Influence of a scattered charged particle on the width of autoionization resonances

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A theoretical description of resonant ionization of an atom by charged particles with allowance for interaction in the final and resonant states is developed. The influence of the distortion of the continuum states of the scattered particle on the width of autoionization resonances is investigated. With allowance for the distortion of the continuum states, an analytic expression is obtained for the time-dependent width of an autoionization resonance. The characteristic dependences of the width of the perturbed resonance on the charge and velocity of the scattered particle and also on the total orbital angular momentum and the magnetic quantum number of the autoionization state are established. It is shown that the integrated yield of the resonance does not depend on allowance for interaction in the final and resonant states. The widths of the lowest autoionization resonances of the helium atom are calculated as functions of the velocity and the magnitude and sign of the charge of the scattered particle. © *1996 American Institute of Physics.* [S1063-7761(96)00201-7]

1. INTRODUCTION

When a charged particle collides with a many-electron atom, autoionization states can be formed that then decay nonradiatively with emission of electrons into the continuous spectrum. The energy spectra of the electrons ejected as a result of autoionization are, as a rule, distorted by the long-range Coulomb interaction between outgoing charged particles. A typical manifestation of this final-state interaction, which in the literature has become known as the post-collision interaction, is a distortion of the Lorentz profile of the resonance lines. Specifically, the lines are displaced, broadened, and acquire a pronounced asymmetry. All these effects have been widely studied, both experimentally and theoretically (see, for example, the reviews in Refs. 1–3), beginning with the first observation of Barker and Berry[4] of the details of the decay of autoionization states in slow ion–atom collisions.

To explain the effects of post-collision interaction observed in the threshold region (defined by $v \ll v_e$, where v and v_e are the velocities of the scattered particle and the autoionization electron, respectively), various theoretical models have been developed: the classical Barker–Berry model,[4] the semiclassical[5,6] and quantum-mechanical[7] models, and also the shake-down model,[8] the quasimolecular adiabatic approach,[9] and more. They are all based on two physical assumptions.

1) The velocity of the autoionization electron is much greater than the velocity of the scattered charged particle, i.e., the interaction with the autoionization electron can be ignored, and the post-collision interaction reduces solely to the interaction between the slow charged particle and the field of the target atom, which changes during the decay process. This has the consequence that the post-collision interaction does not depend on the emission angle of the ejected particles and distorts only the energy distribution of the scattered charged particles and autoionization electrons.

2) The scattered charged particle has no influence on the decay probability of the autoionization state, i.e., the decay takes place with the same width Γ, and the ejected electrons have the same energy distribution as in the absence of the scattered charged particle. The distribution of the ejected electrons changes as a result of interaction of the charged particles during their subsequent motion after the decay of the autoionization state.

Relaxation of the first simplifying restriction leads to the necessity of taking three-particle Coulomb dynamics into account in the final state. This is most clearly manifested when the velocities of the outgoing particles are comparable in magnitude. The key to the solution of this problem is the correct description of the final-state wave function. In Refs. 10–12, three-particle Coulomb dynamics in the final state was described by means of a wave function of a system of three asymptotically free particles that is an approximate solution of the Faddeev–Merkur'ev equations, modified for Coulomb potentials; an analogous wave function obtained in the continuum distorted wave (CDW) approximation was used in Refs. 13 and 14. The general analytic expression for the autoionization amplitude obtained with such a wave function in Ref. 10 simplifies in the case of slow collisions, in which the interaction of the autoionization electron with the scattered charged particle can be ignored, to the corresponding expression for the amplitude obtained in the quasimolecular adiabatic approach.[9] For sufficiently large angles between the outgoing charged particles in the final state, when the interaction energy of the particles as they move apart from each other is less than the kinetic energy of their relative motion, the autoionization amplitude[10] simplifies to the corresponding amplitude obtained earlier in the semiclassical eikonal approximation.[15,16]

The quantum-mechanical description of resonant ionization[10] under conditions of a strong influence of the final-state Coulomb interaction exhibits strong changes in the shapes of the resonance line with changing electron ejection angle that are not present in the semiclassical eikonal

theory.[15,16] Such a singular kinematic situation arises in the case of electron ejection in a direction close to the direction of the outgoing scattered particle with a velocity that exceeds the projectile velocity. In this case, the ejected electron and the scattered particle can interact strongly. Thus in the calculations in Ref. 11 of the energy spectra of electrons ejected as a result of decay of the $(2s^2)^1S$ resonance of the helium atom excited in a collision with protons with velocity $v=1.2$ (in units defined below), qualitatively new effects were observed, namely, a sharp growth in the resonance intensity at small ejection angles as a result of capture of the autoionization electron in the continuum of the scattered particle (this is analogous to electron capture in the continuum of a positively charged ion in the direct channel), and the appearance of an additional maximum in the left-hand wing of the resonance at ejection angles $\theta_e \simeq 1-5°$ due to rescattering of some of the autoionization electrons by a proton.

Recent experimental investigations[17,18] have confirmed the existence of these effects of the post-collision interaction. In Ref. 17, the enhancement of electron intensity in the forward direction is interpreted as a result of "focusing" of the electrons in the Coulomb field of the outgoing ion, and the appearance of the additional maximum in the left-hand wing of the resonance is attributed in Ref. 18 to the interference of the two coherent amplitudes corresponding to the two possible different classical trajectories of the autoionization electron in the field of the outgoing ion. We note however that although the quantum-mechanical description of Refs. 10–12 does predict a sharp growth in the resonance intensity at small ejection angles, the simultaneously obtained enhancement of the electron yields in certain directions is not accompanied by a decrease of the yields in others, with the integrated resonance yield remaining the same. The theory predicts only enhancement of the yield in the forward direction without compensation in other directions.[19,20] The semiclassical model of the post-collision interaction proposed in Ref. 17 also does not give a consistent description of the "Coulomb focusing" effect, since it contains an unphysical singularity in the cross section at zero ejection angle.

The aim of this paper is to develop a theory of the resonant ionization of an atom by charged particles with allowance for interaction in not only the final state but also the resonant state. Allowance for the influence of the scattered particle on the decay of the quasistationary resonant state leads to a modification of the energy and width of the resonant state, which cease to be atomic parameters and become functions of the position of the charged particle. The derived quantum-mechanical model, based on the diagonalization approximation, makes it possible to reproduce the "Coulomb focusing" effect. Moreover, for consistent description of this effect, it is necessary to take into account simultaneously the interaction in the final state and in the resonant state.

Attention is primarily focused in this paper on studying the effect of the scattered particle on the width of autoionization resonances. This effect can be important for sufficiently short-lived autoionization states in the case of high charges and low velocities of the scattered particle. In the following section of the paper, we present the equations of the quantum-mechanical model modified by the interaction of the charged particles, and we solve them in the diagonalization approximation. In Sec. 3, we determine the amplitude of two-step resonance transitions under the assumption that production and decay of the resonance states are independent. We show that the integrated resonance yield does not depend on the interaction in the final and resonant states. In Sec. 4, we obtain an analytic expression for the time-dependent width $\Gamma(t)$ of the autoionization resonance with allowance for the coupling of the resonant states to the continuum distorted by the field of the scattered charged particle. We show that at asymptotically large times, the width of the perturbed autoionization resonance tends to the value Γ_0 determined for an isolated atom, and decreases with time in the same way as the Coulomb field of the outgoing scattered particle in the neighborhood of the excited atom. In Sec. 5, we discuss the results of calculation of the widths of the lowest autoionization resonances of the helium atom as functions of the velocity and of the magnitude and sign of the charge of the scattered particle. Throughout the paper, we employ natural units.

