

ns-ms EXCITATION OF ALKALI ATOMS IN THE GLAUBER APPROXIMATION

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ABSTRACT

We obtain an expression for the scattering amplitude in the Glauber approximation for ns-ms electronic excitation of alkali atoms. The interaction potential between the incident electron, the core electrons and N-1 protons is approximated by an appropriate spherical potential.

RESUMO

Apresentamos uma expressão para a amplitude de espalhamento de Glauber para o processo de excitação eletrônica ns \rightarrow ms dos átomos alcalinos. O potencial de interação entre o elétron incidente, os elétrons do caroço e N-1 é aproximado por um potencial esférico apropriado.

1. Introduction

Calculations of differential cross sections for electron-atom collisions in the region of intermediate incident energy are, generally, complicated and several type of approximations are used. Approximations of the Born type are not satisfactory to describe second order effects and close-coupling approximations are quite involved for this energy region because of the great number of open channels. In 1959 Glauber¹ proposed an approximation for high energy and small scattering angles. When Glauber's approximation is generalized to the problem of composite targets, it corresponds, in some sense, to an approximation complementary to the close-coupling. After Franco's works²⁻⁶ this approximation has been extensively used in atomic problems in the intermediate region of incident energy.

The Glauber approximation, in its formal point of view, has various attractive aspects. As mentioned previously, it is complementary to the close-coupling, in the sense that it takes into account, in an approximated manner, the contribution of all scattering channels⁷⁻¹⁰. It is an eikonal semiclassical approximation for small scattering angles and high energy and in this region the Glauber treatment for composite targets is consistent with the optical theorem, but doesn't satisfy the detailed balance principle. Another important point is the fact that the Glauber approach is essentially a classical approach for the incident electron and exchange terms are not present in the final expression for the scattering amplitude. Some authors⁸⁻¹⁰ proposed modifications in the Glauber formula to describe exchange effects, but these treatments are not

fully satisfactory. This is an important restriction for electronic excitation of atoms in the intermediate energy region, when exchange terms could be fundamental to describe some processes.

Another critical point of the Glauber approach, when used in atomic problems, is the great numerical work related to the many-particle character of the problem. The Glauber approximation without any other additional approximation for the collision problem has been employed to study electron scattering by H, He and Li^{2-7,11-16}. The Glauber expression for the scattering amplitude involves integrals of order $3N+2$, where N is the number of atomic electrons. Franco², Thomas and Chan¹⁷ and others^{7,18,19}, proposed reduction methods for the order of integrals, when the atomic orbitals are approximated by analytical functions of Slater's type. These methods reduce the order of integrals to one, when the interaction between the incident particle and the atom is purely coulombian.

In the present work we present an expression for the scattering amplitude for ns-ms electronic excitation of alkali atoms. Calculations of Glauber cross sections for many-electron atom collisions are very difficult even with the use of Slater's orbitals because of the large number of terms that are present when the reduction methods are used. We use an one-electron approximation to describe the alkali atom, where the interaction of the incident electron with the core electrons and $N-1$ protons is substituted by an appropriate structureless potential.

In section 2 we present the Glauber scattering amplitude, emphasizing some particular points. In section 3 we discuss

the approximation adopted to describe the interaction potential and in section 4 the scattering amplitude for the considered processes is obtained. Finally in section 5 we comment some aspects of this result and the possibility of its generalization to different excitation processes.

2. Theory

We consider the system electron N-electrons neutral atom. Relativistic corrections as well the nuclear motion are not considered. In atomic units ($\hbar = m_e = e = 1$) the hamiltonian for this system is:

$$H = H_a + H_e + V \quad (1)$$

where

$$H_a = -\frac{1}{2} \sum_{j=1}^N \nabla_j^2 - \sum_{j=1}^N \frac{N}{r_j} + \sum_{i>j=1}^N \frac{1}{r_{ij}} \quad (2)$$

is the hamiltonian operator for the atom, and:

$$H_e = -\frac{1}{2} \nabla_{N+1}^2 \quad (3)$$

is the free-electron hamiltonian

$V = V(\vec{r}_1, \dots, \vec{r}_{N+1})$ is the potential that describe the Coulomb interaction between the incident electron (\vec{r}_{N+1}), all the atomic electrons and the nucleus, defined by

$$V = \sum_{j=1}^N V_j, \quad V_j = -\frac{1}{r_{N+1}} + \frac{1}{r_{j,N+1}} \quad (4)$$

