Distortion effects for electron excitation in ion-atom collisions

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Electron excitation from monoelectronic targets by impact of bare ions from low intermediate to high collision energies is theoretically studied by using the symmetric eikonal approximation. In addition, multichannel semiclassical impact-parameter calculations are also carried out. Distortion effects introduced by the projectile charge are shown to appear in the theoretical models at low intermediate collision energies.

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I. INTRODUCTION

The present work deals with the study of single electron excitation by impact of bare projectiles on atomic targets from low intermediate ($v \lesssim v_e$, with v the collision velocity and v_e the electron orbital velocity in the entry channel) to high impact energies ($v > v_e$). These reactions are of main importance in different applied fields, for example in the design of fusion reactors and in the irradiation of biological matter by impact of heavy nuclei.

Thus it is of fundamental interest that a study of these collision processes be carried out with a view to thoroughly understand different intermediate mechanisms. The existence of binding effects, in electron excitation to the continuum of the target at low intermediate impact energies, has been a matter of extensive study by using perturbed stationary states (PSS) and distorted-wave models [1–5]. Binding has been determined to give subtractive Z_P^3 contributions to the total cross sections for asymmetric $Z_P \ll Z_T$ collisions (with Z_P and Z_T the projectile and nuclear charges, respectively.) First Born transition amplitudes present a Z_P dependence, thus resulting in a Z_P^2 dependence of impact-parameter probabilities and total cross sections. So, the Z_P^3 behavior has been interpreted as coming from interferences between first and second orders of the Born approximation [5]. A rough physical picture of the studied mechanism was that at low enough energies, small impact-parameter collisions play the main role in the reaction, producing an effective increase of the electron binding energy and thus decreasing the ionization total cross section [1,2]. Binding effects in electron ionization have also been studied for both asymmetric cases $|Z_P| < Z_T$ and $Z_P > Z_T$ by using the perturbative two-center continuum-distorted-wave–eikonal-initial-state approximation [6–8] (CDW-EIS). Good agreement with existing experimental data was achieved [9]. This good agreement is due to the inclusion of an eikonal phase (associated with the projectile-electron interaction in the entry channel) distorting the initial stationary bound wave function. It is possible to show that the absence of this phase produces severe overestimations of experimental total cross sections at low intermediate impact energies [10]. For the case $Z_P > Z_T$, it has been recently shown [11] that ionization is mostly produced at large enough internuclear distances and that the distortion introduced by the eikonal phase plays a main role in the determination of these distances. So, in this case, we can invoke a *distortion* effect produced by the projectile-charge. Binding has been shown to be represented by the two-center CDW-EIS distorted-wave approximation [6–8]. It must be also noted that within the CDW-EIS model an explicit theoretical Z_P dependence of the total cross sections cannot be obtained.

In electron ionization, tremendous difficulties arise when impact-parameter transition probabilities are calculated for the case in which two-center effects must be taken into account. So, only a qualitative estimation of the relative importance of the contributions coming from different impact parameters has been given. The aim of this work is to study the possible existence of distortion effects due to the projectile charge in reactions of electron excitation to bound states of the target. In this case, the transition probabilities $P(\mathbf{b})$ as a function of the impact parameter $\mathbf{b}$ can be easily calculated.

We use the distorted-wave symmetric eikonal approximation [12] (SE), which has been applied with some success to describe differential and total experimental cross sections for electron excitation [12,13]. In this model, the presence of the projectile in the entry and exit channels is described by distorting the initial and final bound-state wave functions with eikonal phases (associated with the projectile-electron interaction). In order to avoid additional effects due to the presence of passive electrons in multielectron systems, we treat the impact of bare ions on monoelectronic targets.

In Sec. II, a brief description of the theoretical model is given. In Sec. III, impact-parameter probabilities and total cross sections obtained by using the SE approximation are compared with other theoretical results and experimental data. In particular, coupled-channel semiclassical impact-parameter calculations are also carried out in this work. It allows us to study the adequacy of the SE model to represent electron excitation for different systems. Distortion effects are studied in Sec. IV for both cases $Z_P < Z_T$ and $Z_P > Z_T$. Our conclusions are then summarized in the last section. Atomic units will be used except where otherwise stated.

