TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY FOR ELECTRON-ATOM SCATTERING: FINITE BASIS SET CALCULATIONS

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Introduction

Experiments by Sanche et al. [1] have shown that very low energy electrons (3-20 eV) are capable of inducing DNA strand breaks. Present day ab initio scattering methods are unable to describe large DNA fragments because of high computational cost.

(TDD)DFT is a computationally much cheaper method. In collaboration with prof. Kieron Burke (UC Irvine, USA) a scattering method for DFT is being developed.

Scattering with (TD)DFT

The correct procedure is to start from a system that combines the target and the scattering electron [2]. That is, we start from a situation where the electron is bound to the target system, or resides in a resonant state of the target.

We then excite the added electron into the continuum using TDDFT, and calculate the excitation energy. If our target is an atom, and the (N+1)-electron system has a short ranged potential, we can place the atom in a box and obtain the phase shift from the excitation energies.

Atom in a cavity

Putting an atom inside a hard sphere cavity discretizes the continuum. Each positive energy state obtained corresponds to true continuum states, up to the wall radius R.

The scattering phase shift can then be obtained from these “continuum” orbitals, for a long ranged potential such as He, from:

\[ \delta_{nl} = -\frac{F(E_{nl} - \epsilontır, \epsilontır, \epsilontır)}{G(E_{nl} - \epsilonтир, \epsilonтир, \epsilonтир)} \]

where F and G are Coulomb functions and \( \epsilonтир = \sqrt{\epsilontır^2 + \epsilonтир^2} \).

Phase shifts

The phase shifts obtained from a suitably chosen, large BSTO basis set, are equal to the phase shifts obtained using a grid code with a wall placed very far away (the “exact” (TD)DFT results). The finite basis set method does not allow the cavity to be too large, to keep the basis set size manageable and to avoid linear dependency problems. Therefore multiple calculations at different smaller wall sizes need to be performed to fill in the curves.

Conclusion

The phase shift for low-energy electron-atom scattering obtained with TDDFT is remarkably accurate. The atom is placed in a hard-wall cavity to obtain the continuum KS orbitals as pseudo-states.

A finite size basis set with a boundary pre-factor is able to reproduce the exact TDDFT results. Since only small wall radii can be used, different wall sizes are needed to fill in the large, to keep the basis set size manageable and to avoid linear dependency problems.

References


Acknowledgments

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Eberhard Engel, J.W.Goethe-Universität Frankfurt am Main

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