the s-th center. However, this allowance is of little importance in the subsequent treatment because it results only in a redefinition of the nondiagonal parameter of the electron-core interaction ($\varkappa_{01}$, see below), which can be reconstructed from the experimental data on the electron–atom scattering.

[3] Allowance for the interactions with $l_s \neq 0$ is of fundamental importance only in a resonance situtation when autoionizing states of shape-type potential resonances occur in the centers.[7,8] An analysis of the corresponding effects is of intrinsic interest and will be made in a spearate communication.

[4] The role of the Frenkel excitions in these precesses was recently investigated[20] within the framework of the Born approximation.

[5] It should be noted that because of nonanalyticity of the function $Z_0(E, \mathbf{k}_{\parallel})$, the change in the resonance parameters may be abrupt for some values of E and θ.

[6] The possibility of existence of bound electron–exciton complexes in three-dimensional organic crystals was recently confirmed also by Agranovich and Zakhidov.[32]

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