Numerics for Many-Body Systems

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Introduction

Making accurate predictions of many-body systems is paramount to understand the behavior of condensed-matter physics, physical chemistry, and material science. The complexity of the many-body Hamiltonian points toward computational methods as the richest avenue for progress.

$$\hat{H} = -\frac{1}{2}\sum_{i}^{N_e}\nabla_i^2 - \sum_{i}^{N_e}\sum_{I}^{N_n}\frac{Z_I}{|\vec{r}_i - \vec{R}_I|} + \frac{1}{2}\sum_{i}^{N_e}\sum_{j\neq i}^{N_e}\frac{1}{|\vec{r}_i - \vec{r}_j|} + \frac{1}{2}\sum_{I}^{N_n}\sum_{J\neq I}^{N_n}\frac{Z_I Z_J}{|\vec{R}_I - \vec{R}_J|}.$$

Methods

We explore computational progress via two avenues. First, we present a self-consistent Hartree-Fock algorithm tested under the system of electrons in a box with a randomized nuclei distribution of varying number of nuclei and nuclei charge. Second, we develop a many-body Finite Element program using N-Dimensional Cubes. We map each element to a reference cube of edge length 1 and compute the mass and stiffness matrices via the basis of N-D tensor products of the set:

$$\{x_1, 1-x_1, \ldots, x_N, 1-x_N\}$$

We then take the appropriate symmetric or antisymmetric combination in accordance with the bose-einstein statistics of the system.

Results

Hartree- Fock: Plotted to the right are the electron wave functions followed by the electron density and nuclei coordinates for a randomized nuclei distribution. The plots provide strong indication of the success of the self-consistency algorithm, as well as some interesting physical results:

1. Electron wave functions pulled towards positive charge with respect to their unperturbed free particle analogs.
2. Wave-functions with higher expected kinetic energy are displaced less so than those with less kinetic energy.
3. Wave-functions reach their maximum towards the edges of the box.
4. Increasing nuclei charge and the number of nuclei raises the minimum expected kinetic energy of the electrons.

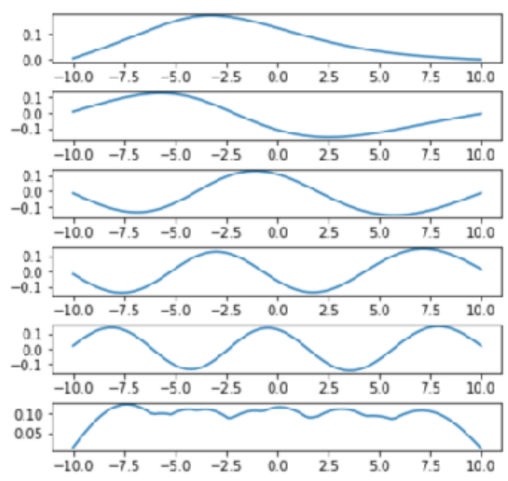
N-D Finite Elements: Plotted towards the bottom right are the first three solutions of the free Hamiltonian for fermions, demonstrating the antisymmetric capabilities of the finite elements. We display the wave functions for 2 electrons in 1 physical dimension for visualization purposes, although the program handles any N electrons.

Discussion

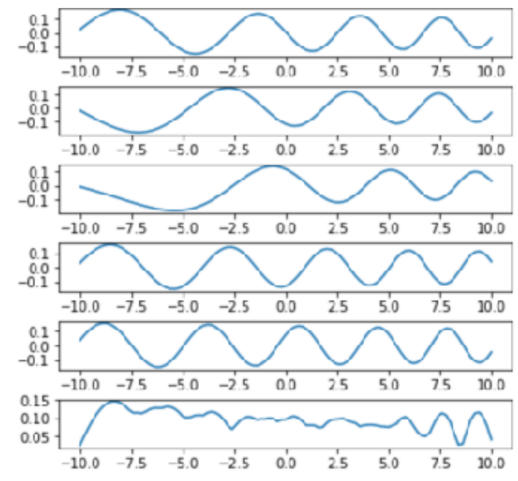
Currently, the dimension of physical space for the N-D finite element program is constrained to 1-D by the dimension of the edge of our N-D cubes. Our current outlook is to generalize the concept of a cube's edge to a higher dimensional space and/or data structure.

