epl A Letters Journal Exploring the Frontiers of Physics

August 2008

EPL, **83** (2008) 43002
doi: 10.1209/0295-5075/83/43002

www.epljournal.org

Effects of mass and electron exchange in H-H scattering

Sumana Chakraborty[1], Y. N. Tiwari[2] and A. S. Ghosh[3(a)]

[1] *Mallabhum Institute of Technology - P.O.-Gosaipur, Bishnupur-722122, Bankura, India*
[2] *Department of Physics, North-Eastern Hill University - Shillong-793022, India*
[3] *Department of Theoretical Physics, Indian Association for the Cultivation of Science Jadavpur, Kolkata-7900032, India*

received 29 May 2008; accepted in final form 5 July 2008
published online 19 August 2008

PACS 34.50.-s – Scattering of atoms and molecules

Abstract – The sensitive change of the singlet scattering length in H-H scattering was found using the Born-Oppenheimer (BO) model when the nuclear mass was replaced by the atomic mass. The mass effect influenced the BO potential immensely. In the close-coupling model, the main inputs to solve the integral equation are the scattering amplitudes for different transitions. The present investigation indicates that the effect of electron exchange in H-H scattering for all the transitions using the nuclear mass survives even in the asymptotic region whereas including the atomic mass this effect diminishes with the increase of energies. In other words, the exchange potential is ill conditioned when the nuclear mass is considered. This is the main reason for the significant change of the scattering length in H-H scattering.

Introduction. – We investigated H-H scattering at ultra cold temperatures using the close-coupling approximation (CCA) model in which the total wave function was expanded in terms of the eigen and pseudostates of the atom [1,2]. We used the nuclear mass in our calculation. This model is *ab initio* and diabatic in nature. The importance of the diabatic contribution has been pointed out in the literature [3,4]. We predicted s-wave singlet and triplet scattering lengths and also low partial-wave cross-sections. Our results are in good accord with the existing theoretical predictions considering the nuclear mass only [5,6]. The mass dependence of the scattering length for the system has also been studied by several authors using the Born-Oppenheimer (BO) formalism. Williams and Julienne [7] obtained a 33% change in the singlet scattering length when they replaced the nuclear mass by the atomic mass. A similar reduction in the scattering length was also reported by Jamieson and Dalgarno [3]. In recent times, Jamieson and Zygelman [4] revisited the H-H scattering and predicted the s-wave singlet scattering length. In that investigation, they considered the atomic mass instead of the nuclear mass. They found that the singlet scattering length obtained by using the atomic mass was 30–35% less than that obtained by the use of nuclear mass. A marginal change in the reduced mass affects the scattering length significantly. They observed that the change of the singlet scattering length was due to the change in the BO potential obtained by using the atomic mass and concluded that the sensitive dependence was most pronounced for the BO potential that supported bound states. Apart from this, the long-range potential as a function of mass was also responsible. In the BO model, the effective potential is the input in any scattering calculation.

Here we employ the close-coupling model where plane-wave scattering amplitudes are the main inputs. In this model, one does not require to calculate the potential separately as it is automatically generated depending on the basis sets employed [1,2]. The effect of the different parts of the potential, including the exchange of electrons of the two hydrogen atoms, can be visualized in our model. Therefore, any change in the scattering amplitude gives rise to the change in the effective potential as well as in the scattering parameters. We try to find the cause of the sensitive dependence of the scattering length in our model without performing the exact calculation. The reason for the discrepancy due to the slight change of the reduced mass of the system should be well reflected in the scattering amplitude that acts as an input in the CCA model. Therefore, we start our investigation from the first-order purely quantum-mechanical model to observe the change in the scattering cross-sections of the H-H system using the atomic mass instead of the nuclear mass.