II. THEORY

Let us consider that a bare projectile impinges on a monoelectronic target promoting the electron from the initial stationary ground state φ_i to a final stationary excited bound state φ_f of the target. We are then concerned with the reaction

$$P^{Z_P+} + T(1s)^{(Z_T-1)+} \to P^{Z_P+} + T(nlm)^{(Z_T-1)+} . \tag{1}$$

Let $\mathbf{R}$ be the position vector of the projectile P relative to the nucleus T, and let $\mathbf{r}_T$ and $\mathbf{r}_P$ be the electron position vectors relative to T and P, respectively. The nuclei are assumed to follow rectilinear trajectories such that $\mathbf{R}=\mathbf{b}+\mathbf{v}t$ describes the time-dependent motion of the nuclei for a given impact parameter.

If we describe the reaction from a frame fixed to the target nucleus the dynamics of the electron is given by solving the time-dependent Schrödinger equation

$$\left[H - i\frac{\partial}{\partial t}\right]\Psi_j^{\pm}(\mathbf{r}_T,t)=0 , \quad j=i,f , \tag{2}$$

where the time-dependent Hamiltonian H is given by

$$H=-\frac{1}{2}\nabla^2_{\mathbf{r}_T}-\frac{Z_T}{r_T}-\frac{Z_P}{r_P}+\frac{Z_P Z_T}{R} \tag{3}$$

and $\Psi_j^{\pm}$ $(j=i,f)$ are the initial and final exact wave functions, which must satisfy the correct boundary conditions [12–14]

$$\lim_{t\to-\infty}\Psi_i^+=\chi_i^+=\Phi_i\exp\left[-i\frac{Z_P}{v}\ln(vr_P+\mathbf{v}\cdot\mathbf{r}_P)+i\frac{Z_PZ_T}{v}\ln(vR-\mathbf{v}\cdot\mathbf{R})\right] , \tag{4}$$

$$\lim_{t\to+\infty}\Psi_f^-=\chi_f^-=\Phi_f\exp\left[i\frac{Z_P}{v}\ln(vr_P-\mathbf{v}\cdot\mathbf{r}_P)-i\frac{Z_PZ_T}{v}\ln(vR+\mathbf{v}\cdot\mathbf{R})\right] . \tag{5}$$

In Eqs. (4) and (5), $\Phi_i=\varphi_i(\mathbf{r}_T)\exp(-i\varepsilon_i t)$ and $\Phi_f=\varphi_f(\mathbf{r}_T)\exp(-i\varepsilon_f t)$, with ε_i and ε_f the initial and final electron orbital energies, respectively. In correspondence with the limits (4) and (5) we can define the post and prior versions of the transition amplitude,

$$\mathcal{A}^+_{\mathrm{if}}(\mathbf{b})=-i\int_{-\infty}^{+\infty}dt\left\langle\chi_f^-(t)\left|\left[H(t)-i\frac{\partial}{\partial t}\right]^{\dagger}\right|\Psi_i^+(t)\right\rangle , \tag{6}$$

$$\mathcal{A}^-_{\mathrm{if}}(\mathbf{b})=-i\int_{-\infty}^{+\infty}dt\left\langle\Psi_f^-(t)\left|\left[H(t)-i\frac{\partial}{\partial t}\right]\right|\chi_i^+(t)\right\rangle , \tag{7}$$

providing that χ_i^+ and χ_f^- do not produce transitions at $t\to+\infty$ and $t\to-\infty$, respectively; it means $\lim_{t\to+\infty}\langle\Psi_f^-|\chi_i^+\rangle=0$ and $\lim_{t\to-\infty}\langle\chi_f^-|\Psi_i^+\rangle=0$ in Eqs. (7) and (6), respectively.

