6. Figure 1 shows the total cross section for the breakup of the negative ion of hydrogen, calculated from (11), together with the experimental and theoretical results obtained by other authors. The parameters for H⁻ were taken from the book by Demkov and Ostrovskiĭ[5] (§1.4). They were: $d = 2.7$ a.u., $\varkappa = 0.231$ a.u. $(\varepsilon = \varkappa^2/2)$. The classical model is valid, in this case, for incident electron energies of 4.20 eV.

It is important to note that no adjustable parameters are used when the cross section is calculated from (11), whereas the data reported by Narain and Jain,[3] which are at present in better agreement with experimental results than any other calculations, were obtained as a result of a very complicated semiempirical calculation. Nevertheless, near the threshold, our simple model of ionization provides good agreement with experiment. Unfortunately, there are no experimental data for other negative ions near the ionization threshold, so that it is difficult to establish the validity of this conclusion.

The reason why the simple classical calculation gives roughly the same result as the relatively sophisticated quantum-mechanical analysis is probably that, as noted by Smirnov,[1] Narain and Jain,[3] and others, the ionization cross section near the threshold depends critically on the choice of the trajectory of the incident electron. In the quantum-mechanical calculation, it is difficult to take the Coulomb interaction rigorously into account, whereas, in the classical approach, this can be done simply and naturally.

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Excitation of autoionization states by electrons near the threshold

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(Submitted December 13, 1976)
Zh. Eksp. Teor. Fiz. **72**, 2079–2089 (June 1977)

The theory of the interaction of a slow quantum particle with a system having an autoionization state is considered. The theory is used to describe a recently observed phenomenon [P. J. Hicks et al., Vacuum **24**, 573 (1974)], namely "interaction after the collision" in the excitation of an autoionization state of an atom by an electron. The roles of various quantum effects in the formation of the resonant structure and in the spectra of the electrons and in the excitation functions of the Rydberg states of the atom are investigated. The possibility of further refining the theory is discussed.

PACS numbers: 34.80.Dp, 32.80.Dz

1. INTRODUCTION

Hicks et al. have observed in 1974[1] a new phenomenon, which occurs when electrons with energy E_i somewhat higher than the energy E_a of excitation of the autoionization states (AS) of an atom are scattered by the atom. An AS manifests itself as a resonant contour in the energy distribution (spectrum) of the electrons knocked out of the atom. It has turned out that the contour shifts towards higher energies with decreasing E_i. Therefore the AS begins to be excited effectively not at $E_i = E_a$, but at a higher incident-electron energy. This new effect was therefore called the "shift of the threshold" in the excitation of AS. Of course, the position of the threshold can be determined only accurate to the level width Γ, but the observed threshold shifts greatly exceed this value.

In the cited paper, this phenomenon was attributed to energy exchange that occurs between the slow scattered electron which has excited the AS and the atomic electron when the two particles move apart. If the lifetime[1)]

0038-5646/77/4506-1092$02.40

of the AS $\tau = 1/\Gamma$ is smaller than or comparable with the characteristic scattering time, then the decay of the AS takes place in the field of the charge, as a result of which the autoionization (fast) electron can be emitted with a larger energy. The resultant decrease of the energy of the slow electron leads to a shift of the corresponding AS structure in the spectrum of the scattered electrons, and can be registered in experiment.[2] The energy of the slow electron can decrease to such an extent that it becomes insufficient to leave the field of the positively charged atomic core. In this case the electron is captured by some state of the Rydberg series of the atom (this being the analog of the associative ionization in the case of the collision of heavy atomic particles). A similar resonant population gives rise to the structure simultaneously observed by two groups of workers[3,4] in the excitation functions of sufficiently high-lying states of the atom.

Bearing the foregoing explanation in mind, the rather inconsistent term "interaction after collision" is frequently used in the literature. The experimental data and the discussion can also be found in[5-9].

When the inelastically scattered electron and the atom move slowly apart, the fast atomic electrons have time to adjust themselves to each position of the slow electron. It is the ratio of the corresponding velocities which constitutes the small parameter whose existence serves as the basis of the scattering theory proposed below. The theory is thus adiabatic, and this makes it possible to use, in the problem of the electron-scattering, the concept of adiabatic terms of a quasimolecule, customarily used in the theory of slow collisions of heavy atomic particles. In our case the quasimolecules are made up of an atom and an immobile electron, and the possibility of the decay brings about a situation wherein the state becomes quasistationary and the term becomes complex.