In eqs. (2)-(4) $r_{jk} = |\vec{r}_j - \vec{r}_k|$ and $r_j = |\vec{r}_j|$

The scattering amplitude in the Glauber approximation is:

$$f_{of}(\vec{k}_o, \vec{k}_f) = \frac{ik_o}{2\pi} \int d^2b \langle \psi_o(\vec{r}_1 \dots \vec{r}_N) | \exp(i\vec{q} \cdot \vec{b}) \{1 - \exp(i\chi(\vec{b}, \vec{r}_1, \dots, \vec{r}_N))\} | \psi_f(\vec{r}_1 \dots \vec{r}_N) \rangle \quad (5)$$

Eq. (5) is the Glauber expression for the scattering amplitude associated to the process of excitation of the atomic state ψ_f from the state ψ_o when the incident electron, initially with momentum \vec{k}_o , is scattered and, asymptotically, has momentum \vec{k}_f .

$\frac{k_o^2}{2} = (E_o - E_\alpha) + \frac{k_\alpha^2}{2}$ where E_o and E_α are the energy of the states ψ_o and ψ_f . $\vec{q} = \vec{k}_o - \vec{k}_f$ is the transferred momentum. $\chi(\vec{b}, \vec{r}_1, \dots, \vec{r}_N)$ is the phase of Glauber:

$$\begin{aligned} \chi(\vec{b}, \vec{r}_1, \dots, \vec{r}_N) &= -\frac{1}{k_o} \int_{-\infty}^{+\infty} dz' V(x, y, z', \vec{r}_1, \dots, \vec{r}_N) = \\ &= \sum_j \chi_j \quad \text{with} \quad \chi_j = -\frac{1}{k_o} \int_{-\infty}^{+\infty} dz' V_j(x, y, z', \vec{r}_j) \end{aligned} \quad (6)$$

The incident electron coordinates are expressed in cartesian coordinates, $\vec{r}_{N+1} = (x, y, z)$, and \vec{b} is the classical impact parameter, projection of \vec{r}_{N+1} over the plane perpendicular to the incident direction, \hat{z} . The integration over z' is made over the \hat{z} axis.

Directly from the eq. (5) it is easy to see that f_{of} involves the determination of integrals of $3N+2$ orders. Some

reduction methods for the order of these integrals were proposed for atomic collisions^{2-7,17-19}. These method assume the atomic functions as described by a linear-combination of Slater orbitals.

For the case of atomic excitation, eq.(5) takes the form:

$$f_{of}(\vec{k}_o, \vec{k}_f) = \frac{i k_o}{2\pi} \int d^2b \exp(i\vec{q} \cdot \vec{b}) \langle \psi_o | \Gamma_1 \cdots \Gamma_N | \psi_f \rangle \quad (7)$$

where

$$\Gamma_j = \exp(i \chi_j) \text{ and } \langle \psi_i | \psi_f \rangle = \delta_{if}$$

was used.

The atomic functions ψ_o and ψ_f are antisymetrized with respect to the change of two electrons coordinates. If these functions are written in terms of one-electron orbitals (central field approximation) eq(7) is composed by $N!$ terms which, eventually, are rearranged. For atoms others than H and He the number of terms which appears in eq(7) is very large and the use of the Glauber approximation is complicated^{11,12}.

For a better understanding of the kind of difficulties involved, it is interesting to particularize our study to the case of excitation of Li (three atomic electrons), and consider the processes associated to each of the Glauber terms.

