Solvated Electron

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Abstract

Increasing attention has been given to the interaction of the solute wave function with solvents. Computing such interactions for a large molecule is expensive. Therefore, the solute-solvent interaction are being investigated here by utilizing a simple model: a solvated electron in water or ammonia. The electron is trapped by the polarization of the medium due to the presence of the electron. Unlike the hydrogen atom, the potential due to the trap depends on the electron inside the trap. Thus, the objective of this project is to develop a simple way to obtain the electron energy and wave function using Mathematica and Maple.

The model for a solvated electron in ammonia was constructed by Jortner in 1958. In his model, the potential energy was divided into two parts: inside and outside of the trap. The potential energy was assumed to be constant inside the trap and the inversely proportional to the distance outside the trap. Jortner's calculation was done by using a Slater function. This project models the trap potential using a uniform solvent and dielectric constant. The calculations were performed using one and two contracted Gaussian functions. Figure 1 shows Jortner's wave function and one and two term Gaussian functions.

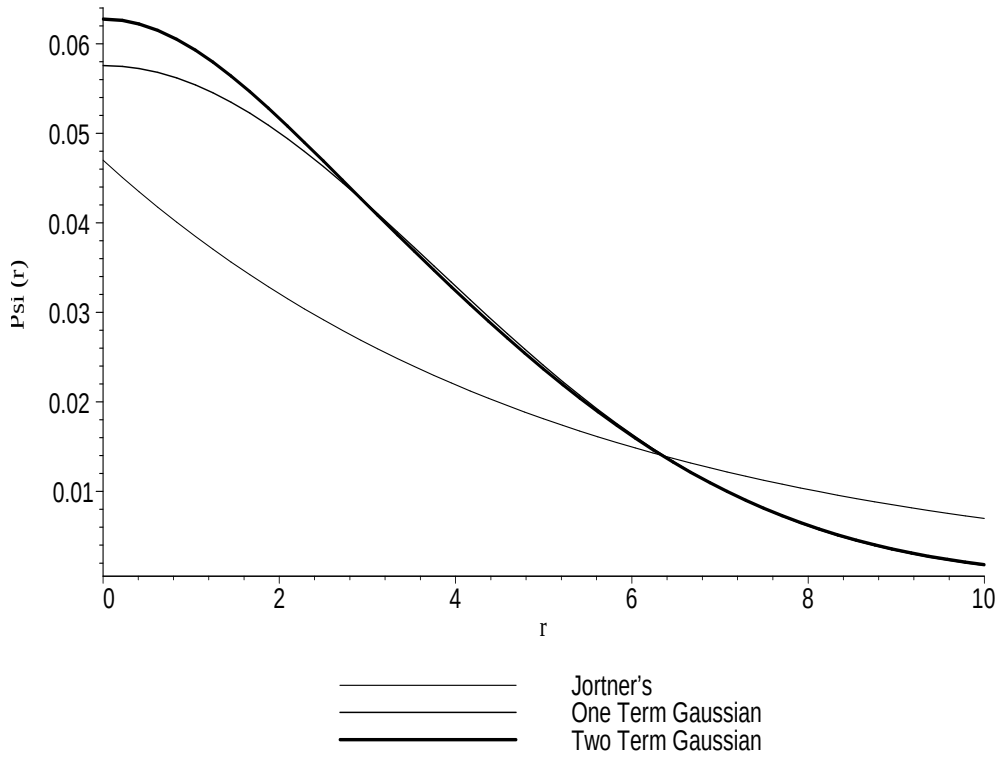

Figure 1: Comparison of calculated wave functions