Optimization of finite difference coefficients for quantum molecular dynamics

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1 Background

Quantum Molecular Dynamics(QMD) provide an accurate information of what happens to individual atoms and molecules during an experiment. The key equation of QMD is Schrödinger equation.

2 Main Goal

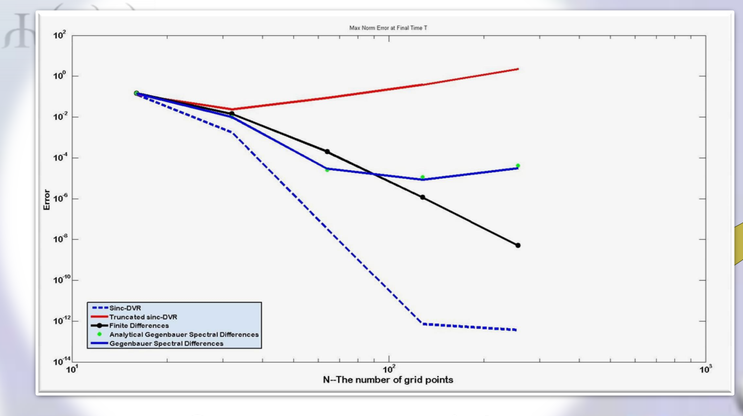
Finding the best approximation of the Hamiltonian operator which is more accurate and sparse

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t}=\left(\frac{-\hbar^2}{2m}\nabla^2+V(r,t)\right)\Psi(r,t)$$

3 Methods

1. Sinc-Discrete Variable Representation
2. Truncated Sinc-Discrete Variable Representation
3. Finite Differences
4. Spectral Differences

4 Results

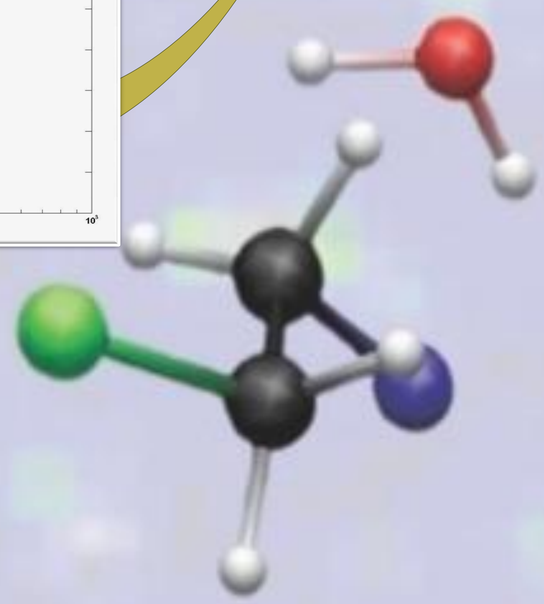


Convergence plot

5 Conclusion

Methods	Accuracy	Execution time
Sinc-DVR	Exponentially convergence	Maximum(4^{th})
Truncated Sinc-DVR	Terrible Accuracy	Average(3^{rd})
Finite Differences	High Accuracy	Average (2^{nd})
Spectral Differences	Exponentially convergence	Minimum(1^{st})

Solving the Analytical Gegenbauer spectral differences in Maple to get better accuracy



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