SPECTRAL LEARNING FOR SOLVING THE SCHRÖDINGER EQUATION FOR MOLECULES

Y. SALEH*, J. EGGERS, V. SANJAY, A. ISKE, A. YACHMENEV, J. KÜPPER

ABSTRACT

Computing the eigenfunctions of the Schrödinger equation in many dimensions is classically based on a Galerkin-approach, where one seeks to approximate the eigenfunctions in the linear span of some given basis set of L^2. Although this method is well-established and we have guarantees for its convergence, it suffers from the curse of dimensionality as the size of the basis set needed to converge the computations scales exponentially with the dimension of the problem. Moreover, this method suffers from a bad scaling as well with the number of computed eigenfunctions.

Here, we present a nonlinear variational pricinple that approximates eigenfunctions in the linear span of *Augmented basis sets*. These sets are constructed using normalising flows [1] where the base distributions are the functions of a standard basis set of L^2. The proposed framework shows more stability during training than nonlinear calculations using standard neural networks [2, 3]. It promises to mitigate the curse of dimensionality and to allow for more accurate computations of eigenfunctions corresponding to high eigenvlaues. We present computations of the vibrational spectra of the water molecule and convergence guarantees under certain assumptions on the potential-energy surface. Moreover, a presepective to use these methods for (ro-)vibrational and dynamics calculations of weakly-bound complexes is outlined.

References

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* Department of Mathematics, Universtät Hamburg, Hamburg, Germany and Center for Free-Electron Laser Science, Deutsches Elektronen-Sychrtron DESY, Hamburg, Germany, yahya.saleh@cfel.de