The general problem of the interaction of a slow quantum particle with a system having a discrete level that interacts with the homogeneous continuum is solved in Sec. 2. Section 3 deals with the simplest choice of the interaction potentials (terms) and the role of the quantum effects in the formation of the contours of the autoionization lines. In Sec. 4, using as an example the experimentally investigated AS $(2p^2)^1D$ in He, the results of the quantum theory and of the Berry formula[10] are compared for a resonant structure both in the excitation functions of the Rydberg states of the atoms and in the spectra of the electrons, and the possibilities of further refinement of the theory are discussed.

Berry's classical theory,[10] which is used by Hicks et al.[1] for a quantitative explanation of the effect of interaction after collision, was initially proposed for the description of the shapes of the autoionization lines of atoms excited in collisions between heavy atomic particles, which broaden as a result of their Coulomb interaction in the course of scattering. The starting point in this theory[11] is the phenomenological equation that describes the change of the probability P of finding the atom in the AS as a result of the decay after a time dt:

$$dP = -\Gamma(t)P\,dt, \qquad (1.1)$$

which can be rewritten in the form

$$\frac{dP}{d\omega} = -\Gamma(t)P\frac{dt}{d\omega}, \qquad (1.2)$$

where ω is the energy of the emitted electron.

To establish the connection between ω and t it is natural to assume that at the instant t the electron is emitted with an energy exactly equal to the real part of the energy of the autoionization term of the quasimolecule: $\omega = E_0(t)$. In particular, in the case of a Coulomb term $E_0(t) = 1/vt + E_a$ (v is the velocity in the scattering) with a constant width Γ, integration of Eq. (1.2) yields the Berry formula—the electron spectrum normalized to unity

$$\frac{dP}{d\varepsilon} = \begin{cases} v\Gamma\varepsilon^{-2}\exp(-\Gamma/\varepsilon v), & \omega > E_a, \\ 0, & \omega < E_a. \end{cases} \qquad (1.3)$$

We have introduced here the quantity $\varepsilon = \omega - E_a$, which is the electron energy reckoned from the position E_a of the autoionization level, i.e., the energy transferred to the outgoing electrons as a result of the interaction after scattering.

The derivation of expression (1.3) actually presupposes a classical description not only of the moving-apart of the particles, but also of the autoionization system. Actually, however, each section of the line contour in the spectrum is made up of contributions of both the center and of the wings of the initial unbroadened line. Since the emission of the electron is coherent, the corresponding amplitudes should be additive. An analysis with allowance for this circumstance, but for a classical description of the scattering, is given in[17].

In the case of excitation of AS by electron impact, the assumption that the slow scattered electron moves after the scattering along a classical trajectory with constant velocity no longer holds. The classical theory is particularly unsuitable for the analysis of the capture of a slow electron in a Rydberg-series state. The quantum-mechanical description of the interaction of a particle with an autoionization system encounters certain difficulties.[12]

2. INTERACTION OF A QUANTUM PARTICLE WITH AN AUTOIONIZATION SYSTEM

The Hamiltonian of the quantum system with one AS and a continuous spectrum can be represented in a diabatic basis in the form[13] (see also[14,17] and the references therein)

$$H = H_0 + \hat{V} = E_0|\varphi\rangle\langle\varphi| + \int d\omega\,\omega|\omega\rangle\langle\omega| + \hat{V}, \qquad (2.1)$$

$$\langle\varphi|\varphi\rangle = 1, \qquad \langle\omega|\omega'\rangle = \delta(\omega - \omega'), \qquad \langle\omega|\hat{V}|\omega'\rangle = 0,$$

where $|\omega\rangle$ are diabatic-continuum states with energy ω, and $|\varphi\rangle$ is a diabatic discrete state with energy E_0 against the background of the continuous spectrum. The operator $\hat{V}$ is responsible for the interaction of the dia-

batic states, which makes the discrete level quasistationary with width $\Gamma = 2\pi |\langle \varphi|V|\omega\rangle|^2_{\omega = E_0}$. For the sake of brevity we shall use the name atom for such a system.

We assume further there is one other quantum particle (we call it the incident or external particle) with mass M and coordinate $\mathbf{R}$, which interacts with the atom. At any fixed position of the external particle, the atom has a Hamiltonian of the type (2.1), in which, all the quantities $(|\varphi\rangle, |\omega\rangle, E_0, \hat{V})$ depend on $\mathbf{R}$ as a parameter. The total Hamiltonian $\mathcal{H}$ is obtained by adding to H the kinetic energy $\hat{T}$ and the potential energy U of the particle

$$\mathcal{H} = H + \hat{T} + U(\mathbf{R}), \qquad \hat{T} = -\frac{1}{2M}\nabla_R^2. \tag{2.2}$$

The solution of the Schrödinger equation $(\mathcal{H} - \mathcal{E})|\Psi\rangle = 0$ for the total energy of the system $\mathcal{E}$ is sought in the form

$$|\Psi\rangle = a(\mathbf{R})|\varphi\rangle + \int d\omega\, b(\omega, \mathbf{R})|\omega\rangle. \tag{2.3}$$