We can always write

$$|\Psi_i^+(t)\rangle=|\chi_i^+(t)\rangle-i\int_{-\infty}^{t}dt'\mathcal{U}(t,t')\times\left[H(t')-i\frac{\partial}{\partial t'}\right]|\chi_i^+(t')\rangle , \tag{8}$$

$$\langle\Psi_f^-(t)|=\langle\chi_f^-(t)|-i\int_{t}^{+\infty}dt'\langle\chi_f^-(t')|\times\left[H(t')-i\frac{\partial}{\partial t'}\right]^{\dagger}\mathcal{U}(t',t) , \tag{9}$$

where $\mathcal{U}(t,t')$ is the evolution operator associated with the Hamiltonian $H(t)$.

If only the first terms of Eqs. (8) and (9) are retained for the calculation of expressions (6) and (7), respectively, first-order approximations of the *symmetric eikonal* model are obtained. It is easy to prove that both versions (post and prior) give the same result for this first-order approximation of the transition amplitude. The prior version is adopted in our calculation.

III. IMPACT-PARAMETER PROBABILITIES AND TOTAL CROSS SECTIONS

Impact-parameter probabilities and total cross sections are obtained by

$$P_{if}(\mathbf{b})=|\mathcal{A}^-_{if}(\mathbf{b})|^2 \tag{10}$$

and

$$\sigma_{if}=\int d\boldsymbol{\eta}|R^-_{if}(\boldsymbol{\eta})|^2 , \tag{11}$$

with $\boldsymbol{\eta}$ the transverse momentum transfer and where the matrix element $R^-_{if}(\boldsymbol{\eta})$ is the Fourier transform of the transition amplitude

$$R^-_{if}(\boldsymbol{\eta})=(2\pi)^{-1}\int d\mathbf{b}\,e^{-\mathbf{b}\cdot\boldsymbol{\eta}}\mathcal{A}^-_{if}(\mathbf{b}) . \tag{12}$$

We mention the well-known fact that the internuclear interaction does not affect the calculation of $P_{if}(\mathbf{b})$ and σ_{if} when the straight-line version of the impact-parameter approximation is used.

In Figs. 1(a) and 1(b), SE cross sections are presented for the reactions

$$H^+ + H(1s) \longrightarrow H^+ + H(2s) \quad (13)$$

and

$$H^+ + H(1s) \longrightarrow H^+ + H(2p) \; . \quad (14)$$

Our SE results are compared with the existing experimental data from Morgan, Geddes, and Gilbody [15] and Schartner, Detleffsen, and Sommer [16] and with other theoretical predictions. The agreement between SE and experiments is very good for the $2p$ case for all energies considered.

