PHYSICAL REVIEW A VOLUME 22, NUMBER 2 AUGUST 1980

Adiabatic effects in atomic inner-shell ionization by heavy charged particles

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(Received 7 December 1979)

The K-shell ionization of a heavy atom by a slow light ion is studied by allowing the initial electron state to relax under the potential of the projectile. General estimates are given for monopole and dipole transitions to continuum states, and for the range of impact parameters that contribute most to the process. The correction to the electron binding is now time dependent, and it is shown that it produces a reduction of the ionization probability for small collision velocities, while at larger velocities the time dependence of the binding may enhance K-shell ionization.

I. INTRODUCTION

The K-shell ionization of a heavy atom when bombarded by an atomic projectile allows the use of several theoretical model for its description, according to the ratio between nuclear charges, and between characteristic projectile and K-electron velocities. This article will treat the Coulomb ionization of K shells, where the model assumes the projectile behaving as a bare charge on its interaction with the electron to be excited, and furthermore, will consider slow projectiles compared with the average velocity of such electron in the target. In order to have a bare projectile acting on the K-shell electrons we impose the restriction

$$Z_1 \ll Z_2 \tag{1}$$

on the nuclear charges (indices 1 and 2 refer to projectile and target nuclei, respectively). The condition of slow collisions is given by

$$v_1 \ll v_{2K}, \tag{2}$$

where the suffix K identifies parameters related to the K-shell electrons.

The impact parameters ρ that contribute most to K-shell excitation in a semiclassical description of the process are given by[1]

$$\rho \sim v_1/\omega_{2K}, \tag{3}$$

where

$$\omega_{2K} = \theta_K Z_2^2/2$$

is the K-shell binding energy, with θ_K representing the nonhydrogenic character of the orbital, and Z_2 is the effective nuclear charge for the motion of each K-shell electron (atomic units are used throughout this paper). A first condition coming out from (2) and (3) is that the projectile must penetrate deeply into the K shell to be able to remove an electron:

$$\rho/a_{2K} = 2v_1/\theta_K Z_2 = 2v_1/\theta_K v_{2K} \ll 1, \tag{4}$$

consequently, the charge Z_1 stays a long time τ inside the K shell, compared with the characteristic orbital period ω_{2K}^{-1}:

$$\tau = a_{2K}/v \gg \omega_{2K}^{-1}. \tag{5}$$

We will now mention the theoretical approaches that have been used to treat collisions described by relations (1) to (5). The general theory for K-shell ionization was first developed along the lines of the plane-wave Born approximation[2] (PWBA). Here the initial and final electron states are assumed undisturbed by the projectile, which is described as a free particle not affected by the internuclear repulsive potential.

The action of the internuclear potential on the nuclear motion was first considered by Bang and Hansteen,[1] who introduced hyperbolic trajectories in a semiclassical approximation (SCA) for the collision, and calculated the transition probability to first order in the projectile-electron interaction. The influence of the target potential on the projectile can also be considered in a quantum formalism by using a distorted-wave Born approximation to the transition amplitude, as done by Pauli and Trautmann.[3]

An alternative approach to inner-shell ionization has been proposed by Kleber,[4] who uses a variational wave function selected so that it can describe approximately nonadiabatic processes; the ionization probability is obtained directly from the asymptotic form of the wave function. It is not easy in this procedure to assess the precision of the results, and furthermore, a previous study of the collision process is necessary in order to propose an appropriate form for the trial function.

The distortion of the initial and final electron states by the projectile may be of importance, since although $Z_1 \ll Z_2$ and consequently the potential set by the projectile is a small perturbation on the K orbital, the collision time is much larger than the electron response time ω_{2K}^{-1}, and the electron can adiabatically adapt its wave function to

the transient potential provided by both the projectile and the target. Several improvements of the SCA were proposed to partially account for this action of the projectile: Brandt, Laubert, and Sellin,[5] and Basbas, Brandt, and Laubert[6] introduced in an approximate way, the correction to the electron-binding energy due to the presence of the projectile, assuming this correction to be independent of the internuclear distance R and equal to its value at the distance of closest approach.

Andersen, Laegsgaard, Lund and Moak[7] went a step further and optimized the K-shell radius, and consequently minimized the binding energy ω_{2K} within the hydrogenic orbital class of functions, when the projectile is at the distance of closest approach.

