Collisions of helium with Rydberg atoms in the presence of static electric and magnetic fields

S. Bivona, R. Burlon, G. Ferrante, and C. Leone
Dipartimento di Fisica e Tecnologie Relative and Istituto Nazionale di Fisica della Materia, Viale delle Scienze, Edificio 18, 90128 Palermo, Italy
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Alignment and orientation effects in collisions of helium with Rydberg atoms due to the presence of static electric and magnetic fields are predicted. Analytical expressions are obtained for the cross sections of the state-to-state transitions within the manifold with the same principal quantum number. For moderate field-induced inelasticity, the curves of the cross sections vs the fields intensity show modulations that are explained in terms of the phase differences accumulated by the wave functions of the states involved in the collision. Due to the presence of the magnetic field, transitions involving inversion of high magnetic quantum numbers are dramatically quenched. The possibility of observing the predicted effects is discussed. The reported analytical cross sections are expected to help in the understanding of the results.

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I. INTRODUCTION

Recently, interesting effects in collisions of rare-gas atoms with Rydberg atoms have been theoretically predicted [1,2]. In particular, the presence of oscillations in the total cross sections of state-to-state transitions as a function of the relative velocity of the colliding atoms was interpreted as the manifestation of interference effects induced by collisions of helium atoms with calcium. The theoretical model on which the predictions are based used the impact parameter method (IPM). Further, some simplifying assumptions were adopted to account for the mechanism responsible for the oscillations. To the best of our knowledge, until now, the above interference effects have not been observed in experiments. The key parameter of the physical process associated with the onset of the oscillations is the ratio $\Delta E/V$, where V denotes the projectile-target relative velocity and ΔE is the collision energy defect which is fixed by the quantum defects of the states involved in the collision event. For $\Delta E \rightarrow 0$ or $V \rightarrow \infty$ the modulations in the cross sections disappear. To observe the predicted phenomena, collisions of rare-gas atoms with Rydberg atoms should be carried out, for a given arrangement, at variable relative velocity of the colliding particles, in order to change the parameter $\Delta E/V$. On the other hand, it is well known that by submitting the colliding system to the action of an external static electric or magnetic field, the energy separation ΔE can be varied and, consequently, modulations of the excitation cross sections should occur at fixed velocities of the colliding particles when the field strength is changed.

It is the aim of the present paper to present a theoretical treatment of alignment and orientation effects in collisions of helium with high-angular-momenta hydrogen Rydberg atoms, germane to those predicted in [1,2], but due to the presence of static electric and magnetic fields. The physical conditions we envisage have a number of advantages: (i) the state of the art in collision experiments of this kind in external fields is very high and well assessed [3]; (ii) a well established theoretical model, the IPM, may be used [4], allowing, in our case, to obtain analytically closed final formulas for the cross sections to be obtained; (iii) inspection of the general formulas for some specific situations and limits gives, in principle, the possibility to trace back precisely the physical reasons for the obtained results without the need to resort to a separate modeling for their interpretation. Concerning the effects of an external static electric field, theoretical studies on angular momentum mixing collisions and on the initial orientation of the relative velocity of the colliding atoms have been performed by Hickman [5] and de Prunele [6], and measurements have been carried out, respectively, by Slusher *et al.* [7] and by Kachru *et al.* [8] in collisions between Xe and Xe Rydberg atoms and Xe and Na Rydberg atoms (see also Ref. [9]).

Below, we first consider the effects of a static electric field on the state-to-state transitions induced by the collision of helium with hydrogen Rydberg atoms. The analysis will be limited to the case in which the relative velocity of the colliding atoms is parallel to the direction of the electric field and the states involved in the collision belong to the same n-manifold. Moreover, within the range of values of the external field strength under consideration, the energy of the Rydberg states is determined by the linear Stark effect, while field-independent wave functions of the excited hydrogen atom states will be assumed. Second, the effects of an additional parallel magnetic field will be considered as well.