2. BASIC EQUATIONS

We consider the collision of a charged particle P^{Z_1} that has positive or negative charge Z_1 with an atom $A(i)$, as a result of which an atomic electron goes over into the continuum:

$$P^{Z_1}+A(i)\rightarrow P^{Z_1}+A^+(f)+e^-. \tag{1}$$

Besides direct ionization transitions, there may also be resonant transitions of an electron into the continuous spectrum through the autoionization levels $|\alpha\rangle = |n_1 l_1, n_2 l_2; LM\rangle$ (n_i and l_i are the principal quantum number and the orbital angular momentum of electron i, and L and M are the total orbital angular momentum and the magnetic quantum number of the autoionization state of the atom):

$$P^{Z_1}+A(i)\rightarrow P^{Z_1}+A^{**}(\alpha)\rightarrow P^{Z_1}+A^+(f)+e^-. \tag{2}$$

To construct the total amplitude for ionization of the atom by the charged particle with allowance for the direct (1) and resonant (2) transitions, it is convenient to represent the space of possible states of the system as a sum of orthogonal Q and P subspaces, putting in the Q subspace the bound states of two-electron excitation of the target atom that are energetically close to the observed autoionization resonances. The subspace P is the complement of Q. We introduce the projection operators $\hat{Q}$ and $\hat{P}$ onto the corresponding subspaces; then the total amplitude for ionization of the atom is determined by the expression[12]

$$t_{fi}=t_{\rm dir}+t_{\rm res} \tag{3}$$

where

$$t_{\rm dir}=\langle \hat{P}\Psi_f^{(-)}|U|\Psi_i\rangle \tag{4}$$

is the amplitude of the direct transitions of the electron to the continuous spectrum, and

$$t_{\rm res}=\langle \hat{P}\Psi_f^{(-)}|\hat{P}\hat{H}\hat{Q}\hat{G}_{\rm res}(E+i0)\hat{T}_{\rm exc}(E+i0)|\Psi_i\rangle \tag{5}$$

is the amplitude of electron transitions to the continuous spectrum via autoionization levels. Here Ψ_i is the wave func-

tion of the initial state of the colliding particles, and the operator $\hat{T}_{\text{exc}}$ determines the t matrix of transition of the atom from the initial state to the resonance states:

$$\hat{T}_{\text{exc}}(E+i0)=\left(1+\hat{Q}\hat{H}\hat{P}\,\frac{1}{E+i0-\hat{P}\hat{H}\hat{P}}\right)U, \tag{6}$$

where U is the interaction potential of the incident particle with the atom in the entrance channel, $\hat{H}$ is the total Hamiltonian, and E is the total energy of the system.

The final-state wave function of the reactions (1) and (2) is determined using the Schrödinger equation

$$(\hat{P}\hat{H}\hat{P}-E)|\hat{P}\Psi_f^{(-)}\rangle=0 \tag{7}$$

with boundary conditions that describe the motion of three asymptotically free charged particles.

The resonance Green's operator describing the relative motion of the scattered particle and atom in the autoionization state is

$$\hat{G}_{\text{res}}(z)=\frac{1}{z-\hat{\mathscr{H}}_{\text{res}}(z)}, \tag{8}$$

where the effective Hamiltonian describing the system in the quasistationary resonant state has the form

$$\hat{\mathscr{H}}_{\text{res}}(z)=\hat{Q}\hat{H}\hat{Q}+\hat{\mathscr{W}}(z), \tag{9}$$

in which the operator

$$\hat{\mathscr{W}}(z)=\hat{Q}\hat{H}\hat{P}\,\frac{1}{z-\hat{P}\hat{H}\hat{P}}\,\hat{P}\hat{H}\hat{Q}$$

is non-Hermitian and depends explicitly on the energy of the system.

We introduce a set of basis state vectors of two-electron excitation of the atom that belong to the Q subspace and diagonalize the atomic Hamiltonian:

$$\langle\Phi_\alpha|\hat{H}_a|\Phi_\beta\rangle=\tilde{E}_{0\alpha}\delta_{\alpha\beta},$$
$$\langle\Phi_\alpha|\Phi_\beta\rangle=\delta_{\alpha\beta}. \tag{10}$$

Then the resonance Green's function corresponding to the Green's operator (8) in the basis representation $\{\Phi_\alpha\}$ satisfies the following system of integrodifferential equations:

$$\sum_\sigma\left[\left(-\frac{1}{2\mu}\nabla_{\mathbf{R}}^2+\tilde{E}_{0\alpha}-E\right)\delta_{\alpha\sigma}+U_{\alpha\sigma}+\hat{\mathscr{W}}_{\alpha\sigma}^{\circ}\right]$$
$$\times\tilde{G}_{\sigma\beta}(\mathbf{R},\mathbf{R}')=-\delta_{\alpha\beta}\delta(\mathbf{R}-\mathbf{R}'), \tag{11}$$

where the matrix elements

$$U_{\alpha\sigma}(\mathbf{R})=\langle\Phi_\alpha(\mathbf{r})|U(\mathbf{r},\mathbf{R})|\Phi_\sigma(\mathbf{r})\rangle \tag{12}$$

determine the direct interaction of the resonant states α and σ in the field of the scattered particle. Here $\mathbf{r}$ is the set of electron coordinates, $\mathbf{R}$ are the coordinates of the scattered particle relative to the center-of-mass position of the atom, and μ is the reduced mass of the scattered particle and the atom.

The integral operator

$$\hat{\mathscr{W}}_{\alpha\sigma}=\left\langle\Phi_\alpha\left|(V+U)\,\frac{1}{E+i0-\hat{P}\hat{H}\hat{P}}\,(V+U)\right|\right|\Phi_\sigma\right\rangle \tag{13}$$

determines the indirect interaction of the resonant states α and σ via the intermediate states of the P subspace; here V is the interelectron interaction potential.

Using the spectral representation for the Green's function in (13), we write the result of applying $\hat{\mathscr{W}}_{\alpha\sigma}$ to a plane wave

$$\hat{\mathscr{W}}_{\alpha\sigma}\circ\exp(i\mathbf{Q}\cdot\mathbf{R})=\sum_\xi\int\frac{d\mathbf{P}}{(2\pi)^3}\langle\Phi_\alpha(\mathbf{r})|(V+U)|$$
$$\times e^{i\mathbf{P}\cdot\mathbf{R}}\Psi_{\mathbf{P},\xi}^{(\pm)}$$
$$\times(\mathbf{r},\mathbf{R})\rangle\langle\langle e^{i\mathbf{P}\cdot\mathbf{R}'}\Psi_{\mathbf{P},\xi}^{(\pm)}(\mathbf{r}',\mathbf{R}')$$
$$\times|(V+U)|\Phi_\sigma(\mathbf{r}')e^{i\mathbf{Q}\cdot\mathbf{R}'}\rangle\rangle/$$
$$\left(E+i0-\frac{P^2}{2\mu}-E_\xi\right), \tag{14}$$

where $\Psi_{P,\xi}^{(\pm)}$ and E_ξ are the wave function and energy of the electron subsystem, and ξ is the set of quantum numbers that characterize the intermediate state of the electron subsystem. The summation over ξ also includes integration over the states of the continuous spectrum of the electrons. In (12)–(14), we use the notation $\langle\ldots\rangle$ for matrix elements in which integration over the coordinates of the scattered particle is not performed; in contrast, in the matrix elements $\langle\langle\ldots\rangle\rangle$ there is integration over all coordinates of the configuration space of the system.