If we want to take into better consideration the distortion of the electron orbital by the projectile, the K-shell radius should be optimized along the nuclear trajectory. Andersen *et al.*[7] suggested that the ionization probability would then increase with respect to the case of optimization at the distance of closest approach. Contrary to this, Basbas, Brandt, and Ritchie[8] concluded that in the region of low collision velocities, the variation of the binding energy along the trajectory may decrease the ionization probability.

In this paper, we will proceed to optimize the K-shell radius as a function of the internuclear distance. This is equivalent to approximating the adiabatic molecular state of the electron in the field of the charges Z_1 and Z_2 by a $1s$ atomic orbital with optimum radius; this will be a very accurate representation of the molecular orbital due to the relation (1) between charges, and to the importance of small internuclear distances for the effectiveness of the excitation, relation (4).

Since the binding and distortion corrections depend on R but not on the particular trajectory considered, we will assume for simplicity a straight-line path, and use first-order time-dependent perturbation theory to obtain the transition amplitudes. Rihan, Müller, and Greiner[9] have shown that for the case of slow collisions between very heavy atoms, second-order terms may be of importance; we will see that accounting for a variable binding produces a change in the results of similar magnitude even for the case of light projectiles. Therefore, this effect should also be considered, along with second-order perturbation contributions, in those collisions between heavy atoms.

The plan of the paper is the following: In Sec. II A we present the formalism of first-order perturbation theory applied to a time-dependent basis; in Sec. II B, we reproduce the condition (3) for an appreciable transition probability, and find that it is directly related to the uncertainty relation between transition energy and time of interaction. In Sec. II C, we obtain the transition amplitude to continuum states represented by Coulomb waves in the field of the optimized charge parameter; the contributions produced by the time dependence of the atomic orbital representing the initial state will be shown to be of the same order as the contributions provided by the potential of the projectile. We will also estimate the transition amplitudes to s and p continuum states and obtain their dependence in impact parameter and collision velocity. In Sec. III, we present the probability of ionization to a continuum s state for hydrogen and carbon projectiles of various energies incident on copper, which shows that for sufficiently low collision energies, the use of a variable charge parameter produces a reduction of the transition probability compared with the results for a static charge. We also give an analytic estimate of the range of velocities where this reduction takes place.

II. THEORY

A. The Schrödinger equation

We will describe each K electron as an independent particle moving in the potential provided by a charge Z_2, modified to take into account the screening produced by the other K electron. The only effect of outer-shell electrons in this model will be to diminish the K-shell binding energy, as given in Eq. (3). The nuclei will be considered as classical particles following straight-line trajectories with constant speed. The Schrödinger equation for the system is

$$\left(H(r,t)-i\frac{\partial}{\partial t}\right)\psi(\vec{r},t)=0\,, \tag{6}$$

where

$$H(\vec{r},t)=-\tfrac{1}{2}\nabla_r^2-\frac{Z_2}{r}-\frac{Z_1}{|\vec{r}-\vec{R}(t)|}\,. \tag{7}$$

Assuming condition (2) to be valid, the natural basis to expand the wave function ψ is the set of molecular adiabatic states, since in the limit of $v_1\to 0$ they are exact solutions of the system. Transitions between states are produced by the time dependence of the basis set, and can be obtained to first order in v_1 (adiabatic approximation).

A different approach to the problem is to expand the wave function in a set of time-independent atomic orbitals that become a convenient basis when $Z_1 \ll Z_2$. Transitions are produced by the perturbing potential, equal to the difference between the total Hamiltonian (7) and the atomic

Hamiltonian. Through the usual formulation of time-dependent perturbation theory, we may then obtain the transition amplitudes to first order in the perturbation.[1,6,7] The adiabatic response of the electron to the projectile potential is neglected in this model, and the difference among the various treatments consists in the type of atomic orbitals used.