II. STATE-TO-STATE CROSS SECTIONS

In this section the state-to-state cross sections will be derived when the collision occurs in the presence of a static external electric field. For the aims of our investigation, the familiar IPM is particularly well suited. According to it, the projectile position $\mathbf{R}$ relative to the target core takes the form $\mathbf{R}(t)=\boldsymbol{\rho}+\mathbf{V}t$ where $\boldsymbol{\rho}$, the impact parameter, is perpendicular to the direction of the static electric field, taken along the z axis, and $\mathbf{V}=\hat{\mathbf{z}}V$ is the relative velocity of the colliding particles with $\hat{\mathbf{z}}$ a unit vector along z. The choice of the parallel geometry allows us to greatly simplify the numerical calculations to be accomplished below. Neglecting the helium polarizability, during the collision event the projectile is treated as a structureless particle interacting only with the Rydberg electron through a potential that, in the Fermi approximation [10], is represented by the zero-range potential

$$W(t) = 2\pi(L_s/\mu)\delta(\mathbf{r} - \mathbf{R}(t)), \quad (1)$$

where $L_s = 1.19a_0$ is the electron-helium scattering length, $\mathbf{r}$ the electron coordinate, a_0 the Bohr radius, and $\mu = m_e m_{\mathrm{He}}/(m_e + m_{\mathrm{He}}) \approx m_e$ the reduced mass of the electron-helium system. With the above assumptions, the Hamiltonian of the target atom in the presence of the static electric field is perturbed by the electron-projectile time-dependent potential $W(t)$, Eq. (1). Therefore, by assuming that at the initial time t_i the atomic state $|\Psi_i\rangle$ is an eigenstate of the Hamiltonian of the hydrogen atom in the presence of the static electric field of intensity F, the transition amplitude at time t to the atomic state $|\Psi_f\rangle$, at first order in W, is

$$T_{if} = -(i/\hbar)\int_{t_i}^{t} \langle \Psi_f | \mathrm{W}(t') | \Psi_i \rangle dt', \quad (2)$$

with $i \neq f$ and $|\Psi_i\rangle$ and $|\Psi_f\rangle$ eigenstates of

$$\hat{H}_0 = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{r} - eFz. \quad (3)$$

For the electric field strengths and the atomic spectrum region taken under consideration in the present paper, the wave functions describing the states involved in the collision may be taken as the field-free hydrogen wave function characterized by the parabolic quantum numbers n_1, n_2, m, with m the magnetic quantum number and $n = n_1 + n_2 + |m| + 1$ the principal quantum number. The electric field effect on the energy of the states $|n, n_1, m\rangle$ is taken into account, at first order in F, by the following expression;

$$E_{n,n_1,m} = -1/(2n^2) + 1.5n(2n_1 - n + |m| + 1)F, \quad (4)$$

while the alignment effects caused by the electric field are accounted for by the permanent electric dipole associated with the atomic states. Note that atomic units are used. By substituting Eq. (1) into Eq. (2), and using $\mathbf{z} = \hat{\mathbf{z}}Vt$, the transition probability amplitude from the state described by the wave function $\Psi_{n,n_{1i},m_i}(\mathbf{r})\exp(-iE_i t)$, for $t_i \to -\infty$, to that described by $\Psi_{n,n_{1f},m_f}(\mathbf{r})\exp(-iE_f t)$, for $t_f \to \infty$, is obtained as

$$T_{if} = -2\pi\, i(L_s/V)\int_{-\infty}^{\infty} \exp(i\Delta E\, z/V)\Psi^*_{n,n_{1f},m_f}(\mathbf{R})\Psi_{n,n_{1i},m_i}(\mathbf{R})dz \quad (5)$$

with $\mathbf{R} = \boldsymbol{\rho} + \mathbf{z}$ and $\Delta E = E_f - E_i$ the inelasticity of the collision. The cross section of the process obtained upon integration over the impact parameter is

$$\sigma(i \to f) = 2\pi\int_0^{\infty} |T_{if}|^2 \rho\, d\rho. \quad (6)$$

In Eq. (5),

$$\Psi_{n,n_{1i},m_i}(\mathbf{r}) = (2^{1/2}/n^2) f_{n_1,m}(\eta/n) f_{n_2,m}(\xi/n)\sqrt{1/2\pi}\exp(im\,\varphi),$$

