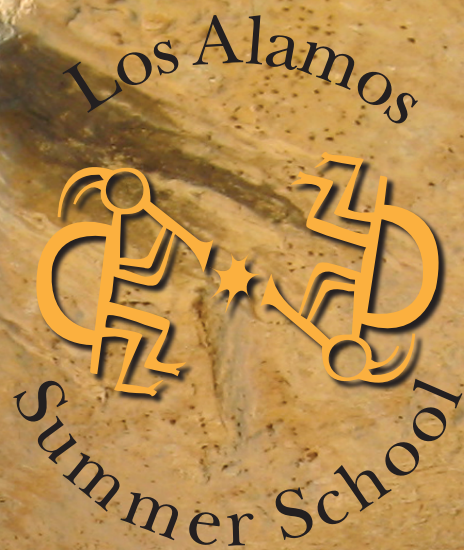


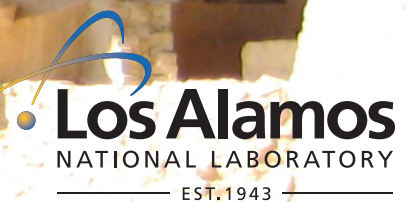


2009

Research Reports

Volume 11

LA-UR-09-06029



UNM

2009 *volume 11*

Los Alamos Summer School Research Reports

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2009 *volume 11*

Los Alamos Summer School Research Reports

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Los Alamos Summer School Research Reports

Preface

This year marked the nineteenth session of the Los Alamos Summer School in Physics, a joint educational project between the University of New Mexico and the Los Alamos National Laboratory (LANL). The National Science Foundation provides funding to the University side through its Research Experience for Undergraduates (REU) site, and this year the LANL Institute for Advanced Studies supports the Laboratory component. In addition, this year we were again pleased to receive support from the Los Alamos National Laboratory's Quantum Institute, and the Department of Energy's ASC program. The School recruits nationwide and the majority of students were junior or senior undergraduates. Twelve students, from a variety of backgrounds and locations, participated in this year's program.

As in previous years, the School employed a dual track of lectures on a wide variety of topics as well as student research projects to give the students their first taste of real research. The lecturers were distinguished scientists from LANL and from UNM, and discussed topics as diverse as climate modeling, high-energy physics, and the latest developments in astrophysics. The research projects, each individually mentored by a LANL scientist, concentrated on a specific problem and allowed the student to experience how research is undertaken at a National Laboratory. Research projects were in many areas of science including atomic physics, high-energy physics, computational neuroscience, and supernovae modeling. Many of the students presented their research at the annual Los Alamos Student Symposium, which was held at UNM-LA on August 4-5, 2009. One student won an outstanding presentation award in the Physics category. All the lecturers and mentors who participated in LASS were volunteers, and we thank them most sincerely for their time and their willingness to participate in the LASS program.

This report collates the research findings of the LASS students in their research experience. Although the short ten-week span of the school usually only allows the students to contribute to a project in progress, or to make a start on a new research project, this year several of the projects are expected to lead to journal publications, leading to advances in the field. More importantly, this summer's experiences have allowed these students to participate in a working research environment, which will be of immense help in deciding their future career paths as they complete their undergraduate education within the coming year. We believe that these project reports demonstrate the remarkable achievements of all the students.

LANL
James Colgan
Norm Magee

UNM
Sally Seidel



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Los Alamos Summer School Class

Paige Martin	Harvard University
Emily Dahlberg	University of Redlands
Simone Brookes	City College of New York
Hadas Friedman	Illinois Institute of Technology
Amy Hass	Humboldt State University
Catherine Lee	Wellesley College
Yvonne Parsons	University of Maryland
Adam Iaizzi	Ithaca College
Evan Li	Harvey Mudd College
Zachary Slepian	Princeton University
Reid Sanders	Clemson University
William Casper	North Dakota State University





Los Alamos Summer School Mentors and Students

Mentor

William Bruno (T-6)

Bogdan Damski (T-4)

David Kilcrease (T-1)

Amy Bauer (T-6)

William Hlavacek/Fangping Mu (T-6)

Steve Valone (MST-8)

Hristo Djidjev (CCS-3)

Cynthia Reichhardt (T-1)

Garrett Kenyon (P-21)

David Roberts/Cristiano Nisoli (T-4)

Ming Xiong Liu (P-25)

Balu Nadiga (CCS-2)