Our aim will be to improve the description of the process by using an atomic expansion that incorporates the main features of the molecular basis; in particular, this is accomplished for small R by introducing a time-dependent optimum charge to the atomic orbitals. We will use this time-dependent atomic basis set to obtain the transition amplitudes, which are due in part to the time dependence of the orbitals, and in part to the perturbing potential acting on them. We therefore separate the total Hamiltonian in a zeroth-order time-dependent part

$$H_0(\vec{r},t)=\tfrac{1}{2}\nabla_{\vec{r}}^2-\alpha(t)/r\,, \tag{8}$$

plus a perturbation

$$V(\vec{r},t)=\frac{\alpha(t)-Z_2}{r}-\frac{Z_1}{|\vec{r}-\vec{R}(t)|}\,. \tag{9}$$

The wave function $\psi(\vec{r},t)$ is expanded in the set of eigenstates of (8)

$$[H_0(\vec{r},t)-E_n(t)]\,\chi_n(\vec{r},t)=0\,, \tag{10}$$

where the χ_n are hydrogenic orbitals for a nuclear charge $\alpha(t)$. Replacing

$$\psi(\vec{r},t)=\sum_n a_n(t)\chi_n(\vec{r},t)\exp\left(-i\int^t E_n(t')dt'\right) \tag{11}$$

into (6) we get

$$i\frac{da_k}{dt}=\sum_n a_n\left\langle\chi_k\left|V-i\frac{\partial}{\partial t}\right|\chi_n\right\rangle \times\exp\left(i\int^t(E_k-E_n)dt'\right). \tag{12}$$

The perturbing potential V admits a multipole expansion

$$V(\vec{r},t)=\frac{\alpha(t)-Z_2}{r} -Z_1\sum_{l,m}\frac{4\pi r_<^l}{2l+1r_>^{l+1}}\,Y_{lm}^*(\hat{R})Y_{lm}(\hat{r})\,. \tag{13}$$

The use of a variable charge parameter in the atomic basis is present only in the monopole contribution to the excitation; Furthermore, the time derivative in (12) that generates transitions due to the nonadiabaticity of the process is also spherically symmetric, and can be rewritten as

$$(E_p-E_n)\left\langle\chi_p\left|\frac{\partial}{\partial t}\right|\chi_n\right\rangle=-\dot{\alpha}\left\langle\chi_p\left|\frac{1}{r}\right|\chi_n\right\rangle,\quad \dot{\alpha}=\frac{d\alpha}{dt}\,. \tag{14}$$

Transition amplitudes are then obtained to first order in the perturbations (13) and (14) by replacing in the right side of (12) $a_n=\delta_{n0}$, where "0" represents the initial $1s$ orbital

$$a_k(\rho,\infty)=-i\int_{-\infty}^{\infty}dt\,V_{k0}(\rho,t)e^{i\delta_{k0}(\rho,t)}\,, \tag{15}$$

where

$$\delta_{k0}(\rho,t)=\int^t dt'(E_k-E_0)\,, \tag{16}$$

$$V_{k0}(\rho,t)=\langle\chi_k|V-i\dot{\alpha}/r(E_k-E_0)|\chi_0\rangle\,, \tag{17}$$

ρ being the impact parameter of the collision.

B. Characteristic values of the collision parameters

We will obtain the conditions under which the transition amplitude $a_k(\rho,\infty)$ will be appreciable by analyzing the integral in (15). There will be a considerable contribution to the integral from a region of t values when the phase δ_{k0} is almost constant in that region (quasicrossing of adiabatic molecular potentials); this will not be our case, because the energy difference between initial and available final states is never small. The other possibility is to have a strong time dependence in the matrix element so that its Fourier expansion presents frequencies ω such that

$$\omega\sim\frac{d\delta_{k0}}{dt}=E_k-E_0\,; \tag{18}$$

there will then be a cancellation between the two phases in (15), and the integration will produce a substantial contribution to a_k (sudden switch of the perturbation). The largest frequencies ω appeaing in the Fourier expansion are the ones that interfere constructively to reproduce the time dependence of the coupling in the region $t\sim t_m$ of maximum time variation of $V_{k0}(t)$; the order of magnitude of those frequencies is

$$\omega\sim\frac{dV_{k0}(t_m)}{dt}\Big/V_{k0}(t_m)\,. \tag{19}$$

We can infer from the behavior of $\alpha(t)$ and from (13) and (14) that the coupling (17) cancels for $R=0$; for $R\gg a_{2k}$ it goes to zero at least as fast as R^{-1}, and in general, its maximum value occurs for R of the order of a_{2k}; we will then assume that for values of R small compared to a_{2k}, the coupling in (15) is a growing function of R that can be represented by an expansion in powers of R. Therefore, the order of magnitude of the second

