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The dependence of scattering length on van der Waals interaction and reduced mass of the system in two-atomic collision at cold energies

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Abstract. The static exchange model (SEM) and the modified static exchange model (MSEM) recently introduced by Ray in *Pramana – J. Phys.* **83**, 907 (2014) are used to study the elastic collision between two hydrogen-like atoms when both are in ground states by considering the system as a four-body Coulomb system in the centre of mass frame, in which all the Coulomb interaction terms in direct and exchange channels are treated exactly. The SEM includes the non-adiabatic short-range effect due to electron exchange. The MSEM added in it, the long-range effect due to induced dynamic dipole polarizabilities between the atoms e.g., the van der Waals interaction. Applying the SEM code in different H-like two-atomic systems, a reduced mass (μ) dependence on the scattering length is observed. Again, applying the MSEM code on H(1s)–H(1s) elastic scattering and varying the minimum values of interatomic distance R_0, the dependence of scattering length on the effective interatomic potential consistent with the existing physics is observed. Both these basic findings in low and cold energy atomic collision physics are quite useful and are being reported for the first time.

Keywords. Scattering length; reduced mass; interatomic potential; elastic collision; van der Waals interaction; non-adiabatic effect.

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The elastic collision between two hydrogen-like atoms is the simplest and the most efficient tool to find basic physics. In the present communication, the H(1s)–H(1s) elastic scattering is studied at low and cold energies to derive the s-wave elastic phase shift and the scattering length using the recently introduced [1] static exchange model (SEM) and the modified static exchange model (MSEM). The SEM includes the non-adiabatic short-range effect due to electron exchange that is repulsive in triplet (−) channel. The MSEM includes the long-range effect due to van der Waals interaction in addition to the short-range effect introduced by the SEM. The centre of mass frame is used to describe the four-body Coulomb system. All the Coulomb interaction terms in direct and exchange channels are calculated exactly to find the Born–Oppenheimer (BO) matrix elements [2] that act as input to find the unknown SEM amplitude, following a coupled-channel methodology introduced by the Calcutta Group [3]. Details of the theory is available in [1–9]. Here, Lippman–Schwinger-type coupled integral equation in momentum space formalism [3] is used. The formally exact Lippman–Schwinger-type coupled integral equation for the scattering amplitude in momentum space is given by [3]

$$f^{\pm}_{n'1\mathrm{s},n1\mathrm{s}}(\vec{k}_\mathrm{f},\vec{k}_\mathrm{i}) = B^{\pm}_{n'1\mathrm{s},n1\mathrm{s}}(\vec{k}_\mathrm{f},\vec{k}_\mathrm{i}) - \frac{1}{2\pi^2}\sum_{n''}\int \mathrm{d}\vec{k}'' \times \frac{B^{\pm}_{n'1\mathrm{s},n''1\mathrm{s}}(\vec{k}_\mathrm{f},\vec{k}'')\, f^{\pm}_{n''1\mathrm{s},n1\mathrm{s}}(\vec{k}'',\vec{k}_\mathrm{i})}{\vec{k}^2_{n''1\mathrm{s}} - \vec{k}''^2 + i\varepsilon}, \tag{1}$$

where $B^{\pm}$ are the well-known Born–Oppenheimer (BO) scattering amplitudes [2] in the singlet (+) and triplet (−) channels, respectively. Accordingly, $f^{\pm}$ indicate the unknown SEM scattering amplitudes for the singlet and triplet states of the two system electrons.

The present interest lays on triplet channel to find the basic physics of cold atomic system.

The BO amplitude for the triplet channel is defined as

$$B^{-}_{n'1\mathrm{s},n1\mathrm{s}}(\vec{k}_\mathrm{f},\vec{k}_\mathrm{i}) = -\frac{\mu}{2\pi}\int \mathrm{d}\vec{R}\mathrm{d}\vec{r}_1\mathrm{d}\vec{r}_2\psi^{*}_\mathrm{f}(\vec{R},\vec{r}_1,\vec{r}_2)V(\vec{R},\vec{r}_1,\vec{r}_2)\psi_\mathrm{i}(\vec{R},\vec{r}_1,\vec{r}_2), \quad (2)$$