We assume that the coupling of the resonant states Φ_α and Φ_σ to the intermediate states of the P subspace in (14) takes place through the "internal" interelectron interaction V with neglect of the "external" potential U of the scattered particle. At the same time, we take into account the distortion of the electron wave functions $\Psi_{P,\xi}^{(\pm)}$ by the field of the scattered particle (the continuum distorted by the scattered particle). This assumption is obviously valid if $R>l_a$, where l_a is the characteristic radius of the atom. In addition, in this region we can ignore the contribution of the possible intermediate states in which an atomic electron is bound to the scattered particle (in the case of a positive charge Z_1).

With allowance for these approximations, we find that the matrix element $\langle\langle\ldots\rangle\rangle$ in (14) has a δ-function singularity at $\mathbf{P}=\mathbf{Q}$. Therefore, we can approximately set $\mathbf{P}=\mathbf{Q}$ in the denominator of Eq. (14) and in the electron wave function $\Psi_{P,\xi}^{(\pm)}$. Integrating over P in Eq. (14) and, finally, setting $\mathbf{Q}=\mathbf{K}$ ($\mathbf{K}$ is the asymptotic momentum of the scattered particle in the final state), we obtain as a result a local approximation of the integral operator (13):

$$\hat{\mathscr{V}}_{\alpha\sigma} \cong W_{\alpha\sigma}(\mathbf{R})$$

$$= \sum_{\xi} \frac{\langle \Phi_\alpha | V | \Psi^{(\pm)}_{\mathbf{K},\xi}(\mathbf{R}) \rangle \langle \Psi^{(\pm)}_{\mathbf{K},\xi}(\mathbf{R}) | V | \Phi_\sigma \rangle}{E_e + \varepsilon_f - E_\xi + i0}$$

$$= \Delta_{\alpha\sigma}(\mathbf{R}) - \frac{i}{2} \Gamma_{\alpha\sigma}(\mathbf{R}), \tag{15}$$

where E_e and ε_f are the energy of the ejected electron and the binding energy of the residual target ion in the final state. Note that the matrix elements $W_{\alpha\sigma}(\mathbf{R})$, which take into account the indirect interaction of the resonant states α and σ via the intermediate states of the distorted continuum, depend on the position of the scattered particle. In the limit $R \to \infty$, the distortion of the continuum by the field of the scattered particle becomes weaker, and the matrix elements $W_{\alpha\sigma}$ do not depend on R.

The decomposition of the matrix elements $W_{\alpha\sigma}$ in (15) into $\Delta_{\alpha\sigma}$ and $\Gamma_{\alpha\sigma}$ corresponds to the decomposition of the energy denominator into real and imaginary parts. It follows from (15) that the matrices $\Delta_{\alpha\sigma}$ and $\Gamma_{\alpha\sigma}$ are Hermitian and the matrix $W_{\alpha\sigma}$ is non-Hermitian, contributions to the non-Hermitian part of the matrix being made only by the open channels determined by the condition $\varepsilon_j < E_e + \varepsilon_f$, where ε_j is the energy of the residual target ion in the jth open decay channel (the total energy of the electron subsystem in channel j is $E_\xi = \varepsilon_j + k^2/2$, where $\mathbf{k}$ is the electron momentum in the distorted continuum).

Ignoring quadratic terms, we linearize the kinetic energy operator in (11),

$$-\frac{1}{2\mu} \nabla^2_{\mathbf{R}} \cong -\frac{\mu v^2}{2} - i\mathbf{v} \cdot \nabla_{\mathbf{R}}, \tag{16}$$

this being equivalent to the use of rectilinear trajectories $\mathbf{R}(t) = \rho + \mathbf{v}t$ in the description of the motion of the scattered particle. Here ρ is the impact parameter, $\mathbf{v} = \mathbf{K}/\mu$ is the velocity of the scattered particle in the final state, and the variable t is the time of motion of the particle.

With allowance for the approximations (15) and (16), the system of integrodifferential equations (11) is transformed into a system of first-order ordinary differential equations:

$$\tilde{G}_{\sigma\beta}(\mathbf{R},\mathbf{R}') = G_{\sigma\beta}(\boldsymbol{\rho},t,t')\,\delta(\boldsymbol{\rho}-\boldsymbol{\rho}'),$$

$$\sum_{\sigma} \left[\left(i\frac{d}{dt} + \mu v^2 + E_e - E_{0\alpha} \right) \delta_{\alpha\sigma} - v_{\alpha\sigma}(\boldsymbol{\rho},t) \right] G_{\sigma\beta}(\boldsymbol{\rho},t,t') = \frac{1}{v}\,\delta_{\alpha\beta}\delta(t-t'), \tag{17}$$

where $E_{0\alpha} = \tilde{E}_{0\alpha} - \varepsilon_f$ is the energy of the α th resonant state of the isolated atom without allowance for coupling to the continuum, relative to the binding energy of the residual target ion.

The resultant system of equations (17) is, essentially, a system of tight-binding equations for the matrix elements of the resonance Green's function that describes the evolution in time of the system of interacting resonances. The interaction of the resonances is determined by the non-Hermitian complex matrix of potentials $[v_{\alpha\sigma}(\rho,t)]$, where the complex interaction potential of the quasistationary resonant states α and σ, $v_{\alpha\sigma}(\rho,t) = U_{\alpha\sigma}(\rho,t) + W_{\alpha\sigma}(\rho,t)$, is the sum of the potential $U_{\alpha\sigma}$ of the direct interaction of the resonances with each other in the field of the scattered particle and the potential of the indirect localized interaction $W_{\alpha\sigma} = \Delta_{\alpha\sigma} - (i/2)\Gamma_{\alpha\sigma}$ of the resonances via the distorted continuum, the latter containing a non-Hermitian part due to the coupling of the resonances to the open decay channels.

In principle, the system of equations (17) can be solved numerically on a restricted basis of autoionization states. However, such an approach is not convenient because of the need for repeated solution of the differential equations (17) to determine the position and shape of the resonances and find their parameters. In many cases, it is physically more advantageous and justified to use the diagonalization method, which was first used in atomic physics in the problem of resonant photoionization.[21] The essence of this method consists of separating out diagonal part of the interaction, $v_{\alpha\sigma} = \delta_{\alpha\sigma} v_{\alpha\alpha}$, and ignoring the off-diagonal part. The effects introduced by the off-diagonal part of the interaction can then be investigated in the framework of perturbation theory.

Making the phase transformation

$$\mathscr{G}(t,t') \to \exp\{i(\mu v^2 + E_e)(t-t')\}\mathscr{G}(t,t') \tag{18}$$

and separating out the diagonal part of the interaction, we represent the system of equations (17) in the matrix form

$$\left(i\frac{d}{dt} - \mathscr{H}(t) \right) \mathscr{G}(t,t') = \frac{1}{v}\,\mathscr{S}\delta(t-t'), \tag{19}$$

where

$$\mathscr{H}(t) = \mathscr{H}_0(t) + \mathscr{V}(t) \tag{20}$$

is the total Hamiltonian of the system of interacting resonances, and is given by the sum of the diagonal matrix of the Hamiltonian of the system of noninteracting resonances,

$$\mathscr{H}_{0\alpha\beta}(t) = \delta_{\alpha\beta} E_{c\alpha}(t), \tag{21}$$

and the nondiagonal matrix of the interaction operator of the resonances with one another:

$$\mathscr{V}_{\alpha\beta}(t) = (1 - \delta_{\alpha\beta}) v_{\alpha\beta}(t). \tag{22}$$

Here

$$E_{c\alpha}(t) = E_\alpha(t) - \frac{i}{2}\,\Gamma_\alpha(t) \tag{23}$$

is the time-dependent complex energy of the αth resonant state (a quasistationary electron term), in which $E_\alpha(t) = E_{0\alpha} + U_{\alpha\alpha}(t) + \Delta_{\alpha\alpha}(t)$ is the real energy of the resonance with allowance for the energy shift $U_{\alpha\alpha}(t)$ in the field of the scattered particle and the energy shift $\Delta_{\alpha\alpha}(t)$ due to the interaction of the level with the distorted continuum. The total width $\Gamma_\alpha(t) = \Sigma_j \Gamma^{(j)}_{\alpha\alpha}(t)$ of the resonance derives from the interaction with the open channels, and $\mathscr{S}$ is the identity matrix. To simplify the expressions, we do not specify the dependence on the impact parameter explicitly.