Student

Paige Martin

Emily Dahlberg

Simone Brookes

Hadas Friedman

Amy Hass

Catherine Lee

Yvonne Parsons

Adam Iaizzi

Evan Li

Zachary Slepian

Reid Sanders

William Casper



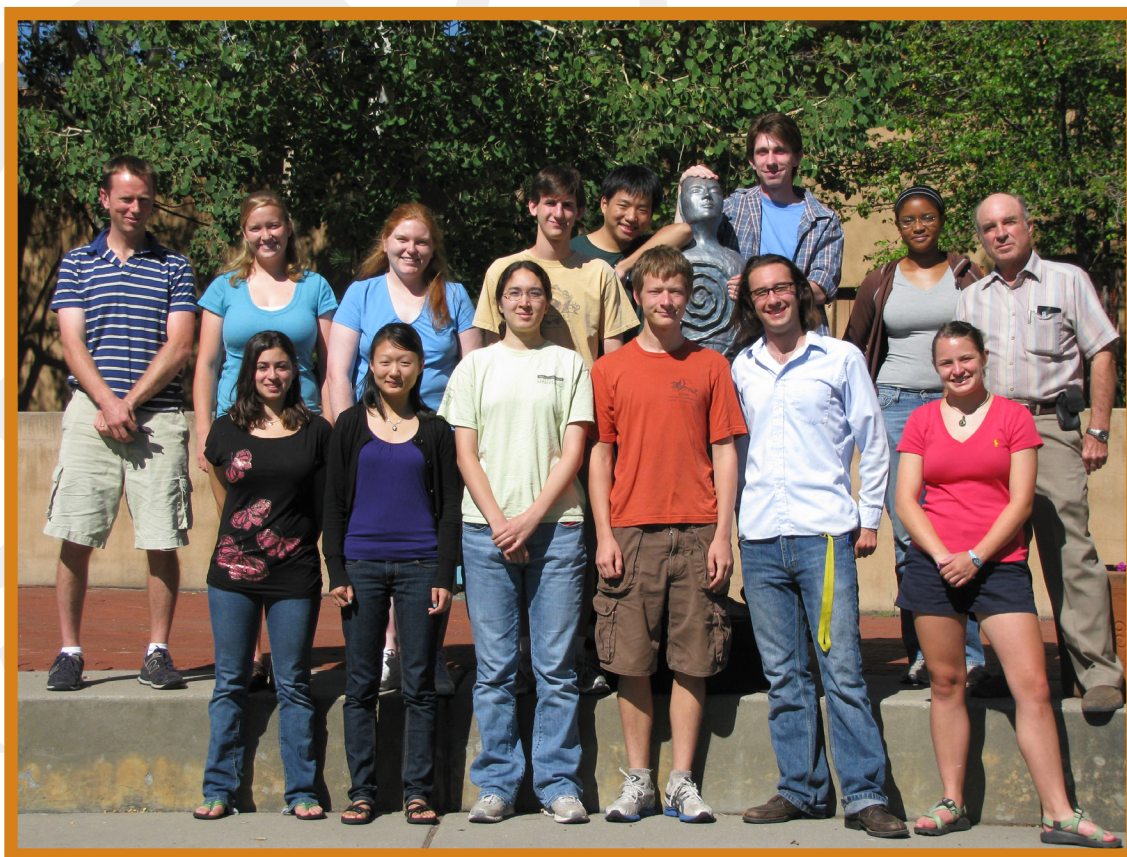
Los Alamos Summer School Lectures

Tom Rescigno (LBNL)	Broken Symmetry in Molecular Scattering
Gary Axen (NM Tech)	Fault Mechanics
Claudia Wilson (NM Tech)	Development of Fuzzy Controllers for Magnetorheological Dampers
Tom Kieft (NM Tech)	Deep Subsurface Geomicrobiology
Ranis Ibragimov (NM Tech)	Fluid Mechanics and Non-linear Waves
Joe Abdallah (T-1)	Atomic Kinetics Modeling
Peter Möller (T-2)	Nuclear Reaction Networks for Astrophysics Applications
Sanjib Gupta (T-2)	Nuclear Astrophysics of Neutron Stars and the r-process
Chris Fryer (CCS-2)	Understanding Nature's Largest Explosions - The Engines Behind Supernovae and Gamma-Ray Bursts
Tim Thomas (UNM)	Novel Computing
Cynthia Reichhardt (T-1)	Local Probes in Superconducting Vortex Matter
Leslie Welser (X-4-PC)	Inertial Confinement Fusion
Gerd Kunde (P-25)	The Quark Gluon Plasma
Charles Reichhardt (T-4)	Realizing Novel Collective Particle Dynamics in Periodic Substrates: from Superconductors to Bacteria
David Roberts (T-4/CNLS)	Spontaneous Synchronization of Coupled Oscillators
Steve Valone (MST-8)	Open System Density Functional Theory and the Millikan Oil-drop Experiment
Balu Nadiga (CCS-2)	An Introduction to Turbulence in the Ocean-atmosphere System
Susan Atlas (UNM)	In Search of H: Lectures on Density Functional Theory
Bill Louis III (P-DO)	Neutrino Physics
Eli Ben-Naim (T-4)	Statistical Physics of Competitions, Statistical Physics of Granular Materials
Garrett Kenyon (P-21)	Computational Neuroscience
James Colgan (T-1)	The Coulomb Three-body Problem
Kent Budge (CCS-2)	Neutrinos in Supernovae



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Los Alamos Summer School Photographs