Electron Wave-functions and Charge Density

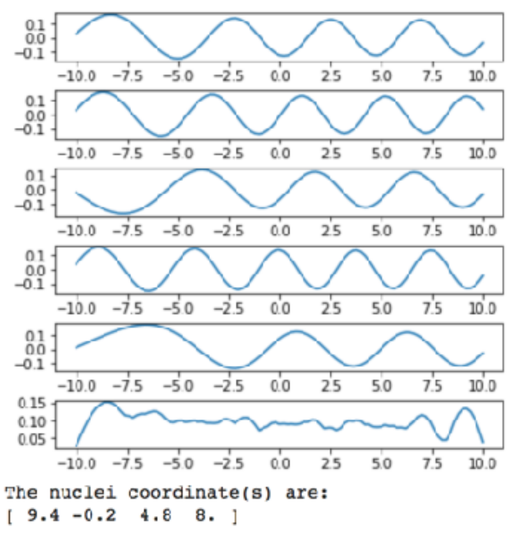
1 Nuclei Z = 3



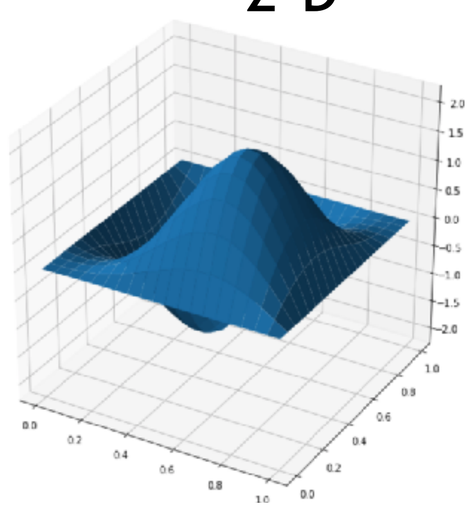
1 Nuclei Z = 35

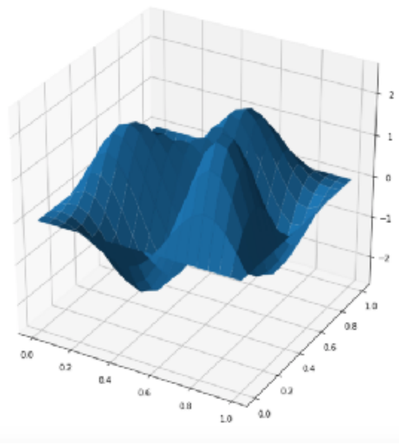


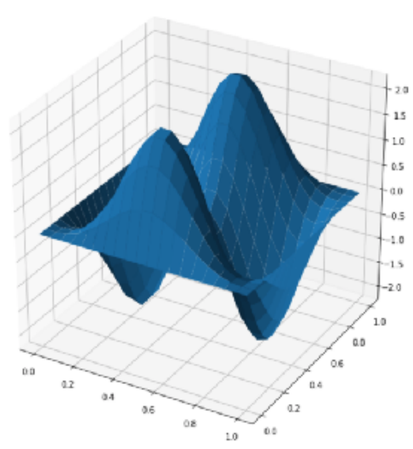
4 Nuclei Z = 3



Free Fermions in 2-D







Literature Cited

Chen, L. (n.d.). Programming of Finite Element Methods in Matlab. *University of California Irvine*.

Johnson, C. (n.d.). *Numerical Solutions of Partial Differential Equations by the Finite Element Method*. Cambridge University Prerss.

Lin, L. (2016). Adaptively Compressed Exchange Operator. *JCTC*, 1–3.

Reddy, C. J., Deshpande, M., Cockrell, C. R., & Beck, F. (n.d.). Finite Element Method for Eigenvalue

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