member in (19) can be determined, and for a straight-line nuclear trajectory we obtain

$$\omega \sim \frac{dR}{dt} \Big/ R \sim v(R^2-\rho^2)^{1/2}/R^2 . \tag{20}$$

The impact parameters of the trajectories that produce an appreciable contribution to the excitation will then be of the order

$$\rho \sim v/\omega \sim v/(E_0 - E_k) . \tag{21}$$

We have then regained the condition proposed by Bang and Hansteen for K-shell excitation, founded now on the uncertainty relation between interaction time and electron energy: The time rate of growth of the perturbation is related to the electron energy level width, which in turn should be of the order of the energy gap between initial and final states in order to have an appreciable transition amplitude.

C. The transition amplitudes

The population of the states of the base χ after the collision is determined by the transition amplitudes (15); they will also represent the probability of ionization of K-shell electrons by a charged projectile if the states χ tend, at large times after the collision, to the correct final continuum one-electron states. More precisely, what is needed for χ is to accurately represent the continuum states of the electron in the region where these orbitals overlap with the initial state, and this is satisfied by the base χ. By using final continuum states on the field of the charge $\alpha(t)$, we are introducing in the outgoing channels the same distortive potential as for the initial channel.

We will describe the continuum hydrogenic states in the field of the charge $\alpha(t)$ as partial waves of the Coulomb wave function

$$\chi_{klm}(\vec{r}, t) = (-i)^l (4\pi/kr) F_l(n, kr) Y_{lm}(\hat{k}) Y_{lm}^*(\hat{r}) , \tag{22}$$

where

$$F_l(n, kr) = N_{kl} e^{-ikr} (2kr)^{l+1} {}_1F_1(l+in, 2l+2, 2ikr)$$

$$= N_{kl} e^{-ikr} \sum_{s=l+1}^{\infty} A^l_{s-l-1}(n) i^{s-l-1} (2kr)^s , \tag{23}$$

$$N_{kl} = e^{n\pi/2} \Gamma(l+1-in)/2(2l+1)! , \quad n = \alpha(t)/k , \tag{24}$$

and the A^l_p are the coefficients of the power expansion of the confluent hypergeometric function ${}_1F_1$, while Y_{lm} and Γ are the usual spherical harmonic and gamma function, respectively.[10]

Let us now investigate which kind of final states are most easily populated during the collision; transitions to continuum s states are produced by the following coupling in (15):

$$M_{k00}(\rho, t) = \langle \chi_{k00} \big| [\alpha(t) - Z_2 - i\dot{\alpha}/(E_k - E_0)]/r - Z_1\Theta(r-R)/r - Z_1\Theta(R-r)/R \big| \chi_0 \rangle , \tag{25}$$

where Θ is the step function. The optimized value of the charge $\alpha(t)$ is obtained by minimizing the binding energy of a $1s$-hydrogenic orbital in the potential provided by the nuclei Z_1 and Z_2 and outer-shell electrons:

$$E_0(t) = \alpha^2(t)/2 - Z_2\alpha(t) - Z_1\{1 - [1+\alpha(t)R]e^{-2\alpha(t)R}\} + \tfrac{1}{2}(1-\Theta_K)(Z_1+Z_2)^2 , \tag{26}$$

where the first two terms are the kinetic and potential energies in the field of the target, the third term is the binding correction due to the projectile, and the last term is the screening provided by the outer electrons, evaluated at the united atom limit since we are interested in values of R much smaller than the K-shell radius. Andersen *et al.*[7] used a charge parameter computed from (26), but taking R equal to the distance of closest approach. Minimizing (26) with respect to $\alpha(t)$, we obtain

$$\alpha(t)(1 - 2Z_1 e^{-2\alpha(t)R}) - Z_2 - Z_1 e^{-2\alpha(t)R} = 0 . \tag{27}$$

It can be inferred from (27) that the optimized charge can be expressed as a power expansion in R:

$$\alpha(t) = Z_1 + Z_2 - 4Z_1(Z_1+Z_2)^2 R^2 + O(R^3) , \tag{28}$$

which, replaced in (25), produces a power-series expansion of this coupling

$$M_{k00}(\rho, t) = A_2(\alpha R)^2 + A_3(\alpha R)^3 + O((\alpha R)^4) ; \tag{29}$$

for $k \ll \alpha$, which comprises the bulk of the ionization process, the coefficients A_i are independent of α.

