Utah State University
DigitalCommons@USU

Undergraduate Honors Theses | Honors Program

5-1-2010

Diffusion Monte Carlo Studies of Quantum Solvation: Finding Nodal Functions of Wavefunctions Using a Genetic Algorithm

Christina Hansen Howell
Utah State University

Recommended Citation
Howell, Christina Hansen, "Diffusion Monte Carlo Studies of Quantum Solvation: Finding Nodal Functions of Wavefunctions Using a Genetic Algorithm" (2010). *Undergraduate Honors Theses.* Paper 52.
http://digitalcommons.usu.edu/honors/52

This Thesis is brought to you for free and open access by the Honors Program at DigitalCommons@USU. It has been accepted for inclusion in Undergraduate Honors Theses by an authorized administrator of DigitalCommons@USU. For more information, please contact becky.thoms@usu.edu.

Diffusion Monte Carlo Studies of Quantum Solvation: Finding Nodal Functions of Wavefunctions Using a Genetic Algorithm

by

Christina Hansen Howell

Thesis submitted in partial fulfillment
of the requirements for the degree

of

HONORS IN UNIVERSITY STUDIES
WITH DEPARTMENTAL HONORS

in

Chemistry with a Professional Emphasis
in the Department of Chemistry and Biochemistry

Approved:

Thesis/Project Advisor Dr. David Farrelly	**Departmental Honors Advisor** Dr. Alvan Hengge
Project Advisor Dr. Vernon Parker	**Director of Honors Program** Dr. Christie Fox

UTAH STATE UNIVERSITY
Logan, UT

Spring Semester, 2010

ABSTRACT

Solvation is important in many chemical reactions since most reactions occur in solution. Recently, progress has been made using helium-4 nanodroplets as the solvent at temperatures close to absolute zero. Because helium-4 is a superfluid it solvates dissolved molecules much differently that does a conventional solvent. This opens up the possibility of performing new types of chemistry in the superfluid environment. However, the nature of the interaction of the dissolved species with the solvent remains poorly understood. The basic question to be answered in this project is: how does the quantum solvent perturb the rotational dynamics of the solute particles? In this project the dissolved molecule will initially be taken to be an HCN molecule. Its behavior as a function of the number of solvent He atoms will be studied. The approach taken is computational and employs the fixed-node quantum diffusion Monte Carlo method. A novel feature is the use of a genetic algorithm to determine the nodal structure of the rotational states of the solute molecule.

ACKNOWLDEGMENTS

During my four years of undergraduate work, I have grown especially fond of the faculty of the chemistry and biochemistry department. The faculty truly went out of their way to help me when I learned I had multiple sclerosis. The compassion and concern that was expressed to me helped me to stay in college and continue working towards my bachelor degree in chemistry. The professors of my chemistry classes have also helped me understand and appreciate all fields of chemistry.

My research project would not have happened without the support and help from my mentor, Dr. Farrelly. He has helped me understand the methods used in computational and theoretical research. Also, I would like to thank Jordan Ramilowski, a graduate student in the lab, who took time from his projects to help me understand FORTRAN programming and how to write a Diffusion Monte Carlo code.

Special thanks go out to my thesis committee members: Dr. Alvan Hengge, Dr. Vernon Parker, and Dr. Christie Fox. They have provided encouragement when I needed it and provided useful advice while I worked on my project. My final thesis would not be the same without their comments and suggestions.

I also want to thank my family and friends who supported me while I earned my undergraduate degree. Their encouragement truly helped me when I doubted myself. And lastly, I want to thank my husband, Broden, who has been my anchor of support. Broden believed in me when I did not and his constant assurance that everything will work out is what truly helped me to succeed.

Christina Hansen Howell

TABLE OF CONTENTS

ABSTRACT…….2

ACKNOWLEDGMENTS……...3

LIST OF FIGURES, EQUATIONS, TALBES, AND SCHEMES……..…5

LIST OF DEFINITIONS…….6

SECTION

1 –BACKGROUND ON SOLVATION…….7

2 – DIFFUSION MONTE CARLO……...10

2.1 RIGID BODY DIFFUSION MONTE CARLO……13

2.2 NODES……..14

2.3 USING A GENETIC ALGORITHM TO FIND NODES…….15

3 – QUANTUM SOLVATION OF HE-HCN……...18

3.1 DMC VERSUS EXACT RESULTS…….20

3.2 SUMMARY AND CONCLUSIONS…….……...22

REFERENCES…….…24

AUTHOR'S BIOGRAPHY……...26

LIST OF FIGURES, EQUATIONS, TABLES, AND SCHEMES

Section 1:

Figure 1 – Gas-phase and solution phase potential energy surface for theS_N2 reaction.

Section 2:

Equation 1 – This is the time-dependent Schrödinger equation for a one-particle, one-dimensional system.

Equation 2 – This is the time-independent Schrödinger equation for a one-particle, one-dimensional system.