Figure (1) shows some of the possible processes. In Fig. (1.a) we present the "direct" excitation process, when the valence electron is excited from the initial level to the final level, and the core wave function relaxes. This process

corresponds to the term:

$$\langle \phi_{1s}(\vec{r}_1) | \Gamma_1 | \phi'_{1s}(\vec{r}_1) \rangle \langle \phi_{1s}(\vec{r}_2) | \Gamma_2 | \phi'_{1s}(\vec{r}_2) \rangle \langle \phi_{2s}(\vec{r}_3) | \Gamma_3 | \phi'_{nl}(\vec{r}_3) \rangle$$

and in the high energy region it reduces to the Born approximation. Figure (1.b) shows a possible "indirect" process: the valence electron (\vec{r}_3) is de-excited to one relaxed core orbital and a core electron is excited to the final level.

This term corresponds to:

$$\langle \phi_{1s}(\vec{r}_1) | \Gamma_1 | \phi'_{nl}(\vec{r}_1) \rangle \langle \phi_{1s}(\vec{r}_2) | \Gamma_2 | \phi'_{1s}(\vec{r}_2) \rangle \langle \phi_{2s}(\vec{r}_3) | \Gamma_3 | \phi'_{1s}(\vec{r}_3) \rangle$$

3. Collisions with Alkali Atoms: Approximation to the Atomic Problem

In several aspects the alkali atoms behaves as an one-electron atom. In the central field approximation the alkali-
ne is described by a core with complete shells and one valence electron. An approximation usually adopted in atomic physics is to substitute the interaction between the valence electron and the core electrons and N-1 protons by an average spherical potential. We can write the interaction between the incident electron and the atomic electrons and the nucleus as:

$$V(\vec{r}_1, \dots, \vec{r}_{N+1}) = -\frac{1}{r_{N+1}} + \frac{1}{|\vec{r}_{N+1} - \vec{r}_N|} + V_c \quad (8)$$

where \vec{r}_N is the valence electron coordinates and V_c describes the interaction of the incident electron and the N-1 core elec

trons and N-1 protons

$$V_C = \frac{N-1}{r_{N+1}} + \sum_{i=1}^{N-1} \frac{1}{|\vec{r}_{N+1} - \vec{r}_i|} \quad (9)$$

The frozen-core approximation is obtained when the relaxation effects are not considered and V_C is approximated by an average core potential defined by:

$$\langle V_C \rangle = \langle \phi_C | V_C | \phi_C \rangle$$

The inert frozen-core approximation¹³ corresponds to put $\langle V_C \rangle = 0$.

At large distances from the atom the interaction is of the form²⁰:

$$V_I = -A \exp(-\lambda r_{N+1}) / r_{N+1} \quad (10)$$

where A and λ are, respectively, the depth and the range of the potential, and are determined by the asymptotic behavior of $\langle V_C \rangle$.

The approximation adopted in this work is to consider $V_C = V_I$ in all space and describe the interaction of the incident electron and the atom by the approximate potential:

$$V(\vec{r}_1, \dots, \vec{r}_{N+1}) = -\frac{1}{r_{N+1}} + \frac{1}{|\vec{r}_{N+1} - \vec{r}_N|} - \frac{A \exp(-\lambda r_{N+1})}{r_{N+1}} \quad (11)$$

corresponds

This corresponds to consider approximately the "indirect" contributions to the excitation process.

4. Collisions with Alkali Atoms: Glauber Amplitude

Using the approximation described in section 3 for the interaction potential the Glauber phase defined by eq(6) is:

$$\chi = \chi_H + \chi_C \quad (12)$$

where χ_H is the Glauber phase for the electron-hydrogen collision and χ_C is the core contributions. The analytical expressions for χ_H and χ_C are^{2-6,21,22}:

$$\chi_H = \frac{1}{k_0} \int_{-\infty}^{+\infty} dz' \left(\frac{1}{r_{N+1}} - \frac{1}{|\vec{r}_{N+1} - \vec{r}_N|} \right) = \frac{2}{k_0} \ln \frac{|\vec{b} - \vec{s}|}{b} \quad (13)$$

and

$$\chi_C = \frac{1}{k_0} \int_{-\infty}^{+\infty} dz' \frac{A \exp(-\lambda r_{N+1})}{r_{N+1}} = \frac{2A}{k_0} K_0(\lambda b) \quad (14)$$

\vec{s} is the projection of \vec{r}_N in the plane perpendicular to the direction of incidence (\hat{z}) and K_0 is the Modified Bessel function²².

