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Interatomic Potential Structures in Highly Ionized Scattering Systems

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Abstract

The interatomic potential of the ion-atom scattering system I^{N+}–I at small intermediate internuclear distances is calculated for different charge states N from atomic Dirac–Focker–Slater (DFS) electron densities within a statistical model. The behaviour of the potential structures, due to ionized electronic shells, is studied by calculations of classical elastic differential scattering cross-sections.

1. Introduction

The interatomic potential as a tool for the description of elastic scattering between ions and atoms has been studied by many authors [1] and it is known quite well in the two extreme ranges of internuclear distances where the forces of the electrons, surrounding the colliding nuclei, can be described by screening functions. But as soon as the internuclear distance becomes comparable to the expectation values of the electron shell radii the interatomic forces depend on the actual distribution of the charge density, the potential contains structures due to the electronic shell structure in the two-centre many-electron system.

Loftager et al. [2] have shown that these shell structure effects can be observed in various scattering systems. They measured well defined structures in the elastic differential scattering cross-section for small angle scattering with impact energies from 2.5 to 400 keV.

2. Our method

We calculated the interatomic potential in a density functional approach. For a given internuclear separation $R = |\mathbf{r}_1 - \mathbf{r}_2|$ the total system energy is in atomic units

$$E = V_{NN} + V_{Ne} + V_{ee} + T_e \tag{1}$$

where

$$V_{NN} = \frac{Z_1 \cdot Z_2}{R} \tag{2}$$

is the potential energy of the bare nuclei,

$$V_{Ne} = -\int \left(\frac{Z_1}{|\mathbf{r} - \mathbf{r}_1|} + \frac{Z_2}{|\mathbf{r} - \mathbf{r}_2|} \right) \rho(\mathbf{r})\, \mathrm{d}^3 r \tag{3}$$

the electron–nucleus interaction energy,

$$V_{ee} = \frac{1}{2} \int \frac{\rho(\mathbf{r}) \cdot \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3 r\, \mathrm{d}^3 r' - \kappa_a \int \rho^{4/3}\, \mathrm{d}^3 r \tag{4}$$

the electron–electron interaction energy, where the first term is the direct part and the second the exchange part in Slater approximation, and

$$T_e = \kappa_k \int \rho^{5/3}\, \mathrm{d}^3 r \tag{5}$$

the kinetic energy term, which is based on the statistical Thomas–Fermi (TF) theory of the atom [3]. The constants κ_a and κ_k are in atomic units

$$\kappa_a = \alpha_x \cdot \frac{3}{2} \left(\frac{3}{\pi} \right)^{1/3} \tag{6}$$

$$\kappa_k = \tfrac{3}{10} (3\pi^2)^{2/3} \tag{8}$$

where we use $\alpha_x = 0.7$.

For the electron density ρ of the scattering system we take the sum of the densities of the separated collision partners

$$\rho = \rho_1^{DFS} + \rho_2^{DFS} \tag{8}$$

These atomic and ionic electron densities have been calculated by using good SCF Dirac–Fock–Slater (DFS) wavefunctions. To get the scattering potential energy we have to subtract from the total system energy the total energies of the separated particles

$$V(R) = E(R) - E_1 - E_2 \tag{9}$$

so

$$V(R = \infty) = 0$$

3. Results and discussion for I^{N+}–I

As the electron shell structure effect on the interatomic potential is very small in an absolute plot, we choose an ordinate that is relative to the average Lenz–Jensen [4] potential of the system I–I, as suggested by Loftager et al. [2]. The Lenz–Jensen potential fits the overall behaviour of many-electron systems quite well but does not take into account the effects of electronic shell structure. Its analytic form is in atomic units

$$V_{LJ} = \frac{Z_1 \cdot Z_2}{R} \cdot \phi(y) \tag{10}$$

with the screening function

$$\phi(y) = \exp(-y)(1 + b_1 y + b_2 y^2 + b_3 y^3 + b_4 y^4) \tag{11}$$

Here the coefficients are $b_1 = 0.9839$, $b_2 = 0.4272$, $b_3 = 0.0115$, $b_4 = 0.012\,88$. The variable is $y = (9.67 \cdot R/a)^{1/2}$ with the screening length $a = 0.8853\ (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$ in atomic units. Fig. 1 shows the quantity $(V - V_{LJ}) \cdot R$ as function of the internuclear distance for the system I^{N+}–I with ionizations 7+, 17+, and 25+ for one scattering partner. The ionized particles are assumed to be in the ground state. In this plot the electronic shell structure effects show up in the region between 0.1 and

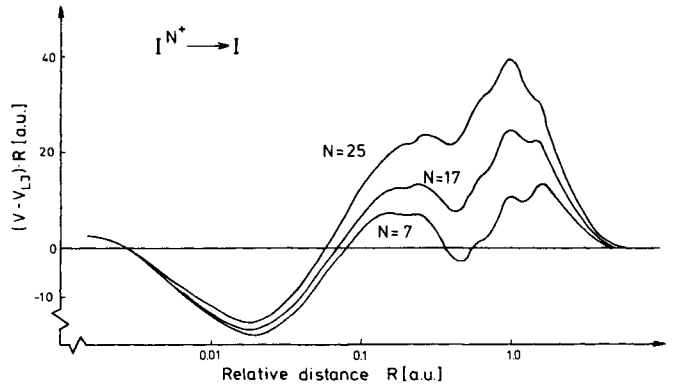

Fig. 1. Relative interatomic potential curves for the ionized scattering system I^{N+}–I.