LASS Class of 2009

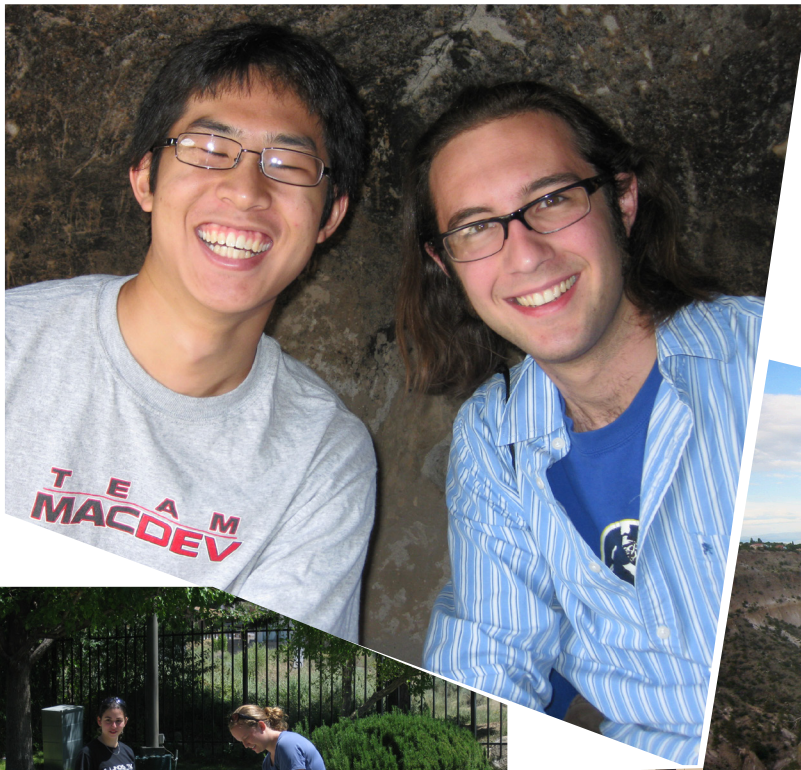
Back row left to right: James Colgan (LANL), Paige Martin, Amy Hass, Zachary Slepian, Evan Li, William Casper, Simone Brookes, Norman Magee (LANL)

Front row left to right: Hadas Friedman, Catherine Lee, Yvonne Parsons, Reid Sanders, Adam Iaizzi, Emily Dahlberg



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Los Alamos Summer School Titles of Papers

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Anisotropy in Depinning of Stripes Particles on Quenched Disorder

Adam Iaizzi

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Theoretical Division,

Los Alamos National Laboratory, Los Alamos, NM

(Dated: August 14, 2009)

We use computer simulations to study driven pattern forming systems, such as a 2D electron gas or charged colloidal particles. We consider charged particles interacting with a long-range repulsive Coulomb force and a short range attraction as well as with randomly distributed local potential wells representing impurities in the substrate. Starting from an initially striped state, we compare the difference between driving the particles parallel and perpendicular to the stripe orientation. We show that for a drive applied perpendicular to the stripes the force necessary to depin the particles is significantly higher than for a drive applied parallel to the stripes. This is due to the significant energy cost of breaking up the stripes and reorienting them in the direction of the drive. We also observe hysteresis in the velocity-force curves. We compare our results to recent experimental data on 2D electron gases. Other applications of these systems could include producing logic devices that have different I-V curves for different current directions.

INTRODUCTION

A wide variety of systems, due to competing interactions between their constituent particles, can spontaneously form patterns such as stripes and labyrinthine structures. These are called pattern forming systems. Some examples include animal stripes and the superconducting/normal states in type I superconductors; for more examples see Seul and Andelman[1].

Recently there have been experiments that show anisotropy in electron transport in a two-dimensional electron gas (2DEG) in the quantum hall effect. A 2DEG is observed in a GaAs/AlGaAs interface of very high purity. The sample is cooled to very low temperatures (on the order of 150 mK) and subjected to a high magnetic field (on the order of several Tesla)[2] normal to the plane of the gas. Electrons start to spin in cyclotron orbits: this localizes the electrons' wave functions so they act like particles. At energy levels above $N=1$ interactions between their wave functions' allow electrons to experience a short-range attractive force to one another. This combination of the long and short range Coulomb repulsion and a intermediate range attraction enables the electrons to form a triangular lattice known as a Wigner solid.

Experiments, such as Ref.[2] show evidence of anisotropy in a two-dimensional electron gas in the quantum hall effect. Samples at less than 150 mK subjected to magnetic fields between 1 and 3 Tesla showed a marked anisotropy in resistivity Ref.[2] The anisotropy was very strong in the $N=2$ through $N=5$ Landau Levels (LL), while it was completely absent in the $N=1$ LL (where the short-range electron attraction is impossible). Others, such as Göres[3] have even shown that the anisotropy is consistent with a striped electron state.

Motivated by these experiments, we simulate localized electrons in a striped configuration in two-dimensions.

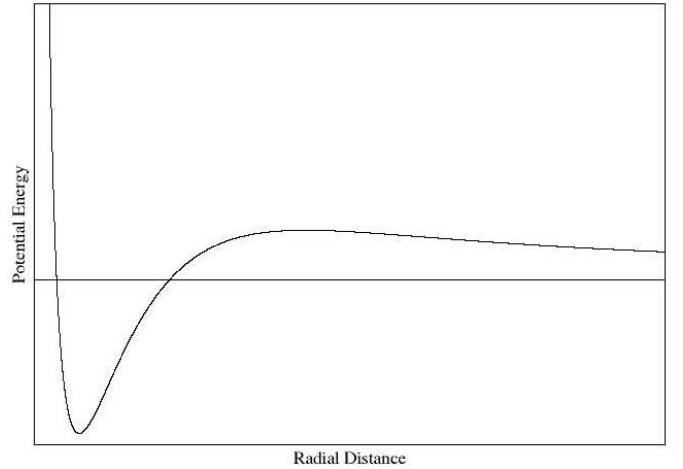


FIG. 1: Electron-electron interaction potential. At very short and at long distances the Coulomb force dominates; however, in an intermediate region, the short-range attraction dominates and there is a potential well at finite distance. This potential is completely symmetric and isotropic.

