



Multibody Energy States With exact electron-electron interactions

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Abstract

In a class on quantum mechanics in 1964 at LSU a question was asked whether the potential energies of a multibody could be added up to give the energy state. It was stated that Vanagas was somewhat successful in using 2 body states. In 1971 two hypotheses were made using current Hilbert Space applied to the multibody Schrödinger's Equation and the wave functions derived. The ground states of atoms with atomic number $Z=2-20$ were calculated and agreed with Hartree-Fox iterations. The success was due to the exact electron-electron interactions.

Key Words

Physics; Quantum Mechanics; Multibody Energy States; Multibody Schrödinger's Equation Solution;

Introduction

The material here presented uses the Texas Method of solving mathematical theorems. A few lemmas are required before the derivation of the solution of the multibody Schrödinger's Equation.

The derivative of a function of x offset by a constant c with respect to x is equal to the derivative with respect to x offset by c . From the definition of the derivative: $\lim_{x \rightarrow c} \frac{|F(x-c)-F(x'-c)|}{|x-x'|} = \lim_{x \rightarrow c} \frac{|F(x-c)-F(x'-c)|}{(x-c)-(x'-c)}$.

From Goldstein Classical Mechanics near the end of chapter 1 can be found the Virial Theorem which says statistically $2T=-V$ or $2E=V$. This holds for the S orbitals and the peak of the P orbitals.

From Hilbert space with T, V and E as Hermitian operators with positive signed eigenvalues, the Schrödinger's Equation for the hydrogen atom is given by $T-V=-E$ and with the same eigenfunctions $V-T=E$ by multiplying both sides of the equation by -1 .

The possibility of independent distances between N points where $n=N(N-1)/2$ is shown by a rotation tensor acting on an n dimensional vector yielding an $n+1$ dimensional vector conserving the distance d except for the last distance which varies independently.

$$\begin{vmatrix} a_{11} & a_{1n-1} & a_{1n} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ a_{n1} & a_{nn-1} & a_{nn} \end{vmatrix} \times \begin{vmatrix} 1 & \dots & \cos(\theta) & a_{1n}\sin(\theta) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \dots & \cos(\theta) & a_{n-1}\sin(\theta) \\ 1 & \dots & \cos(\theta) & a_{nn}\cos(\theta) \end{vmatrix} =$$

$$A^*T=B$$

$$d_i^2 = a_{i1}^2 + a_{i2}^2 + \dots + (a_{in}\sin(\theta))^2 + (a_{in}\cos(\theta))^2$$

$$A_{ij}^*T_{ij} = B_{ij}$$

$$\begin{vmatrix} a_{11} & \sin(\theta)a_{1n} & \cos(\theta)a_{1n} \\ \cdot & \cdot & \cdot \end{vmatrix}$$



solution is well known and is not done explicitly in the derivation. The second derivative returns the equation to a dot product scalar sum of the two varieties of terms d^2 and d^*d as shown in the derivation. Setting the equation plus the potential energy V to an unknown E times ψ gives the separated Schrödinger's Equation by dividing by the function ψ resulting in a series of independent terms each of which may be set equal to a constant E_{ij} whose sum is a constant E . Each term is a hydrogen equation and is given. E is the energy state of the atom. Note the e-e solution is below. The ψ function is solved to be the product of hydrogen wave functions.

Results

Ground states of atoms found in the Handbook of Chemistry and Physics compared to ground states calculated from the above derivation.

Z	E0	E6	E sawf	E HBCP	%error
2	81.6	2.6	79	79	0.0%
3	214.2	8.3	205.9	205.2867	0.3%
4	421.6	19.1	402.5	402.5354	0.0%
5	714	36.6	677.4	677.54	0.0%
6	1101.6	62.5	1039.1	1041.018	-0.2%
7	1594.6	98.3	1496.3	1502.637	-0.4%
8	2203.2	145.8	2057.4	2066.402	-0.4%
9	2937.6	206.6	2731	2745.903	-0.5%
10	3808	282.2	3525.8	3550.808	-0.7%
11	4803.8	374.3	4429.5	4470.897	-0.9%
12	5937.5	484.5	5453	5513.738	-1.1%
13	7215.7	614.5	6601.2	6681.209	-1.2%
14	8644.8	765.9	7878.9	7978.725	-1.3%
15	10231	940.3	9290.7	9411.34	-1.3%
16	11981	1139.4	10841.6	10979.88	-1.3%
17	13902	1364.7	12537.3	12691.81	-1.2%
18	16000	1618	14382	14551.74	-1.2%
19	18281	1901	16380	16550.14	-1.0%
20	20753	2214.7	18538.3	18693.41	-0.8%
21	23421	2561.5	20859.5	20985.43	-0.6%
22	26282	2943	23339	23434.67	-0.4%