The formulated theory has been adapted to the description of the adiabatic case, when the velocity of the external particle is small. Accordingly, we neglect in the equations for the functions $a(\mathbf{R})$ and $b(\omega, \mathbf{R})$ the matrix elements of the operators ∇_R and ∇_R^2 between the different basic states $|\varphi\rangle$ and $|\omega\rangle$

$$-\frac{1}{2M}\nabla_R^2 a(\mathbf{R}) + (E_0(\mathbf{R}) + U(\mathbf{R}))a(\mathbf{R}) + \int d\omega\, V_\omega(\mathbf{R})b(\omega, \mathbf{R}) - \mathcal{E}a(\mathbf{R}) = 0, \tag{2.4}$$

$$-\frac{1}{2M}\nabla_R^2 b(\omega, \mathbf{R}) + (\omega + U(\mathbf{R}))b(\omega, \mathbf{R}) + V_\omega^*(\mathbf{R})a(\mathbf{R}) - \mathcal{E}a(\mathbf{R}) = 0, \tag{2.5}$$

$$V_\omega = \langle\varphi|\hat{V}|\omega\rangle.$$

Obviously, the energies ω of the continuum states are reckoned now from the lower limit of the continuous spectrum, the role of which is played by $U(\mathbf{R})$.

We write down the formal solution of Eq. (2.5) in terms of the Green's function G^+ corresponding to outgoing waves at large R:

$$\left[-\frac{1}{2M}\nabla_R^2 + U(\mathbf{R}) - E\right]G^+(\mathbf{R}, \mathbf{R}', E) = \delta(\mathbf{R} - \mathbf{R}'), \tag{2.6}$$

$$b(\omega, \mathbf{R}) = -\int d\mathbf{R}'\, G^+(\mathbf{R}, \mathbf{R}', \mathcal{E} - \omega)V_\omega^*(\mathbf{R}')a(\mathbf{R}'). \tag{2.7}$$

In the right-hand side of (2.7) we could add the solution of the homogeneous equation, which would mean that initially the populated states were those of the diabatic continuum. It will be assumed henceforth, however, that only the state $|\varphi\rangle$ was initially populated. Substituting the last equation in (2.4), we obtain in the general case an integro-differential equation for the function $a(\mathbf{R})$, in the form of a Schrödinger equation with a complex nonlocal potential

$$-\frac{1}{2M}\nabla_R^2 a(\mathbf{R}) + (E_0(\mathbf{R}) + U(\mathbf{R}))a(\mathbf{R})$$

$$-\int d\mathbf{R}'a(\mathbf{R}')\int d\omega\, V_\omega(\mathbf{R})V_\omega^*(\mathbf{R}')G^+(\mathbf{R}, \mathbf{R}', \mathcal{E} - \omega) - \mathcal{E}a(\mathbf{R}) = 0. \tag{2.8}$$

In the case of interest to us we can reduce this equa-

tion to a differential equation, whereby greatly simplifying the investigation of the actual problems. Indeed, we shall assume that the matrix element $V_\omega(\mathbf{R})$ of the interaction depends little on ω, and take it outside the sign of integration with respect to $d\omega$. In addition, if the energy region of interest to us is far from the lower boundary of the continuous spectrum, then we can extend the integration with respect to $d\omega$ in (2.8) to include the entire axis (we emphasize that the foregoing approximations are perfectly analogous to those used in the nonstationary quantum problem[13-14,17]). We can then use the known general identity for the Green's functions (see, e.g., the book of Baz', Zel'dovich, and Perelomov[15]; our definition of the Green's function differs in sign from that assumed in formula (3.3), Chap. 4 of that monograph):

$$\int dE\, G^+(\mathbf{R}, \mathbf{R}', E) = \pi i\delta(\mathbf{R} - \mathbf{R}'), \tag{2.9}$$

so that (2.8) takes on the form of the Schrödinger equation for $a(\mathbf{R})$ with a complex local potential $E(\mathbf{R})$ that represents the energy of the quasistationary term:

$$-\frac{1}{2M}\nabla_R^2 a(\mathbf{R}) + (E(\mathbf{R}) - \mathcal{E})a(\mathbf{R}) = 0, \tag{2.10}$$

$$E(\mathbf{R}) = U(\mathbf{R}) + E_0(\mathbf{R}) - \tfrac{1}{2}i\Gamma(\mathbf{R}), \qquad \Gamma(\mathbf{R}) = 2\pi|V(\mathbf{R})|^2. \tag{2.11}$$

We note that the dependence of $V_\omega(\mathbf{R})$ on ω can be regarded as approximately taking into account if we calculate in the expression for $\Gamma(\mathbf{R})$ the value of $V_\omega(\mathbf{R})$ at $\omega = E_0(\mathbf{R})$. In addition, the shift of the position of the term, due to its interaction with the continuum, can be regarded as included in $E(\mathbf{R})$.