where η, ξ, φ are the parabolic coordinates and

$$f_{k,m}(x) = \sqrt{\frac{k!}{(k+|m|\,!)}} L_k^{|m|}(x)\exp\left(-\frac{x}{2}\right)x^{|m|/2} \quad (7)$$

with $L_k^{|m|}(x)$ the associated Laguerre polynomials [11]. The integral giving T_{if} may be evaluated analytically. As shown in the Appendix, the result of the integration is obtained in terms of modified Bessel functions of the second kind. By further integration over the impact parameter, as prescribed by Eq. (6), an analytical closed form of the cross section is arrived at, which is too involved to be reported here. In the simplest case, when the initial state is a so-called circular state with quantum numbers $n_1 = n_2 = 0, m = n - 1$, the cross section of the process in which the atom makes a transition to the state with $n_{1f} = 1, n_{2f} = 0, m_f = m - 1$ is obtained as

$$\sigma(n,0,m \to n,1,m-1) = \left(\frac{2\pi Ls}{V}\right)^2 \left(\frac{(2m)!}{n\ m!}\right)^4 \frac{(2m+1)^2}{2(4m+1)!}(\cos^2\chi)^{2(m+2)} \times \left[\frac{2m+1}{4} - \frac{2m(m+1)}{4m+3}\cos^2\chi\right], \quad (8)$$

where $\cos^2\chi = [1 + (n\Delta E/2V)^2]^{-1}$. In the Appendix, it will be shown that the cross sections $\sigma(i \to f)$ may be expressed as combinations of powers of cos χ. Moreover, it is not difficult to show that the ratio $n\Delta E/(2V)$ may be cast in the form $\Delta E/\Delta E_m$ where ΔE_m is the maximum value of the energy that may be exchanged in an elastic collision between a heavy particle and an electron moving, respectively, with initial velocities V and $v_e \gg V$ with $v_e = 1/(2n)$, the average electron velocity in the state with principal quantum number n. In our calculations $\Delta E/\Delta E_m$ will be taken less than unity.

III. RESULTS

We note that the cross sections given by Eq. (6) are independent of the signs of ΔE, m_i, and m_f. From Eq. (5) it clearly follows that the transition amplitude, for fixed velocity of the projectile, is determined by the overlap of the wave functions of the states involved in the collision event, and by the modulating factor $\exp(i\Delta Ez/V)$. As ΔE may be changed by varying the field strength, the modulation and, hence, the cross sections may be controlled by the external field. More precisely, the overlaps of the wave functions, for the values of the field strength taken under consideration in the present work, are not modified by the presence of the field. In the ρ-z plane, their maxima and minima are located in the boxes formed by the nodal lines of the wave functions, as illustrated in Fig. 1 where, as an example, the overlap between the states with $n = 15$, $n_{1i} = 5$, $m_i = 5$, $n_{1f} = 6$, $m_f = 6$ is shown. Instead, the phase factor $\exp(i\Delta Ez/V)$ weighting the overlap along the line $\rho = \rho_0$, ρ_0 being a given impact parameter, changes by varying ΔE, altering appreciably the result for the transition amplitude. This effect is illustrated in Fig. 2 where the transition probability times the impact parameter, $\rho|T_{if}|^2$, as a function of ρ is plotted for different values of the field strength. It turns out that, when the field strength varies, the major modifications take place when the trajectory of the projectile intersects the maxima of the absolute values of the

