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Atomic polarisabilities, hyperpolarisabilities and the factorisation of molecular interactions[1] J.M. ROSSI, B.A. RIGSBEE[2], K.G. ROLLIN, M.W.J. BROMLEY, Department of Physics and Computational Science Research Center, San Diego State University, San Diego CA, JIM MITROY, School of Engineering, Charles Darwin University, Darwin, NT, Australia — The properties of one and two-electron atoms and their molecules are calculated numerically using configuration interaction and perturbative methods. Firstly, we present calculations of the dynamic dipole and hyperpolarisabilities of the ground and low-lying excited states of atoms emphasising low-energy fields of interest in atomic clocks, and high-energy excitations that probe near Rydberg states. Theoretical expressions will be presented that factorise the long-range dispersion forces between two atoms into their individual scalar and tensor dipole polarisabilities at imaginary frequencies. This method yields C_6 dispersion coefficients in agreement with the latest theoretical values for both homo-nuclear and the hetero-nuclear interactions, eg. Li($2s$)-H($1s$). The application of this methodology to di-atomic molecular symmetries involving non-s-wave atomic states will be emphasised.

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