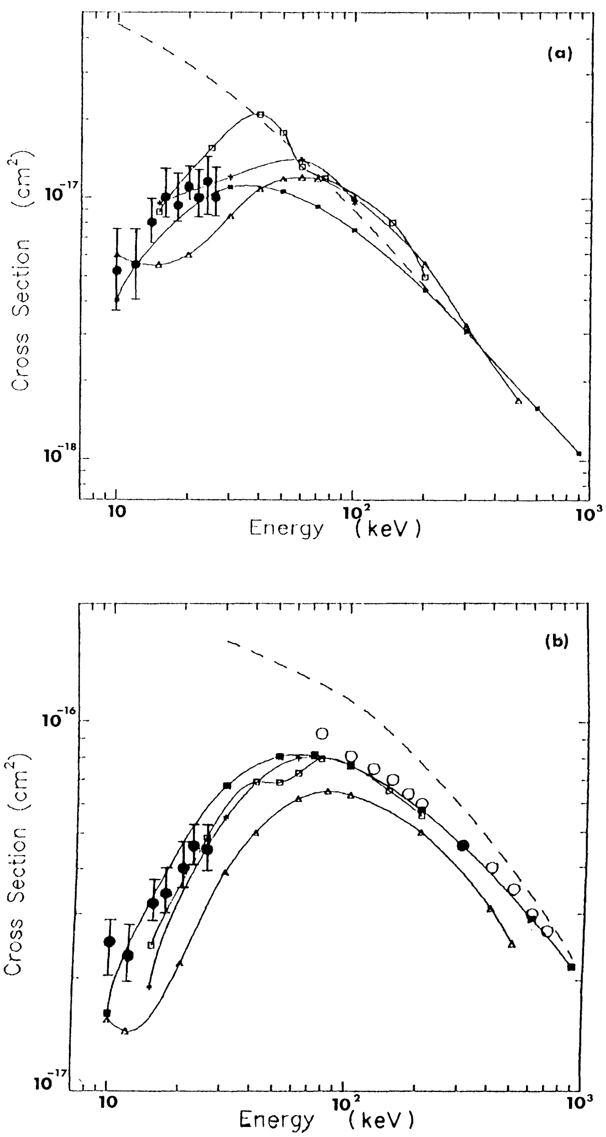

FIG. 1. (a) and (b) Cross sections for excitation of H(1s) by protons to the $2s$ and $2p$ final states, respectively. Theoretical results: ■, present SE; ★, PSS from Reading, Ford, and Becker [18]; □, PSS from Shakeshaft [17]; △, 2OPT from Lüdde and Dreizler [19]; — — —, B1, present work. Experimental data: ●, Morgan, Geddes, and Gilbody [15]; ○, Schartner, Detleffsen, and Sommer [16].

Agreement is also achieved with perturbative stationary states calculations from Shakeshaft [17] and Reading, Ford, and Becker [18]. On the contrary, calculations with a two-center optical-potential model [19] (2OPT) underestimate the measured data. For the $2s$ case only a few experimental points exist in the low-energy region. More important discrepancies between the results obtained with different theoretical models (our SE calculations, the PSS from Refs. [17] and [18] and the 2OPT from Ref. [19]) are observed. Even when SE slightly underestimates the experimental data, it follows the general trend of measured points. For the two analyzed cases the first-order Born approximation (B1) gives a pronounced overestimation of the reactions when the collision energy decreases. SE calculations for excitation to the $n=2$ shell, by proton impact on H(1s) targets, have been previously presented [12,13].

In Figs. 2(a) and 2(b), cross sections are shown for the asymmetric collision processes

$$H^+ + Li^{2+}(1s) \longrightarrow H^+ + Li^{2+}(2s) \quad (15)$$

and

$$H^+ + Li^{2+}(1s) \longrightarrow H^+ + Li^{2+}(2p) \; . \quad (16)$$

No experimental data are available for these reactions. Present SE calculations are compared with theoretical PSS [20] and one-center optical-potential [21] (1OPT) results. In both physical cases, the 1OPT predictions underestimate the PSS ones. SE cross sections agree with the PSS results for the $2p$ case and with the 1OPT ones for the $2s$ case.

Impact-parameter-weighted probabilities $bP_{if}(\mathbf{b})$ are introduced in Figs. 3(a) and 3(b) for the reactions (13) and (14) at 100-keV and 40-keV impact energies, respectively. For the 100-keV case, SE results are in close agreement with the ones obtained by using the 1OPT approximation. In order to test the SE model at lower collision energies we have also carried out multichannel semiclassical impact-parameter calculations (see, for example, Shingal [22]) for 40-keV proton impact on ground-state hydrogen atoms. The total wave function of the system was expanded in terms of a total of 44 atomic states on the target and the projectile nucleus (for details of the hydrogen-atom basis set see Shingal, Bransden, and Flower [23]).

It must be also noted that this PSS model explicitly includes charge-exchange channels, excluded in the SE approximation. However, good agreement is found between the PSS and the SE calculations.

In Fig. 3(c) impact-parameter-weighted probabilities are presented for the collision systems

$$He^{2+} + H(1s) \longrightarrow He^{2+} + H(2s) \; , \quad (17)$$

$$He^{2+} + H(1s) \longrightarrow He^{2+} + H(2p) \; , \quad (18)$$

at a 40-keV impact energy. As in the previous case presented in Fig. 3(b), PSS calculations have also been developed for this work (Fritsch, Shingal, and Lin [24]).

A good agreement is obtained for excitation to the $2p$ state. However, this is not true for $2s$ excitation. It must be also noted that the $2p$ reaction, in general, dominates the process of excitation to the $n=2$ shell, which we will deal with in Sec. IV.

