Polarisabilities and long-range atom-atom interactions of atoms and ions

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Synopsis Effective oscillator strength distributions are systematically generated and tabulated for the alkali atoms, the alkaline-earth atoms, the alkaline-earth ions, the rare gases and some miscellaneous atoms. These effective distributions are used to compute dipole, quadrupole, and octupole static polarisabilities. These polarisabilities can be used to determine the long-range C_6, C_8 and C_{10} atom-atom interactions for the dimers formed from any of these atoms and ions, and we present example tables of some combinations. A relativistic description of the structure of heavy alkali atoms and alkali-like ions using S-spinors and L-spinors has been developed and results of the dynamic polarisabilities of Sr^+ will be presented.

The long-range interaction between two spherically symmetric atoms can be written in the form [1]

$$V(R) \approx -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} + \dots , \qquad (1)$$

where the C_n parameters are the London/van der Waals dispersion coefficients. There are two complementary approaches to the computation of the dispersion coefficients. One approach uses oscillator strength sum-rules, while the second utilizes Casimir-Polder relations and uses the dynamic polarisabilities computed at imaginary energies. These approaches can be regarded as complementary to each other.

The key to the first approach is to generate an oscillator strength distribution that incorporates excitations to bound excited states and to the continuum states. In practice, the oscillator strength distributions are best termed 'effective' oscillator strength distributions. One might find that the lowest few excited states are accurately represented by the distribution, however the higher bound states and continuum states are approximated with a set of discrete effective oscillator strengths and energies. The oscillator strength distributions can be derived from *ab initio* structure calculations, experimental information such as refractive indices, atomic transition rates and photo-ionization cross sections.

The Casimir-Polder relation is reliant on being able to calculate the dipole and multipole dynamic polarisabilities at imaginary frequencies. One way to calculate a dynamic polarisability is to use oscillator strength sum-rules in conjunction with a previously determined oscillator strength distribution.

We will report effective oscillator strength distributions and dynamic polarisabilities for a number of spherically symmetric atoms and ions [3]. The atoms presented are the noble gases, the alkali atoms and hydrogen, the singly-charged alkaline-earth ions and the alkaline earth atoms. The long-range atom-atom interaction coefficients C_6, C_8 and C_{10} are also presented for any dimer formed from these atoms and ions. A previous tabulation of dynamic polarisabilities for many of these atoms does exist [2]. This previous tabulation only gave the dynamic dipole polarisabilities, while the present tabulation extends this to the quadrupole and octupole polarisabilities that are needed in the evaluation of C_8 and C_{10}. The C_8 and C_{10} dispersion coefficients are typically included in analysis of diatomic spectra aimed at characterizing the inter-atomic potential curve.

A relativistic description of the structure of heavy alkali atoms and alkali-like ions using S-spinors and L-spinors has been developed [4]. The core wavefunction is defined by a Dirac-Fock calculation using an S-spinors basis. The S-spinor basis is then supplemented by a large set of L-spinors for the calculation of the valence wavefunction in a frozen-core model. The numerical stability of the L-spinor approach is demonstrated, and we present the dynamic polarisabilities of the low-lying states of Sr^+.

We also report here on C_6, C_8, D_8, and C_{10} dispersion coefficients of Ps (positronium) interactions with atoms, along with those of H, D, T interactions with Li and Be^+ isotopes.

References

[1] J. Mitroy, M.W.J. Bromley 2003 *Phys. Rev. A* **68** 052714

[2] A. Derevianko, S.G. Porsev, J.F. Babb 2010 *At. Data Nucl. Data Tables* **96** 323

[3] J. Jiang, J. Mitroy, Y. Cheng, M.W.J. Bromley 2015 *At. Data Nucl. Data Tables* **101** 158

[4] J. Jiang, J. Mitroy, Y. Cheng, M.W.J. Bromley 2016 *Phys. Rev. A* **94** 062514

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