Solving Eq. (2.10) with the corresponding boundary conditions and substituting the result in (2.7), we obtain the wave function of the system. Its asymptotic form gives the amplitudes of the different processes. To find them it is convenient to use an integral representation for the Green's function in terms of the eigenfunctions of the discrete $\Phi_n(\mathbf{R})$ and continuous $\Phi_E(\mathbf{R})$ spectra for the potential $U(\mathbf{R})$:

$$G^+(\mathbf{R}, \mathbf{R}', E) = \sum_n \frac{\Phi_n(\mathbf{R})\Phi_n(\mathbf{R}')}{E - E + i0} + \int dE' \frac{\Phi_{E'}(\mathbf{R})\Phi_{E'}(\mathbf{R}')}{E' - E + i0} \tag{2.12}$$

(additional summation over the omitted quantum numbers, for example the orbital angular momentum, is implied here). In the final state, the atom is always in the continuum, i.e., it becomes ionized, and the incident particle may turn out to be bound in the potential $U(\mathbf{R})$ or free with energy E. The scattering amplitudes for these cases are respectively

$$F_n = \frac{1}{(2\omega)^{1/4}}\int d\mathbf{R}(\Gamma(\mathbf{R}))^{1/2}\Phi_n(\mathbf{R})a(\mathbf{R}), \qquad \omega = \mathcal{E} - E_n, \tag{2.13}$$

$$F(k) = \frac{1}{(2\omega)^{1/4}}\left(\frac{M}{k}\right)^{1/2}\int d\mathbf{R}(\Gamma(\mathbf{R}))^{1/2}\Phi_E(\mathbf{R})a(\mathbf{R}), \tag{2.14}$$
$$E = k^2/2M, \quad \omega = \mathcal{E} - E,$$

where the function $a(\mathbf{R})$ is assumed to be normalized relative to the incident wave of the incoming particles.

At first glance, the results appear to be in the form

of a perturbation theory in the interaction $V(\mathbf{R}) = (\Gamma(\mathbf{R})/2\pi)^{1/2}$ that leads to the decay of the AS. Actually, however, they have a different meaning. Assuming adiabatically, the derivation of Eq. (2.8) for the function $a(\mathbf{R})$ is exact. Further simplifications, which lead to (2.10), are likewise not connected with the smallness of the interaction, and make use of the fact that the autoionization level is far from the end point of the continuous spectrum. The transition to a perturbation theory in terms of V is connected with the neglect of the width $\Gamma(\mathbf{R})$ in Eq. (2.10). If, in addition, we assume in formulas (2.13) and (2.14) that the width is independent of $\mathbf{R}$, then we obtain in these expressions the same matrix elements which arise in the "jolting" theory, where instantaneous removal of the autoionization electron from the atom is assumed.[5] We note, however, that the method proposed in that paper for introducing the damping into the function $a(\mathbf{R})$ is correct (cf. Sec. 3).

3. COULOMB INTERACTION IN SCATTERING

The theory developed in Sec. 2 could in principle have been included in the more general description of the entire process of excitation and decay of an AS of an atom. In the present paper it is assumed that the process can be broken up into two independent stages.[6] The first, the excitation of the AS, will be characterized by a certain cross section σ_{ex}, which is not calculated in the present paper. For the second stage—the moving part of the excited electron and atom, accompanied by the decay of the AS—we confine ourselves to consideration of only the s-wave radial motion of the scattered electron. Indeed, since the potential of the interaction of the electron with the atom in the AS decreases with increasing distance more rapidly than the Coulomb potential, an inelastically scattered electron in the near-threshold region is mainly in the s state.[15] When the particles move apart, exchange of angular momentum takes place between the scattered and atomic electrons, but its probability is small.[4] Thus, for the scattered electron we arrive at the one-dimensional problem considered in Sec. 2.

Inasmuch as the scattered electron is slow and the autoionization electron is fast, exchange of electrons in scattering would mean a large energy transfer between them, but this has low probability and can be disregarded.

At large distances, a Coulomb attraction ($U \sim -1/R$) acts between the scattered electron and the ionized atom, and the potential of the interaction of the electron with the atom in the AS decreases much more rapidly (like $1/R^4$). In the simplest approximation, the latter interaction can be neglected, as well as the distortion of the Coulomb potential at short distances

$$U(R) = -1/R, \quad E(R) = E_a - \tfrac{1}{2}i\Gamma. \tag{3.1}$$

We shall assume also that the width of the term is constant and equal to the width of the AS of the isolated atom: $\Gamma(R) = \Gamma$.