Using these approximations we reduce the collision problem with alkali atoms to an electron- "hydrogen" - core potential problem.

Using eqs(13) and (14) in (5):

$$f_{of}(\vec{k}_o, \vec{k}_f) = \frac{ik_o}{2\pi} \int d^2_{b < \psi_f} \exp(i\vec{q} \cdot \vec{b}) \left\{ 1 - \left(\frac{|\vec{b} - \vec{s}|}{b} \right)^{2in} \exp\left(\frac{2i A K_0(\lambda b)}{k_o} \right) \right\} \quad (15)$$

or, for the case of atomic excitation, and integrating over the core electron coordinates:

$$f_{of} = \frac{ik_o}{2\pi} \int d^2b \langle \phi_f(\vec{r}_N) | \exp(i\vec{q} \cdot \vec{b}) \left(\frac{|\vec{b}-\vec{s}|}{b} \right)^{2i\eta} \exp\left(\frac{2i A K_o(\lambda b)}{k_o}\right) | \phi_o(\vec{r}_N) \rangle$$

with $\eta = 1/k_o$ for electronic collisions and $\phi_j(\vec{r}_N)$ the j -orbital of the valence electron.

Considering only ns-ms excitations and the atomic wave functions described by an appropriate linear combination of Slater orbitals, we can use the method proposed by Thomas and Chan¹⁶ to reduce the order of the integrals. The generalization for others excitations processes is possible.

The atomic orbitals ϕ_o and ϕ_f are written as:

$$\phi_o = \phi_{ns} = \frac{1}{\sqrt{4\pi}} \sum_{j=1}^n a_j r^{j-1} \exp(-\alpha_j r)$$

$$\phi_f = \phi_{ms} = \frac{1}{\sqrt{4\pi}} \sum_{j=1}^m b_j r^{j-1} \exp(-\beta_j r)$$

Since relaxation effects are not considered we have the orthogonality condition for the atomic orbitals:

$$\langle \phi_o | \phi_f \rangle = \delta_{fo}$$

or, expressing the above condition in terms of the coefficients a_j , b_k and $\gamma_{ij} = \alpha_i + \beta_j$:

$$\sum_{ij} a_i b_j \frac{(i+j)!}{\gamma_{ij}^{i+j+1}} = 0 \quad (16)$$

The scattering amplitude is:

$$f_{of} = \frac{ik_0}{8\pi} \sum_{j=1}^n \sum_{k=1}^m \int d^2b \exp(i\vec{q} \cdot \vec{b}) \exp\left(\frac{2i A K_0(\lambda b)}{k_0}\right) a_{j,b_k} \int d^3r \left[r^{j+k-2} \exp(-\gamma_{jk} r) \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} \right] \quad (17)$$

Introducing the generator function I_0 , defined by:

$$I_0(\gamma, \vec{b}) = \int d^3r \frac{\exp(-\gamma r)}{r} \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} \quad (18)$$

we can use the method of Thomas and Chan¹⁶ to reduce the order of the integrals that appear in eq(17):

$$I_0(\gamma, \vec{b}) = 4 \pi \gamma^{-2} - 8 \pi i \eta e^{i\pi\eta} b^{-2i\eta} \gamma^{-2i\eta} \mathcal{L}_{2i\eta-1,0}(i\gamma b) \quad (19)$$

where $\mathcal{L}_{\mu,\nu}(iz)$ is the modified Lommel's function with argument iz , defined by^{11,17}:

$$\mathcal{L}_{\mu,\nu}(iz) = s_{\mu,\nu}(iz) - \exp\left(\frac{i\pi\mu}{2}\right) 2^{\mu-1} \Gamma\left(\frac{1+\mu+\nu}{2}\right) \Gamma\left(\frac{1+\mu-\nu}{2}\right) I_\nu(z)$$

$\Gamma(x)$ is the Gamma function, $s_{\mu,\nu}$ is the Lommel function and I_ν the modified Bessel function²³.