From the figures, it can be observed that the cross sections are dominated by impact parameters of the order or larger than the mean initial orbital radius r_K. We call them *intermediate* or *large* impact parameters, respectively. For a fixed collision energy, the dominant impact parameters become larger as the projectile nuclear charge Z_P increases [see Figs. 3(b) and 3(c)]. A similar behavior has been recently obtained [25] for Z_P increasing up to $Z_P=30$, using the SE approximation and a numerical evaluation of the Schrödinger equation (2). So, the studied excitation reactions are not dominated by small impact parameters ($b \ll r_K$).

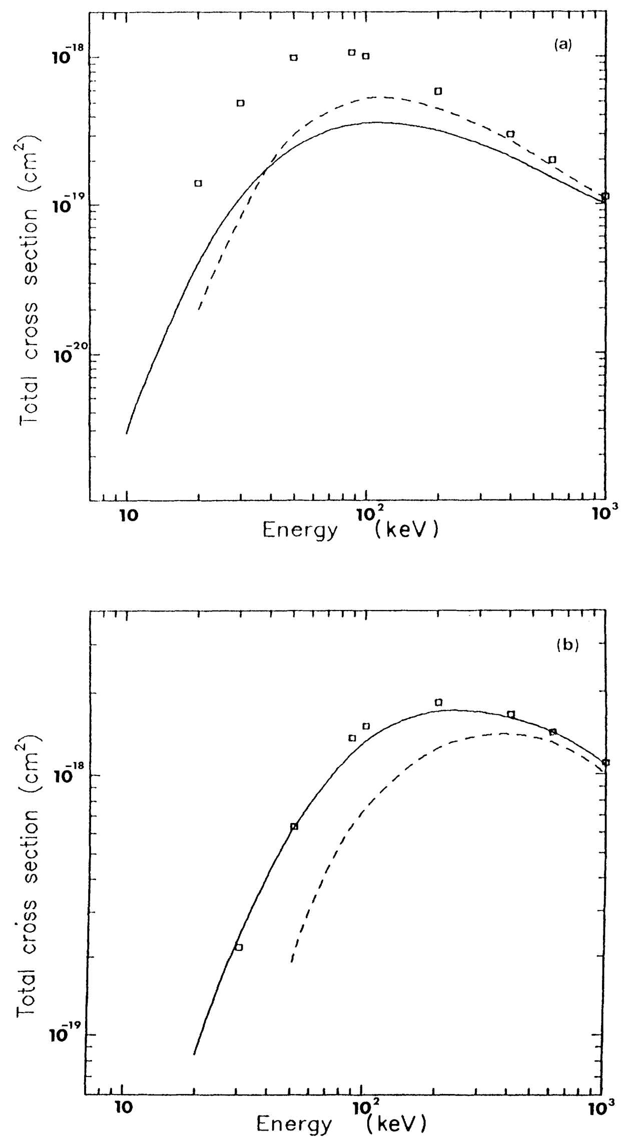

FIG. 2. (a) and (b): Cross sections for excitation of $Li^{2+}(1s)$ by protons to the $2s$ and $2p$ final states, respectively. Theoretical results: ——, present SE; — — —, 1OPT from Ast, Lüdde, and Dreizler [21]; □, 59 atomic orbitals PSS from Ermolaev and McDowell [20].

IV. DISTORTION EFFECTS

In the present section we analyze the possible existence of distortion effects in electron excitation to the $n=2$

