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Numerical Method for a Confined Atomic System

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Introduction

Quantum Confinement is a relatively new subject matter in quantum mechanics. Although the principle has existed for some time, the problem of quantum confinement has raised numerous issues pertaining to boundary conditions in elementary quantum mechanics and how they should apply to real problems. Quantum confinement traps the atom in a cavity whose dimensions are small enough to alter its properties. Sommerfeld and Welker were the first to take notice that a hydrogen atom confined in a sphere with infinite non-penetrable walls problem can be solved exactly. In previous works, physicist used the time-independent Schrodinger equation with boundary conditions to obtain exact results. The Schrodinger equation is a partial differential equation that describes how the quantum state of a physical system changes with time. There is the time-dependent equation and the time-independent equation. The time-dependent equation, the most general equation, gives a description of a system evolving with time while the time-independent equation describes stationary states. In real situations, the cavity the atom or molecule is being held in is never fully impenetrable. Hench forth, this research focuses on what happens when the hydrogen atom leaves captivity.

Methods and Material

Materials used for this research program comprised the program Eclipse that was used for the computer programing language C++. This project studied the effects after a hydrogen atom is released out of a container using a very simple model of confinement that describes the reality of a hydrogen atom in captivity. The following definitions and descriptions are essential to understanding the results presented in this paper. Schrodinger equation is used as a method of determining wave functions systematically. The wave function ψ(r,t) can be calculated from a partial differential equation called the Schrodinger wave equation where r relates to space coordinates and t relates to time. The time dependent Schrodinger equation gives a description of a system evolving with time while the time independent Schrodinger equation predicts that wave functions can form standing waves. The general solution of the time-dependent Schrodinger equation can be expressed as a sum of separable solutions.

Results

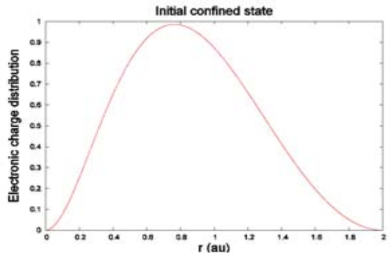

Figure 1: Initial confined state where r (au) is the distance from the electron to the nucleus

K	E_k	$\lvert d_k{}^2 \rvert$
1	-0.50000	0.665940
2	-0.12500	0.056265
3	-0.05556	0.014275
4	-0.03125	0.005837
5	-0.02000	0.002945
6	-0.01389	0.001691

Table 1: Energy, E_k, in au of the unconfined states in au and probability |〖d_k〗^2 | that the atom reach each state after the cage is removed.

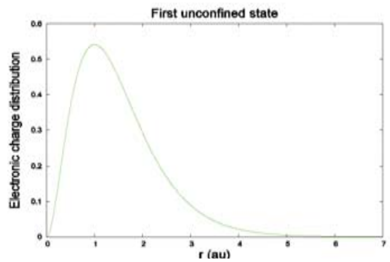

Figure 2: Electronic charge distribution of the first unconfined state of the hydrogen atom as a function of the electron-nucleus distance

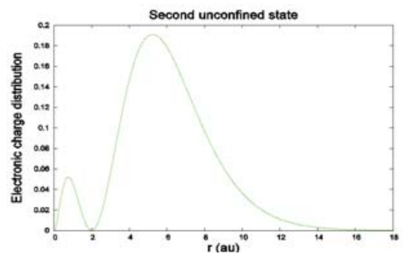

Figure 3: Electronic charge distribution of the second unconfined state of the hydrogen atom as a function of the electron-nucleus distance

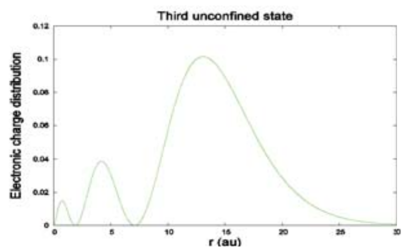

Figure 4: Electronic charge distribution of the third unconfined state of the hydrogen atom as a function of the electron-nucleus distance

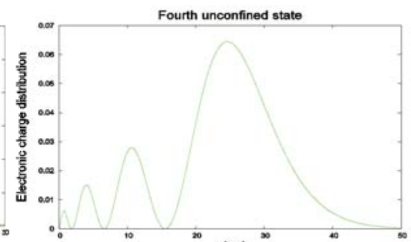

Figure 5: Electronic charge distribution of the fourth unconfined state of the hydrogen atom as a function of the electron-nucleus distance

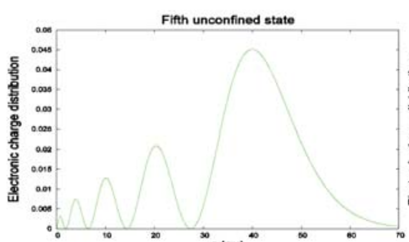

Figure 6: Electronic charge distribution of the fifth unconfined state of the hydrogen atom as a function of the electron-nucleus distance

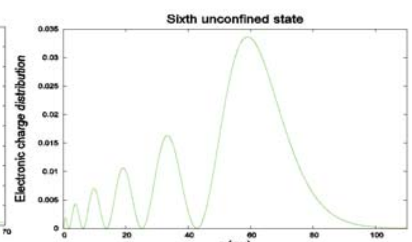

Figure 7: Electronic charge distribution of the sixth unconfined state of the hydrogen atom as a function of the electron-nucleus distance

Results

The results focused on what would happen to the atom when it was taken out of its cavity. Figures 1 – 7 were calculated by using B-Splines where E=2au and l=0. Figures 2-7 are the result of the unconfined hydrogen atom while Figure 1 shows the exact results for the hydrogen atom in captivity. Our results showed that after the confinement is removed, the atom can be in a state of higher energy (k=1), equal energy (k=2), or even lower energy (k>2). Only minor modifications are required in the code to consider l>0. For other values of the angular momentum, the results can be obtained the same way. The results reported in Table 1 show that the probability decreased as the energy of the possible final state increases. The highest probability is found for the ground sate. The atom can reach any of the states indicated and others with a smaller probability not indicated in the table. We observe a deep decrease in the probability from the first possible final state (k=1) and the others. Note that the energy of the final state is not the same as the energy of the initial confined state. The energy is not conserved because the system is not isolated because the removal of the cage is an external interaction with the system.

Summary and Conclusion

By using B-Splines along with matrix diagonalization linear algebra methods we solved the time-dependent Schrodinger equation by using the solution of the time-independent Schrodinger equation. This study has been carried out over the simplest atom. We computed the probability of the hydrogen atom once the cage is eliminated. It is described by any of the Eigen solutions of the free hydrogen atom. We have considered the case of a hydrogen atom enclosed by a spherical cavity of radius of 2 au. The highest probability of the ground state of the unconfined atom is that the probability decreased for the other excited states. Figures 2-7 show the hydrogen atom as it progressed from its excited state. Our results showed that our hypothesis was correct; once the hydrogen atom was released from a confined state it would decrease from its excited state and go off into infinity.

Acknowledgments

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