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Full Length Research Paper

Discrete singular convolution for Lennard-Jones potential using Shannon kernel

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In this paper, the idea of discrete singular convolution (DSC) as a viable computation method for analyzing physical systems has been underlined. Discrete singular convolution has been used for solving the Schrödinger equation for water molecules, subject to the Lennard Jones potential, and the DSC differentiator has been used for obtaining the energy eigen-states of water, for a given grid size for discretization, along with the Shannon kernel for approximation of the singular delta-type kernel in the problem.

Key words: Discrete singular convolution, computational methodology, Schrödinger equation, Lennard Jones potential.

INTRODUCTION

In the world of computational methodology, one has global and local methods for analysis. Global methods are more accurate and localized than local methods. However, local methods are more useful for handling particular kinds of problems, especially those involving certain boundary conditions.

Discrete singular convolution (DSC) is a potential numerical approach for solving computational problems. Wei worked on the application of this method for problems such as the use of discrete singular convolution for solving the Fokker-Planck equation (Wei, 1999) analyzing the nonlinear dynamic response of laminated plates (Civalek, 2013) and free vibration analysis of multiple-stepped beams (Duan and Xinwei, 2013). The purpose of this paper is to use the DSC algorithm for the numerical solution of the Schrodinger equation for solving for the energy eigen values of the Schrodinger equation for the Lennard Jones potential in water using the Shannon kernel. This is along the lines drawn by *Wei* in his seminal paper on the topic (Wei, 2000).

The Lennard Jones potential has been a subject of interest among physicists with the associated computational methods used to analyze it. Huacuja et al. (2007) have analyzed the molecular configurations which minimize the Lennard Jones potential. Barr et al. (1995) and McGeoch (1996) have established the plinth of computational analysis in terms of statistical and experimental aspects of algorithms. As per one of the main criteria for computational methods, one needs to optimize the resources available in one's disposal for the evaluation or analysis of a problem. For studying problems involving either sample size approaching to infinity or a discontinuity in any variable, one needs to devise a way to circumvent this problem using the tools available. Barr et al. (1995), McGeoch (1996), Pattengale et al. (2009) and Terán-Villanueva et al. (2013) have proposed a set of principles that allow us to extract scientific knowledge from these methods. This includes relevant computational experiments, as per the literature related to the given subject, which must be reproducible and should relate with other studies carried out in the relevant field.

Solving the Schrödinger equation is a non-deterministic polynomial (NP) type of problem. This means that if the

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problem's solution can be guessed in some polynomial time, but no rule is followed on how to make the guess for the solution Arkady (2013). None of the instances of the equation's guessed solutions have yielded an algorithm for exactly solving this equation in a polynomial or reasonable number of steps for any quantum system. It is in this context that the idea of discretizing the Schrödinger equation for solutions becomes worth noting. For this one could use the idea of convolution, as in the case of discrete singular convolution (DSC), explained in the following section. More importantly, going by McGeoch's formulation, one needs to test the relevance of Wei's DSC algorithm for solving for the Schrodinger equation for more complex systems than the Morse potential for iodine.

DISCRETE SINGULAR CONVOLUTION

Discrete singular convolution is a general approach for numerically solving problems involving singular convolution such as in Hilbert transforms and Abel Transforms. Using the appropriate kernel, one can use the formalism to solve a number of physical problems. The discrete singular convolution approach is based on the theory of distributions. Let W be a distribution and $f(x)$ be an element of the space of test functions for the kernel. If W is a singular kernel, we can define what is known as the singular convolution:

$$F(x) = W * f(x) = \int_{-\infty}^{\infty} W(x-y) f(y) dy$$

One such kernel is the singular kernel of the delta type (δ). One must remember that the Dirac Delta function is a generalized function itself and not strictly a function, as per the conditions satisfied by functions. Since these are singular kernels, one cannot use them in computation methods. To overcome this problem, one defines a sequence of functions that are approximations of the distribution:

$$\lim_{\alpha \to \alpha_0} W_\alpha(x) \to W(x)$$

Here α_0 is the generalized limit. For a singular kernel of the delta type, one has a delta sequence.

Delta sequence

Any sequence of functions $f_n(x)$ which converges to the Delta function for $n \to \infty$. One can define the approximation to the convolution as:

$$F_\alpha(x) = \sum_j W_\alpha(x - x_j) \times f(x_j)$$

Here, $\{x_j\}$ represents the set of points for which the algorithm is defined. One must note that this algorithm is valid only for smooth approximations of the Kernel. One kernel of the Delta type is the Shannon kernel, which is defined as:

$$\frac{\sin(\alpha(x - x_0))}{(x - x_0)}$$

One often defines an algorithm sampling element or the *Nyquist* frequency for discrete singular convolution. It can be defined as:

$$\alpha = \frac{\pi}{\Delta}$$

One can then define the Shannon kernel as:

$$\frac{\sin(\frac{\pi}{\Delta}(x - x_0))}{\frac{\pi}{\Delta}(x - x_0)}$$

DSC approach for Schrodinger equation

We have a grid representation for the coordinate so that the potential part of the Hamiltonian is made diagonal. One can represent the Hamiltonian in the matrix form:

$$H(x_i, x_j) = -\frac{\bar{h}^2}{2m} \delta_\alpha{}''(x_i - x_j) + V(x_i)\delta_{ij}$$

where

$$\delta_\alpha{}''(x_i - x_j) = \frac{d^2}{dx^2}[\delta_\alpha(x - x_j)]|_{x=x_i}$$

and

$$\delta_\alpha(x - x_j) = \frac{\sin(\frac{\pi}{\Delta}(x - x_j))}{\frac{\pi}{\Delta}(x - x_j)}$$