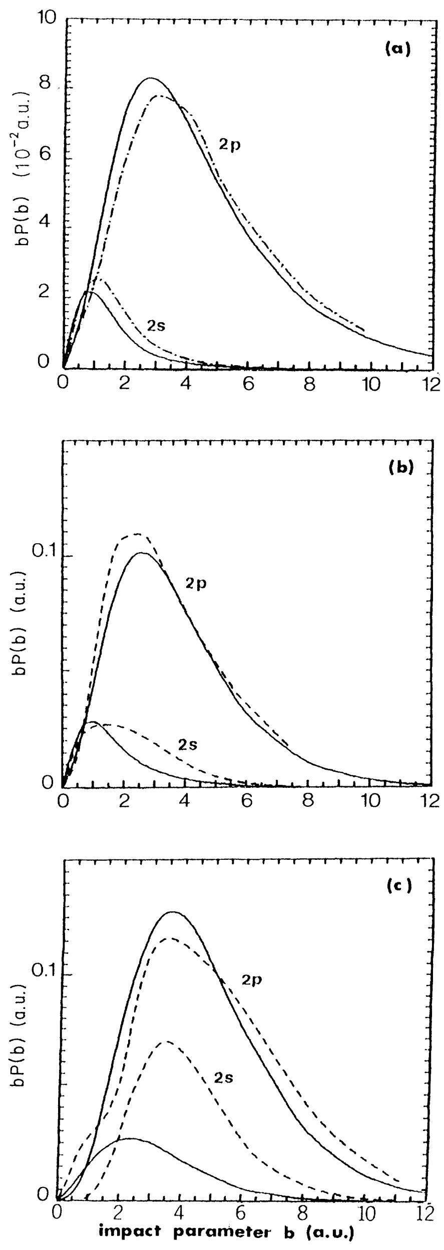

FIG. 3. Impact-parameter-weighted probabilities vs impact parameter. (a) Excitation of $H(1s)$ to the $2s$ and $2p$ states by 100-keV protons. Theoretical results: ——, present SE; —·—·—·, 1OPT from Ast, Lüdde, and Dreizler [21]. (b) Same as in (a) but for 40-keV protons. Calculations: ——, present SE; — — —, present PSS. (c) Same as in (a) but for 40-keV/amu α particles. Calculations: ——, present SE; — — —, present PSS.

shell of the target. First, we focus our attention on the impact of bare projectiles on heavier targets ($Z_T > Z_P$). This is the case studied by Basbas, Brandt, and Laubert [1,2] in which binding effects in electron ionization were introduced, to our knowledge, for the first time. As is well known, the B1 approximation for electron excitation gives a Z_P^2 dependence for the transition probabilities and total cross sections. Distortion effects are determined as deviations from this behavior. Let us consider the collision systems

$$P^{Z_P+} + \mathrm{Ne}^{9+}(1s) \longrightarrow P^{Z_P+} + \mathrm{Ne}^{9+}(n=2) , \qquad (19)$$

with $Z_P = 1,2,3,5$. For these asymmetric systems we can assume that the electron-capture channels will not play a main role in the determination of the excitation cross sections.