There are large numbers of the first-Born (FBA) calculations for the H-H scattering system [8–18]. The

(a) E-mail: tpasg@iacs.res.in

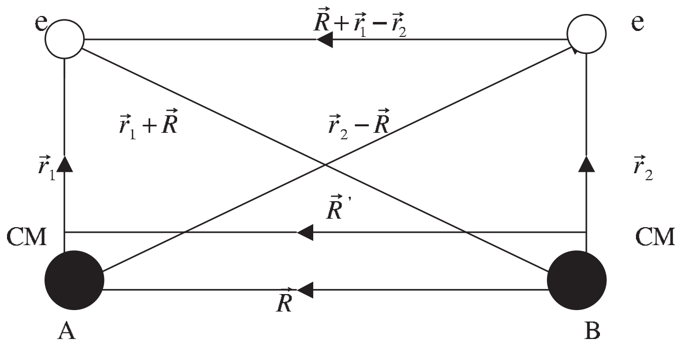

Fig. 1: The coordinate system of the H-H scattering employed here. Here CM stands for the centre of mass of the atom.

first-Born calculations for the single-excitation (when one of the H-atom is in excited state) and double-excitation (when both H-atoms are in excited states) cross-sections were carried out by several authors [8–13]. They considered the nuclear mass only and neglected the electron exchange effect. There are also some first-order calculations by impact parameter formalism in which the effect of electron exchange were taken partially [14–18].

We perform the first-order matrix elements considering the atomic mass as well as the nuclear mass. Moreover, the present model includes the effect of electron exchange explicitly following the Pauli exclusion principle. The main motivation of this work is to find the effect of mass and electron exchange on the scattering parameters. Here, we present the elastic as well as single- and double-excitation cross-sections up to $n = 2$ states in the energies region from 50 eV to 1 MeV.

Theory. – In fig. 1 we illustrate the coordinate system of the H-H scattering employed in the present work. The atom A is the projectile and the atom B is the target atom and $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of two electrons with respect to their respective nucleus. $\vec{R}$ is the inter nuclear distance and $\vec{R}'$ is the distance between the center of mass of the two atoms. The first-Born direct-scattering amplitude of the H-H system considering the atomic mass for the transition $\mathrm{H}_A(1s) + \mathrm{H}_B(1s) \to \mathrm{H}_A(n_1'l_1'm_1') + \mathrm{H}_B(n_2'l_2'm_2')$ is given by

$$f^B = -\frac{\mu}{2\pi}\int e^{-i\vec{k}_f\cdot\vec{R}'}\varphi^*_{n_1'l_1'm_1'}(\vec{r}_1)\,\varphi^*_{n_2'l_2'm_2'}(\vec{r}_2) \times V_{int.}e^{i\vec{k}_i\cdot\vec{R}'}\varphi_{1s}(\vec{r}_1)\,\varphi_{1s}(\vec{r}_2)\,\mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\mathrm{d}\vec{R}, \quad (1)$$

where

$$\vec{R}' = \vec{R} + \frac{m}{M_A+m}\vec{r}_1 - \frac{m}{M_B+m}\vec{r}_2 \quad (2)$$

and the reduced mass of the system $\mu = \frac{(M_A+m)(M_B+m)}{M_A+M_B+2m}$.

Here M_A and M_B are the masses of the proton of the atom A and of the atom B, respectively, and m denotes the electron mass.

Here,

$$V_{int.} = \frac{Z_A Z_B}{R} - \frac{Z_A}{|\vec{R}-\vec{r}_2|} - \frac{Z_B}{|\vec{R}+\vec{r}_1|} + \frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|}, \quad (3)$$

Z_A and Z_B denote the charges of the nucleus for A and B atoms, respectively.