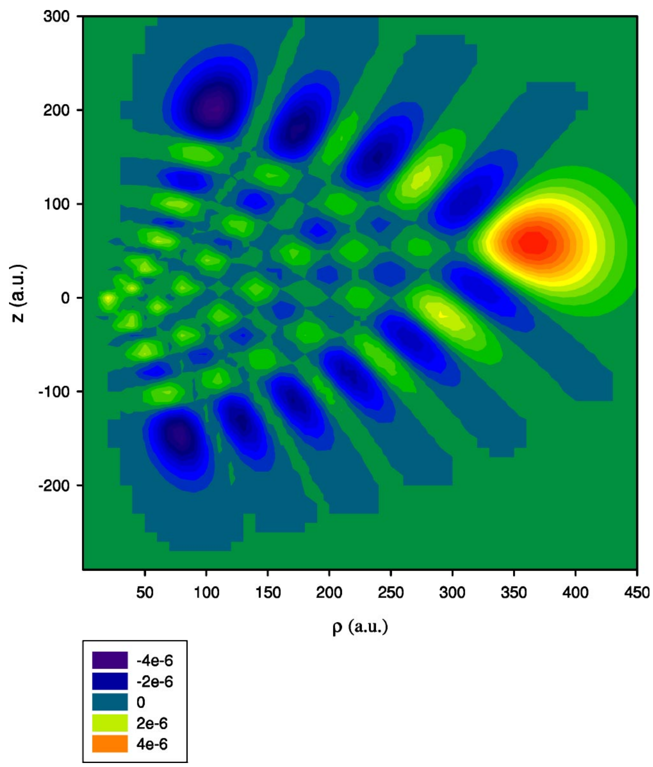

FIG. 1. (Color online) Contour plot of the overlap between the wave functions of the states $|15,5,5\rangle$ and $|15,6,6\rangle$. Note the nodal lines describing parabolas.

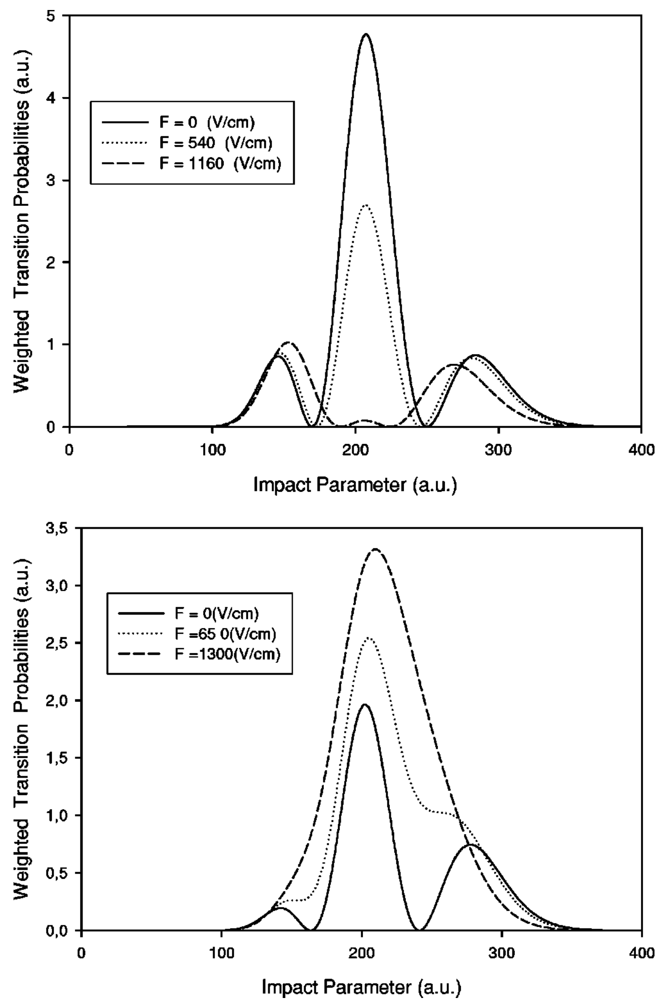

FIG. 2. (a) Weighted transition probabilities from the state $|15,0,14\rangle$ to the state $|15,0,13\rangle$ vs the impact parameter, for different values of the electric field F. The relative velocity of the colliding atoms is $V=10^5$ cm/sec. (b) As for (a) for transition from the state $|15,0,14\rangle$ to the state $|15,0,12\rangle$.

overlaps. The effect of the electric field on the cross sections for transitions involving some selected states is shown in Fig. 3. All the curves have been obtained for relative velocities $V=10^5$ cm/sec. For the range of field strength taken under consideration, the field effect is not univocal even if, by further increasing the ratio $\Delta E/V$, the cross sections are expected to suffer severe reduction due to fast oscillations of the phase factor $\exp(i\Delta Ez/V)$, irrespective of the two states involved in the collision.