We test the anisotropy of transport by comparing the average velocity of electrons when they are driven along the stripes to when they are driven against (normal to) the stripes. We do this for a variety of pin strengths.

Our data show significant and consistent anisotropy when pinning forces of 0.10 or greater are used. The simulations also show a sharp depinning feature in the I-V curves consistent with Figure 1c. of Csáthy et al[4].

METHODS

Each simulation is a box of dimensions approximately 31 by 34 with randomly distributed pins and periodic boundary conditions. Pins are modeled as parabolic potential wells that represent impurities and flaws in the

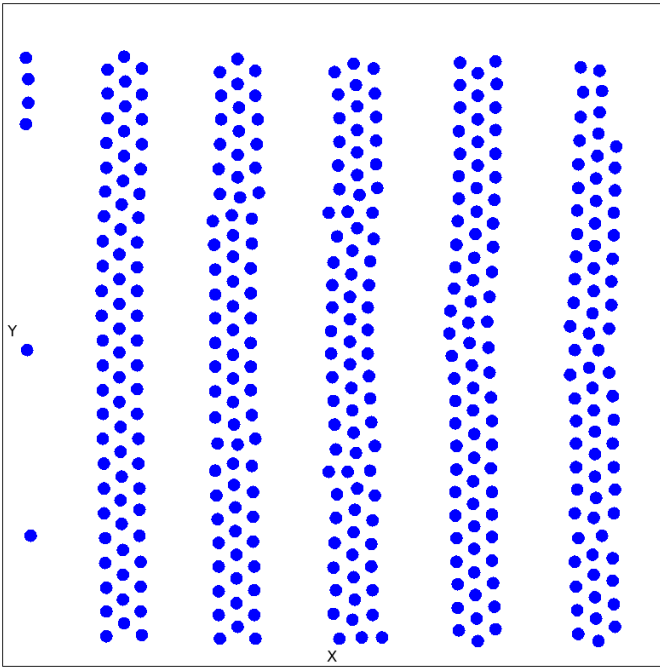


FIG. 2: The stripes formed by annealing. Due to the dimensions of the sample and the density of the particles we obtain stripes in the vertical direction. To study the anisotropy we drive the particles either along the orientation of the stripes, or normal to the stripes.

sample that would attract electrons. Although the distributed is random, the same random distribution is used for each run. The overdamped equation of motion is

$$f = f_{ij} + f_p + f_d = \eta v$$

where f_{ij} represents the sum of all the pairwise particle interactions, f_p represents the force from the pin if the particle is interacting with one, and f_d represents the external driving force (analogous to an applied voltage).

We treat electrons as point particles that interact in two ways: there is a long range Coulomb repulsion that varies with the inverse of the radial distance between the particles, and a short-range attractive force that varies like a decaying exponential with radial distance. These potentials combine to form:

$$V_i = \frac{1}{r} + B e^{-(\kappa r)}$$

This equation produces a potential minimum at finite distance, as shown in Figure 1. The force on each particle is a sum of the pairwise interactions with every other particle in the sample box. The infinite range Coulomb force is treated using the Lekner method[5].

Our simulations start with particles already arranged in stripes, as shown in Figure 2. We build these stripes by starting with randomly arranged particles (and no pins) and doing a simulated anneal. For our simulations we

set temperature to zero on an absolute scale because the effects we are interested in are not made more interesting by adding Brownian motion. In Lilly's experiment, the effect was, in fact destroyed at temperatures about 150 mK[2]. We vary the pinning force in different simulations. We study the anisotropy by running two simulations for each pinning force. In one simulation we apply a drive along the x-direction $F_d = F_d \hat{x}$, which is normal to the stripes. In the second simulation, we apply the drive in the y-direction, parallel to the stripes, $F_d = F_d \hat{y}$.

In each simulation we start with no applied drive. After a number of time steps (160,000 in most of our data), we increase the driving force by a small increment ($0.00005 \leq \Delta f_d \leq 0.001$). The larger pinning forces required larger increments to be completed in a reasonable amount of time, while smaller pinning forces require smaller increments obtain sufficiently high resolution. We allow the simulation to continue until the particles had all depinned and the measured the depinning force.

RESULTS

We process our data in several ways, one of which is constructing velocity-force (v-F) curves by averaging all of the velocities of all of the particles over a single force interval. Using these curves, we can set a threshold for what driving force we consider to be 'depinned.' Velocity-force curves are equivalent to current-voltage (I-V) curves because the average velocity of the particles is analogous to current and driving force is the equivalent of applied voltage.

Figures 3-5 are some selected I-V curves. In Figure 3 we display the lower limit of the pinning forces we investigated. When $f_p < 0.05$ there is no anisotropy at all. In this regime the pinning force is so weak that the stripes only flow *elastically*. Since the stripes never break up, there is no energy cost associated with breaking them up and the I-V curves for the X and Y driven stripes are identical. Even this regime, both curves still display rather sharp depinning followed by Ohmic behavior, consistent with Figure 1c of Ref. [4];

In Figure 4 we can see anisotropy: the y-driven electrons depin somewhat smoothly around $f_d = 0.0019$, while the x-driven electrons do not depin until $f_d = 0.0024$, when they depin sharply. This is a roughly 30% difference in critical force, which is reasonably outside of error.

