Study of Numerical Methods to Solve the Quantum Mechanical Three-Body Problem

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STUDY OF NUMERICAL METHODS TO SOLVE THE QUANTUM MECHANICAL THREE-BODY PROBLEM

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HELIUM

- The helium atom with two electrons serves as a model for many other three-body problems in atomic physics.
- Unlike hydrogen, it is the simplest system that cannot be solved exactly in the nonrelativistic limit; but it displays many of the complications found in multi-electron atoms.
- Thus, it has been researched extensively since the beginnings of quantum theory.

TYPES OF PRECISION

- Single Precision : 4 bytes

  PI = 3.14159274

- Double Precision : 8 bytes

  PI = 3.1415926535897931

- Quadruple precision: 16 bytes

  PI = 3.14159265358979323846264338327950280

- Double Quadruple (DQ) precision : 32 bytes

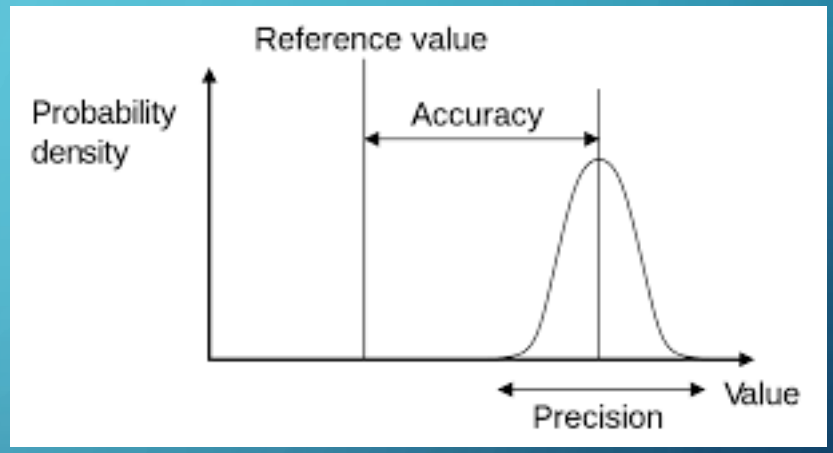
  PI = 3.14159265358979323846264338327950279747906809813729557300450433187429 67E0

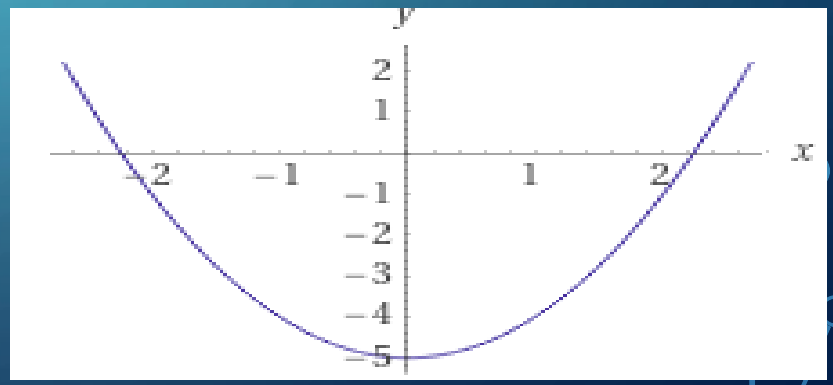
WHY ARE WE USING THE DQ PRECISION?

1. To increase the numerical accuracy from 32 to 70 figures, which is the maximum machine accuracy
2. Since there is loss of 10 to 15 figures while calculating in quadruple precision (32 figures), this is solved by using double quadruple precision.

THREE METHODS OF CALCULATION

- There is no exact solution yet for calculating the energies of threes-body systems due to the complexity of the system; there are only approximations that become very close to the exact solutions to the Schrodinger equation.
- In this project we are comparing the accuracy of three methods using double quadruple precision, The more negative the eigenvalue (energy) the closer it is to the true value, because the calculated value is an upper bound for the true value
- These calculations depend on the derivatives of the energy with respect to nonlinear parameters, using Newton Method to find the zeros of the derivatives. Hence the smaller the derivative the closer the energy gets to the true eigenvalue





In this project, we compare the accuracy and speed of three methods of calculating eigenvalues (energies) of helium:

- Power Method
- Tridiagonalization method
- Jacobi's method

By transferring Dr. Drake's Fortran program from quadruple version to double quadruple precision (dq) using David Bailey's module. This increases the numerical accuracy from 32 decimal digits in quadruple precision to 70 decimal digits in dq-precision - the machine epsilon is 7×10^{-70}.

HOW THE THREE METHODS OF CALCULATION USED?