Before closing this section, we observe that for collisions involving rare-gas atoms other than helium, because of the effects due to their higher polarizability, Eq. (1) is likely to become inadequate for describing the Rydberg-electron–rare-gas interaction.

Although a discussion of such effects is beyond the aims of the present work, we remark that Lebedev and Fabrikant [14] have shown how to account for them. Working within the impulse approximation (IA) approach, they used the electron–rare-gas scattering amplitude provided by the modified effective range theory [15,16] to incorporate the long-range interaction due to the higher polarizability of the heavier noble gases. Moreover, within the IA method, calculations have been carried out for Xe-Ca collisions [1] by using an approximate expression of the electron–rare-gas-atom scattering amplitude given in [16]. As already remarked in the Introduction, the numerical results obtained in [1] displayed the presence of oscillations in the curve showing the state-to-state transition cross sections as a function of the velocity of the colliding atoms. In the case of our concern, the external fields would not affect the Rydberg-electron–rare-gas interaction, but only the initial and final atomic state energies. Therefore, oscillatory behavior of the state-to-state transition cross section as a function of the external field intensity is expected too for rare-gas projectiles heavier than helium.

IV. EFFECTS DUE TO A STATIC WEAK MAGNETIC FIELD

As the cross sections given by Eq. (7) are invariant under inversion of the sign of ΔE and of the magnetic quantum numbers, the cross sections of the transitions from a circular state to one of the four states characterized by $m=\pm(n-1)$ and n_1 equal to either 0 or 1 turn out to be equal. If the colliding system is submitted to an additional uniform static magnetic field, parallel to the electric field, the symmetry with respect to the inversion of m breaks down. In fact, assuming such a strength of the field that the diamagnetic effects may be neglected, and ignoring spin-flip transitions, the inelasticity of the collision, ΔE, takes the following form:

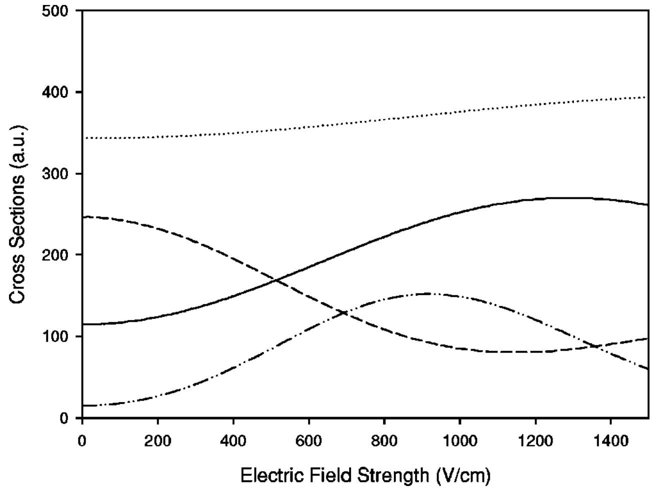

FIG. 3. State-to-state cross sections $\sigma(n_{1i},m_i;n_{1f},m_f)$ as a function of the electric field strength at the relative velocity $V=10^5$ cm/sec. Dotted line, $\sigma(0,14;1,13)$. Dashed line, $\sigma(0,13;1,13)$. Full line, $\sigma(0,14;0,12)$. Dash-dotted line, $\sigma(0,14;0,10)$.

$\Delta E=1.5n[2(n_{1i}-n_{1f})+|m_i|-|m_f|)]F+(m_i-m_f)\gamma$, with $\gamma=(B/B_0)$, where the magnetic field intensity B is measured in gauss and $B_0=4.7\times10^9$ G. The additional paramagnetic term is a measure of the orientation effect brought about by the magnetic field in the collision event. To evaluate this last effect, the cross sections calculated by Eq. (8) at $F=500$ V/cm, as a function of the magnetic field strength, are shown in Fig. 4. The cross sections of the transitions with $m_i-m_f=1$ are slightly influenced by the presence of the magnetic field, while sizable modifications occur for transitions with inversion of the sign of the magnetic quantum number, especially when the magnetic field strength increases. The behavior of the curves at the highest values of B considered in Fig. 4 shows the stabilizing effect of the magnetic field on the projection of the electron angular momentum along the direction of the field. So the quenching of the cross sections, when the magnetic field strength is high, is a measure of the freezing of the magnetic quantum number operated by the magnetic field during the collision event. For relatively low field strength ($B\leqslant 2$ kG) and $m_f=-m_i+1$, the features of the curves are similar to those of Fig. 2, and oscillations of the cross sections may appear.