Figure 5 shows the I-V curves for $f_p = 1.00$, the highest pinning force we examined. The anisotropy is even larger: the critical force in the y direction is $f_d = 0.030$, while the critical force in the x direction is $f_d = 0.057$, a difference of 90%. Once again, the x-driven stripes exhibit a sharp depinning behavior while the y-driven stripes depin more gradually. This is because it takes energy to break up the

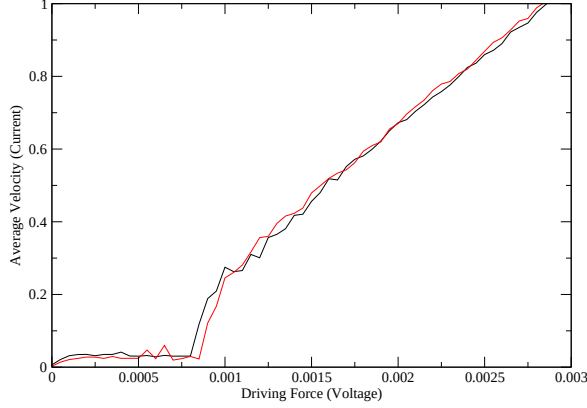


FIG. 3: Velocity-force curves for X and Y driven runs with $F_p = 0.05$. The pinning force is not sufficiently strong to break up the stripes and there is no anisotropy. In black is the I-V curve for particles driven in the X direction, against the stripes; in red is the I-V curve for particles driven in the Y direction, parallel to the stripes.

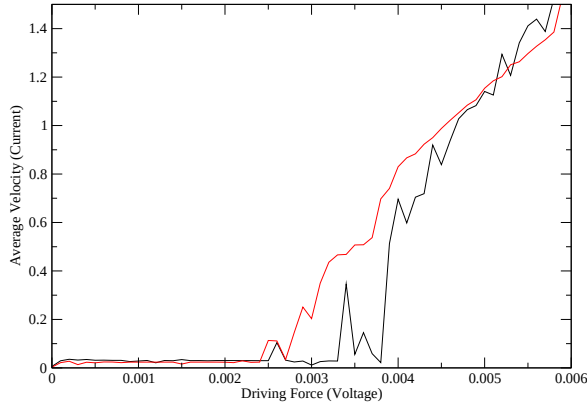


FIG. 4: Velocity-force curves for X and Y driven runs with $F_p = 0.15$. In black is the I-V curve for particles driven in the X direction, against the stripes; in red is the I-V curve for particles driven in the Y direction, parallel to the stripes.

stripes.

We examine each I-V curve and determine the critical depinning force. An average velocity $\bar{v} = 0.40$ is the threshold we use. We only consider the particles to be depinned when their average velocity permanently exceeds the threshold value. This allows us to eliminate cases where noise would affect our results. We plot the results in Figure 6. Although the data is noisy: it generally shows the trends we are looking for: the critical force for X and Y driven stripes increases with increas-

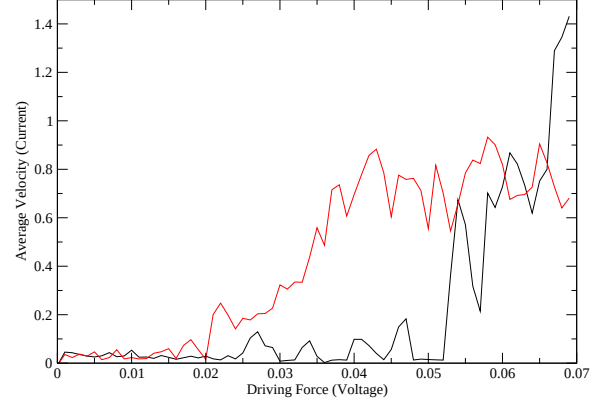


FIG. 5: Velocity-force curves for X and Y driven runs with $F_p = 1.00$. In black is the I-V curve for particles driven in the X direction, against the stripes; in red is the I-V curve for particles driven in the Y direction, parallel to the stripes.

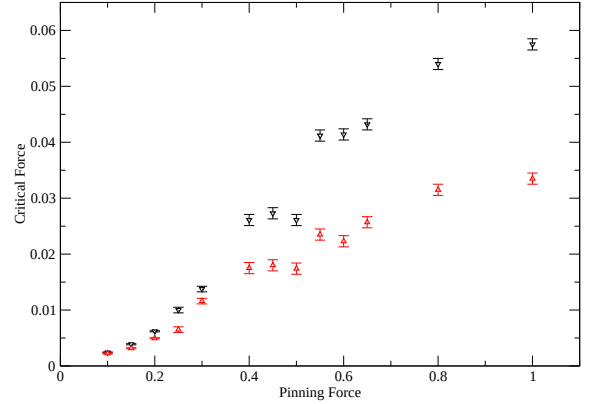


FIG. 6: Critical depinning force for particles driven in the X direction (in black) and the the Y direction (in red).

ing pinning force. There is also a consistent and strong anisotropy: the y-driven particles always depin before the x-driven particles. This anisotropy grows with increasing pinning force. We suspect that at sufficiently high pinning strength, the anisotropy would disappear because the energy of the stripes would be insignificant compared with the energy of the pins.