By virtue of causality,

$$\mathscr{G}(t,t') = -\frac{i}{v}\,\theta(t-t')\mathscr{S}(t,t'), \tag{24}$$

where

$$\theta(x)=\begin{cases}1, & x\geq 0,\\ 0, & x<0.\end{cases}$$

It follows from causality that the operator for the evolution of the system in time satisfies the homogeneous equation and initial condition

$$i\frac{d}{dt}\mathscr{S}(t,t')=\mathscr{H}(t)\mathscr{S}(t,t'),$$

$$\mathscr{S}(t',t')=\mathscr{S}. \tag{25}$$

To zeroth order in the interaction, $\mathscr{V}(t)=0$, or, in the diagonalization approximation, the evolution operator of the system can be written in the explicit form

$$\mathscr{S}_0(t,t')=\exp\left(-i\int_{t'}^{t}d\tau\mathscr{H}_0(\tau)\right) \tag{26}$$

or

$$\mathscr{S}_{0\alpha\beta}(t,t')=\delta_{\alpha\beta}\exp\left(-i\int_{t'}^{t}d\tau E_{c\alpha}(\tau)\right),$$

since for $\tau\neq\tau'$, the commutator $[\mathscr{H}_0(\tau),\mathscr{H}_0(\tau')]$ vanishes. The diagonal operator (26) describes the independent evolution in time of the system of noninteracting autoionization states. Allowance for the interaction of the resonance states with one another leads to nonvanishing off-diagonal matrix elements of the evolution operator $\mathscr{S}$ and, accordingly, to a mixing of the different autoionization states during temporal evolution. As is shown in Refs. 22 and 23, allowance in the dipole approximation for Stark mixing of the two closely spaced autoionization states $(2s2p)^1P$ and $(2p^2)^1D$ of the helium atom leads to an initial distortion of the angle and energy distributions of the autoionization electrons. In this paper, we restrict ourselves to the zeroth approximation in the interaction of the resonant states with one another; this interaction is negligible for sufficiently distant resonant states, for example, for the autoionization state $(2s^2)^1S$ of the helium atom.

3. RESONANT IONIZATION AMPLITUDE

Let $f_{\alpha i}(t')$ be the complex amplitude for excitation of the αth autoionization state at time t'. The excitation amplitude $f_{\alpha i}(t')$ is determined by the t matrix of transitions of the system from the initial state $|i\rangle$ to the autoionization states $|\alpha\rangle$:

$$f_{\alpha i}(t')=\exp\{-i(\mu v^2+E_e)t'\}\langle\Phi_\alpha|\hat{T}_{\rm exc}(E+i0)|\Psi_i\rangle. \tag{27}$$

Then the amplitude of the resonance transitions (5) in the diagonalization approximation (26) has the form

$$t_{\rm res}=-\frac{iv}{(2\pi)^3}\sum_\alpha\int d\rho\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt' f_{f\alpha}(t)\exp\left(iE_e t-i\int_{t'}^{t}d\tau E_{c\alpha}(\tau)\right)f_{\alpha i}(t'). \tag{28}$$

Here

$$f_{f\alpha}(t)=\langle\Psi_f^{(-)}|V|\Phi_\alpha\rangle \tag{29}$$

is the matrix element of the amplitude for decay of the αth autoionization state as a result of transition of the system to the final state $|f\rangle$ at time t; the final-state wave function is $|\Psi_f^{(-)}\rangle=\exp(-i\mu v^2 t)|\hat{P}\Psi_f^{(-)}\rangle$.

We note that the formation and decay of the autoionization states in (28) are not independent processes but are correlated in time. In the theory of resonance reactions, one usually makes the hypothesis that the formation and decay of resonant states are independent, it being assumed that the mean lifetime $\tau_{\rm dec}=\Gamma_\alpha^{-1}$ is much greater than the effective interaction time of the colliding particles, during which the excitation of the states occurs. To obtain the amplitude (28) neglecting temporal correlation, we expand the excitation amplitude as a Fourier integral

$$f_{\alpha i}(t')=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\varepsilon\,\exp(-i\varepsilon t')\tilde{f}_{\alpha i}(\varepsilon). \tag{30}$$

Then, with allowance for (30), the point of stationary phase, which makes the main contribution to the integral over t', is determined by $\varepsilon=E_\alpha(t')$. In (30), we approximately set $\tilde{f}_{\alpha i}(\varepsilon)\simeq\tilde{f}_{\alpha i}[E_\alpha(t')]$ and obtain

$$f_{\alpha i}(t')=\tilde{f}_{\alpha i}[E_\alpha(t')]\delta(t'),$$

i.e., in the limit we have a δ-function excitation of the autoionization state at $t'=0$. With such a δ-function approximation of the real excitation amplitude, the amplitude for the resonance transitions factorizes and simplifies to the form

$$t_{\rm res}=-\frac{iv}{(2\pi)^3}\int d\boldsymbol{\rho}\int_0^\infty dt\,\exp(iE_e t+i\mathbf{Q}_\perp\boldsymbol{\rho})\sum_\alpha A_{f\alpha}(\boldsymbol{\rho},t)A_{\alpha i}(\boldsymbol{\rho}), \tag{31}$$

where

$$A_{f\alpha}(\boldsymbol{\rho},t)=f_{f\alpha}(\boldsymbol{\rho},t)\exp\left(-i\int_0^t d\tau E_{c\alpha}(\boldsymbol{\rho},\tau)\right),$$

$$\tilde{f}_{\alpha i}(E_\alpha(0))=\exp(i\mathbf{Q}_\perp\boldsymbol{\rho})A_{\alpha i}(\boldsymbol{\rho}).$$

In (31), we have explicitly separated out the significant dependence of the amplitude on the energy E_e in the neighborhood of the autoionization resonances and on the scattering angle θ_p of the incident particle ($Q_\perp=M_p v\theta_p$, where M_p is the mass of the incident particle). With allowance for (13), the cross section for resonant ionization can be integrated over energy E_e and scattering angle θ_p. As a result, we obtain the following expression for the differential (with respect to the electron ejection angle) yield of resonances:

$$\frac{d\sigma_{\rm res}}{d\Omega_e}=\sum_\alpha\int d\boldsymbol{\rho}K_{\alpha\alpha}(\boldsymbol{\rho})|A_{\alpha i}(\boldsymbol{\rho})|^2+\sum_{\alpha\neq\alpha'}\int d\boldsymbol{\rho}K_{\alpha\alpha'}(\boldsymbol{\rho})A_{\alpha i}(\boldsymbol{\rho})A^*_{\alpha' i}(\boldsymbol{\rho}), \tag{32}$$

where the factor $K_{\alpha\alpha'}$, which modifies the differential yield of the resonances, depends on the product of the decay amplitudes of the resonant states α and α':

$$K_{\alpha\alpha'}(\boldsymbol{\rho})=2\pi k_e\int_0^\infty dt A_{f\alpha}(\boldsymbol{\rho},t)A^*_{f\alpha'}(\boldsymbol{\rho},t). \tag{33}$$

In deriving (32), we have set the lower limit of integration for the variable E_e to $-\infty$, since the resonance width is much less than the resonance energy, and the integral over E_e converges rapidly; in addition, in (33) $k_e=(2E_\alpha)^{1/2}$, where E_α is the energy of the unperturbed autoionization state.