$\vec{k}_i$ and $\vec{k}_f$ are the initial and final momenta of the system. On performing integration over $\mathrm{d}\vec{R}$, we get

$$f^B = -\frac{2\mu}{Q^2} I_1 \times I_2, \quad (4)$$

where

$$I_1 = \int e^{i\frac{m}{M_A+m}\vec{Q}\cdot\vec{r}_1}\varphi_{n_1'l_1'm_1'}(\vec{r}_1)\left\{Z_A - e^{-i\vec{Q}\cdot\vec{r}_1}\right\} \times \varphi_{1s}(\vec{r}_1)\,\mathrm{d}\vec{r}_1, \quad (5)$$

$$I_2 = \int e^{-i\frac{m}{M_B+m}\vec{Q}\cdot\vec{r}_2}\varphi^*_{n_2'l_2'm_2'}(\vec{r}_2)\left\{Z_B - e^{i\vec{Q}\cdot\vec{r}_2}\right\} \times \varphi_{1s}(\vec{r}_2)\,\mathrm{d}\vec{r}_2 \quad (6)$$

with $\vec{Q} = \vec{k}_i - \vec{k}_f$ the momentum transfer.

Integration I_1 and I_2 are straightforward for any arbitrary final state.

The plane-wave exchange scattering amplitude for the $(1s1s)$ to $(n_1'l_1'n_2'l_2')$ transition is given by

$$g^B = -\frac{\mu}{2\pi}\int e^{-i\vec{k}_f\cdot\vec{R}_f}\varphi^*_{n_1'l_1'm_1'}(\vec{R}-\vec{r}_2)\varphi^*_{n_2'l_2'm_2'}(\vec{R}+\vec{r}_2) \times V_{post}e^{i\vec{k}_i\cdot\vec{R}'}\varphi_{1s}(\vec{r}_1)\,\varphi_{1s}(\vec{r}_2)\,\mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\mathrm{d}\vec{R}, \quad (7)$$

where

$$\vec{R}_f = \vec{R} + \frac{m}{M_A+m}(\vec{r}_2 - \vec{R}) - \frac{m}{M_B+m}(\vec{R}+\vec{r}_1). \quad (8)$$

The post interaction potential is

$$V_{post} = \frac{Z_A Z_B}{R} - \frac{Z_A}{r_1} - \frac{Z_B}{r_2} + \frac{1}{\left|\vec{R}+\vec{r}_1-\vec{r}_2\right|}. \quad (9)$$

Neglecting terms containing the factor $\frac{m}{(M+m)}$ (here $M = M_A = M_B$) in eqs. (1) and (7) we get the corresponding scattering amplitudes by considering only the nuclear mass of the system. The evaluation for the exchange matrix elements is not straightforward as in the case of the direct scattering amplitude. Two-dimensional integrations have been carried out numerically to evaluate the exchange scattering amplitudes.

The total spin-averaged Born (SAB) cross-section is given by

$$\sigma^{SAB} = \frac{1}{4}\sigma^{B^+} + \frac{3}{4}\sigma^{B^-}, \quad (10)$$

where

$$\sigma^{B^\pm} = 2\pi\frac{k_f}{k_i}\int\left|f^B \pm g^B\right|^2 \mathrm{d}(\cos\theta), \quad (11)$$

$\sigma^{B+}$and σ^{B^-}denote the singlet and triplet total cross-section, respectively.

The first-Born (FBA) cross-section is defined as

$$\sigma^{FBA} = 2\pi\frac{k_f}{k_i}\int\left|f^B\right|^2 \mathrm{d}(\cos\theta) \quad (12)$$

Table 1: Total direct single- and double-excitation cross-sections (σ^{FBA} in units of πa_0^2) for the H-H scattering system. (The bracketed (−) terms denote the powers of 10 by which each entry should be multiplied.)