where $V(\vec{R},\vec{r}_1,\vec{r}_2)$ represents the Coulomb interaction: V_Direct is for the direct channel and V_Exchange is for the exchange or rearrangement channel; μ is the reduced mass of the system. $\vec{R}$ is the internuclear separation and $\vec{r}_1$, $\vec{r}_2$ are the coordinates of two electrons from their corresponding nuclei with charges $+Z_1$ and $+Z_2$ in a.u. so that

$$V_\mathrm{Direct}(\vec{R},\vec{r}_1,\vec{r}_2) = \frac{Z_1Z_2}{R} - \frac{Z_1}{|\vec{R}-\vec{r}_2|} - \frac{Z_2}{|\vec{R}+\vec{r}_1|} + \frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|}, \quad (3)$$

$$V_\mathrm{Exchange}(\vec{R},\vec{r}_1,\vec{r}_2) = \frac{Z_1Z_2}{R} - \frac{Z_1}{|\vec{r}_1|} - \frac{Z_2}{|\vec{r}_2|} + \frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|}. \quad (4)$$

The initial and final-state wavefunctions are defined respectively as

$$\psi_\mathrm{i} = \mathrm{e}^{i\vec{k}_\mathrm{i}\cdot\vec{R}'}\phi_{1\mathrm{s}}(r_1)\eta_{1\mathrm{s}}(r_2), \quad (5)$$

$$\psi_\mathrm{f} = (1-P_{12})\mathrm{e}^{-i\vec{k}_\mathrm{f}\cdot\vec{R}'}\phi_{1\mathrm{s}}(r_1)\eta_{1\mathrm{s}}(r_2), \quad (6)$$

where $\phi_{1\mathrm{s}}(r_1)$ and $\eta_{1\mathrm{s}}(r_2)$ are two atomic wavefunctions and P_{12} is the exchange or antisymmetry operator.

$\vec{R}'$ represents the CM coordinates of the system in the direct channel so that

$$\vec{R}' = \vec{R} + \frac{m_\mathrm{e}}{m_\mathrm{A}+m_\mathrm{e}}\vec{r}_1 - \frac{m_\mathrm{e}}{m_\mathrm{B}+m_\mathrm{e}}\vec{r}_2, \quad (7)$$

where m_A, m_B are the masses of two positrons and m_e is the electron mass. The CM coordinates of the system in the rearrangement channel is defined by $\vec{R}_\mathrm{f}$ and can be expressed as

$$\vec{R}_\mathrm{f} = \vec{R} + \frac{m_\mathrm{e}}{m_\mathrm{A}+m_\mathrm{e}}(\vec{r}_2-\vec{R}) - \frac{m_\mathrm{e}}{m_\mathrm{B}+m_\mathrm{e}}(\vec{r}_1+\vec{R}). \quad (8)$$

The long-range matrix element due to van der Waals interaction that is added to BO amplitude in MSEM theory is

$$B_\mathrm{van} = -\frac{\mu}{2\pi}\int \mathrm{d}\vec{r}_1 \int \mathrm{d}\vec{r}_2 \int \mathrm{d}\hat{R} \int_{R=R_0}^{\infty} \mathrm{d}R\cdot R^2 \times \left[\psi^{*}_\mathrm{f}(\vec{R},\vec{r}_1,\vec{r}_2)\left\{-\frac{C_\mathrm{W}}{R^6}\right\}\psi_\mathrm{i}(\vec{R},\vec{r}_1,\vec{r}_2)\right], \quad (9)$$

where C_W is the van der Waals coefficient [10] and R_0 is the minimum value of the interatomic distance. The s-wave elastic triplet phase shift and the corresponding scattering length are calculated by following the standard procedure described in refs [1–9].