If we replace the variable parameter $\alpha(t)$ by its united atom limit the matrix element (25) reads

$$\langle \chi_{k00} \big| Z_1\Theta(R-r)(1/r - 1/R) \big| \chi_0 \rangle ; \tag{30}$$

since the additional terms that appear in (25) are of the same order as (30), we conclude that the use of a time-dependent atomic basis will introduce appreciable corrections to existing calculations.

D. Monopole and dipole transition amplitudes

The probability amplitude for transitions to continuum s states is obtained by substituting (29) in (15) and performing the integration along the nuclear trajectory. Since we are interested in low-energy collisions where only impact parameters much smaller than the K-shell radius are im-

portant, we will only consider, to get an order of magnitude of the transition amplitude, the case $\rho \to 0$ which facilitates the time-integration; furthermore, and since the relative change of the binding energy $E_0(t)$ along the trajectory is of the order of Z_1/Z_2, we can approximate δ_{k0} by a linear function of time valid at least for $Z_1 \ll Z_2$. With these assumptions (15) results

$$a_{k00}(\rho \sim 0) = -i\int_{-\infty}^{\infty} \frac{dx}{v}\,[A_2(\alpha|x|)^2 + A_3(\alpha|x|)^3]\,e^{-i\beta x}, \qquad (31)$$

where $\beta \sim \alpha^2/v$, $x = vt$.

The integral (31) can be solved term by term if a convergence factor $e^{-\gamma|x|}$ is used; we should notice that an expansion such as (29) can also be written as the product of $e^{-\alpha|x|}$ times a series similar to (29), we are then free to add a convergence factor of the type indicated, with $\gamma \lesssim \alpha$, and still keep the form (29) for the expansion of M_{k00}. We perform the integration of the nth term of this expansion: Writing $n = 2p + q$, where $q = 0(1)$ indicates that n is even(odd), the order of magnitude of the integral is[10]

$$-i\int_{-\infty}^{\infty} \frac{dx}{v}\,A_n(\alpha|x|)^n \cos\beta x\, e^{-\gamma|x|} = \frac{iA_n}{v}\frac{n!}{(\beta^2+\gamma^2)^{(n+1)/2}}\cos[(n+1)\arctan\beta/\gamma] \sim A_n\alpha^{-2}(v/\alpha)^{2p+1}(\gamma/\alpha)^{1-q}. \qquad (32)$$

From (32) we conclude that since $\gamma \lesssim \alpha$, the order of magnitude of (31) is independent of γ:

$$a_{k00}(\rho \sim 0) \sim A_3\alpha^{-2}(v/\alpha)^3. \qquad (33)$$

We will now consider transitions to continuum p states. They are described by the following matrix element [see Eq. (13)]:

$$M_{k1m}(\rho, t) = -\tfrac{4}{3}\pi Z_1 Y_{1m}(\hat{R})\langle \chi_{k1m}|\,(r\Theta(R-r)/R^2 + R\Theta(r-R)/r^2)Y_{1m}(\hat{r})\,|\chi_0\rangle \qquad (34)$$

using the expansion (23) for χ_{k1m} the result can be expressed in terms of a power series in αR

$$M_{k1m}(\rho, t) = Y_{1m}(\hat{R})[B_1(\alpha R) + B_3(\alpha R)^3 + B_4(\alpha R)^4 + O((\alpha R)^5)], \qquad (35)$$

where the coefficients B_i are also independent of α for the important case of $k \ll \alpha$. The calculation of the transition amplitude (15) in the limit $\rho \to 0$ involves integrations similar to (31): Owing to the absence of a quadratic term we can not extract from M_{k1m} a factor $e^{-\alpha R}$ and still keep an expansion with the same form of (35). Therefore, the convergence factor used in (32) for the integration of the linear term of (35) should satisfy $\gamma \ll \alpha$. The case $m = 1$ gives the same result (33), but with a factor $\alpha\rho$ produced by the spherical harmonic $Y_{11}(\hat{R}) \sim \rho/R$ in (35):

$$a_{k11}(\rho \sim 0) \sim B_3\,\alpha\rho\alpha^{-2}(v/\alpha)^3. \qquad (36)$$