Under the foregoing assumptions, the one-dimensional equation (2.10) has a solution that decreases at large

R, in the form of a damped plane wave; we normalize this solution at $R = 0$ (we put henceforth $M = 1$):

$$a(R) = \exp(ik'R), \tag{3.2}$$

$$k'^2/2 = \mathscr{E} - E_a + \tfrac{1}{2}i\Gamma, \quad k_0' = \operatorname{Re}k', \quad \gamma = \operatorname{Im}k' > 0. \tag{3.3}$$

Using the well known expressions for the Coulomb wave functions of the continuous spectrum, we calculate the integral (2.14):

$$F(k) = \left[\frac{\Gamma}{k(2\omega)^{1/2}(1-e^{-2\pi/k})}\right]^{1/2}\frac{1}{-\omega+E_a-i\Gamma/2}$$
$$\times \exp\left\{-\frac{1}{k}\operatorname{arctg}\frac{2\gamma k}{k_0'^2-k^2+\gamma^2}+i\xi\right\}, \tag{3.4}$$
$$\xi = \frac{1}{k}\ln\frac{(k_0'-k)^2+\gamma^2}{(k_0'+k)^2+\gamma^2}, \quad \frac{k^2}{2}=\mathscr{E}-\omega=\mathscr{E}-E_a-\varepsilon.$$

The differential cross section (with respect to the energy transfer) of the atom ionization via an intermediate resonant state is equal to

$$\frac{d\sigma}{d\varepsilon} = \sigma\,\frac{1}{k_0'(1-e^{-2\pi/k})}\frac{\Gamma}{\varepsilon^2+\Gamma^2/4}\exp\left\{-\frac{2}{k}\operatorname{arctg}\frac{2\gamma k}{k_0'^2-k^2+\nu^2}\right\}. \tag{3.5}$$

Just as in Sec. 1, it is convenient to introduce the probability density of the energy transfer in scattering, $dP/d\varepsilon = (d\sigma/d\varepsilon)/\sigma_{ex}$, for which we obtain, taking (3.3) into account

$$\frac{dP}{d\varepsilon} = \frac{1}{k_0'(1-e^{-2\pi/k})}\frac{\Gamma}{\varepsilon^2+\Gamma^2/4}\exp\left\{-\frac{2}{k}\operatorname{arctg}\frac{\gamma k}{\varepsilon+\gamma^2}\right\}. \tag{3.6}$$

The values of k_0' and γ can be obtained from (3.3)

$$k_0'^2 = \mathscr{E}-E_a+[(\mathscr{E}-E_a)^2+(\Gamma/2)^2]^{1/2}, \quad \gamma=\Gamma/(2k_0'). \tag{3.7}$$

Let us consider a case of practical importance, when the difference between the energy of the incident electron and the unshifted excitation threshold of the AS greatly exceeds the width: $\mathscr{E}-E_a \gg \Gamma/2$. Then the quantity $k_0' = [2(\mathscr{E}-E_a)]^{1/2} = v$ has the meaning of the electron velocity on a horizontal autoionization term. If furthermore $(\Gamma/\varepsilon)(k/k_0') \ll 1$, then we can replace the arctangent in (3.5) by its argument

$$\frac{dP}{d\varepsilon} = \frac{1}{v(1-e^{-2\pi/k})}\frac{\Gamma}{\varepsilon^2+\Gamma^2/4}\exp\left\{-\frac{\Gamma}{v[\varepsilon+(\Gamma/2v)^2]}\right\}. \tag{3.8}$$

If we consider in the cross section that wing of the autoionization which is formed in the classically allowed region, i.e., if we assume that $\omega - E_a \gg \Gamma/2$, and also put $1 - e^{-2\pi/k} \approx 1$, then (3.7) goes over into the Berry formula (1.3). The Berry formula cannot be used, however, for the center of the line, nor for the other (classically forbidden) wing $\omega - E_a \ll -\Gamma/2$ (a fact that follows also from the derivation of this formula—see Sec. 1). Indeed, it does not permit a transition in the limit into a Lorentz contour at large v and leads at $\varepsilon = 0$ ($\omega = E_a$) to a vanishing of the cross section $d\sigma/d\varepsilon$ with all its derivatives with respect to ε. Actually, the cross section vanishes exactly at $\omega > \mathscr{E}$, this being connected with the energy conservation law. The limiting value of the cross section as $\omega \to \mathscr{E}$, which can be obtained by letting k tend to zero in (3.6), is different from zero, as is typical of a Coulomb interaction. Formula (3.6) is free

of the shortcomings of the Berry formula.