The H-like two-atomic systems of interest for studying the reduced mass dependence of scattering lengths using the SEM code are: (i) muonium (Mu) and Mu, (ii) Mu and H, (iii) Mu and deuterium (D), (iv) Mu and tritium (T), (v) H and H, (vi) H and D, (vii) H and T, (viii) D and D, (ix) D and T and (x) T and T. The reduced masses (μ) of these systems in atomic units are respectively (i) $\mu = 103.9$, (ii) $\mu = 186.7$, (iii) $\mu = 196.7$, (iv) $\mu = 200.2$, (v) $\mu = 918.5$, (vi) $\mu = 1224.5$, (vii) $\mu = 1377.6$, (viii) $\mu = 1836.5$, (ix) $\mu = 2203.7$, (x) $\mu = 2754.5$. To vary the strength of van der Waals interaction in the MSEM code for H(1s)–H(1s) elastic scattering, the values of R_0 are varied from $2a_0$ to $20a_0$ to study the s-wave elastic phase shifts. As two atoms cannot occupy the same space at a time, the minimum value of interatomic distance is chosen as $2a_0$.

Both the codes [1] are used to calculate the triplet (−) s-wave elastic phase shift (δ_0^-) and the corresponding cross-section in the energy region with $k =$ 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 a.u. The variation of $k\cot\delta_0^-$ vs. k^2 following the effective range theory for $R_0 = 2a_0$, $3a_0$, $4a_0$, $5a_0$, $6a_0$, $7a_0$, $8a_0$, $9a_0$, $10a_0$, $11a_0$, $12a_0$, $15a_0$, $20a_0$ are presented in figure 1. All the MSEM curves are represented by solid lines; the bottom one is the MSEM data when $R_0 = 2a_0$ and the top solid curve is for $R_0 = 20a_0$. The dotted line represents the SEM data [5]. All the curves are gradually laying upwards systematically as the value of R_0 gradually increased from $2a_0$ to $20a_0$; at $R_0 = 20a_0$, the MSEM curve almost coincides with the SEM curve (dotted line) indicating almost no contribution of long-range effect. The triplet scattering lengths corresponding to different values of R_0 are presented in table 1 and compared with the SEM data and other available data [11–15]. The MSEM data improve gradually towards the reported scattering lengths as the strength of van der Waals interaction is increased gradually decreasing the value of R_0. The findings are

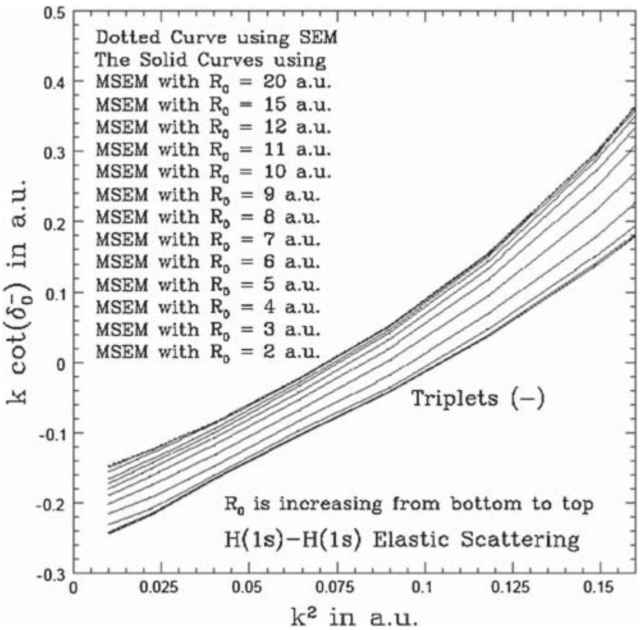

Figure 1. The $k \cot \delta_0^-$ vs. k^2 plot for H(1s)–H(1s) elastic scattering using SEM and MSEM codes for $R_0 = 2a_0$, $3a_0$, $4a_0$, $5a_0$, $6a_0$, $7a_0$, $8a_0$, $9a_0$, $10a_0$, $11a_0$, $12a_0$, $15a_0$, $20a_0$.

consistent with the basic physics as the stronger attractive potentials cause shorter scattering lengths and the stronger repulsive potentials cause longer scattering lengths [16]. The long-range van der Waals interaction is always attractive. In addition, the larger reduced masses of the system make the interaction stronger [16].