Energy (eV)	$1s2p$		$2s2s$		$2s2p$		$2p2p$	
	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass
50	0.2436 (−5)	0.9736 (−3)	0.5148 (−15)	0.1823 (−12)	0.5802 (−17)	0.1964 (−9)	0.6606 (−19)	0.2785 (−6)
70	0.1399 (−4)	0.8366 (−3)	0.1459 (−13)	0.4626 (−12)	0.2492 (−15)	0.3242 (−9)	0.4302 (−17)	0.3034 (−6)
100	0.7852 (−4)	0.8019 (−3)	0.3717 (−12)	0.1417 (−11)	0.9563 (−14)	0.5214 (−9)	0.2487 (−15)	0.3196 (−6)
200	0.1525 (−2)	0.2295 (−2)	0.1149 (−9)	0.1192 (−9)	0.6241 (−11)	0.1295 (−8)	0.3429 (−12)	0.3325 (−6)
500	0.2860 (−1)	0.2991 (−1)	0.9205 (−7)	0.9234 (−7)	0.1278 (−7)	0.2512 (−7)	0.1797 (−8)	0.3283 (−6)
1000	0.1032	0.1047	0.6417 (−5)	0.6436 (−5)	0.1769 (−5)	0.1987 (−5)	0.4957 (−6)	0.9103 (−6)
2000	0.1688	0.1701	0.1672 (−3)	0.1675 (−3)	0.8940 (−4)	0.9207 (−4)	0.4898 (−4)	0.5192 (−4)
5000	0.1360	0.1366	0.1963 (−2)	0.1965 (−2)	0.2368 (−2)	0.2388 (−2)	0.3005 (−2)	0.3049 (−2)

and

$$\sigma^{Ex} = 2\pi \frac{k_f}{k_i} \int \left| g^B \right|^2 \mathrm{d}(\cos\theta) \qquad (13)$$

is the exchange cross-section.

In the ion-atom and atom-atom scattering system, the differential cross-section is sharply peaked in the forward direction. At high energies the total cross-section comes from the milli-radian region. Sufficient care has been taken to obtain the total cross-section.

Results and discussion. – Here we are interested to see the effect of mass as well as the effect of electron exchange on the first-order elastic and inelastic ($n \leqslant 2$) scattering cross-sections. We also calculate the first-Born total cross-section (σ^{FBA}) to see the mass effect. Except for the elastic and $1s2s$ single excitation total cross-sections (not shown) the difference between the two sets of the FBA results (one with the nuclear mass and the other with the atomic mass) for each transition up to $n = 2$ (table 1) is significant and with the increase of the incident energy the difference decreases. The two sets of results coincide beyond the incident energy of 5 keV.

Now we consider only the exchange scattering cross-sections for all the transitions (σ^{Ex}). The total cross-sections only for the g^B (eq. (13)) are evaluated separately to see the effect of mass explicitly. The elastic, and single- and double-excitation exchange cross-sections using nuclear and atomic masses are found to differ from each other in the energy region 1 keV to 1 MeV (table 2). With the increase of energy, the exchange scattering cross-sections with nuclear mass are found to differ significantly from the results involving the atomic mass for each excitation processes. It is well known that the effect of exchange dies out with the increase of energy. Using the atomic mass, this feature has been explicitly shown. In other words, the exchange scattering cross-sections including the nuclear mass are not physically correct.

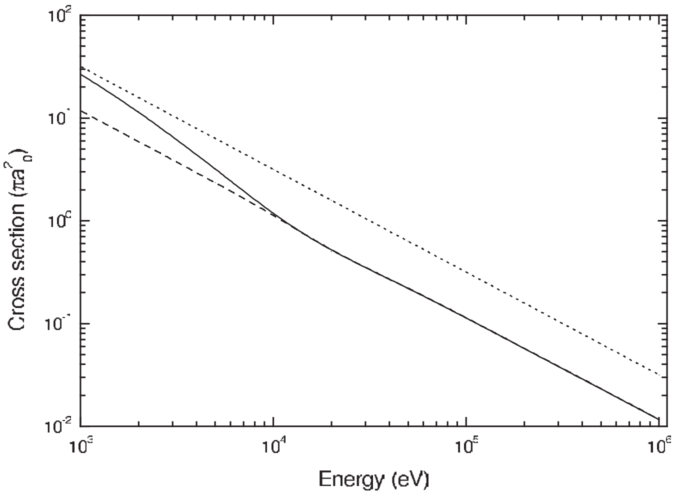

Fig. 2: The total elastic cross-section (in unit of πa_0^2) for the H-H scattering system. Curves: dashed line (σ^{FBA} elastic); dotted line (σ^{SAB} with nuclear mass); solid line (σ^{SAB} with atomic mass).