The case with $m = 0$ presents an asymmetric factor x in the integrand coming from $Y_{10}(\hat{R}) \sim x/R$, then the contribution to the integral (15) comes from the sine function of the phase $e^{i\delta_{k0}}$,

$$-i\int_{-\infty}^{\infty} \frac{dx}{v}\,B_n(\alpha|x|)^n \sin\beta x\, e^{-\gamma|x|} = -i\frac{B_n}{v}\frac{n!}{(\beta^2+\gamma^2)^{(n+1)/2}}\sin[(n+1)\arctan\beta/\gamma] \sim B_n\alpha^{-2}(v/\alpha)^{n+q}(\gamma/\alpha)^q; \qquad (37)$$

since for the linear term γ should be negligible, we obtain from (35) and (37) that

$$a_{k10}(\rho \sim 0) \sim B_4\alpha^{-2}(v/\alpha)^4, \qquad (38)$$

and this result is also independent of the convergence factor used.

Equations (33), (36), and (38) provide us with estimates for the transitions to s and p continuum states: We see that the dipole contributions (36) and (38) are a factor $v/\alpha \sim \alpha\rho$ smaller than the monopole transition (33) in the region $\rho \ll 1/\alpha$, $k \ll \alpha$. This result has its origin in the fact that a slow projectile must come close to the target nucleus in order to produce a noticeable perturbation of the $1s$ orbital, but then such a perturbation will appear as a population of electron orbitals that have an appreciable electron density around the target, which as we see from (22) and (23), corresponds to s states. We also see from (32) and (37) that there is an additional condition necessary to have an appreciable transition amplitude, namely, that the R dependence of the coupling has to produce a constructive interference of the elementary contributions to the amplitude summed along the nuclear trajectory. From this respect we see that if we use the nuclear charge Z_2 in place of the parameter $\alpha(t)$ in Eqs. (8)–(13), the coupling will present a term in $(\alpha R)^0$, which does not produce a contribution to an $a_{k00}(\rho)$ because its integration along the trajectory cancels, as shown by (32), with $\gamma \to 0$. This tells us that the inclusion of the binding effect (replacing Z_2 by a constant parameter $\alpha \cong Z_1 + Z_2$) will modify the transition amplitude, but it will conserve its order of magnitude, given in both cases by (33). Incidentally, the result (33) can be derived from the treatment of Bang and Hansteen[1] for the case of $\rho \to 0$, $k \ll \alpha$ applied to their expression (3.12) of the differential cross section for a straight-line path.

III. RESULTS

We obtain the transition amplitude $a_{k00}(\rho)$ [Eq. (15)] for excitation to a continuum s state; this is the main channel for the ionization of a K-shell electron at low collision velocities, as was shown in Sec. II D. We will compare the results obtained for $a_{k00}(\rho)$ by performing numerically the quadrature of (15), and considering both the cases of an optimized charge $\alpha(t)$ along the straight-line trajectory, and a constant $\alpha(0)$ equal to the optimum value at the point of closest approach, thus reproducing the calculations of Andersen *et al.*[7] By comparing the results obtained in the two cases, we test the accuracy of taking a constant binding correction along the trajectory.

In Fig. 1, we show the ionization probabilities

$$I_p = \frac{2}{(2\pi)^3}\int d^3k\ |a_{k00}(\rho)|^2 \tag{39}$$

for hydrogen and carbon projectiles of various energies incident on copper targets. It can be immediately seen that both collision systems present a region of energies where the ionization probability calculated with a variable $\alpha(t)$ is appreciably smaller than for the case of a constant $\alpha(0)$; this seems to confirm the conclusions of Basbas *et al.*[8] on the influence of a variable charge on the results at low velocities. An analysis of the numerical computations indicates that the difference between the two calculations comes from the binding energies corresponding to each approach, $E_0(\alpha(t))$ and $E_0(\alpha(0))$, while the presence of a variable charge in the shape of the wave functions produces a negligible difference over the use of the static optimum charge.