Figure 2 – This is a representation of the DMC algorithm by a flow diagram.

Section 2.1:

Equation 3 – Rigid Body DMC equation.

Figure 3– Diffuse rotations around space-fixed axes.

Section 2.2:

Figure 4 – Example of a node.

Section 2.3:

Figure 5 – This is a visual representation of the GA. The GA has five basic steps: 1) initial populations are designed, 2) the fitness of each population is evaluated, 3) A new population referred to as the offspring is created from two parent populations, 4) the new population is replaced into the existing population, and 5) the offspring populations are tested.

Section 3

Figure 6 – Helium nanodroplets can contain up to several thousand atoms. Shown here is a NO molecule surrounded by helium atoms.

Section 3.1:

Table 1 – He-HCN Energies (cm^{-1}).

Figure 7 – Density maps of $|\Phi^{(a),(b)}(r)|^2$ for the HCN–He binary complex. Panels (a)–(d) are obtained from matrix diagonalization and panels. In (a) and (b), Φ =0. The densities have all been scaled to have a maximum value of unity. In color: the color bar shows the range of density values and applies to all four frames.

Figure 8 – GA node. Preliminary results indicate that the genetic algorithm node is fairly close in agreement with the true node.

Table 2 – Comparison of exact and GA energies.

Section 3.2:

Table 3 – Summary of the He-HCN energies using the DMC and DMC-GA method.

DEFINITIONS:

Diffusion Monte Carlo (DMC): A numerical method that is used to solve the Schrödinger equation. The DMC is a quantum Monte Carlo method that implements a random walk algorithm to solve the Schrödinger equation and provides a way to obtain the ground state energy and ground state wave function.

FORTRAN (Formula Translation): It is a high-level language meaning it uses English-like commands and instructions. It uses a complier to translate the FORTRAN program into a binary code that the computer understands.

Microsolvation: The addition of solvent molecules one at a time to the reaction.

Potential Energy Surface (PES): Describes the energy of a molecule in terms of its structure.

Schrödinger Equation: Incorporates both wavelike behavior and particle-like behavior to describe the electron. Solving this equation yields wave functions known as mathematical functions that describe the behavior of the electron.

Solvation: Clustering of solvent particles around solute particles; interaction between the solvent and the solute.

Superfluid: means a fluid with zero viscosity. Superfluids have all their atoms in the same quantum state which allows all the atoms to have the same momentum, thus allowing them to move without friction.

Wavefunction: probability patterns used to describe the motion of the electron; describes the behavior of the electrons.

Section 1 – Background on Solvation

The mechanism how solvation affects the progress of a chemical reaction is an important research topic. This area in chemistry requires understanding for several reasons: 1) most chemical reactions take place in solution (i.e., liquid phase is used more frequently in organic chemistry and in living systems), 2) there are many solvent effects in chemistry systems, and 3) relatively little is known about the detailed dynamical mechanisms of solution phase reactions compared to gas-phase reactions.

Recently, solution phase reactions are becoming open to computational study and simulation in order to study solvent effects. Thus, the role of the solvent can be revealed by learning about the behavior of the reaction in the gas-phase [1]. Solvation can be found in organic systems such as the S_N2 reaction all the way up to quantum systems. However, solvation in a quantum system behaves differently than in a classical system.

In a classical system, solvent particles cluster around the solute particles to separate the solute particles from each other. This process allows the solute particles to dissolve in the solvent. Solvation can have a large effect on the enthalpy, $\Delta H°$, and the entropy, $\Delta S°$, of a reaction. This can be illustrated when a polar solvent solvates a polar reactant and the freedom of movement of the solvent molecules is reduced. Solvents also affect the rate of a reaction depending on its polarity and if one of the rate-determining reactants is charged [2]. An example of solvation affecting a classical system can be seen in an S_N2 reaction.

The effect of solvation on S_N2 reactions can be seen in the potential energy surfaces [3] and the dynamical mechanisms by microsolvation [4] (Figure 1). The generic chemical reaction, $X^- + RY \rightarrow RX + Y^-$, represents an S_N2 reaction. In figure 1, the R group in the generic S_N2 reaction is a methyl group.

