Application of high-precision computation in atomic and molecular physics

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Abstract: The variational method complemented with the use of explicitly correlated Gaussian basis functions has been demonstrated to have the capacity of calculating the properties of few-body systems with high precision. We originally developed the confined variational method to precisely determine the scattering parameters of theelastic scattering of electron, positron and positronium from few-body atoms and molecules in the low energy region. As its application, our results for the zero-energy scattering of e-H_2 and e^+-H_2 are in the best agreement with the experiments. In addition, our precise calculation for the Ps-H have resolved the confusion between the Kohn variational method and R-matrix method.

In the second part, we will talk about our work on the long-range interaction of atoms and ions. Based on the continuum model, we studied the long-range interaction between a pair of parallel pristine graphenesheets at zero temperature. The asymptotic form of the obtained potential density, $E(D)\sim -D^{-3}-O(D^{-4})$, consistent with therandom phase approximation and Lifshitz theory indicates that neglectance of the anisotropy is the reason that the widely used Lennard-Jones potential approach and dispersion-corrections indensity functional theory give a wrong asymptotic form of $E(D)\sim -D^{-4}$.

Resume: Dr.Jun-Yi Zhang got his B.S. from Nanhua Univ.(1997), Master from Jilin Univ.(2001), Ph. D. from Univ. of New Brunswick(2006). He worked as research associate in Charles Darwin Univ. from 2006-2010, then he did his postdoctoral research in King Abdullah Univ. of Science and Technology, Saudi Arabia from 2011 to present.