The first sum in (32) takes into account the contribution to the differential yield of the individual resonant states without allowance for their interference. The second sum over α and α' includes the interference contribution of the fairly closely spaced resonant states α and α'. The interference contribution of the isolated resonant states is negligible, since in this case

$$A_{f\alpha}(t)A_{f\alpha'}(t)\propto\exp\left\{-i\int_0^t d\tau[E_\alpha(\tau)-E_{\alpha'}(\tau)]\right\}$$

contains a rapidly oscillating factor. The factor (33) governs the angular dependence of the differential yield, and the nature of this dependence is determined by the form of the final-state wave function in the matrix element (29) of the decay amplitude. Allowance for final-state interaction modifies the decay matrix element and leads accordingly to a distortion of the angular distributions (32) of the autoionization electrons. On the other hand, allowance for interaction in the resonant state changes the resonance width and energy and also affects the angular distributions (32).

Consider the integrated yield of an isolated resonance, for example, the $(2s^2)^1S$ resonance of the helium atom. We integrate the factor $K_{\alpha\alpha}$ over the electron ejection angle:

$$K^I_{\alpha\alpha}(\boldsymbol{\rho})=\int d\Omega_e K_{\alpha\alpha}(\boldsymbol{\rho}\Omega_e)$$

$$=\int_0^\infty dt\Gamma^{(f)}_{\alpha\alpha}(\boldsymbol{\rho},t)\exp\left\{-\int_0^t d\tau\Gamma_\alpha(\boldsymbol{\rho},\tau)\right\}, \tag{34}$$

where

$$\Gamma^{(f)}_{\alpha\alpha}(\boldsymbol{\rho},t)=2\pi k_e\int d\Omega_e|f_{f\alpha}(\boldsymbol{\rho},t,\Omega_e)|^2$$

is the partial width of decay of the resonant state α to the final state f. If the resonance can decay through several channels, (34) must be summed over all possible decay channels of the resonant state. As a result, we find that the total width is $\Sigma_f\Gamma^{(f)}_{\alpha\alpha}=\Gamma_{\alpha'}$, where Γ_α is the total decay width of the resonant state α, and we have the integrated factor $K^I_{\alpha\alpha}(\boldsymbol{\rho})=1$. Thus, the integrated yield of the isolated resonance is equal to the excitation cross section of the resonant state α:

$$\sigma_{\mathrm{res},\alpha}=\int d\boldsymbol{\rho}|A_{\alpha i}(\boldsymbol{\rho})|^2.$$

We emphasize that to obtain this result it is important that we simultaneously take into account in an appropriate manner the interaction in the final state and in the resonant state.

We now consider the contribution of the interference terms in (32) to the integrated yield. We integrate the factor $K_{\alpha\alpha'}$ over the electron ejection angle:

$$K^I_{\alpha\alpha'}(\boldsymbol{\rho})=\int d\Omega_e K_{\alpha\alpha'}(\boldsymbol{\rho},t)$$

$$=\int_0^\infty dt\Gamma^{(f)}_{\alpha\alpha'}(\boldsymbol{\rho},t)\exp\left(-i\int_0^t d\tau[E_\alpha(\tau)-E_{\alpha'}(\tau)]\right.$$

$$\left.-\frac{1}{2}\int_0^t d\tau[\Gamma_\alpha(\tau)+\Gamma_{\alpha'}(\tau)]\right), \tag{35}$$

where

$$\Gamma^{(f)}_{\alpha\alpha'}(\boldsymbol{\rho},t)=2\pi k_e\int d\Omega_e f_{f\alpha}(\boldsymbol{\rho},t,\Omega_e)f^*_{f\alpha'}(\boldsymbol{\rho},t,\Omega_e)$$

is the matrix element of the indirect interaction of the resonant states α and α' via continuum states. Thus, $K^I_{\alpha\alpha'}$ is proportional to the non-Hermitian part of the interaction potential resulting from the coupling of the resonant states to the open decay channels (15), the part of the interaction that we ignored in the diagonalization approximation. Therefore, remaining consistently in the framework of the diagonalization approximation, we must ignore the interference terms in (32), and the total integrated yield is equal to the total excitation cross section of the resonant states:

$$\sigma_{\mathrm{res}}=\sum_\alpha\int d\boldsymbol{\rho}|A_{\alpha i}(\boldsymbol{\rho})|^2.$$

We investigate in more detail the situation in which $\Gamma^{(f)}_{\alpha\alpha'}(\mathbf{R})$ can be neglected. As wave function of the continuous spectrum, we take the final-state wave function used in the calculations of Refs. 10–12:

$$\Psi^{(-)}_f=\hat{A}[\varphi_f\psi^{(-)}_{\mathbf{k}_{23}}(\mathbf{r}_{23})\Phi^{(-)}(\nu_{12},\xi_{12})\Phi^{(-)}(\nu_{13},\xi_{13})]. \tag{36}$$

Here φ_f is the wave function of the residual ion, $\psi^{(-)}_{\mathbf{k}_{23}}(\mathbf{r}_{23})$ is the Coulomb wave function of the electron in the field of the residual ion, $\hat{A}$ is the operator of (anti)symmetrization with respect to the electron coordinates,

$$\Phi^{(-)}(\nu_{ij},\xi_{ij})=f^{(-)}_c(\nu_{ij})\,{}_1F_1(i\nu_{ij},1,-i\xi_{ij}) \tag{37}$$

are the distorting factors that take into account the Coulomb interaction in the final state between particles i and j, where

$$f^{(-)}_c(\nu)=\exp(-\pi\nu/2)\Gamma(1-i\nu)$$

is the Coulomb normalization factor, ${}_1F_1(a,c,z)$ is the confluent hypergeometric function,

$$\nu_{ij}=Z_iZ_jm_{ij}/k_{ij},\quad \xi_{ij}=k_{ij}r_{ij}+\mathbf{k}_{ij}\mathbf{r}_{ij},$$

m_{ij}, $\mathbf{k}_{ij}$, and $\mathbf{r}_{ij}$ are the reduced mass, relative momentum, and position vector for the pair of particles i and j, respectively, and Z_i is the charge of particle i. Subscripts 1, 2, and 3 denote the scattered particle, the ejected electron, and the residual ion, respectively.