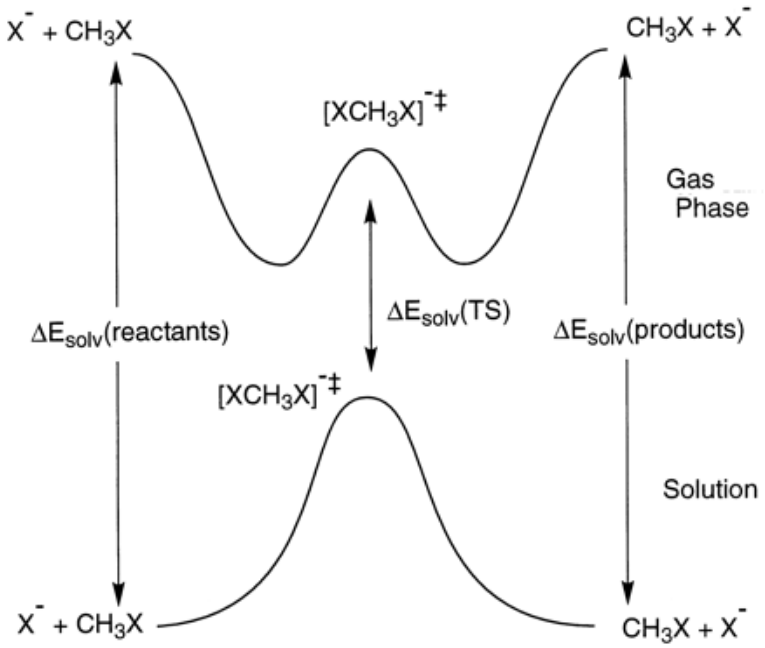


Figure 1. Gas-phase and solution phase potential energy surface for theS_N2 reaction [3].

The reaction barrier in the gas phase has a lower reaction barrier than the barrier in the solution phase. This is due because the charge in the transition state is delocalized over a smaller area; thus, charge localized ions are better solvated then charge delocalized ions.

Usually, a molecule dissolved in a liquid is not expected to rotate freely as it might in the gas phase. However, in an ultracold droplet of helium-4 atoms, coherent molecular rotation over many periods is possible and normal for helium-4 [5]. Helium-4 is unique since it behaves as a superfluid meaning a fluid with zero viscosity. Some other superfluid characteristics of helium-4, better termed superfluid phenomena, are an extremely high heat conductivity, He fountain, film flow and creep, and quantized vortices [6].

Due to the superfluid nature of helium-4, this quantum solvent is a gentle solvent and works well for ultraclean nanolaboratories [6]. Although this helium-droplet matrix has many benefits, there is one shortcoming of the matrix which is an apparent increase in the moments of inertia of solvated molecules compared to their gas-phase values. This shortcoming is not quite understood and emphasizes the importance of understanding the dynamics of how molecules become

solvated in a small droplet of quantum solvent [5].

The quantum system being studied in this project is an HCN molecule solvated by He atoms. Because helium-4 is a superfluid it solvates dissolved molecules much differently than a conventional solvent and, thus, little is understood about the interaction of the solvent with the dissolved species. The basic question to be answered is how would solvation affect a quantum system, and more specifically how does the quantum solvent perturb the rotational dynamics of the solute particles?

The question will be answered computationally by using diffusion Monte Carlo Studies that employs a fixed-node approximation and a genetic algorithm. Thus, the main result will be a theoretical understanding of solvent interactions.

Section 2 – Diffusion Monte Carlo

In 1926, Erwin Schrödinger, an Austrian physicist, formulated an equation that used both the wavelike and particle-like behavior of the electron to describe the behavior and energies of that submicroscopic particle called the Schrödinger equation (Equation 1 and Equation 2). Thus, quantum mechanics or wave mechanics was born. When the equation is solved, wave functions or mathematical functions are obtained that describe the electron's behavior. Wave functions can be thought as probability patterns used to describe the motion of the electron.

$$i\hbar\frac{d\Psi(x,t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi(x,t)}{dx^2}V(x,t)\Psi(x,t)$$

Equation 1. This is the time-dependent Schrödinger equation for a one-particle, one-dimensional system.

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

Equation 2. This is the time-independent Schrödinger equation for a one-particle, one-dimensional system.

The time-dependent Schrödinger equation allows one to calculate the future wave function at any time as long as one knows the wave function at time t_0. The probability of the electron's location in an allowed energy state is found by the square of the wave function, Ψ^2. Thus Ψ^2 is known as the probability density or the electron density.

In a few idealized situations, the Schrödinger equation can be solved analytically. However, for situations that are not idealized or trivial, there are numerical methods that are used to solve the Schrödinger equation such as the Diffusion Monte Carlo (DMC) method. The DMC is a quantum Monte Carlo method that implements a random walk algorithm to solve the Schrödinger equation.

The Diffusion Monte Carlo (DMC) describes the ground states of quantum systems and

provides a way of evolving time into imaginary time to obtain a solution of the Schrödinger equation. Thus, the ground state energy and ground state wave function of the system being studied can be obtained.

The DMC can be formulated in 3 steps which are: 1) Imaginary time Schrödinger equation, 2) Monte Carlo Integration, and 3) Continuous estimate of the ground state energy and sampling of the ground state wave function [7].

1) The first step expresses the time-dependent Schrödinger equation as a series expansion in terms of the eigenfunctions of the Hamiltonian. This is followed by the transformation of real time to imaginary time by introducing $t = i\tau$. The solution of the imaginary time Schrödinger equation is expressed as a series of transients in which the longest transient relates to the ground state of the system.

