Fully Quantum Calculation of Dielectric Virial Coefficients for Noble Gases

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We present our recent results on the ab-initio calculation of dielectric and refractive virial coefficients of noble gases; we developed a systematic path-integral approach that can in principle be applied to coefficients of any order, including exchange effects at low temperatures. We show that in the case of the second dielectric virial coefficient, our approach is in perfect agreement with the standard wavefunction-based method for helium isotopes, neon and argon.In the case of the third dielectric virial coefficient, one of the necessary inputs – the three-body polarizability – is not yet available for any gas. We use state-of-the-art potentials and pair polarizabilities to calculate the values of the third dielectric virial coefficient of helium isotopes and argon, discussing the effect of the missing three-body polarizability in the framework of the superposition approximation. The effect of the propagated uncertainties from potentials and pair polarizability is also analyzed in detail, pointing out the areas where improvement in electronic-structure calculations will have the greatest effect on the accuracy of the dielectric virial.