In Figure 7 we see some novel and unanticipated behavior: at high drives the anisotropy reappears. When we watch the x-driven electrons in motion we see that the stripes break up and the particles flow in rivers. As the drive increases, the particles flow as clumps and then partially reorder into stripes in the direction of the drive, as

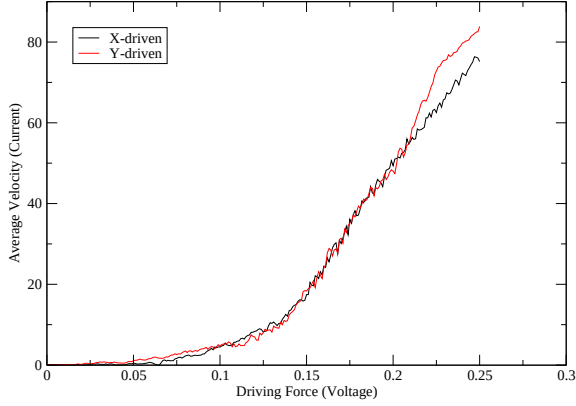


FIG. 7: Velocity-forces curves for X and Y driven runs with $F_p = 1.00$ (the highest tested). As the driving force increases, the Y driven stripes depin, followed by the X driven stripes. At a second critical drive, they converge, and finally, at high drive, they diverge again. This divergence is not anticipated from theory. This curve was constructed using 80,000 time steps per force increment.

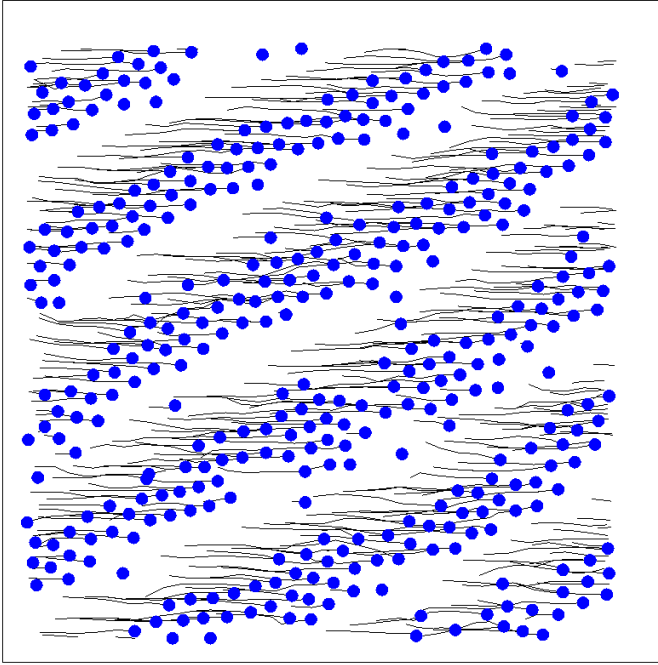


FIG. 8: X-Driven particles at high drive. Stripes reform but at an angle to the drive, rather than parallel to it.

expected. Stripes form at an angle to the drive, as shown as Figure 8. In the y-direction the stripes break up, the particles flow plastically in rivers and then clumps, and finally they reorder into stripes in the direction of the drive. When the I-V curves are converged, the electrons are flowing isotropically in clumps (isotropic both

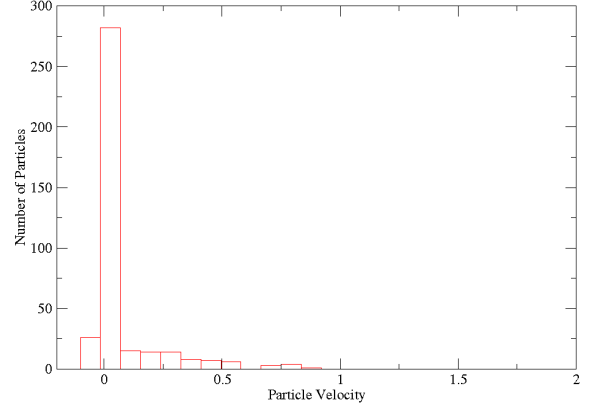


FIG. 9: Velocity distribution for x-driven particles at $f_d = 0.100$, for $f_p = 1.00$. The total number of particles is 380.

in sense of the x and y driven simulations being converged and the individual simulations being isotropic: having no directional structures).

We find that the x-driven electrons do not form stripes parallel to the drive in the way that the y-driven electrons do. A possible explanation has to do with the inherent width and spacing of the stripes. The stripes form in the y-direction because the dimensions of the box are fine tuned to allow the stripes to form in that direction; they fit best in they vertical orientation. The stripes have an intrinsic width and have a certain amount of space between them. It is possible that the stripes do not fit horizontally so they orient themselves as close as they can get to the horizontal direction.

We also examine the velocity distributions of the particles at a given driving force. This is another technique to understand how the particles are flowing. The distribution usually takes the shape of a bimodal distribution, with one peak around zero and one peak at finite velocity. Figures 9-12 are sample velocity distributions from the x-driven particles in Figure 7 with $f_p = 100$. Note that the velocities in theses figures are not directly comparable with the velocities shown in the I-V curves because they are normalized differently. In Figure 9 the particles are still mostly pinned with the vast majority clustered around zero velocity.

In Figure 10, a little less than half the particles are depinned. The bimodal distribution indicates plastic flow. The moving particles have a approximately Gaussian velocity distribution, centered around $\bar{v} \approx 0.5$.