2) The second step uses "replicas" which are imaginary particles. The wave function is calculated through diffusive displacements and birth-death processes applied to the replicas. These replicas are distributed in the space of the system and the replicas converge to the probability density which represents the ground state wave function. These diffusive displacements are done by the computer using random number generators.

3) The third step involves sampling the wave function after each time step. The replicas provide an approximate to the wave function and the ground state energy of the system at any given time. First, one begins with an estimate of the ground state

energy, and by using the replicas the estimate is improved by the diffusive displacements and birth-death processes. Eventually the estimate converges to the ground state energy and the distributed replicas converge to the wave function.

The steps used to formulate the DMC method are used to write a working code for the system being studied. Figure 2 represents the series of steps that are taken in the DMC algorithm. Briefly, the DMC algorithm will be discussed.

After defining the parameters that will be used in the computer program, one initializes the replicas. Upon initializing the replicas, the code enters a loop containing three routines: walk, branch, and count. A test is done after the routines to determine if the replica should be kept, copied, or killed. Once the test indicates good results, then the ground state energy is obtained.

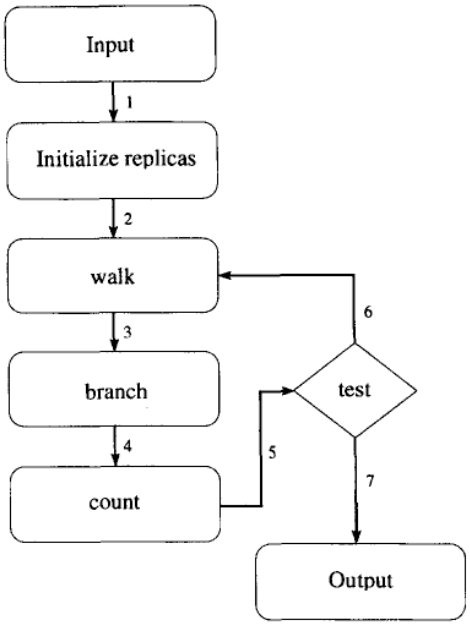


Figure 2. This is a representation of the DMC algorithm by a flow diagram [7].

Section 2.1 Rigid Body Diffusion Monte Carlo

Due to the large disparity in the strengths of the intramolecular and intermolecular interactions the molecules can be treated as rigid bodies (rigid body DMC) [5,8]. In rigid body DMC (Equation 3) excited rotational states can be computed using the fixed-node method [9].

Equation 3. Rigid Body DMC equation.

$$\overbrace{\Psi_T = \left\{ \prod_{i=1}^{N} \Xi(R_{il}, \theta_{il}, \phi_{il}) \right\} \left\{ \prod_{i<j}^{N} e^{t(r_{ij})} \right\}}^{Boson-Symmetric} \underbrace{\varphi(\alpha, \beta, \gamma)}_{Rotor}$$

One of the biggest challenges all DMC methods face is how to calculate excited states since in the fixed-node implementation of DMC the nodal surfaces must be known in advance.

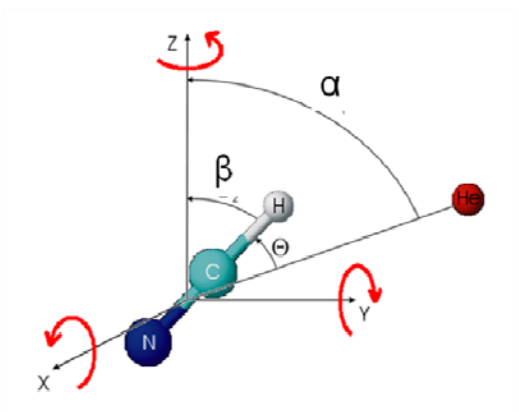


Figure 3. Diffuse rotations around space-fixed axes.

Treating HCN-He as a rigid rotor is depicted in Figure 3. The Cartesian Coordinates are used for the center of mass for the rigid rotor and the solvent atom. The rotations are done around the principal axes of the rigid rotor.

Section 2.2 Nodes

The probability density or the square of the wavefunction, , provides information about the electron orbitals. Thus, the probability density ultimately gives the probability of finding an electron at a given point in space. When the probability density is zero, this point is called a node, meaning that there is zero probability of finding the electron in that space (Figure 4).

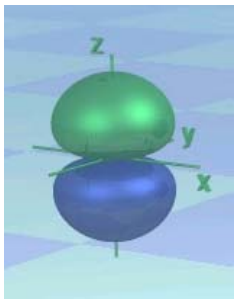


Figure 4. Example of a node that is located at the origin of the coordinate system. The green and blue regions indicate regions where there is a probability of finding an electron there.

The node of a system must be known in order to know the wavefunction; thus, the most immediate problem is how to obtain estimates of the nodal surfaces of unknown excited state wavefunctions. In rigid body DMC excited rotational states can be computed using the fixed-node method.