The $k \cot \delta_0^-$ vs. k^2 plot for H-like two-atomic systems with different reduced masses is presented in figure 2. The bottom curve is for the Mu–Mu system with reduced mass $\mu = 103.9$ a.u. and top one for T–T system with the reduced mass $\mu = 2754.5$ a.u. All the other curves lie gradually above the other with the gradual increase of reduced masses. An interesting and systematic resemblance is observed between the reduced mass and the scattering length of the system. The variation of the calculated scattering length with the corresponding reduced mass of the system is presented in table 2. In Ps–Ps system, $\mu = 1$ and the triplet scattering length is 3.25 a.u. using the present code [6]. The findings are consistent with the basic physics [16] because the static exchange potential in triplet channel is repulsive and the larger reduced mass makes the interaction stronger. Accordingly, the scattering length is gradually increasing with the increase of reduced mass of the system.

It should be noted again that the present SEM theory includes only the non-adiabatic short-range effects and there is no contribution of long-range interaction in it. But at low and cold energies, the long-range van der Waals interaction has an important role in addition to short-range non-adiabatic effects. So inclusion of both these effects are extremely useful to describe the cold energy atomic collision processes. It could provide better information if van der Waals interaction is included in all the systems with different reduced masses. However, in the literature no data are available for the van der Waals coefficients to study the H-like two-atomic systems described here. The data using the appropriate values of the van der Waals coefficients for different two-atomic systems in MSEM code could explain more accurately the unexplained findings such as the electron-like behaviour of Ps [17] and the occurrence of Bose–Einstein condensation (BEC) [18] in Rb_{85}– Rb_{85} system with $\mu = 78048.5$ a.u. It should be noted that in electron–atom and positronium–atom collisions, the system reduced masses are almost equal; as the atoms become heavier, the two reduced masses exactly coincide. Again, the reduced mass for the Rb_{87}–Rb_{87} system is $\mu = 79884.5$ a.u. and for the Rb_{85}–Rb_{87} system is $\mu = 78955.8$ a.u., both are greater than the reduced mass of Rb_{85}–Rb_{85} system. It would be extremely useful to include the first excited 2s and 2p states of both the atoms in the coupled-channel methodology for more accurate data; indeed it is a very difficult and extremely labourious job. On the other hand, it would be useful to introduce the first excited 2s state of both the atoms following the coupled-channel

Table 1. The scattering length in atomic units using SEM and MSEM for different values of R_0 in H(1s)–H(1s) elastic scattering.

Scattering length in atomic unit (a.u.)														
Using	Using MSEM with $R_0 =$													
SEM	$20a_0$	$15a_0$	$12a_0$	$11a_0$	$10a_0$	$9a_0$	$8a_0$	$7a_0$	$6a_0$	$5a_0$	$4a_0$	$3a_0$	$2a_0$	Data of others
5.88, 5.90[a]	5.80	5.68	5.26	5.11	4.89	4.63	4.38	4.03	3.77	3.68	3.63	3.60	3.58	2.04[a], 1.91[b], 1.22[c], 1.34[d], 1.3[e]

[a][11]; [b][12]; [c][13]; [d][14]; [e][15].