V. CONCLUDING REMARKS

In summary, by using the impact parameter method, analytical expressions of the cross sections of the state-to-state transitions within manifolds with the same principal quantum number have been obtained. For moderate field-induced energy differences, the curves of the cross sections vs the field strength show modulation features that are explained in terms of the phase differences accumulated by the wave functions of the states involved in the collision. It has been shown that, due to the presence of the magnetic field, transitions involving inversion of high magnetic quantum numbers are dramatically quenched. The results of the calculations may be extended to the case of collisional state-to-state excitation of Rydberg states of alkali-metal atoms with, practically, zero quantum defects. By using external fields with parameters well within the experimental state of the art, the possibility of investigating the reported field effects on Rydberg alkaline-metal atoms is open. In particular, advantage may be taken of the experimental demonstrations ([3] and references therein, [13]) that it is possible to produce targets of oriented elliptic Rydberg atoms of sufficient density and arbitrary degree of ellipticity to perform atomic-collision and spectroscopic studies.

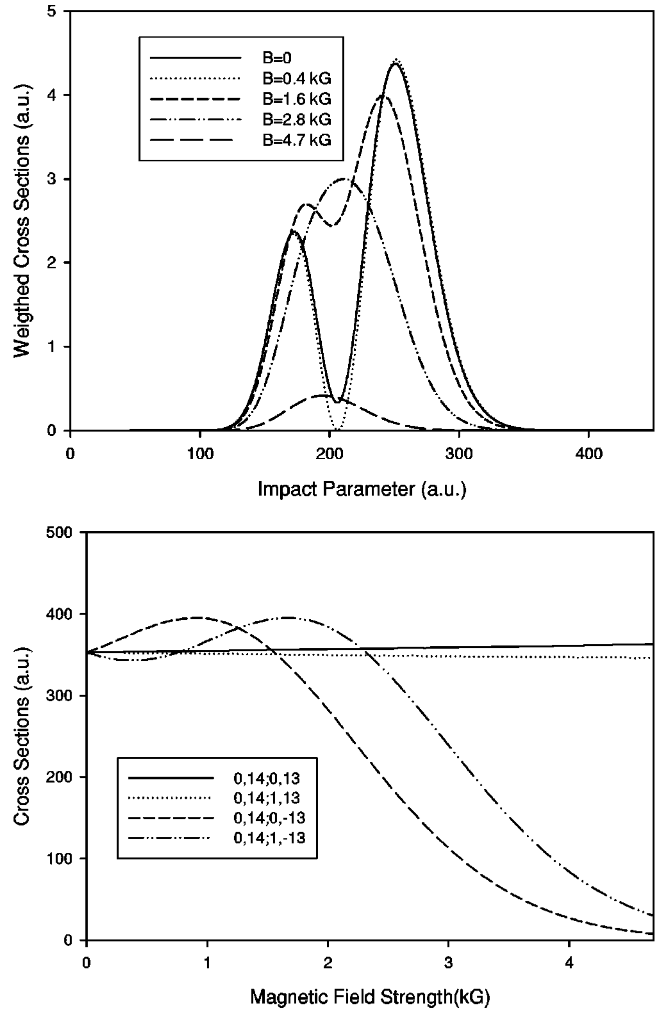

FIG. 4. (a) As for Fig. 2(a), for transition from the state $|15,0,11\rangle$ to the state $|15,1,-13\rangle$, for different values of the magnetic field and for $F=500$ V/cm. (b) State-to-state cross sections $\sigma(n_{1i},m_i;n_{1f},m_f)$ as a function of the magnetic field strength at the relative velocity $V=10^5$ cm/sec.