The fixed-node approximation in DMC is based on the knowledge that the wavefunction goes to zero when it approaches an infinite potential barrier or a node [9]. This approximation allows one to compute excited state levels by imposing a predefined nodal surface. A rejection step in the approximation method is used in order to reject, or kill, any walkers that cross the nodal surface and, thus, making those rejected walkers retain their previous position.

Section 2.3 Using a Genetic Algorithm to Find Nodes

Generic algorithms (GA) are a part of what is known as evolutionary computing meaning that a solution to a problem solved by genetic algorithms is evolved. It was inspired by Darwin's theory about evolution which is why GA mimics the biological processes of natural selection and reproduction [10]. Natural selection refers to how certain members of a population, with traits that make them more likely to survive, are able to successfully reproduce yielding a new population with members of that common trait.

Before a GA is used, the parameters of the system being studied are encoded into a string of binary digits that is referred to as the population. Once this step is done, the GA is applied to the population (see Figure 5).

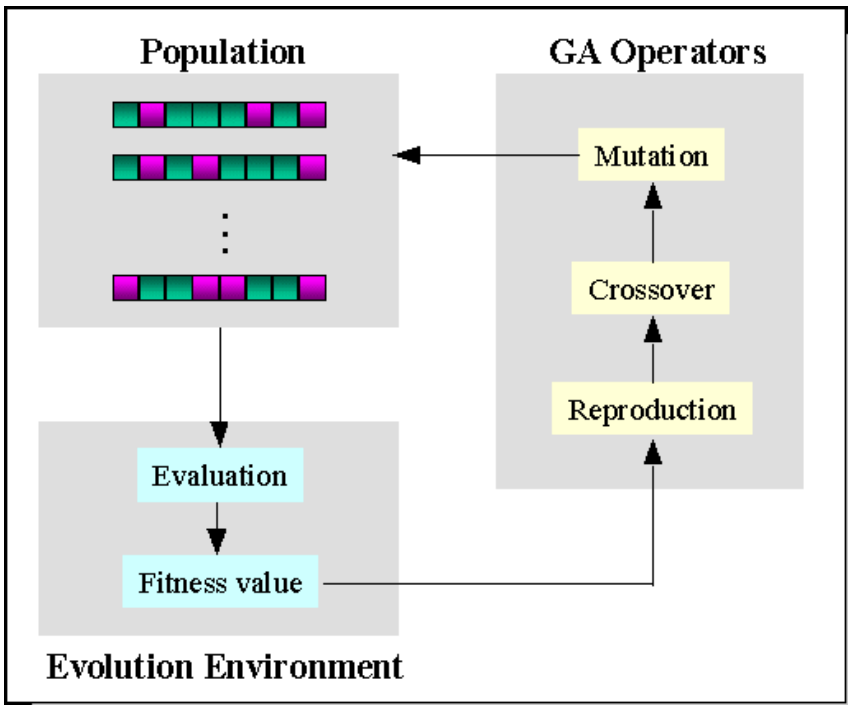
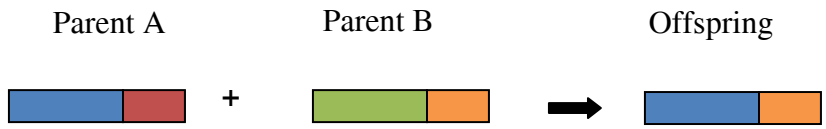


Figure 5. This is a visual representation of the GA. The GA has five basic steps: 1) initial populations are designed, 2) the fitness of each population is evaluated, 3) a new population referred to as the offspring is created from two parent populations, 4) the new population is replaced into the existing population, and 5) the offspring populations are tested [11].

A genetic algorithm follows this basic outline [12]:

1) Initial design populations are generated or created. These need to be suitable solutions for the problem being studied.
2) Evaluate the fitness of each population.
    a) The fitness is determined by the specifications of the problem and measures the success of the population in life. In nature, organisms that have a low chance of reproducing have a low fitness while organisms with a high chance of reproducing have a high fitness. Thus, in GA the fitness of each population or string refers to how well each population will be at reproducing a new population.
3) Create a new population by repeating the following steps:
    a) Select 2 parent populations according to their fitness
        i. Only high fitness populations will be selected since they have the greatest probability of producing offspring that will be more successful than the previous generation. Two high fitness strings create a new population or offspring by exchanging parts of their binary digits that make up their strings.
    b) Crossover

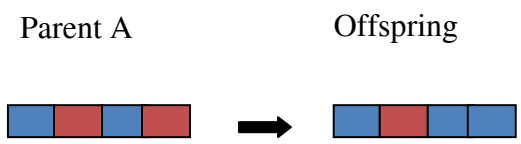
    A crossover is a basic operator of GA. Below is an example of single-point crossover.