In Figure 11 the majority of particles are depinned and moving with an average velocity of $\bar{v} \approx 0.8$. The velocities of the depinned particles appear approximately Gaussian.

Finally, in Figure 12 nearly all of the particles have

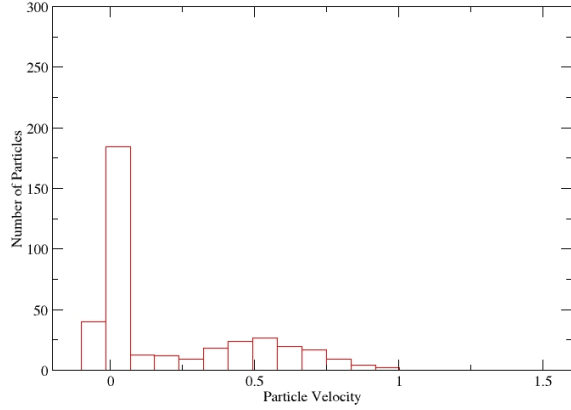


FIG. 10: Velocity distribution for x-driven particles at $f_d = 0.150$, for $f_p = 1.00$. The total number of particles is 380.

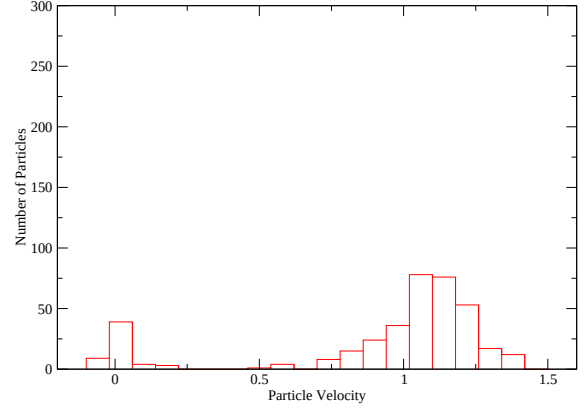


FIG. 12: Velocity distribution for x-driven particles at $f_d = 0.240$, for $f_p = 1.00$. The total number of particles is 380.

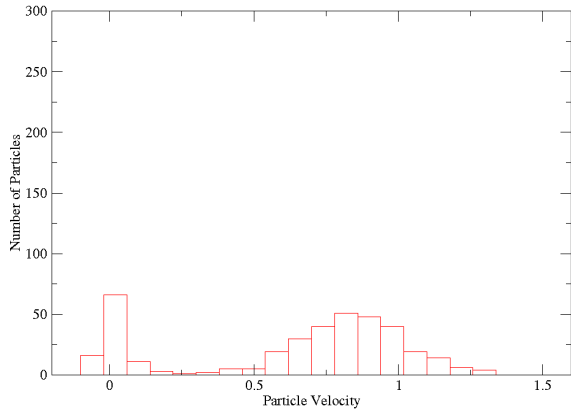


FIG. 11: Velocity distribution for x-driven particles at $f_d = 0.200$, for $f_p = 1.00$. The total number of particles is 380.

depinned with $\bar{v} \approx 1.1$. One of the interesting features of these distributions is that the electrons' behavior is *non-ohmic*. As the driving force increases, the electrons' average speed increases. This seemed to warrant further investigation. Figure 13 is the average velocities of the depinned particles, ignoring the particles with velocities below a cutoff we set at $v_{cutoff} = 0.2$. This seems to confirm the trend from the velocity distributions: the average velocity of the moving particles increases with the driving force. It is also surprising that Figure 13 exhibits almost no anisotropy.

From Figure 14 it is apparent that the source of the anisotropy is not the velocity of the particles, but the number of depinned particles. When the y-stripes first depin, they carry more of the particles with them. The

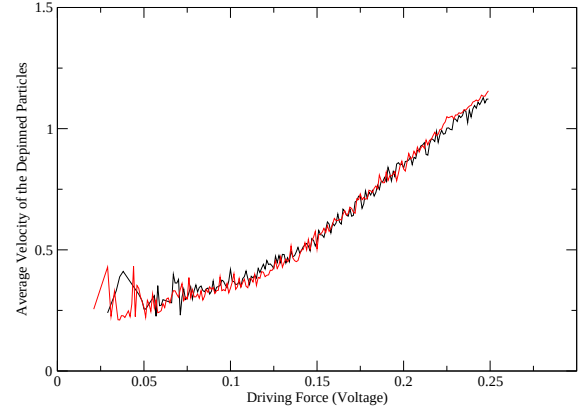


FIG. 13: Average velocity of depinned particles (particles with velocities of $v < 0.2$ were ignored) for x-driven particles with $f_p = 1.00$. The black curve represents x-driven particles; the red curve represents y-driven particles.

reason the y-stripes diverge at high drive is that when they reorder they pull all of the particles along, while some of the x-driven particles get left behind.

Future work may include investigation of the hysteresis shown in Figure 1c of Ref. [4]. We would also like to change our simulations in a way that allows direct comparisons to Göres' results on current-induced anisotropy, shown in Figure 1 of Ref. [3].