2.0 atomic units. The minima at 0.02 a.u. are due to the analytic form of the Lenz–Jensen potential. One can see that with increasing ionization the screening is reduced and the peak structures, which result from the electronic shell overlap, are varying slightly in height, due to the different outer shell population, and in position, due to the shrinking of the ionized partner's wavefunction with increasing N.

To get a correspondence to experimental data we calculated the classical elastic scattering function $\theta(b)$ in the centre-of-mass (c.m.) system

$$\theta(b) = \pi - 2b\int_{R_0}^{\infty} \frac{dr}{r^2\sqrt{1 - b^2/r^2 - V(r)/E_{0\,cm}}} \tag{12}$$

where θ is the c.m. scattering angle, b the impact parameter, R_0 the distance of closest approach and $E_{0\,cm}$ the c.m. impact energy. The elastic differential scattering cross-section is given by

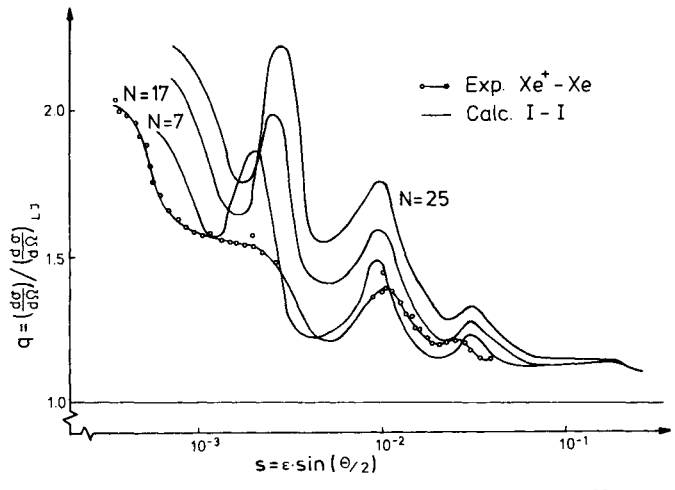

Fig. 2. Calculated differential scattering cross-sections for I^{N+}–I and experimental data from [2] for Xe^+–Xe.

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \frac{1}{|d\theta/db|} \tag{13}$$

In Fig. 2 results are shown for $E_{0\,cm}$ from 25 to 400 keV. A scaled plot is used where the small angle cross-sections for different impact energies fall on one curve, as worked out by Lindhard et al. in their LNS-theory [5]. The abscissa is dimensionless: $s = \epsilon \cdot \sin(\theta/2)$ with $\epsilon = (E_{0\,cm} \cdot a)/(Z_1 \cdot Z_2)$. The ordinate is the reduced differential scattering cross-section

$$q = \left(\frac{d\sigma}{d\Omega}\right) \Big/ \left(\frac{d\sigma}{d\Omega}\right)_{LJ} \tag{14}$$

where LJ indicates the value for the original Lenz–Jensen potential. The curve for $N = 7$ can be compared to the measurement of the system Xe^+–Xe [2]. The agreement is quite good except for the peak at $s = 2 \times 10^{-3}$. This one is smeared out by inelastic processes during the collision which are not separated by the experiment. The two curves for $N = 17$ and $N = 25$ show the development of the cross-section for increasing ionization. As there are no experimental data available for these highly ionized systems, we predict a general increase of the cross-section while the peak structure will change only slightly to higher s-values. Only the peak at very small s, which is enhanced in our model, will be lowered significantly by ionization and charge transfer during the collision.

4. Conclusion

In this communication we get an interpretation of the structures in interatomic potentials for the elastic scattering of atoms with highly charged ions. We show that with a simple statistical model rather good interatomic scattering potentials can be calculated which allow us to predict even detailed structures in elastic scattering cross-sections for scattering systems with various charge states.

Acknowledgement

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References

1. For a general review see Torrens, I. M., Interatomic Potentials. Academic Press, New York and London (1972).
2. Loftager, P., Besenbacher, F., Jensen, O. S. and Sørensen, V. S., Phys. Rev. **A20**, 1443 (1979).
3. Gombas, B., Handbuch der Physik (Edited by S. Flügge), **36**, p. 109. Springer, Berlin (1956).
4. Lenz, W., Z. Phys. **77**, 713 (1932); Jensen H., Z. Phys. **77**, 722 (1932).
5. Lindhard, J., Nielsen, V. and Scharff, M., K. Dan. Vid. Selsk. Mat.-Fys. Medd. **36**, No. 10 (1968).