This means that one point on the binary string is selected and is where the beginning of the string up to the point from parent A is kept and the remaining part from the point to the end is supplied by parent B for the offspring.

c) Mutation

A mutation refers to when one of the bits, either the 0 or the 1, is inverted to the other digit. This idea is represent below where the last red segment is mutated to a blue segment.



d) Accepting

Accepting refers to how the offspring is placed into the new population.

4) Use the newly generated population for a further run in the algorithm
5) Test the new populations and if the end condition is satisfied then stop.
    a) If not, repeat again starting at step 2.
        i. New populations will be continued to be pursued until the success of the next population does not significantly improve from the previous population.

GA works by fitting a cubic spline through the guessed points to map where the node is located. Eventually, the energies on each side of the node should be the same [9]. This is represented by a fitness function: E1 – E2 = 0.

Section 3 – Quantum Solvation of He-HCN

Understanding how solvation affects the dynamics of a chemical environment is an important research topic because relatively little is known about the solution phase dynamics compared to gas-phase dynamics. A molecule dissolved in a liquid is not normally expected to rotate freely as it might in the gas phase. However, in ultracold 0.37 K droplet of helium-4 coherent molecular rotation over many periods is not only possible, it appears to be the norm.

Helium is a unique substance since it exists as a liquid at absolute zero. Below 2.17 K helium-4 behaves as a superfluid, meaning a fluid with zero viscosity. Because superfluids have all their atoms in the same quantum state, the atoms all have the same momentum allowing them to move without friction.

Nanodroplets of helium-4 contain anywhere from a few to thousands of atoms (Figure 6). These nanodroplets can easily pick up atoms or molecules and form complexes with them on the surface or in the interior [13]. Helium-4 nanodroplets are considered to be the ultimate spectroscopic matrix since they exhibit little matrix broadening [14].

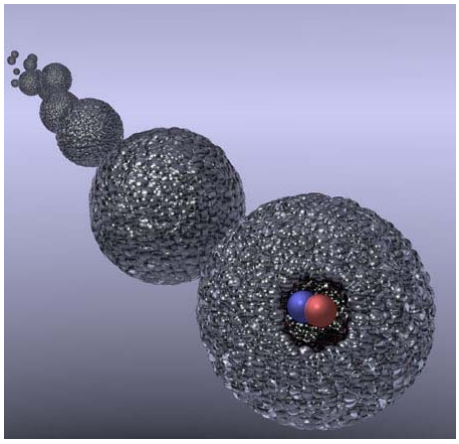


Figure 6. Helium nanodroplets can contain up to several thousand atoms. Shown here is a NO molecule surrounded by helium atoms [15].

Due to the superfluid properties, helium-4 nanodroplets offer the potential to be ultracold, ultraclean nanoreactors or microscopic cryogenic chambers where new chemical species can be synthesized and characterized, high-resolution spectroscopy of van der Waals complexes can be performed, complexes of biomolecules can be created, reaction intermediates or precursors can be isolated, chemical reactions can be monitored, and the nature of superfluidity in finite-sized systems can be studied [5].

Using helium-4 as a solvent allows the possibility to perform new types of chemistry in a superfluid environment since it solvates dissolved molecules differently [16]. The solute molecule in this project is an HCN molecule and its behavior will be studied as the number of solvent He atoms are added. The interaction of the solute and solvent will be investigated using computational methods such as the DMC method and a genetic algorithm.

Section 3.1 – DMC versus Exact Results

Obtaining He-HCN energy (cm^{-1}) for the ground state level by DMC produces fairly reasonable results. However, DMC is not a good approximation to the level (1,0,1) (Table 1). This is because the rigid rotor nodal surface is a poor approximation to the true node (figure 7). Thus, using DMC along with the genetic algorithm is a better approximation to the true node.

Level (j,l,J)	Close Coupling	DMC
(0,0,0)	**-8.867**	**-8.87 ± 0.20**
(1,0,1)	**-5.554**	**-6.38 ± 0.22**

Table 1. He-HCN Energies (cm^{-1}).

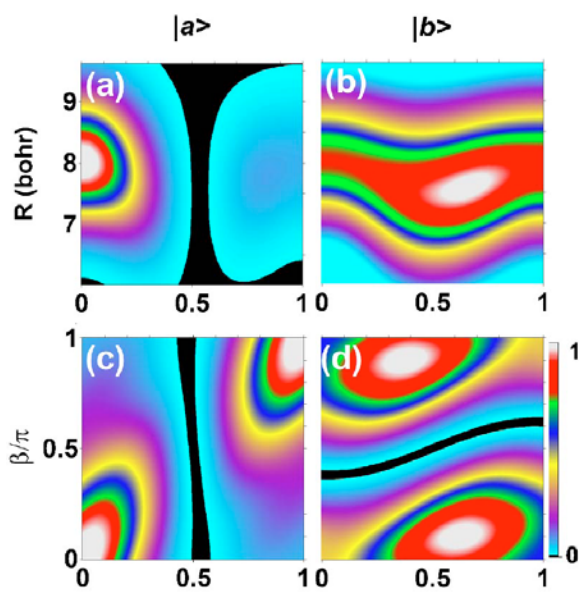


Figure 7. Density maps of $|\Phi^{(a),(b)}(r)|^2$ *for the HCN–He binary* complex. Panels (a)–(d) are obtained from matrix diagonalization and panels. In (a) and (b), Φ =0. The densities have all been scaled to have a maximum value of unity. In color: the color bar shows the range of density values and applies to all four frames [5].

