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From scattering phase-shift computations to the determination of thermophysical and transport properties: van der Waals interactions and beyond

Owing to their huge importance, scattering processes by van der Waals pairs have repeatedly been revisited over the last two decades, permitting nowadays by means of high-accuracy interaction potentials to account for the ever-growing sophistication of the experiments. In that context, the computation of phase shifts is usually a critical issue since this quantity can permit to access to a large variety of physical properties, such as cross section, viscosity or thermal conductivity. Although subtle at a first glance, approaches enabling to calculate quantum-mechanical scattering phase-shifts only give a relative definition due to the arbitrariness of the arctan function. In contrast this trait is fundamental when Virial coefficients have to be determined since the need for absolute scattering phase shift is mandatory.

In that context, we have put forward a novel formula intended for absolute phase-shift calculations and we show how our formula can tackle situations involving van der Waals interactions. The formula relies on Lippmann-Schwinger (LS) or Volterra equations and phase-functions concepts and permits to definitely close the problem of the arbitrariness of the arctan function. Furthermore, also important is the ability of our approach to be extended to potentials of any range. This step forward can be achieved by a renormalization of the complex LS equation. Even potentials decaying as slowly as the Coulomb's one which range is infinite can be tackle with our method.

Choix de session parallèle

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