- ***Jacobi's method*** is the slowest, but the most numerically stable (1 to 1.5 min). It is used to find the complete set of eigenvalues of a symmetric matrix by repeated exact diagonalization of a 2 x 2 matrix formed by two diagonal elements and the matching largest off-diagonal element. This process is iterated until it converges.
- ***Tri-diagonalization method*** (about 20 seconds). It reduces a Hermitian matrix to tridiagonal form that is then diagonalized to find the complete set of eigenvalues and eigenvectors.
- ***Power method*** with inverse iteration (2-3 seconds): it converges to the single eigenvalue that is closest to an initial guess and corresponding eigenvector.

COMPARING THE THREE METHODS - RESULTS

N=2 omega = 5 number of terms = 166 Basis set sizes: 56 56 54

Tridiagonalization:

-2.12384308569438746037391606774407980582945603774312859353171492038535585E0

Jacobi's

-2.12384308569438746037391606774407980582945603774312859353171492039079925E0

Power Method

-2.12384308569438746037391606774407980582945603774312859353171492038521102E0

COMPARING CALCULATIONS

Energy level n = 2 (P-state: angular momentum = 1)

-2.123843086498093 (Dr. Drake's previous calculation using quadruple precision)

-2.123843086498101353584574505977314768654705305692076568167693181341304 5E0

(current calculations using double quadruple precision)

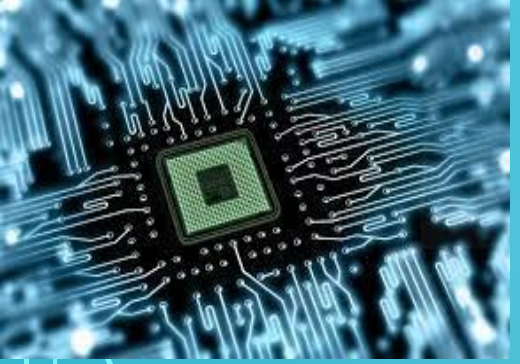
Energy level n = 15 (S-state: angular momentum = 0)

-2.00226424127026347 6 (Hiroyuki Nakashima, Yuh Hijikata and Hiroshi Nakatsuji calculations using ICI method)

-2.00226424127026347765315195066595537126434732710756049792973078605240 75E0

(our current calculations using double basis sets with the Power Method)

New World Record!



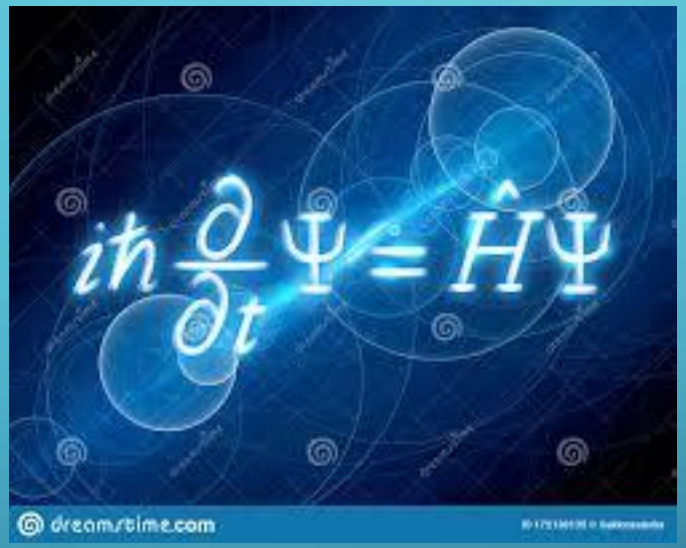
IMPORTANCE AND APPLICATION OF HIGH PRECISION CALCULATIONS

- The progress of civilization and technology is determined by how accurately we can measure things starting from steam engines → microchips → quantum computing.
- High precision calculation will develop many current used applications and instruments such as the global positioning system (GPS), and gravitometer.
- Finding high precision calculations for physical universal constants such as Rydberg Constant, and Fine Structure Constant.

PLANNED FUTURE RESEARCH

Our current calculations of Helium energy are not including quantum electrodynamic and relativistic corrections, so we are planning to include these corrections so we can compare our calculations with the experimental measured values.

Thank you



REFERENCES

- *G.W.F Drake. Atomic, Molecular, and Optical Physics Handbook*

2006

ISBN : 978-0-387-20802-2

- *G.W.F Drake. Long-Range Casimir Forces*

1993

ISBN : 978-1-4899-1230-5

- *G.W.F Drake lectures. http://drake.sharcnet.ca*
- *Hiroyuki Nakashima, Yuh Hijikata and Hiroshi Nakatsuji . The Journal of Chemical Physics*

J. Chem. Phys. ***128****, 154108 (2008); https://doi.org/10.1063/1.2904871*