By making some simplifications in the calculations, we will be able to obtain an analytic result for the transition amplitude $a_{k00}(\rho)$, and then to obtain the range of collision velocities for which the use of a variable binding decreases the ionization probability: The matrix element (25) that couples the $1s$ orbital to a continuum s state can be solved exactly

$$M_{k00}(\rho,t) = -i8\pi N_0 N_{k0}\frac{(\alpha-ik)^{in-1}}{(\alpha+ik)^{in+1}}\left(1-\frac{i\dot{\alpha}}{E_k-E_0}\right) + Z_1 e^{-(\alpha-ik)R}S_k(R,\alpha), \tag{40}$$

where

$$S_k(R,\alpha) = \sum_{m=1}^{\infty} A^*_{m-1}(n)(-2ik)^{m-1} \times\left(\sum_{s=0}^{m+1}\frac{(m+1)!}{s!}\frac{R^{s-1}}{(\alpha-ik)^{m+2-s}} - \sum_{s=0}^{m}\frac{m!}{s!}\frac{R^s}{(\alpha-ik)^{m+1-s}}\right). \tag{41}$$

To show the R dependence in a simpler way it is convenient to make some rearrangements on the summations (41)

$$S_k(R,\alpha) = \sum_{s=2}^{\infty}\frac{[R(\alpha-ik)]^s}{s!}\sum_{m=1}^{s+1}A^*_{m-1}(n)(-2ik)^{m-1}\frac{m!}{(\alpha-ik)^{m+1}} - R^{-1}\sum_{s=3}^{\infty}\frac{[R(\alpha-ik)]^s}{s!}\sum_{m=1}^{s-2}A^*_{m-1}(n)(-2ik)^{m-1}\frac{(m+1)!}{(\alpha-ik)^{m+2}} - [1+2ik/(\alpha-ik)]^{-1-in}/(\alpha-ik)^2. \tag{42}$$

From (40) and (42) we see clearly that the coupling obeys the expansion (29) at small R.

To estimate the influence of a variable binding on the transition amplitude, we will simplify the integral in (15) by approximating the binding energy $-\frac{1}{2}\alpha^2(t)$ with the first two terms of its expansion at the point of closest approach

$$a_{k00}(\rho) = -i\int_{-\infty}^{\infty} dt\, M_{k00}(\rho,t)e^{-i\delta_{k0}(\rho,t)}, \tag{43}$$

where, using (16) and (28)

$$\delta_{k0}(\rho,t) \equiv \epsilon_{k0}\frac{x}{v} + \beta\frac{x^3}{v}, \tag{44}$$

where $\epsilon_{k0} = E_0(\alpha(0)) - E_k$ and $\beta = -\frac{4}{3}Z_1(Z_1+Z_2)^3$. Since we know that transitions are produced for values of $R \sim v\alpha^{-2}$ [Eqs. (18) and (20)], the last term of (44) is of the order of $(Z_1/\alpha)(v/\alpha)^2 \ll 1$, we can then approximate

$$e^{i\delta_{k0}(\rho,t)} = e^{i\epsilon_{k0}x/v}\left[1+i\beta\frac{x^3}{v}+\left(\frac{\beta^2x^6}{v^2}\right)\right]. \tag{45}$$

From (32), (37) and (40) we see that the largest order contribution to (43) comes from the R^2 term of $S_k(R,\alpha)$ in (42). Thus, the estimation of the transition atmplitude $a_{k00}(\rho)$ with the correction introduced by the variable binding is, in the limit of $\rho \to 0$:

$$a_{k00}(\rho) \cong -Z_1 8\pi N_0 N_{k0} \times\int_{-\infty}^{\infty}\frac{dx}{v}e^{-(\alpha-ik)R}\frac{R^2}{6}e^{i\epsilon_{k0}x/v}\left(1+i\beta\frac{x^3}{v}\right). \tag{46}$$

Replacing in (46) the complete results for the integrals (32) and (37) we obtain the range of velocities for which the use of a variable binding produces a reduction of the ionization probability:

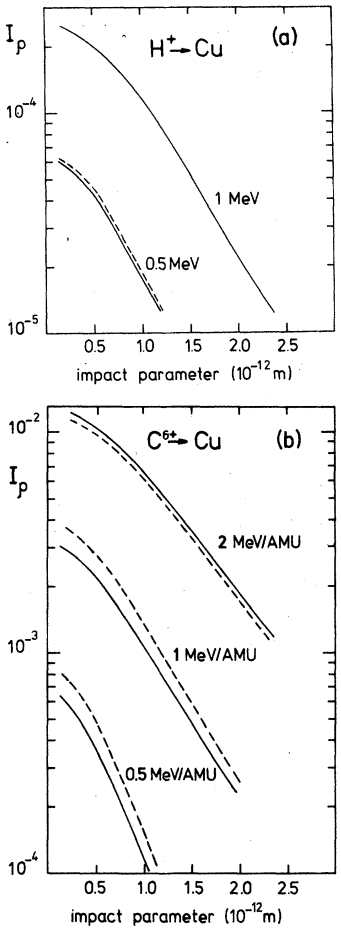

FIG. 1. K-shell ionization probability I_p vs impact parameter for H^+ and C^{6+} ions bombarding Cu targets. Solid curves are obtained when the charge parameter of the electron wave function is optimized along the projectile trajectory; for the dashed curves this parameter is fixed to its value at the distance of closest approach. Both curves coincide for 1-MeV H^+ projectiles.

$$0 < v/\alpha < 1/2\sqrt{3} \ . \tag{47}$$

This shows that for $v/\alpha \ll 1$, where our results are valid, there is a reduction in the ionization probability (39) due to the presence of a variable binding. Performing an accurate numerical calculation of the right side of (43), as shown in Fig. 1, produces a reduction of probability for a somewhat smaller range of velocities than in (46).

IV. CONCLUSIONS

We have studied the excitation probability of a K-shell electron interacting with a slow light ion that follows a straight-line trajectory. Our interest was to determine the corrections on the results introduced by the use of time-dependent electron orbitals, able to adiabatically adjust to the potential of the projectile. For low velocity collisions, transitions are produced while the projectile is well inside the K shell. It can then be assumed that we only need an accurate description of electron orbitals near the target nucleus. There a description of K-shell electrons as independent particles is justified. Furthermore, the one-electron two-center molecular orbitals which are the natural basis needed to include the electron adiabatic response into the formalism, were replaced by atomic orbitals with a variational charge parameter; we gained in simplicity without losing in rigor, since both basis sets are almost identical when the internuclear distance is much smaller than the K-shell radius. The transition amplitude was calculated considering both the perturbation on the initial state produced by the potential of the projectile and the time dependence of the unperturbed basis.

The order of magnitude of the impact parameters that give appreciable transition amplitudes was obtained from the time-energy uncertainty relation (the perturbation has to change fast enough to produce an energy uncertainty for the electron to reach the available final states). The result obtained (21) confirms the assumed relation between impact parameters and collision velocities, that was suggested by the outcome of previous calculations.[1,11]

The transition amplitudes to continuum s and p states were also estimated analytically in terms of impact parameters and collision velocities; dipole transition amplitudes were found to be much smaller than the dominant monopole contribution to ionization at low velocities.

The transition amplitude to continuum s states was calculated assuming an optimized charge parameter along the trajectory, and the time dependence of the initial state orbital produces an appreciable contribution to the process. The matrix element of the transition was solved analytically, while the integration along the trajectory was performed numerically. The use of a time-varying charge parameter diminishes the resulting ionization probability for sufficiently low collision velocities; the effect is more marked for heavier projectiles, and the range of velocities where it lowers the ionization probability was estimated. The results obtained confirm the prediction of Basbas *et al.*,[8] who made a qualitative estimation of the influence of a time-dependent binding on the probability of ionization; they also are consistent with measurements of nickel K-shell ionization cross sections by carbon projectiles[12-14] that fall below the theoretical curve for a static binding correction at low collision velocities.

Our results also show that at higher collision velocities the ionization probability will be increased by the presence of a variable binding; in general, the sign of the correction introduced by a variable binding will depend on the detailed interferences among the elementary contributions to the amplitude along the trajectory, and these depend on the collision velocity.

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