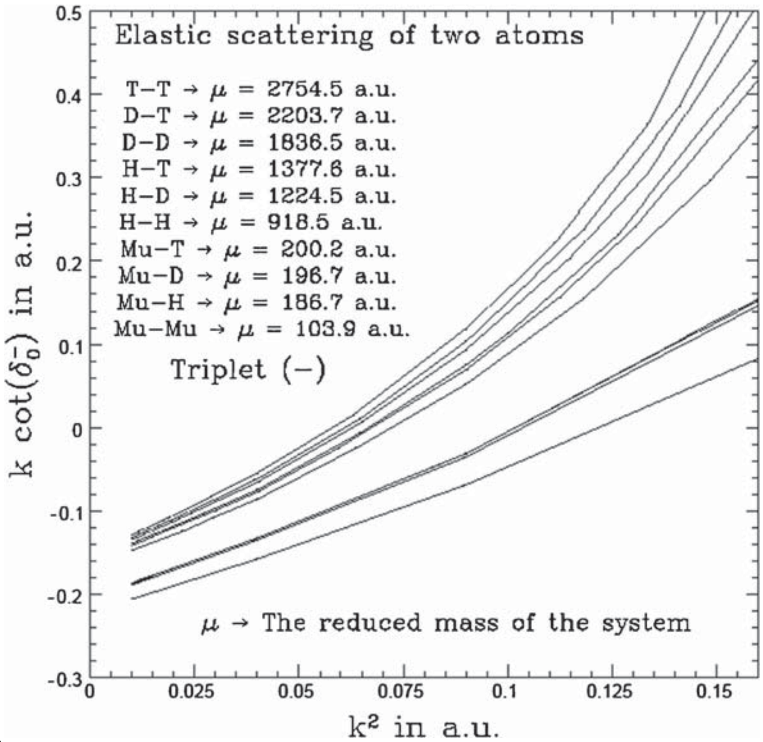

Figure 2. $k \cot \delta_0^-$ vs. k^2 curve for different H-like two-atomic systems. The reduced masses of the systems are increasing gradually from bottom to top curves.

Table 2. The variation of the triplet scattering length with the reduced mass of different H-like two-atomic systems.

System	Mu–Mu	Mu–H	Mu–D	Mu–T	H–H	H–D	H–T	D–D	D–T	T–T
Reduced mass (a.u.)	103.9	186.7	196.7	200.2	918.5	1224.5	1377.6	1836.5	2203.7	2754.5
Scattering length (a.u.)	4.54	4.76	4.88	4.95	5.88	6.25	6.37	6.58	6.68	6.90

methodology in the MSEM code to include a majority of the non-adiabatic short-range effects.

In conclusion, we report for the first time, the reduced mass dependence of scattering length in two-atomic collision at low and cold energies. Using the SEM theory in H-like two-atomic systems with reduced masses in the range 103.9–2754.4 a.u., it is observed that with the increase of reduced mass of the system, the scattering length increases almost proportionately. Again, applying the MSEM theory in H(1s)–H(1s) elastic scattering, the variation of scattering length with the strength of attractive van der Waals interaction that is consistent with the existing physics, is observed. The most accurate calculation using the methods described above could provide more accurate informations.

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References

[1] H Ray, *Pramana – J. Phys.* **83**, 907 (2014)
[2] H Ray and A S Ghosh, *J. Phys. B* **29**, 5505 (1996); *ibid.* **30**, 3745 (1997)
[3] A S Ghosh, N C Sil and P Mandal, *Phys. Rep.* **87**, 313 (1982)
[4] H Ray *et al*, *The effect of van der Waals interaction in elastic collision between Ps(1s) and H(1s)*, arXiv:1308.1939 (2013)
[5] H Ray, *The collision between two hydrogen atoms*, arXiv:1311.3132 (2013)
[6] H Ray, *The collision between two ortho-positroium (Ps) atoms: A four-body Coulomb problem*, arXiv:1409.3371 (2014); *Pramana – J. Phys.* **86**, 1077 (2016)
[7] H Ray, *The collision between positronium (Ps) and muonium (Mu)*, arXiv:1501.00260 (2015); *J. Phys. Conf. Ser.* **618**, 012008 (2015)

[8] H Ray, *The atom and atom scattering model to control ultracold collisions*, arXiv:1206.5476 (2012)
[9] H Ray, *The effect of long-range forces on cold-atomic interaction: Ps-H system*, arXiv:1103.4915 (2011)
[10] J Mitroy and M W J Bromley, *Phys. Rev. A* **68**, 035201 (2003)
[11] A Sen, S Chakraborty and A S Ghosh, *Europhys. Lett.* **76**, 582 (2006)
[12] M J Jamieson, A Dalgarno and J N Yukich, *Phys. Rev. A* **46**, 6956 (1992)
[13] M J Jamieson and A Dalgarno, *J. Phys. B* **31**, L219 (1998)
[14] C J Williams and P S Julienne, *Phys. Rev. A* **47**, 1524 (1995)
[15] N Koyama and J C Baird, *J. Phys. Soc. Jpn* **55**, 801 (1986)
[16] R J Drachman, Private communication during August–September 2015 at GSFC, NASA, Greenbelt, Maryland, USA
[17] S J Brawley, S Amritage, J Beale, D E Leslie, A I Williams and G Laricchia, *Science* **330**, 789 (2010)
[18] S Chaudhuri, S Roy and C S Unnikrishnan, *Curr. Sci.* **95**, 1026 (2008)