It is of interest to trace in greater detail the role of the different factors in the formation of the contour of the autoionization line. We assume first that $k^2/2 \gg \varepsilon$, so that the energy of the scattered electron changes relatively little as a result of the interaction following the scattering. In the region $\varepsilon \gg \Gamma/2$, both the autoionization system and the scattered particles can be regarded as classical (Sec. 1), and the Berry formula is valid. The region $\Gamma/2 \gtrsim \varepsilon \gg (\Gamma/2v)^2$ calls already for a quantum description of the autoionization system, but the scattered particle can still be regarded classically. In the corresponding theory,[17] to calculate the contour (for both wings) it suffices to specify the difference between the autoionization term and the boundary of the continuous spectrum, and not their absolute variations, so that the expression for $dP/d\varepsilon$ takes the form

$$\frac{dP}{d\varepsilon} = \frac{\Gamma}{v(\varepsilon^2+\Gamma^2/4)} \exp\left\{-\frac{2}{v}\operatorname{arctg}\frac{\Gamma}{2\varepsilon}\right\}. \tag{3.9}$$

Finally, a quantum description of the entire system is needed in the region $\varepsilon \lesssim (\Gamma/2v)^2$, and also at $k^2/2 \sim \varepsilon$, i.e., when the energy transfer is comparable with the energy of the slow electron.

We proceed now to the cross sections for the capture of a slow scattered electron into a bound state. Calculating the integral (2.13) with the wave functions of the bound s states in a Coulomb field and with the function (3.2), we obtain

$$F_n = \frac{1}{n^{3/2}} \frac{\Gamma^{1/2}}{E_a - \mathscr{E} + E_b - i\Gamma/2} \left[\frac{k_0'^2+(\gamma-1/n)^2}{k_0'^2+(\gamma+1/n)^2}\right]^{n/2} e^{i\xi}, \tag{3.10}$$

$$\xi = -\frac{n}{2}\operatorname{arctg}\frac{2k_0'/n}{\gamma^2-1/n^2}$$

where n is the principal quantum number and $E_b = 1/(2n^2)$ is the binding energy. The cross section for the excitation of the state of an atom with a principal quantum number n via an intermediate resonant state will be designated σ_n. At large n, the density of the Rydberg states, in the energy scale, is equal to n^3, so that the quantity $n^3\sigma_n$ at $E < 0$ has a meaning analogous to $d\sigma/d\varepsilon$ at $E > 0$. The energy transfer in scattering is conveniently characterized by the quantity $dP/d\varepsilon = n^3\sigma_n/\sigma_{ex}$:

$$\frac{dP}{d\varepsilon} = \frac{1}{k_0'} \frac{\Gamma}{\varepsilon^2+\Gamma^2/4} \left[\frac{k_0'^2+(\gamma-1/n)^2}{k_0'^2+(\gamma+1/n)^2}\right]^n$$

$$= \frac{1}{k_0'} \frac{\Gamma}{\varepsilon^2+\Gamma^2/4} \exp\left\{-2n\operatorname{arth}\frac{\gamma/n}{\varepsilon+\gamma^2}\right\}, \tag{3.11}$$

where now

$$\varepsilon = \mathscr{E} - E_a + E_b \tag{3.12}$$

and the variable can be taken to be the energy $\mathscr{E}$.

If we put $1 - e^{-2\tau/k} \approx 1$ in (3.6), then (3.10) can be obtained from (3.6) by analytic continuation in the final momentum of the slow electron ($k = i/n$), not only at large n but also at small ones. The Berry formula (with allowance for (3.12)) is obtained from (3.11) under the same assumptions as from (3.6). Thus, the Berry result describes approximately the transitions of the in-

cident particle into bound states as well as into the continuum.

4. DISCUSSION OF RESULTS AND CONCLUSION

In measurements of the excitation functions of the Rydberg states, the final energy of the incident electron is fixed. Nienhuis and Heidemann[6] have called attention to the fact that in the experiment the spectra of the free electrons are also obtained at a fixed final energy of the scattered electron $k^2/2 = \mathscr{E} - \omega$. The variable in both cases is the initial energy $E_i = \mathscr{E}$ of the incident electron or, equivalently, the energy transfer ε.