The genetic algorithm finds a family of nodes. It can be seen that the He-HCN energy from the DMC-GA node is in better agreement with exact results than the DMC node (Figure 8, Table 2). Future work will concentrate on improving the fitness function to get better global agreement with the true node.

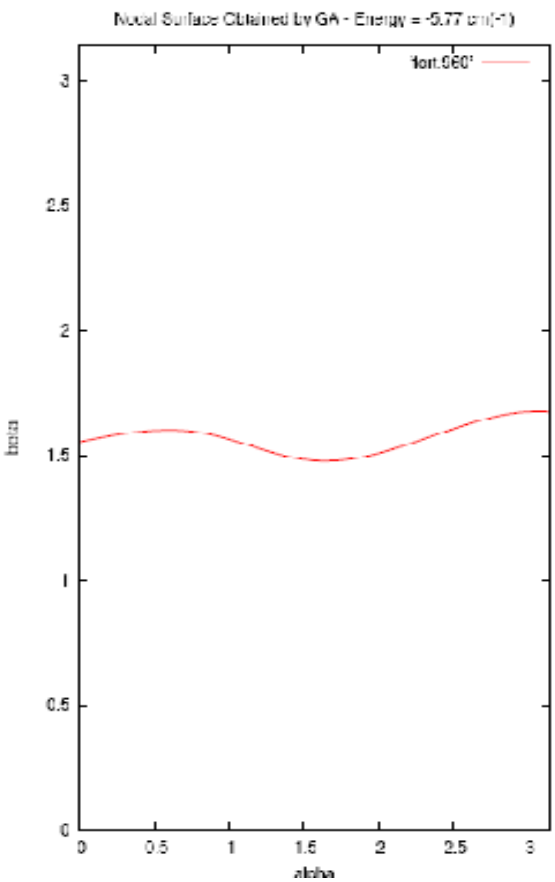


Figure 8. GA node. Preliminary results indicate that the genetic algorithm node is fairly close in agreement with the true node.

Level (j,l,J)	Close Coupling	DMC-GA Node
(1,0,1)	**-5.554**	**-5.55 ± 0.25**

Table 2. Comparison of exact and GA energies.

Section 3.2 – Summary and Conclusions

One of the main goals of this project was to develop a method of finding nodal functions of wavefunctions using a genetic algorithm with the DMC method. Finding nodal functions can be time consuming so having a new method that finds them quicker is extremely important. The system He-HCN is just an example that was used to determine the accuracy of this developed method.

In order to solve the Schrödinger equation for the He-HCN system, a numerical method called the Diffusion Monte Carlo (DMC) is employed. DMC solves the Schrödinger equation by implementing a random walk algorithm to obtain the ground state energies and ground state wavefunction of the system. To understand more about the system, the excited state energies and wavefunction are investigated.

In rigid body DMC excited rotational states can be computed using the fixed-node method. However, the node of the system must be known in order to know the wavefunction; thus, the most immediate problem is how to obtain estimates of the nodal surfaces of unknown excited state wave functions. The fixed-node approximation allows one to compute excited state levels by imposing a predefined nodal surface.

In the previous section, it was shown that using just the DMC method to calculate the ground state energy of He-HCN is quite accurate. On the other hand, using the DMC method to calculate the excited state energy of He-HCN is not a good approximation (Table 3). To improve this approximation, the genetic algorithm was used to determine the nodal structure of the rotational states of the solute molecule and to help understand the nodal topology better. The DMC-GA method proved to be quite effective considering how accurate it came to the actual excited state energy of He-HCN system (Table 3).

Level (j,l,J)	Close Coupling	DMC	DMC-GA
(0,0,0)	**-8.867**	**-8.87 ± 0.20**	**N/A**
(1,0,1)	**-5.554**	**-6.38 ± 0.22**	**-5.55 ± 0.25**

Table 3. Summary of the He-HCN energies using the DMC and DMC-GA method.

The idea behind the DMC-GA method is fitting a cubic spline through guessed points by the genetic algorithm to map where the node is located. It is proposed that the energies on each of side of the node should be same since the number of walkers initialized on one side of the node should equal the same number of walkers initialized on the other side of the node. To see if this method works, it was used on the system He-HCN where the excited state energies were already known. From the results presented in Table 3, it can be seen that the DMC-GA method does provide a reasonable nodal function for the system. This method will be applied to other systems already studied to see how accurate it can obtain the nodal function before it is applied to systems with unknown excited state energies and wavefunctions.