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APPENDIX

Here we outline the evaluation of the transition amplitude and cross section defined, respectively, by Eqs. (5) and (6) of the main text. Though rather involved, the following derivation is felt to be useful to obtain different, specific cases. By introducing the parabolic coordinates $\xi=R+z$ and $\eta=R-z$, the impact parameter may be written as $\rho=\sqrt{\eta\xi}$. For fixed $\rho, z=(\xi-\rho^2/\xi)/2$ and Eq. (5) is cast in the form

$$T_{if}=-2\pi i(L_s/V)\exp[i(|m_i|-|m_f|)\varphi](1/\pi n^4)I_0 \qquad \text{(A1)}$$

with

$$I_0=(1/2)\int_0^\infty d\xi\,\exp[i\alpha(\xi-\rho^2/\xi)/n] \times f_{n_{1i},m_i}\left(\frac{\xi}{n}\right)f_{n_{2i},m_i}\left(\frac{\rho^2}{n\xi}\right)f_{n_{1f},m_f}\left(\frac{\xi}{n}\right)f_{n_{2f},m_f}\left(\frac{\rho^2}{n\xi}\right)(1+\rho^2/\xi^2) \qquad \text{(A2)}$$

and $\alpha=n\Delta E/2V$. By putting $\rho/n=\tilde{\rho}$, $\xi=n\tilde{\rho}\tau$ and using the definitions of $f_{n,m}$ given by Eq. (7) and of the associated Laguerre polynomials $L_n^{|m|}(x)=\Sigma_{l=0}^{n}c_{n,|m|}^{l}x^l$ with

$$c_{n,|m|}^{l}=(-1)^l\frac{(n+|m|)!}{n!\,|m|!}\frac{n(n-1)\cdots(n-l+1)}{(|m|+1)(|m|+2)\cdots(|m|+l)(l)!},$$

$$c_{n,|m|}^{0}=\frac{(n+|m|)!}{n!\,|m|!},$$

Eq. (A2) is written as

$$I_0=(1/2)nN_{if}\tilde{\rho}^{(|m_i|+|m_f|+1)}\sum_{l_1=0}^{n_{1i}}\sum_{l_2=0}^{n_{2i}}\sum_{l_3=0}^{n_{1f}}\sum_{l_4=0}^{n_{2f}}c_{n_{1i},|m_i|}^{l_1} \times c_{n_{2i},|m_i|}^{l_2}c_{n_{1f},|m_f|}^{l_3}c_{n_{2f},|m_f|}^{l_4}\tilde{\rho}^{(l_1+l_2+l_3+l_4)}I_c(\alpha), \qquad \text{(A3)}$$

where

$$N_{if}=\sqrt{\frac{n_{1i}!}{(n_{1i}+|m_i|)!}}\sqrt{\frac{n_{2i}!}{(n_{2i}+|m_i|)!}} \times\sqrt{\frac{n_{1f}!}{(n_{1f}+|m_f|)!}}\sqrt{\frac{n_{2f}!}{(n_{2f}+|m_f|)!}}$$

and

$$I_c(\alpha)=\int_0^\infty x^{(l_1+l_3-l_2-l_4)}\exp\left(-\tilde{\rho}(1+i\alpha)x-\tilde{\rho}\frac{(1-i\alpha)}{x}\right) \times(1+x^{-2})dx. \qquad \text{(A4)}$$

By using ([12], p. 340),

$$\int_0^\infty x^{(\nu-1)}\exp\left(-\gamma x-\frac{\beta}{x}\right)dx=2\left(\frac{\beta}{\gamma}\right)^{(\nu/2)}K_\nu(2\sqrt{\beta\gamma}),$$