Let Φ_{LM} and $\Phi_{L'M'}$ be the wave functions of two energetically closely spaced resonant states, for example, the $(2s2p)^1P$ and $(2p^2)^1D$ states of the helium atom. We take into account the fact that the electrons in a autoionization state are concentrated near the nucleus of the atom, and

therefore in the calculation of the decay matrix elements (29) we can in the distorting factors (37) set $r_{23}=0$, i.e., $\mathbf{r}_{12}=-\mathbf{R}$, $\mathbf{r}_{13}=\mathbf{R}$, and $\Gamma_{LM,L'M'}(\mathbf{R})$ takes the form

$$\Gamma_{LM,L'M'}(\mathbf{R})=C\sqrt{\Gamma_{L0}\Gamma_{L'0}}|\Phi^{(-)}(\nu_{13},\xi_{13})|^2 \times\int d\Omega_e Y_{LM}(\Omega_e)Y^*_{L'M'}(\Omega_e)|\Phi^{(-)} \times(\nu_{12},\xi_{12})|^2, \quad (38)$$

where $C=e^{i\varphi}$ is a phase factor, and Γ_{L0} is the width of the unperturbed resonant state $|LM\rangle$. Since the velocity of the residual ion in the final state is low, $v_3\simeq 0$, it follows that

$$\mathbf{k}_{13}=m_{13}\mathbf{v}, \quad \mathbf{k}_{12}=m_{12}\mathbf{v}'_e,$$

where $\mathbf{v}'_e=\mathbf{v}_e-\mathbf{v}$ is the electron velocity in the frame of the scattered particle, and

$$\xi_{13}=m_{13}(vR+v^2t), \quad \xi_{12}=m_{12}(v'_eR-\mathbf{v}'_e\mathbf{R}).$$

It follows from (38) that $\Gamma_{LM,L'M'}(\mathbf{R})=0$ under conditions of weak interaction of the electron and the scattered particle, when the amplitude of the distorting factor satisfies $|\Phi^{(-)}(\nu_{12},\xi_{12})|=1$. If we ignore the ρ dependence of $\Gamma_{LM,L'M'}(\rho,t)$ and set $\rho=0$, then $\Phi^{(-)}(\nu_{12},\xi_{12})$ does not depend on the azimuthal ejection angle, and $\Gamma_{LM,L'M'}(0,t)\sim\delta_{MM'}$, i.e., the interaction of resonant states with different magnetic quantum numbers, including ones that belong to a single term, $L=L'$, is negligible.

4. WIDTH OF AUTOIONIZATION RESONANCES

If the states of the distorted continuum that interacts with the discrete resonant states are described by the same wave functions as the final state (36), then the instantaneous value of the perturbed width of the resonance will be determined by the expression (38), in which it is necessary to set $L=L'$, $M=M'$, $\Gamma_{L0}=\Gamma_{L'0}=\Gamma_0$, $C=1$. In the amplitude (31), the instantaneous width of the resonance is integrated with respect to the time over the interval $(0,t)$, and therefore it is more convenient to work with the width of the resonance averaged over the interval $(0,t)$, which is more directly related to the physical characteristics of the decay process:

$$W_{LM}(t)\equiv\bar{\Gamma}_{LM}(\rho=0,t)/\Gamma_0 =\int d\Omega_e|Y_{LM}(\Omega_e)|^2\mathfrak{F}(t,\Omega_e), \quad (39)$$

where we have introduced the width distortion function

$$\mathfrak{F}(t,\Omega_e)=\frac{1}{t}\int_0^\infty d\tau\varphi_c(\tau,t)|\Phi^{(-)}(\nu_{13},a_{13}\tau)\Phi^{(-)} \times(\nu_{12},a_{12}\tau)|^2. \quad (40)$$

Here $\varphi_c(\tau,t)=\theta(\tau)-\theta(\tau-t)$ is a cutoff function, equal to 1 for $\tau\in(0,t)$ and 0 for $\tau\notin(0,t)$; $a_{13}=2m_{13}v^2$, $a_{12}=m_{12}(v'_ev-\mathbf{v}'_e\mathbf{v})$. In limiting cases we have: As $t\to\infty$, the measure of the set of directions in which $\mathfrak{F}(t,\Omega_e)\neq 1$ tends to zero, reflecting the weakening of the distortion of the continuum states, and the perturbed width of the resonance tends to its unperturbed value Γ_0; in the limit $t\to 0$, the perturbation of the width is determined by the product of the squares of the moduli of the Coulomb normalization factors averaged over the electron ejection angle:

$$W_{LM}(0)=|f_c^{(-)}(\nu_{13})|^2\int d\Omega_e|Y_{LM}(\Omega_e)|^2|f_c^{(-)}(\nu_{12})|^2. \quad (41)$$

Note that when we take into account only the phase distortions of the continuum states, in particular in the framework of the semiclassical eikonal approximation, $\mathfrak{F}(t,\Omega_e)\equiv 1$, and the width of the resonance is unchanged. If we approximate the cutoff step function by an exponential function of the form $\varphi_c(\tau,t)=\exp(-\tau/t)$, then $\mathfrak{F}(t,\Omega_e)$ can be expressed in terms of the Lauricella hypergeometric function of four variables $F_A^{(4)}$ (Ref. 24):

$$\mathfrak{F}(t,\Omega_e)=|f_c^{(-)}(\nu_{13})|^2|f_c^{(-)}(\nu_{12})^2F_A^{(4)}(1,i\nu_{13}, -i\nu_{13},i\nu_{12},-i\nu_{12};1,1,1,1;ia_{13}t, -ia_{13}t,ia_{12}t,-ia_{12}t). \quad (42)$$

In the special case when the interaction of a pair of particles can be ignored, for example, the interaction of the scattered particle and the residual ion ($\nu_{13}\equiv 0$), $F_A^{(4)}$ simplifies to the Lauricella hypergeometric function of two variables $F_A^{(2)}(1,i\nu_{12},-i\nu_{12};1,1;ia_{12}t,-ia_{12}t)$, which, in turn, can be expressed in terms of Gauss's hypergeometric function and

$$\mathfrak{F}(t,\Omega_e)=F(\nu_{12},a_{12}t) \equiv|f_c^{(-)}(\nu_{12})|^2\exp(2\nu_{12}\tan^{-1}(a_{12}t))\ {}_2F_1 \times\left(i\nu_{12},-i\nu_{12},1,\frac{(a_{12}t)^2}{(a_{12}t)^2+1}\right). \quad (43)$$

We use the following two-dimensional integral representation for the function $F_A^{(4)}$ (Ref. 24):

$$F_A^{(4)}=\frac{1}{|\Gamma(i\nu_{12})\Gamma(1-i\nu_{12})|^2}\int_0^1\int_0^1 dt_1dt_2t_1^{i\nu_{12}-1}(1-t_1)^{-i\nu_{12}}t_2^{-i\nu_{13}-1}(1-t_2)^{i\nu_{13}}\frac{1}{1+it(t_1-t_2)}\exp(\nu_{13}[\tan^{-1}(a_{12}t(t_1-t_2)+a_{13}t)-\tan^{-1}[a_{12}t(t_1-t_2)-a_{13}t)]]_2F_1\left(i\nu_{13}-i\nu_{13},1,\frac{(a_{13}t)^2}{(a_{13}t)^2+[1+ia_{12}t(t_1-t_2)]^2}\right). \quad (44)$$

We expand the integrand in (44) in an asymptotic series up to terms of first order in $(a_{13}t)^{-1}$:

$$\mathfrak{F}(t,\Omega_e)=(1-2\nu_{13}/a_{13}t)F(\nu_{12},a_{12}t). \quad (45)$$

Bearing in mind that $F(\nu,X)=1-2\nu/X$ to first order in X^{-1}, we approximately determine the width distortion function for all values of t in a form factorized in the pairwise interaction of particles:

$$\mathfrak{F}(t,\Omega_e)=F(\nu_{13},a_{13}t)F(\nu_{12},a_{12}t).$$

Then the distorted width of the resonance is

$$W_{LM}(R=vt) = F(\nu_{13},a_{13}t)\int d\Omega_e |Y_{LM}(\Omega_e)|^2 F(\nu_{12},a_{12}t). \tag{46}$$