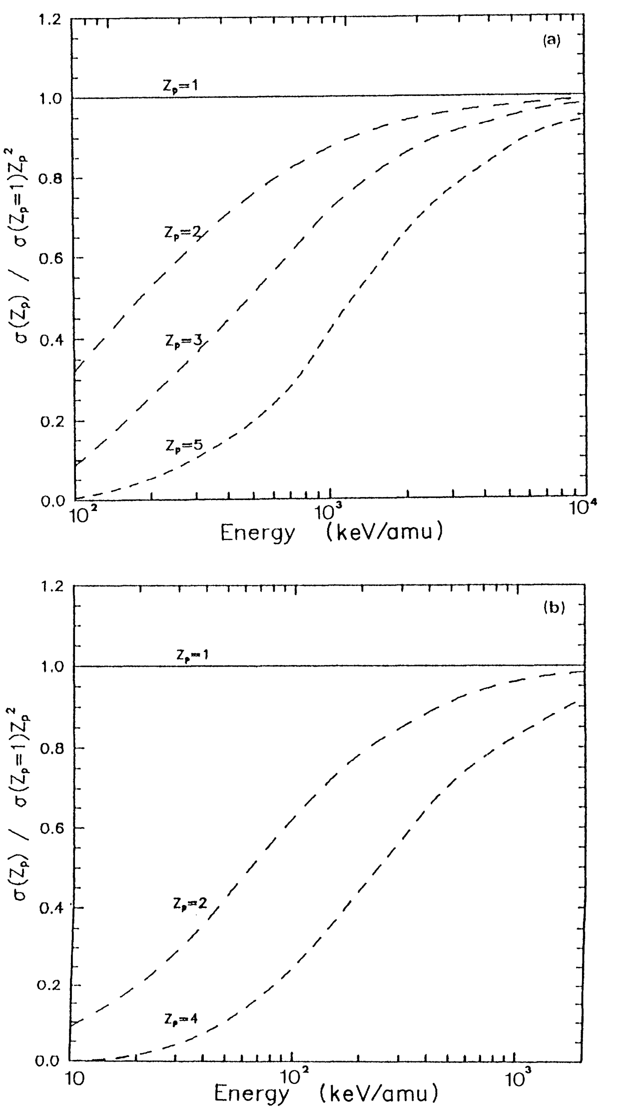

FIG. 4. Cross-section ratio $\sigma(Z_P)/[\sigma(Z_P=1)Z_P^2]$ vs impact energy. All curves correspond to SE results, present work. (a) $P^{Z_P+} + \mathrm{Ne}^{9+}(1s) \longrightarrow P^{Z_P+} + \mathrm{Ne}^{9+}(n=2)$. (b) $P^{Z_P+} + \mathrm{H}(1s) \longrightarrow P^{Z_P+} + \mathrm{H}(n=2)$.

In Fig. 4(a) the excitation-cross-section ratio $\sigma_{if}(Z_P)/[Z_P^2 \sigma_{if}(Z_P=1)]$ is presented, where with $\sigma_{if}(Z_P)$ we indicate the cross section for impact of a projectile with charge Z_P. It is obvious that in the B1 approximation this ratio always equals 1. It is shown that when the SE approximation is used the ratio decreases as Z_P increases, and the effect is more pronounced when the collision energy decreases. This is similar to the qualitative behavior observed before for electron ionization at low enough impact velocities.

In order to study the origin of the decrease in the excitation-cross-section ratio, we analyze the impact-parameter dependence of the probabilities $P_{if}(\mathbf{b})$ at fixed collision velocities. In Fig. 5(a) we present the quantity