Eq. (A4) is reduced to a combination of modified Bessel functions K_ν:

$$I_c(\alpha)=2\,\exp(-il\chi)\left[e^{-i\chi}K_{l+1}\left(2\tilde{\rho}\sqrt{1+\alpha^2}\right) + e^{i\chi}K_{l-1}\left(2\tilde{\rho}\sqrt{1+\alpha^2}\right)\right], \qquad \text{(A5)}$$

with

$$l=l_1+l_3-l_2-l_4,\quad e^{(-i\chi)}=\frac{1-i\alpha}{\sqrt{1+(\alpha)^2}}. \qquad \text{(A6)}$$

By using Eqs. (A3) and (A5), the transition probability amplitude is obtained as combinations of terms of the kind $\cos[(i-j)\chi]K_i(z)K_j(z)$ giving rise to interference effects due to the energy difference, induced by the external field, between the states involved in the collision event. For $\Delta E=0, \alpha=0$ and the interference effects disappear.

In order to evaluate the cross section of state-to-state transition, use is made of the following relation [12], p. 693:

$$\int_0^\infty z^\beta K_i(z)K_j(z)dz=\frac{2^{(\beta-2)}}{\beta!}\Gamma\left(\frac{\beta+1+i+j}{2}\right)\Gamma\left(\frac{\beta+1+i-j}{2}\right) \times\Gamma\left(\frac{\beta+1-i+j}{2}\right)\Gamma\left(\frac{\beta+1-i-j}{2}\right). \qquad \text{(A7)}$$

In our case, β, i, j, and the arguments of the Γ function turn out to be integer numbers.

Equation (6) together with Eqs. (A2), (A5), and (A7) gives

$$\sigma(i\to f)=\pi\left(\frac{L_s}{Vn^2}\right)^2N_{if}^2\sum_{L,L'}\frac{C(L,L',i,f)}{\beta!\,\sqrt{(1+\alpha^2)^{\beta+1}}}\{\cos[(l-l')\chi] \times f(l,l')+2\cos[(l-l'+2)\chi]g(l,l')\}$$

where l is defined in Eq. (A6) and

$$\sum_{L,L'}\equiv\sum_{l_1=0}^{n_{1i}}\sum_{l_2=0}^{n_{2i}}\sum_{l_3=0}^{n_{1f}}\sum_{l_4=0}^{n_{2f}}\sum_{l_1'=0}^{n_{1i}}\sum_{l_2'=0}^{n_{2i}}\sum_{l_3'=0}^{n_{1f}}\sum_{l_4'=0}^{n_{2f}};$$

$$C(L,L',i,f)=c_{n_{1i},|m_i|}^{l_1}c_{n_{2i},|m_i|}^{l_2}c_{n_{1f},|m_f|}^{l_3}c_{n_{2f},|m_f|}^{l_4}c_{n_{1i},|m_i|}^{l_1'} \times c_{n_{2i},|m_i|}^{l_2'}c_{n_{1f},|m_f|}^{l_3'}c_{n_{2f},|m_f|}^{l_4'};$$

$$\beta=l_1+l_2+l_3+l_4+l_1'+l_2'+l_3'+l_4'+2(|m_i|+|m_f|)+3;$$

$$l'=l_1'-l_2'+l_3'-l_4',$$

$$f(l,l')=(l_1+l_3+l_1'+l_3'+|m_i|+|m_f|+2)!\,(l_1+l_3+l_2'+l_4' +|m_i|+|m_f|+1)!\,(l_2+l_4+l_1'+l_3'+|m_i|+|m_f|+1)! \times(l_2+l_4+l_2'+l_4'+|m_i|+|m_f|)!\;+(l_1+l_3+l_1'+l_3' +|m_i|+|m_f|)!\,(l_1+l_3+l_2'+l_4'+|m_i|+|m_f|+1)! \times(l_2+l_4+l_1'+l_3'+|m_i|+|m_f|+1)!\,(l_2+l_4+l_2'+l_4' +|m_i|+|m_f|+2)!$$

$$g(l,l')=(l_1+l_3+l_1'+l_3'+|m_i|+|m_f|+1)!\,(l_1+l_3+l_2'+l_4' +|m_i|+|m_f|+2)!\,(l_2+l_4+l_1'+l_3'+|m_i|+|m_f|)! \times(l_2+l_4+l_2'+l_4'+|m_i|+|m_f|+1)!$$

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