Note that for $R=0$ (46) is identical to (41). We consider the asymptotic behavior of (46) in the limit $R\to\infty$ in the case of an S resonance. Since

$$F(\nu,X)=\begin{cases} 1-2\nu/X, & X\gg 1, \\ |f_c^{(-)}(\nu)|^2, & X\ll 1, \end{cases}$$

we interpolate $F(\nu,X)$ with the rational function

$$F_{\text{int}}(\nu,X)=1-\frac{2\nu}{X+a(\nu)},$$

where

$$a(\nu)=\frac{2\nu}{1-|f_c^{(-)}(\nu)|^2}.$$

With this interpolation,

$$W_{L=0}(R)=F_{\text{int}}(\nu_{13},a_{13}t)\left(1-\int_0^2 dy\,\frac{\nu_{12}(y)}{X_{12}(y)+a[\nu_{12}(y)]}\right), \tag{47}$$

where we have introduced the new variable of integration $y=1-\cos(\theta_e)$, and θ_e is the electron ejection angle. Note that $\nu_{12}(y)$ is a "slow" and $X_{12}(y)=a_{12}(y)t$ a "fast" function of the variable of integration, since $X_{12}(y)$ contains the large parameter $R=vt$. At the same time, $X_{12}(y)$ increases rapidly over the interval (0,2) from $X_{12}(0)=m_{12}(|v_e'|-v_e')R$, where $v_e'=v_e-v$, to $X_{12}(2)=2m_{12}(v+v_e)R$. If $2\pi|\nu_{12}(y)|>1$, then the slowly varying function $a(\nu_{12}(y))$ can be approximately set equal to π^{-1} for $\nu_{12}<0$ and $2\nu_{12}$ for $\nu_{12}>0$. With allowance for this approximation, the remaining integral in (47) can be calculated analytically.[25] For example, in the case $\nu_{12}<0$ in the limit $R=vt\to\infty$ we have

$$\bar{\Gamma}_{L=0}(R)=\Gamma_0\left(1-\frac{1}{2}\frac{V_{13}(R)}{E}-\frac{1}{2}C(R)\frac{V_{12}(R)}{E_0}\right), \tag{48}$$

where

$$C(R)=\ln\frac{(v+v_e+|v_e'|)\pi vR}{(v+v_e)[(|v_e'|-v_e')\pi R+v/v_e]},$$

$$V_{ij}(R)=\frac{Z_iZ_j}{R},$$

$E_0=m_{12}v_e^2/2$, $E=m_{13}v^2/2$. It follows from (48) that the perturbed part of the resonance width is proportional to the charge of the scattered particle, and decreases asymptotically with increasing distance as the Coulomb potential of the interaction of the scattered particle with the autoionization electron and the target residual ion.

By virtue of the decay, the amplitude for occupation of the autoionization state decreases with the time as

$$e-\frac{\bar{\Gamma}(R)t}{2}.$$

Therefore, using Eq. (48), we can assess the effect of the distortion of the line width on the integrated yield of the autoionization electrons by means of the factor

$$K_{wd}=\exp\left(-\frac{1}{2}\,\xi\,\ln\frac{E_0}{\Gamma_0}\frac{8\pi}{1+v_e/v}\right) \tag{49}$$

for $v<v_e$. Here $\xi=(\Gamma_0/E_0)(Z_1/v)$ is the characteristic parameter that determines the range in which width distortion may be important.

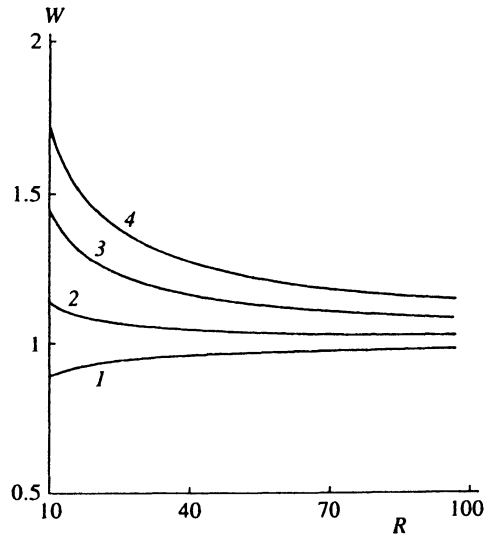

FIG. 1. Dependence on the internuclear separation R of the relative width $W(R)$ of the $(2s^2)^1S$ resonance of the helium atom decaying in the Coulomb field of scattered ions with different charges Z_1 and velocity $v=1.0$. Curves 1–4 correspond to calculations with the charges $Z_1=-1$, 1, 5, and 10, respectively.

5. DISCUSSION OF NUMERICAL RESULTS

In Fig. 1, we present the results of calculations in accordance with Ref. 46 of the relative width $W(R)=\bar{\Gamma}_{LM}(R)/\Gamma_0$ of the $(2s^2)^1S$ resonance of the helium atom ($E_0=1.222$, where E_0 is the unperturbed resonance energy, and $\Gamma_0=0.005$) excited in a collision with ions possessing velocity $v=1$ and charge Z_1 of both signs and different magnitudes, as a function of the internuclear separation $R=vt$. In making the calculations, we ignored the interaction of the scattered ion with the residual ion. By virtue of Eqs. (41) and (48), the influence of the interaction of heavy particles can be significant only over a short time interval $(0,\Delta)$, where $\Delta\sim m_{13}^{-1}$ ($m_{13}\gg 1$), modifying $W(0)$ by a factor $|f_c^{(-)}(\nu_{13})|^2$. It can be seen that with increasing charge Z_1 the influence of distortion of the resonance width by the Coulomb field of the scattered ion increases, and can be substantial at large $Z_1\sim 10$. At the same time, $W(R)$ varies monotonically with distance from the value (41) at $R=0$ to 1 in accordance with (48) as $R\to\infty$. The nature of the perturbation of the resonance width differs qualitatively depending on the sign of the charge Z_1: the width of the resonance increases in the field of

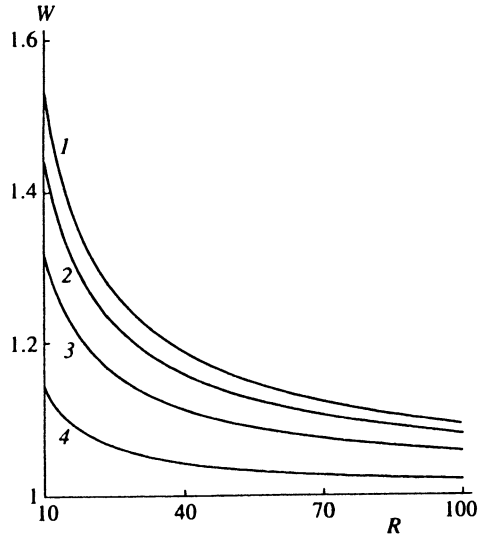

FIG. 2. Dependence of the relative width $W(R)$ of the autoionization state $(2s^2)^1S$ of the helium atom on the velocity of the scattered ion. The ion charge is $Z_1=5$. Curves 1–4 correspond to calculations with the velocities $v=0.5$, 1.0, 1.5, and 2.0, respectively.