To highlight the effects of mass and electron exchange, we calculate the total elastic cross-sections in the energy range 50 eV to 1 MeV. Figure 2 represents the first-Born (FBA) elastic cross-sections along with the corresponding spin-averaged Born cross-sections (SAB) with the nuclear and the atomic masses. The present SAB cross-sections including the mass effect are higher in magnitude than the FBA predictions at low and medium energies. With

Table 2: Total exchange single- and double-excitation cross-sections (σ^{Ex} in units of πa_0^2) for the H-H scattering system. (The bracketed terms denote the powers of 10 by which each entry should be multiplied.)

Energy (eV)	$1s1s$		$1s2p$		$2s2s$		$2p2p$	
	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass	Nuclear mass	Atomic mass
1000	0.2820 (2)	0.2287 (2)	0.6418	0.8526	0.3360 (−3)	0.1530 (−3)	0.1428 (−1)	0.6545 (−1)
2000	0.1410 (2)	0.9271 (1)	0.3094 (1)	0.8645	0.3080 (−2)	0.2444 (−2)	0.2242 (−1)	0.9616 (−1)
5000	0.5640 (1)	0.1980 (1)	0.4749 (1)	0.4605	0.1986 (−1)	0.1001 (−1)	0.4235	0.1022
10000	0.2816 (1)	0.3492	0.3406 (1)	0.5897 (−1)	0.2737	0.6963 (−3)	0.3705 (1)	0.3414
20000	0.1409 (1)	0.2634 (−1)	0.1937 (1)	0.5589 (−1)	0.3415	0.1607 (−3)	0.6803 (1)	0.1349
50000	0.5638	0.8770 (−2)	0.8110	0.3452 (−1)	0.2923	0.2599 (−4)	0.5799 (1)	0.3338 (−2)
100000	0.2819	0.2968 (−2)	0.4086	0.7895 (−2)	0.4918	0.5512 (−5)	0.4082 (1)	0.6996 (−4)
200000	0.1410	0.5168 (−3)	0.2047	0.1280 (−2)	0.4774	0.1365 (−5)	0.2559 (1)	0.1406 (−5)
500000	0.5639 (−1)	0.3597 (−4)	0.8193 (−1)	0.1051 (−3)	0.2838	0.9981 (−7)	0.1202 (1)	0.2031 (−7)
1000000	0.2820 (−1)	0.4507 (−5)	0.4097 (−1)	0.1609 (−4)	0.1617	0.1231 (−7)	0.6372	0.1210 (−8)

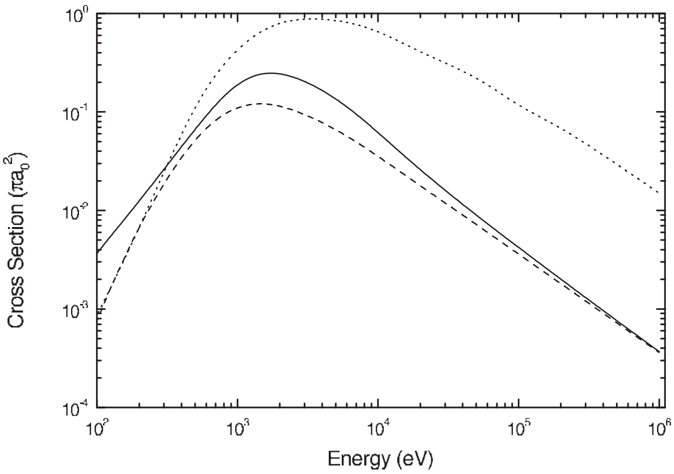

Fig. 3: The total inelastic ($1s1s$-$1s2s$) cross-section (in unit of πa_0^2) for the H-H scattering system. Curves: dashed line (σ^{FBA}); dotted line (σ^{SAB} with nuclear mass); solid line (σ^{SAB} with atomic mass).