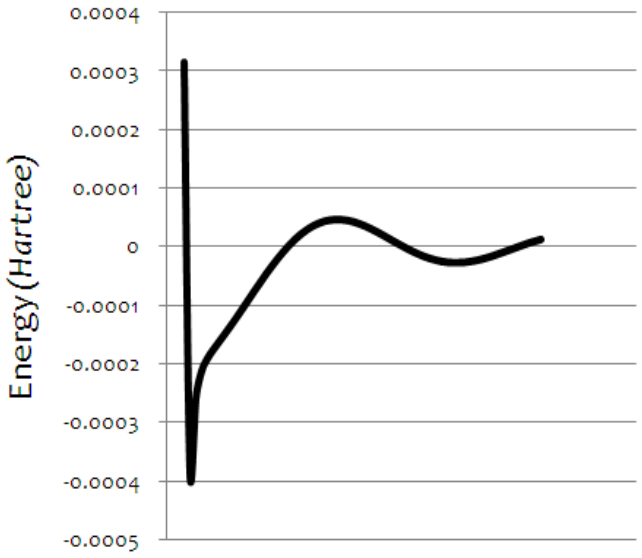
in this case.

Lennard Jones potential

Lennard-Jones potential describes the interaction between uncharged molecules. It is mildly attractive as two molecules approach each another from a distance,

Table 1. Energy Eigenvalues *(in Hartree)*

1.005E+03	8.074E-06	-2.730E-05	2.890E-06
2.294E-01	2.477E-06	-2.730E-05	1.282E-05
3.142E-04	-2.913E-06	-2.661E-05	2.156E-05
-3.876E-04	-7.982E-06	-2.523E-05	2.890E-05
-2.592E-04	-1.259E-05	-2.340E-05	3.509E-05
-2.122E-04	-1.668E-05	-2.106E-05	3.991E-05
-1.906E-04	-2.018E-05	-1.821E-05	4.335E-05
-1.755E-04	-2.294E-05	-1.505E-05	4.542E-05
-1.619E-04	-2.523E-05	-1.161E-05	4.633E-05
-1.484E-04	-2.661E-05	-7.982E-06	4.587E-05
-1.344E-04	2.913E-06	-4.312E-06	4.450E-05
-1.202E-04	6.285E-06	-6.400E-07	4.220E-05
-1.055E-04	9.381E-06	-6.124E-05	3.876E-05
-9.060E-05	1.216E-05	-4.679E-05	3.486E-05
-7.569E-05	-3.326E-05	-2.025E-05	3.005E-05
1.379E-05	1.945E-05	-8.166E-06	2.500E-05



Graph 1. Plot of eigenvalues obtained.

but is strongly repulsive when they are close to each other. The 12:6 Lennard Jones potential form is given as:

$$V = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

METHODOLOGY

In this work, discrete singular convolution methodology was used to analyze the system of water molecules, subject to the conditions:

$$\sigma = 0.3166 \times 10^{-9} m$$
$$\varepsilon = 1.08 \times 10^{-21} J/mol$$

To begin with, the Hamiltonian matrix was obtained for the system, using the DSC-Hamiltonian matrix formulation (A), using the Shannon kernel, for the parameters,

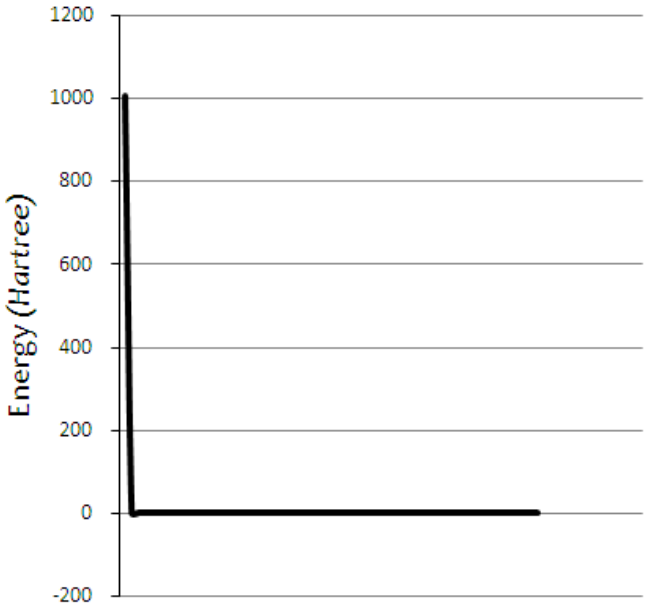
$$\Delta = 1 \times 10^{-12} m$$
r = 0.942×10^{-10} m.

the mean bond length of water.

Thereafter, the diagonalization of the matrix was carried out to obtain the eigen vectors of the given system, subject to the Lennard Jones potential.

RESULTS

For 64 grid-points for the DSC evaluation, the following eigen values were found in Table 1. Magnifying Graph 1, one finds these interesting characteristics. The representation for the entire range of eigenvalues gives us a graph similar to that for the Wigner Distribution (Graph 2). Wigner distribution is the probability



Graph 2. Wigner Distribution.

distribution on the interval $[-R, R]$ whose probability density function is a semicircle of radius R centered at (0, 0), and given by:

$$f(x) = \begin{cases} \frac{2}{\pi R^2}\sqrt{R^2 - x^2}, -R \le x \le R \\ 0, R < |x| \end{cases}$$

This distribution arises as the limiting distribution of eigen values of symmetric matrices whose size approaches

infinity. The given data complies with this distribution, and increasingly so as the number of grid points are increased from 16 to 64.

Conclusion

The discrete singular convolution method was studied and used for finding the eigen values of water molecules under the influence of the Lennard Jones potential.

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