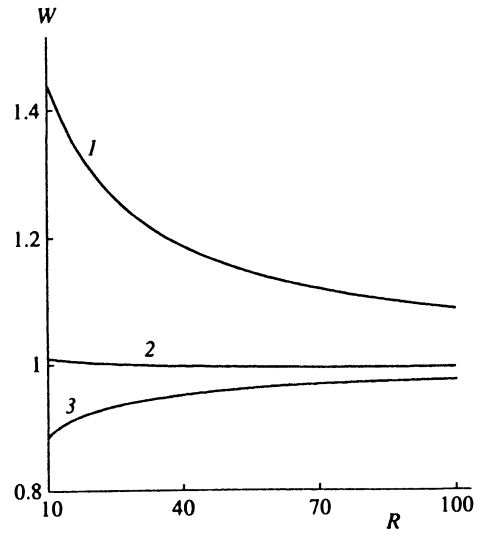

FIG. 3. Dependence of the relative width $W(R)$ of the autoionization state $(2s^2)^1$ of the helium atom on the velocity of the scattered electron. Curves 1–3 correspond to calculations with velocities $v=0.25$, 0.5, 1.0, respectively.

a positive charge but decreases in the field of a negative charge. The increase (decrease) of the resonance width in the case of positive (negative) charge Z_1 leads by virtue of (33) and (34) to a decrease (increase) in the differential and integrated resonance yields, and this compensates the increase (decrease) resulting from allowance for the final-state interaction in such a way that the integrated yield of the resonance is unchanged when simultaneous allowance is made for interaction in the final state and in the resonant state. Note, however, that exact cancellation does not occur [if we take into account the approximation of the cutoff step function by an exponential function in the derivation of the expression (46)].

Figure 2 gives the results of calculations of $W(R)$ for the $(2s^2)^1S$ resonance of the helium atom for different velocities of the scattered ion, $v=0.5$–2, and charge $Z_1=5$. It can be seen that with increasing collision velocity the effect of width distortion decreases monotonically. Moreover, the nature of this dependence does not change as the velocity v approaches $v_e=(2E_0)^{1/2}=1.563$, the velocity of the autoionization electron in the continuum. As a result of exact averaging of $F(\nu_{12}, a_{12}\, t)$ over the electron ejection angle in (46), the singularity in the behavior of the integrand at $v=v_e$ is completely smoothed.

We made a similar calculation of the width of the $(2s^2)^1S$ resonance of the helium atom for a light scattered particle (electron) at velocities $v=0.25$, 0.5, 1.0 (Fig. 3). The light projectile particle is interesting in that the nature of the distortion of its resonance width is determined by the superposition of the interactions of the scattered particle with the residual ion and autoionization electron in the continuum, since in this case the mass parameters $m_{13}\cong 1$ and $m_{12}\cong 0.5$ are comparable in magnitude. In the calculation, we did not allow for exchange between the scattered electron and the autoionization electron. It can be seen that the superposition of the interactions leads to more complicated behavior of the width of the resonance as a function of the collision velocity. One can identify two qualitatively different kinematic velocity ranges in which one of the pairs of particles in the continuum dominates. At low velocities $v<0.5$, the attractive potential between the scattered electron and the residual ion dominates, and this leads to an increase in resonance width. At $v\simeq 0.5$, the interactions of the scattered electron with the residual ion and the autoionization electron cancel one another, and distorted the resonance width is weakly distorted. In contrast, at high velocities $v>0.5$ the repulsive potential between the scattered electron and the autoionization electron dominates, and the resonance width decreases.

With allowance for the distortion of the continuum state by the scattered particle, the width of the autoionization state acquires a dependence on the magnetic quantum number M. To determine the dependence of the resonance width on M, we calculated $W_{LM}(R)$ for various values of M $(W_{L,M}=W_{L,-M})$ of the $(2p^2)^1D$ resonance $(E_0=1.298$, $\Gamma_0=0.00263)$ of the helium atom excited in a collision with ions with charge $Z_1=5$ and velocity $v=1.0$ (Fig. 4). The calculations revealed different dependences of $W_{LM}(R)$ on the distance: whereas $W_{L,M=0}(R)$ decreases smoothly with increasing R, $W_{1,M\neq 0}(R)$ tends more rapidly to 1 the larger the value of M. Moreover, for $R\gg 1$ we have $|\Delta W_{L,M=0}(R)|\gg|\Delta W_{L,M\neq 0}(R)|$, where $\Delta W_{L,M}(R)=W_{L,M}(R)-1$. For a rough estimate of the L,M dependence of $\Delta W_{L,M}(R)$, we can extract the slowly varying spherical harmonic $Y_{LM}(\Omega_e)$ at the point $\theta_e=0$ in front of the integral in (46). As a result, we obtain $\Delta W_{L,M}(R)=\delta_{M0}(2L+1)\Delta W_{L=0}(R)$ for $R\gg 1$.

6. CONCLUSIONS

In this paper, we have developed a theory of the resonant ionization of an atom by charged particles with allowance for interaction in the final and resonant states. We have obtained

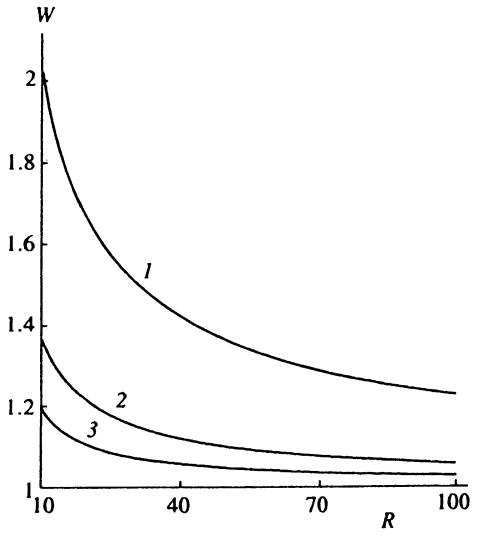

FIG. 4. Dependence of $W(R)$ on the magnetic quantum number M of the autoionization state $(2p^2)^1D$ of the helium atom. The charge and velocity of the scattered ion are $Z_1=5$ and $v=1.0$. Curves 1–3 correspond to $M=0$, 1, 2, respectively.

a system of equations for the temporal evolution operator of the system of interacting resonant states that can be explicitly solved in the diagonalization approximation. In the diagonalization approximation, the amplitudes for occupation of the autoionization states evolve in time independently of one another. The amplitude of resonant ionization is determined with neglect of temporal correlations between the processes of formation and decay of the autoionization states. We have shown that the total cross section for resonant ionization or the integrated yield of autoionization electrons calculated with such an amplitude are determined by the total probability for excitation of the resonant states, and do not depend on the effects of the interaction in the final state and resonant state.

We have investigated influence of distortion of the continuum states by the scattered particle on the width Γ of a quasistationary state. We have shown that Γ, which has been regarded in all previous theories of the post-collision interaction as a free parameter, becomes, when the interaction in the resonant state is taken into account, a function of the position of the scattered particle that can differ appreciably from the width of the autoionization state in the isolated atom for small separations between the atom and the scattered particle. We have obtained a simple analytic expression for the time-dependent width $\Gamma_{LM}(t)$ of the autoionization resonance. We have established the characteristic dependences of $\Gamma_{LM}(t)$ on the velocity and charge of the scattered particle and also on the orbital angular momentum L and the magnetic quantum number M of the resonance.

Our theoretical description makes it possible to calculate the energy and angular distributions of autoionization electrons with allowance for interaction in the final and resonant states. It is of considerable interest to study the effects of the joint influence of interaction in the final and resonant states on the angle and energy spectra of the autoionization electrons. In addition, it is necessary to develop the theory beyond the diagonal approximation. This will make it possible to describe consistently the excitation and decay of closely spaced interfering autoionization states.

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