REFERENCES:

[1]. Chandrasekhar, J., and Jorgensen W.L. Energy profile for a nonconcerted S_N2 reaction in solution. *J. Am. Chem. Soc.,* 107, (1985), 2974-2975.

[2]. Olmstead, W.N., and Brauman, J.I. Gas-phase nucleophilic displacement reactions.*J. Am. Chem. Soc.,* 99:13, (1977), 4219-4228.

[3].Chabinyc M.L., Craig, S.L., Regan, C.K., and Brauman, J.I. Gas-Phase Ionic Reactions: Dynamics and Mechanism of Nucleophilic Displacements. *Science 279,* (1998) 5538, 1882-1886.

[4]. Lu, Y., Handoo, K.L, Parker, V.D. Non-steady-state kinetic study of the S_N2 reaction between p-nitrophenoxide ion and methyl iodide in aprotic solvents contating water. Evidence for a 2-step mechanism. *Org. Biomol. Chem.,* 1, (2003), 36-38.

[5]. Mikosz, A.A., Ramilowski, J.A. ,and Farrelly D. Quantum solvation dynamics of HCN in a helium-4 droplet. *JCP* 125, (2006) 014312, 1-10.

[6]. Toennies, P., Vilesov, A.F., and Whaley, B. Superfluid helium nanodroplets: an ultracold nanolaboratory. *Physics Today.* February (2001), 31-37.

[7]. Kosztin, I., Faber B., and Schulten K. Introduction to the diffusion Monte Carlo method. *Am. J. Phys.,* 64 (5), (1996) 633-644.

[8]. Buch, V. Treatment of rigid bodies by diffusion Monte Carlo: Application to the para-H2---H20 and ortho-H2---H20 clusters. *J. Chem. Phys., 97 (1),* (1992), 726-729.

[9]. Petit, A.S., and McCoy, A.B. Diffusion Monte Carlo Approaches for Evaluating Rotationally Excited States of Symmetric Top Molecules: Application to $H3O^+$ and $D3O^+$. *J. Phys. Chem.* 113 (2009) 12706-12714.

[10]. Rennard, Jean-Philipppe. Introduction to Genetic Algorithms. [cited 2010 April 9]. Available from: http://www.rennard.org/alife/english/gavintrgb.html.

[11]. An Educational Genetic Algorithms Learning Tool. [cited 2010 March 25]. Available from: http://ewh.ieee.org/soc/es/May2001/14/Begin.htm.

[12]. Obitko, Marek. Genetic Algorithms. [cited 2010 April 9]. Available from: http://www.obitko.com/tutorials/genetic-algorithms/

[13]. Toennies, J.P. and Vilesov A.F. Superfluid Helium Droplets: A Uniquely Cold Nanomatrix for Molecules and Molecular Complexes. *Angew. Chem. Int. Ed.* 43 (2004) 2622 – 2648.

[14]. Ramilowski, J.A., Mikosz, A.A, and Farrelly, D. Rotational Structure of Small 4He Clusters Seeded with HF, HCl, and HBr Molecules. *J. Phys. Chem.,* 111 (2007), 12275-12288.

[15]. Physics News Graphics [cited 2010 March25]. Available from: http://www.aip.org/mgr/png/images/droplets450.jpg.

[16]. Viel, A., and Whaley, K.B. Quantum structure and rotational dynamics of HCN in helium clusters. *J. Chem. Phys.* 115 (22), (2001), 10186-10198.

AUTHOR'S BIOGRAPHY:

Christina Hansen Howell was born and raised in Logan, Utah. After graduating valedictorian from Logan High School, she attended Utah State University on a Presidential Scholarship. As a freshman, she declared her major to be chemistry with a professional emphasis. While taking her major requirements, she discovered that mathematics was just as fascinating as chemistry and declared it as her minor.

During her four years at Utah State, she was involved with undergraduate research. For two years she worked with Dr. Joan Hevel, and was able to get a publication out on one of her research projects. After she took physical chemistry, she learned how exciting quantum mechanics can be; thus, in her senior year she switched into Dr. David Farrelly's lab to do research in physical chemistry.

She took time from school to train and run the Top of Utah marathon and the Boston marathon. As she became more involved with campus activities, running marathons was put on a hold. While at Utah State, she lived and breathed chemistry since she was involved with the chemistry and biochemistry club where she was the president for two years, taught Chemistry 1210 supplemental instruction, and was a teacher's assistant to Chemistry 1220 for an entire year.

After she graduates in May 2010, she will start the Master of Education program at Utah State University in August 2010. This degree will allow her to teach chemistry at a high school level where she can share her passion for chemistry to the students.