The table gives the sawf ground state E_0 for the first 20 atoms of atomic number Z . The next column is the energy state with the electrons in the 6th orbital E_6 . The next column is $E_{\text{sawf}} = E_0 - E_6$ which compares to about 1% with the next column ground state from the Handbook of Chemistry and Physics. It appears the E_6 correction is due to accepted calculations stopping at the 5th or 6th orbital. The difference for $Z=11-20$ is explained by the nuclear spin:

Main quantum number n correction from nuclear spin..Orbital capacities are 2,16,36...Not 2,8,8,18,18...

The main quantum number n is 1 for the first row of the periodic table and $n=2$ for the second row and is thought to change to 3 for the third row for new states. However the nuclear spin flips providing 8 new states with $n=2$ in the third row. Each higher row is off also.

Electron -Electron Solution

Solve the electron - positron Schrödinger's Equation noting the energy is $1/2$ because of the reduced mass. From group theory the energy equation is $T - V = -E$ and multiplying both sides by -1 the energy is found to be positive:

$$V - T = E.$$

The wave functions are the same and the energy is $13.6x/(n^2)/2$. x is unknown but may be solved for in a element of atomic number Z . From the Virial Theorem (Classic Mechanics by Goldstein (index)) statistically:



$$V=2E$$

The potential energy is $V=Z/r$ and $V=13.6x/n^2$. $r = n^2/(13.6x)$. From the solution for the hydrogen atom for r we see $x = 2Z$. Thus for e-e $E=13.6Z/n^2$ and from the triangle inequality we can solve for the range of n and the longest distance will give the most negative total energy. The distance is bounded by the nucleus electron distance (a greater bond). For N electrons $mass=1/2$:

$$n!/(n-2)!2!(1/2)=n(n-1)2/2! =n(n-1)\Rightarrow n(n-1)13.6Z/m^2$$

m is found by the triangular inequality from the nuclear-electron r which is the stronger bond.

$$m^2=(n1^2 + n2^2)$$

Summary

The Texas Method of mathematical proof has been applied to the second order differential equation, the Schrödinger's Equation discovering an exact electron-electron solution and an exact total solution within a zero perturbation. Application to chemical processes will require further study. A finding of the correction of the main quantum number n is important showing a correction needed for all current quantum iterative models.

References

Handbook of Chemistry and Physics 87th Edition 2006-2007 Experimental Values 10-203

James W Goodman biography

Over 50 hours of graduate physics and math courses.

BS physics

Followed the solution of the hydrogen Schroedinger equation.

Solved the hydrogen equation using group theory.

Studied Hilbert Space and QM group theory.

Graded Hilbert Space group theory theorems.

89 percentile physics GRE

Member of Mensa

1971 The design of this digital cell phone is proprietary information for the Bell System.

1972 The Schoedinger equation was studied with the idea of writing down the potential energy between each pair of particles and adding them up.

1972 Two new assumptions were written down and from this the Schoedinger equation was solved. The electron electron interaction was solved exactly. The ground state energy of the first 10 elements was found exactly correct. New physics was found for the rest of the elements. The nuclear spin had been omitted.

1979 Bell needed a power forecasting and record keeping system. The secret was to use an exponential growth curve fitted to the three high values of the amperage. The statistical theory says that more users cause more mips cause more amps.

1980's described the DSL to Bell and asked them to provide for students to hook up to the Internet. At that time the high-speed available was 2400 bits per second. DSL provided 1 million bits per second.

1980's from study of the Aluminum gallium arsenide laser showed Cox cable how to turn around the repeaters. It shows that with the voltage below lasing the laser is a receiver.

1980's from study of calculus of statistics and study of traffic engineering with the Bell System pointed out the problem with too many users on one T1 Line. At high usage after supper 10 users on one T-1 line would get about 100,000 bits per second. This increased the demand for DSL's.



1990's Suggested from a sawf study to Lockheed Martin the alloy LiAl for the skin of the shuttle tank. They used the Super Lightweight Tank for years. Each pound saved would put a pound added to the load in orbit.

2013 most reactions go through many energy states. Each difference in energy state represents gain or loss of a photon. The highest gain is the activation energy. The sum of the losses is the heat of formation. The greatest loss is the bond strength