The same authors have shown that, after a scale transformation of the energies, the Berry expression depends only on two real variables. The quantum result no longer permits such a reduction. We consider below by way of example the structure that can be connected with the $(2p^2)\,^1D$ state of the He atom ($E_a = 59.90$ eV, $\Gamma = 0.072 \pm 0.01$ eV), for which there is the largest amount of experimental data. In Fig. 1, for a resonant structure in the cross sections for the excitation of the Rydberg states of the atom (Fig. 1a) and in the spectra of the emitted electrons (Fig. 1b), are compared the results given by the Berry formula (1.3) (dashed) and by the quantum-mechanical formulas (3.6) and (3.11) (solid curves). The larger difference occurs near the maximum in the low-energy part of the contour, corresponding to below-the-barrier population. The positions of the maxima of the structure, calculated from these formulas, differ insignificantly. Thus, for the excitation of a state with $n = 4$, the maximum corresponds to a value $E_i - E_a = \varepsilon - E_b = 0.0662$ eV in accordance with the Berry formula, and 0.0599 eV in accordance with the quantum formula. Although the relative difference reaches here 10%, for an energy transfer $\varepsilon = E_i - E_a - E_b$ it turns out to be small, since the latter is determined mainly by the value of E_b.

The structure width at half maximum, as a function of the final energy of the incident electron, is shown in Fig. 2 both for the spectra and for the cross sections
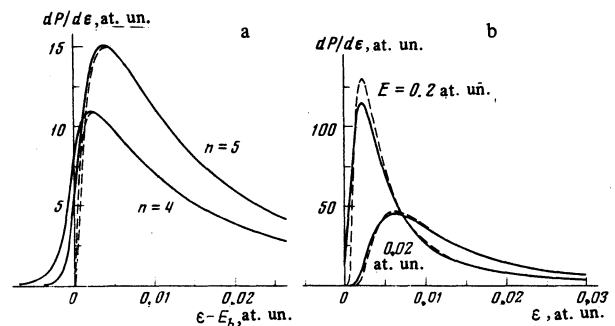

FIG. 1. The function $dP/d\varepsilon$, which characterizes the probability of transfer of energy ε between electrons as a result of interaction in scattering after the excitation of the autoionization state; $\Gamma = 0.072$ eV $= 0.00265$ at. un.: a—upon excitation of the Rydberg states of an atom with principal quantum numbers $n = 4$ and 5; $E_b = 1/2n^2$; b—in the spectrum of the emitted electrons at a fixed energy of the scattered electron $E = 0.2$ and 0.02 at. un. Solid lines—quantum theory (3.11) and (3.6); dashed—the Berry formula (1.3).
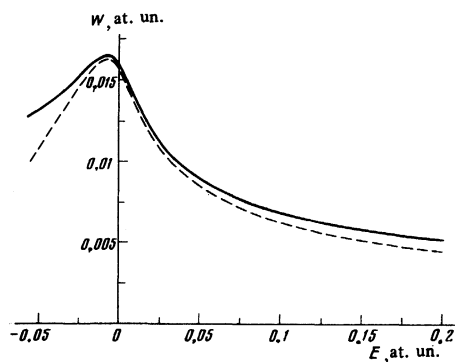
FIG. 2. Width W of the resonant structure at half height for the excitation functions ($E < 0$) and the spectra ($E > 0$) at Γ = 0.072 eV. The final energy of the scattered electron E is fixed. Solid lines—quantum theory, dashed—Berry formula.

of the excitation. For the final states of an incident electron having a small absolute value of the energy (both in the discrete and in the continuous spectrum), the classical and quantum results are again close. At large $E > 0$, the Berry formula gives a width that tends to zero, whereas the quantum-mechanical result approaches the width of the AS of the isolated atom. For $n = 4$, the difference between the results for the width is ~10%.

The relatively small difference between the results of the classical and quantum theory is due to the smallness of the level width Γ. The characteristic energy parameter $(\Gamma/2v)^2$, which determines the importance of the quantum effects for the motion of the scattered electron (Sec. 3), turns out to be small even at the smallest v attainable in experiment (where the energy resolution is characterized by a quantity on the order of 0.01 eV). The quantum effects in the decay of AS are more substantial and determine the difference in the width and shape of the structure. For levels with larger width, the situation can change. It is also possible that when the variation of the terms is made more precise the quantum effects acquire a larger significance (see the discussion that follows).

As shown by Nienhuis and Heidemann,[6] the Berry formula does agree sufficiently with experiment. The quantum theory, when the simplest potentials are chosen for the electron interaction with the atom, does not improve this agreement. However, the approach developed here admits of such an improvement and makes it possible to take into account different physical effects which may turn out to be important for concrete atoms and AS. The results of Sec. 3 of the present paper should serve in this case as the starting point. Certain trends in the development of the theory will be briefly discussed below.

Besides providing a quantitative refinement, allowance for the distortion of the Coulomb potential $U(R)$ at short distances might be of interest also from the point of view of the general assessment of the role of quantum effects. It is known that the quasiclassical approximation frequently yields exact results for a pure Coulomb interaction, and this may be the cause of the relative

smallness of the quantum effects for the scattered electron.