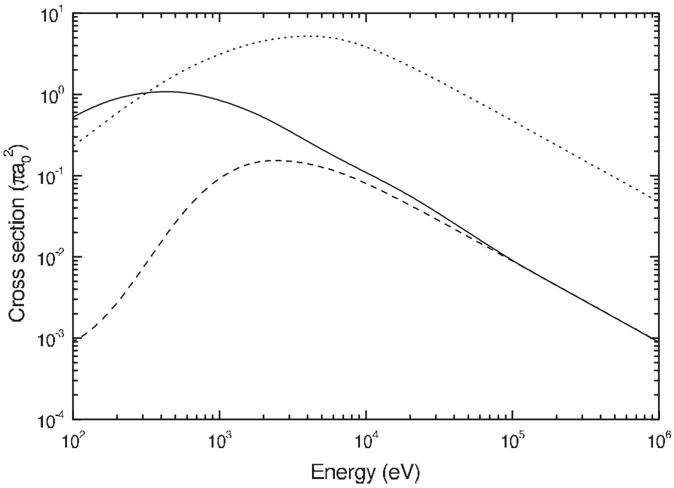

Fig. 4: The total inelastic ($1s1s$-$1s2p$) cross-section (in unit of πa_0^2) for the H-H scattering system. Curves: dashed line (σ^{FBA}); dotted line (σ^{SAB} with nuclear mass); solid line (σ^{SAB} with atomic mass).

the increase of energy, the difference between the two sets of results decreases. Both the results coincide beyond 10 keV. The effect of exchange vanishes at high energies. The elastic SAB cross-section with the atomic mass reflects the correct physical feature. On the other hand, the SAB cross-section with the nuclear mass differs from other two sets of results at all energies and survives in the asymptotic energy region. It has been noticed that the SAB cross-section is very much sensitive to the marginal change of the reduced mass in the atom-atom scattering system. In the ion-atom scattering system, the charge transfer cross-section is also found to be influenced appreciably due to the mass factor.

The total SAB cross-sections using both the nuclear and atomic masses for single- and double-excitation transitions (figs. 3–5) are compared with their corresponding total