Of course:

$$\int d^3r r^{j+k-2} \exp(-\gamma_{jk} r) \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} = (-1)^{j+k-1} \left. \frac{\partial^{j+k-1} I_0(\gamma, \vec{b})}{\partial \gamma^{j+k-1}} \right|_{\gamma = \gamma_{jk}} \quad (20)$$

Using eqs(18), (19), (20) and the recurrence relations for the modified Lommel's functions¹⁶, we obtain the scattering amplitude:

$$f_{of} = \frac{ik_o}{8\pi^2} \sum_{j=1}^n \sum_{k=1}^m a_j b_k 4\pi \left[(j+k)! \gamma^{-j-k-1} \int d^2b \exp\left(\frac{2i A K_o(\lambda b)}{k_o}\right) - 2i\eta e^{i\pi\eta} \sum_{\ell=0}^{j+k-1} i^{j+k-\ell-1} \frac{(-1)^{j+k-\ell}}{2i\eta(2i\eta+1)} \prod_{p=0}^{\ell} (2i\eta+p+1) \prod_{q=0}^{j+k-\ell-1} (2i\eta-2q) \int d^2b \exp\left(\frac{2i A K_o(\lambda b)}{k_o}\right) b^{-2i\eta+j+k-\ell-1} \gamma^{-2i\eta-2-\ell} \mathcal{L}_{2i\eta-j-k+\ell, j+k-\ell-1}^{(i\gamma b)} \right]_{\gamma=\gamma_{jk}} \quad (21)$$

Using the orthogonality condition expressed by eq(16) the first term in eq(21) is zero. Using the relation²²:

$$\int_0^{2\pi} \exp(im\psi) \exp(i\vec{q} \cdot \vec{b}) d\psi = 2\pi \exp(im(\psi_q + \frac{\pi}{2})) J_m(qb)$$

with $\vec{q} = (q, \psi_q)$ and J_m the Bessel function, the final expression for the Glauber scattering amplitude is given by:

$$f_{of} = \frac{k_o e^{i\pi\eta}}{2i\eta+1} \sum_{j=1}^n \sum_{k=1}^m \sum_{\ell=0}^{j+k-1} a_j b_k \frac{\gamma^{-2i\eta-2-\ell} (-i)^{j+k-\ell} (j+k-1)!}{\ell! (j+k-\ell-1)!}$$

$$\prod_{p=0}^{\ell} (2i\eta+p+1) \prod_{q=0}^{j+k-\ell-1} (2i\eta-2q) \int_0^{\infty} db \exp\left(\frac{2i A K_0(\lambda b)}{k_0}\right) J_0(qb) b^{-2i\eta+j+k-\ell} d_{2i\eta-j-k+\ell, j+k-\ell-1}^{(i \gamma_{jk} b)} \quad (22)$$

When $b \gg \max\{1/\gamma_{jk}, 1/q, 1/\lambda\}$ the integrand has the asymptotic behavior:

$$\exp\left(\frac{2i A}{k_0} \sqrt{\frac{\pi}{2\lambda b}}\right) b^{-3/2} \cos\left(qb - \frac{\pi}{4}\right) \quad (23)$$

5. Conclusions

- The effects due to the core electrons are expressed by the factor:

$$\exp\left(\frac{2i A K_0(\lambda b)}{k_0}\right)$$

When $A = 0$ (or, $V_I=0$) we obtain an expression for the scattering amplitude of ns - ms electronic excitation of hydrogen, or alkali atoms in the inert frozen-core approximation.

- The introduction of core effects decreases the inert frozen-core scattering amplitude.

- To generalize the method to compute the expression for a general excitation $n\ell \rightarrow n'\ell'$ it is only necessary to consider the angular part of the atomic orbitals and define new generators functions^{11,17}.

- The integrand in eq(22) presents an asymptotic behavior adequate for numerical calculations. This is a direct consequence of the fact that the orthogonality condition was explicitly taken into account in eq(21) and spurious divergence are avoided.

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FIGURE CAPTIONS

Figure 1 - Some possible processes of excitation of lithium.

(1a) represents the "direct" excitation

(1b) represents an "indirect" excitation