A refinement of the potential of the interaction of the electron with the atom in the AS uncovers an interesting possibility of taking into account the quasistationary state of the negative ion (if a quasibound state is present in the corresponding potential). Such states of the He⁻ ion lie near the AS of the He atom, but their role has been discussed so far only qualitatively.[4,9,12] Of course, the choice of the pseudopotential $E(R)$ is not a trivial question.

As indicated by Read,[8] a slow electron knocked out from the internal shell of the atom by an x-ray photon of energy close to threshold can exchange energy effectively with a fast electron emitted by an atom as a result of the Auger effect. In this case, both the autoionization term $E(R)$ and the end point of the continuous spectrum $U(R)$ are determined at large distances by the Coulomb interaction. A similar situation arises when the AS of positive ions are excited by electron impact.

One can expect the width of the AS of the atom to increase in the presence of a pointlike change, although in principle the opposite is possible, as shown recently by Dalidchik and Slonim,[16] who considered the Stark effect on AS in the zero-radius approximation for the interaction of an electron with an atomic system. Allowance for the $\Gamma(R)$ dependence can greatly alter the shape of the contour of the autoionization line.

The contours of the autoionization lines near the threshold are substantially different from Lorentzian, making the interpretation of the experimental data difficult. Allowance for the interference between direct ionization by electron impact and the resonant mechanism considered in the present paper could be useful here.

The influence of several closely-lying autoionization levels can be taken into account in a manner similar to that used in the nonstationary case[14,17]; we then obtain the multichannel problem for the slow scattered electron. The transfer of orbital momentum in the scattering can be described in similar fashion.

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Translated by J. G. Adashko

Relativistic and radiative corrections to the energy of the ground state of an atom

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(Submitted December 15, 1976)
Zh. Eksp. Teor. Fiz. **72**, 2090–2099 (June 1977)

Feynman vacuum diagrams with a non-zero chemical potential renormalized in a certain manner are used to obtain relativistic and radiative corrections to the energy of the ground state of an atom. Corrections are obtained in the lowest (second) order of perturbation theory which are the sum of contributions of the Lamb shift, vacuum polarization and the Breit correction for the electrons of an atom in an effective external field. Numerical calculations are carried out for a number of neutral atoms using both the semiclassical and the nonrelativistic approximations.

PACS numbers: 31.30.Jv

§1. INTRODUCTION

In connection with the increase in the accuracy of experimental investigations and the improvement of calculational methods recently there has been a growth in the interest in relativistic corrections to the theory of a many-electron atom. In their simplest form they are taken into account by means of the relativistic equations of the Hartree-Fock self-consistent field based on the Dirac equation (cf., for example, Ref. 1). A further improvement in the calculation requires the solution of two theoretical problems. Firstly, it is necessary to have a convenient apparatus for the calculation of the energy of a many-electron relativistic atom taking into account the retarded interaction between electrons. Secondly, it is necessary to carry out a renormalization of the mass and of the charge of the electron. These problems are interconnected, since a convenient calculation of the energy first of all presupposes just the possibility of carrying out a program of renormalization without operating in the intermediate stages with divergent nonphysical quantities.

It should be emphasized that no difficulties of principle exist in carrying out the program of renormalization for an atom. The corresponding many-electron Green's function in an external field can evidently be renormalized in the usual manner. However, to extract in a simple manner from such a Green's function the value of the energy of the atom appears to be possible only in the simplest cases of one- or two-electron atoms.[2,3] For a greater number of electrons the equations for the many-electron Green's function are very complicated

and no one has succeeded in finding a simple algorithm for calculating the corrections to the energy using perturbation theory. We note in this connection that the well-known Gell-Mann–Low formulas[4] contain differentiation with respect to the bare charge and the obviously noncovariant time cut-off and are therefore inappropriate for use with renormalized quantities.

Earlier Labsovskiĭ and one of the authors of the present paper proposed a method of calculating the renormalized energy of the atom consisting of extracting from the renormalized many-electron Green's function the effective Hamiltonian for the interaction between electrons.[5] The interaction potential in this case turned out to be nonlocal and nonunique. The principal disadvantage of such a method, along with its certain artificiality, is associated with the fact that in this case each Feynman diagram is in fact counted twice: once as a contribution to the potential, and a second time as an iteration of the potential in the lowest order in determining the energy. This leads to a sharp increase in the amount of calculation. However, this method also has serious advantages—thus, it encounters no difficulty with degenerate ground states and enables one to determine also the excited energy levels.

For the calculation of the energy of a nondegenerate ground state of the electron shell of an atom a more natural and simple method of calculation appears to be one based on the quantum-field-theoretic technique with a given non-zero chemical potential μ. The renormalization and the determination of the energy for relativistic Fermi-systems in the case of zero external field and