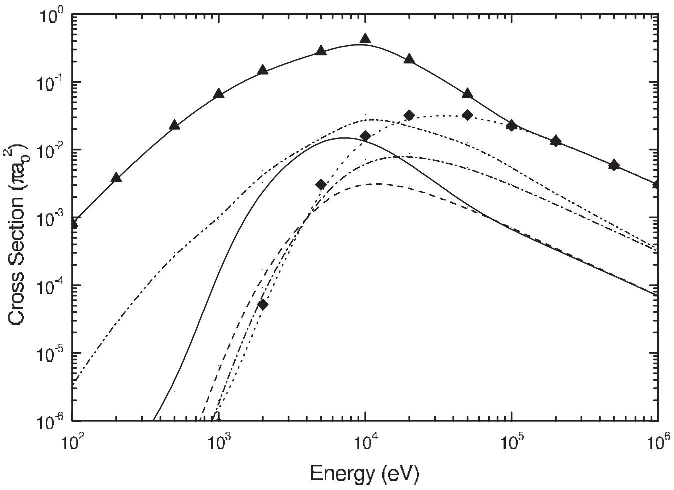

Fig. 5: The double-excitation ($1s1s$-$2s2s$, $1s1s$-$2s2p$, $1s1s$-$2p2p$) total cross-section (in unit of πa_0^2) for the H-H scattering system. Curves: dashed line (σ^{FBA} of ($1s1s$-$2s2s$)); solid line (σ^{SAB} with atomic mass of ($1s1s$-$2s2s$)); dash-dotted line (σ^{FBA} of ($1s1s$-$2s2p$)); dash–double-dotted line (σ^{SAB} with atomic mass of ($1s1s$-$2s2p$)); dotted line with solid square (σ^{FBA} of ($1s1s$-$2p2p$)); solid line with solid triangle (σ^{SAB} with atomic mass of ($1s1s$-$2p2p$)).

FBA cross-sections. The characteristic features of the SAB cross-section for each transition are very much similar to those of elastic results. The total cross-sections obtained for different transitions involving the atomic mass and electron exchange are found to be physical.

Conclusion. – We report, for the first time, the total elastic and excitation cross-sections in H-H scattering at intermediate energies employing the plane-wave model in which the effect of electron exchange is included explicitly. To see the effect of mass, calculations are carried out considering the nuclear mass as well as the atomic mass. We notice that the short-range electron exchange effect for any transition survives asymptotically when the nuclear mass is used. On the other hand, with the use of atomic mass this effect diminishes with the increase of energy as expected. In the CCA model, the short- and long-range potential is generated automatically [1,2] by using a proper basis set. In terms of the potential scattering, the exchange part of the short- and long-range effective potential is expected to predict the correct scattering length replacing the nuclear mass by the atomic mass. We conclude that the short- and long-range potentials are both responsible for the overestimation of the scattering length when the mass effect $\frac{m}{(M+m)}$ is neglected. We plan to study the H-H scattering system using our full CCA model in the near future considering the atomic mass instead of the nuclear mass.

REFERENCES

[1] Sen A., Chakraborty S. and Ghosh A. S., *Europhys. Lett.*, **76** (2006) 582.
[2] Chakraborty S., Sen A. and Ghosh A. S., *Eur. Phys. J. D*, **45** (2007) 261.
[3] Jamieson M. J. and Dalgarno A., *J. Phys. B*, **31** (1998) L219 and other references cited therein.
[4] Jamieson M. J. and Zygelman B., *Phys. Rev. A*, **64** (2001) 032703.
[5] Koyama N. and Baired J. C., *J. Phys. Soc. Jpn.*, **55** (1986) 801.
[6] Jamieson M. J., Dalgarno A. and Kimura M., *Phys. Rev. A*, **51** (1995) 2626.
[7] Williams C. J. and Julienne P. S., *Phys. Rev. A*, **47** (1993) 1524.
[8] Bates D. R. and Griffing G. W., *Proc. Phys. Soc. London, Ser. A*, **66** (1953) 961.
[9] Bates D. R. and Griffing G. W., *Proc. Phys. Soc. London, Ser. A*, **67** (1954) 663.
[10] Bates D. R. and Griffing G. W., *Proc. Phys. Soc. London, Ser. A*, **68** (1955) 90.
[11] Pomilla Frank R. and Milford S. N., Grumman Research Department Report Rethpage, New York (1965) RE-210.
[12] Pomilla Frank R. and Milford S. N., *Astrophys. J.*, **144** (1966) 1174.
[13] Pomilla Frank R., *Astrophys. J.*, **148** (1967) 559.
[14] Bottcher C. and Flannery M. R., *J. Phys. B*, **3** (1970) 1600.
[15] Belkic Dz and Gayet R., *J. Phys. B*, **8** (1975) 442.
[16] Mc Laughlin B. M. and Bell K. L., *J. Phys. B*, **18** (1985) L861.
[17] Riley M. E. and Ritchie A. B., *J. Phys. B*, **33** (2000) 5177.
[18] Hansen J. P. and Dubois A., *J. Phys. B*, **31** (1998) L861.