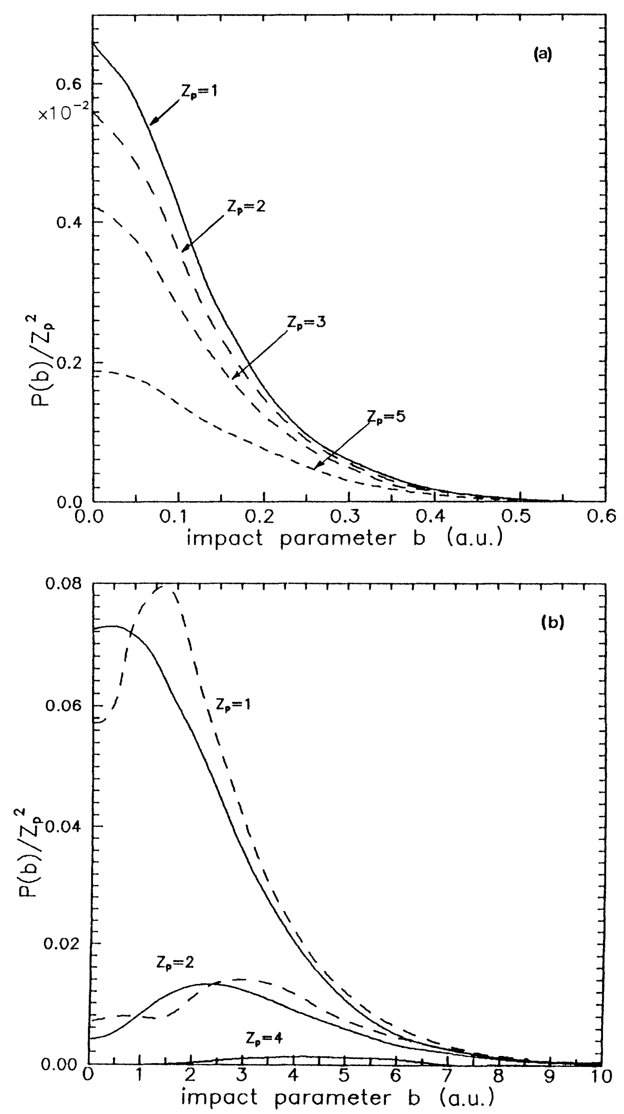

FIG. 5. Impact-parameter probabilities divided by Z_P^2 vs impact parameter. (a) SE result for the reaction $P^{Z_P+} + \mathrm{Ne}^{9+}(1s) \longrightarrow P^{Z_P+} + \mathrm{Ne}^{9+}(n=2)$ at 1000 kev/amu. (b) $P^{Z_P+} + \mathrm{H}(1s) \longrightarrow P^{Z_P+} + \mathrm{H}(n=2)$ at 40 kev/amu: ——, SE; — — —, PSS. Both present work.

$P_{if}(\mathbf{b})/Z_P^2$ for the reactions (19), as a function of b, at a 1000-keV/amu impact energy. If the B1 approximation is used, the same curve would be obtained for all Z_P. However, in the SE approximation $P_{if}(\mathbf{b})/Z_P^2$ drastically decreases for any value of the impact parameter when Z_P increases. It is easy to show again that the total cross sections are dominated by $b \gtrsim r_K$ contributions. The electron evolves in the simultaneous presence of the projectile and target potentials. Distortions in the entry and exit channels introduce this two-center effect in the SE approximation. The SE approximation partially contains all orders of the Born series and unfortunately it is not possible to obtain an explicit expression for the Z_P dependence like the one obtained with the Born series. Nevertheless, it can be concluded that the decrease in the excitation-cross-section ratio comes in SE from Z_P^n contributions with $n > 2$.

In the case $Z_P > Z_T$ we have studied the collision systems

$$P^{Z_P +} + \mathrm{H}(1s) \longrightarrow P^{Z_P +} + \mathrm{H}\ (n=2)\ , \tag{20}$$

with $Z_P = 1,2,4$. An even more pronounced decrease of the cross-section ratio and $P_{if}(\mathbf{b})/Z_P^2$ is now observed as Z_P increases. This fact can be seen in Figs. 4(b) and 5 (b) where SE calculations for the reactions (20) are presented. In Fig. 5(b) the quantity $P_{if}(\mathbf{b})/Z_P^2$ is calculated for a 40-keV/amu impact energy. As has been shown in Sec. III, impact parameters larger than r_K give the dominant contribution to the total cross sections.

It must be noted that in the case $Z_P > Z_T$ charge exchange can influence the final excitation channels. Even when PSS calculations include explicit charge-transfer states and SE do not, similar behavior for the quantity $P_{if}(\mathbf{b})/Z_P^2$ is observed when obtained using any of the two models [see Fig. 5(b)]. So, the PSS calculations support the possible existence of distortion effects for the case of impact of heavy projectiles on lighter targets.

V. CONCLUSIONS

Electron excitation in ion-atom collisions is studied by using the SE approximation. The model is shown to give an appropriate description of the reaction for different collision systems. With such a goal in mind SE cross sections and impact-parameter probabilities are compared with other theoretical predictions and with existing experimental data.

It is shown that electron excitation is a reaction dominated by impact parameters of the order of or larger than the mean initial orbital radius. So, the simultaneous presence of the projectile and target potentials (two-center effect) is well described by distorting the initial and final bound wave function with projectile eikonal phases. As a consequence, impact-parameter probabilities and total cross sections deviate from the Z_P^2 law predicted by the first-order Born approximation. At low intermediate collision energies it is observed that the ratio $\sigma(Z_P)/[\sigma(Z_P=1)Z_P^2]$ decreases as Z_P increases. PSS calculations support the possible existence of these distortion effects predicted by the SE approximation. A similar behavior for the total cross sections has been previously obtained for electron ionization. The origin of this behavior has been shown to come from binding effects [1–3]. It has also been proven that the distorted-wave CDW-EIS model (where the initial bound state is distorted by a projectile eikonal phase, like in the excitation SE model) describes these binding effects [6–8]. Therefore one is tempted to identify distortion and binding effects for electron excitation. However, additional theoretical and experimental work is necessary to determine a possible connection between both descriptions and to confirm the predictions given by the SE approximation.

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