In summary, we have investigated anisotropy transport of striped electron states. The data shows a sharp depinning behavior consistent with Figure 1c of Ref. [4]. We have observed anisotropy in the I-V curves as seen in Ref. [2] and in the depinning of the particles. The ve-

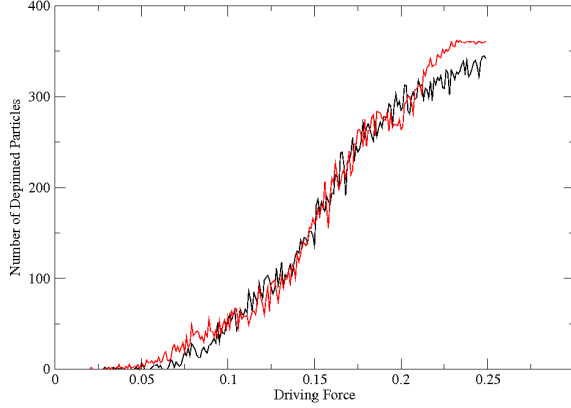


FIG. 14: Number of depinned particles for x-driven particles with $f_p = 1.00$. The black curve represents x-driven particles; the red curve represents y-driven particles.

locities of the depinned particles are isotropic. However, there *is* anisotropy in the number of particles depinned. Our results suggest that a electron stripe configuration

does exist in a 2DEG in the quantum hall effect.

ACKNOWLEDGMENTS

This research would not have been possible without the mentoring and assistance of Dr. Cynthia Reichhardt and Dr. Charles Reichhardt and the support and sponsorship of Norm Magee, James Colgan and the Los Alamos Summer School, funded the National Science Foundation.

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 - [3] J. Göres G. Gamez, J.H. Smet, L. Pfeiffer, K. West, A. Yacoby, V. Umansky, and K. von Klitzing Phys. Rev. Lett. **99** 246402(2007)
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Automated receptor docking of Testing automated docking of μ opioid ligands

Amy A. Hass, Fangping Mu (mentor), and Chang-Shung Tung

Abstract

The three-dimensional structure and binding modes of representative mu-opioid ligands have been investigated using molecular modeling techniques. A homology model of the μ opioid receptor was built. Using the docking program Autodock 4, 155 ligands with high affinity were docked to the homology model of the μ opioid receptor, and the docking score of each was recorded. No correlation was found between docking scores and the known protein-ligand affinity values, casting doubt on Autodock free energy estimation as a reliable measure of binding energy. Since binding affinity and docking score should be directly proportional, Autodock's free energy equation is investigated next. After reviewing software documentation, we conclude that the docking process is far too delicate for the primitive Autodock, based as it is upon semiempirical equations, to compute accurately.

Introduction

G-protein coupled receptors, or GPCR, are involved in the operation of 30% of all commercial drugs.¹ Without GPCRs, the pharmaceutical industry would suffer greatly. These receptors are membrane-bound proteins, and 3D structures are difficult to measure. In spite of their essential roles, only a few GPCR 3D structures have been solved. Without structural information, it becomes much harder to design drugs or divine functions for members of the GPCR group. Only about 30 different GPCRs are currently engaged pharmaceutically, reflecting the paucity of information available on these receptors. Enormous therapeutical potential could be waiting in the remaining GPCR population.

One GPCR in particular, the μ opioid receptor, could prove vital to the battle against drug and alcohol addiction. The μ opioid receptor is known to play a part in the 'high' drug abusers experience, and tweaking this receptor may ease the withdrawal stage. Drugs produce their effect by binding to the μ opioid receptor. This leads to phosphorelation of a compound within the cell. If the drug agonist were blocked by an antagonist compound, the drug would be neutralized. By binding more tightly to the receptor, the antagonist would keep the agonist from having any effect. To design new, more effective drugs, the first step is to find a good antagonist for the μ opioid receptor. Since this is currently next to impossible through x-ray crystallography, alternative methods must be called upon.

Homology Modeling of μ -receptor

Traditionally, x-ray diffraction techniques are the method of choice for discerning a molecule's structure, however GPCRs, such as the μ opioid receptor, are notoriously recalcitrant to this technique. GPCRs reside within the membrane of a cell, poking through the top and bottom of the cell's lipid membrane. A small molecule will bind to the receptive area of the GPCR from outside the cell, and a chain reaction will precipitate phosphorylation of another molecule inside the cell. The functional structure of a molecule depends heavily on the medium in which it naturally exists, which is, in this case, the cell's lipid bilayer. It is not possible with the current technology to crystallize a μ -receptor in the same shape as it exists in the cell membrane. Since the shape of a molecule is often critical to its function, alternative methods are sought.

In the situation when the target structure is not available, in silico methods can provide an alternative for deriving the target structure. Homology modeling is based on a simple assumption that proteins with homologous amino acid sequences adopt similar 3D structures. This assumption allows for the prediction of the 3D structures of these proteins based solely on their amino acid sequences and the 3D structures of proteins with homologous amino acid sequences. In addition, when combined with other modeling procedures, homology modeling can be applied beyond the normal usage of the method and successfully model structures of various biomolecules. GPCRs share many structural features,

including a bundle of seven transmembrane α helices connected by six loops of varying lengths. A BLAST search (<http://www.ncbi.nlm.nih.gov/blast/Blast.cgi>) of the human mu-opioid receptor (mu-OR) amino acid sequence against all proteins in the PDB shows a relatively high homology of human mu-OR with bovine rhodopsin (PDB accession code: 3C9M) and the squid rhodopsin (PDB accession code: 2ZIY). The sequence homology between the bovine and the squid rhodopsins is relatively low (< 20% identity), the structures between the two molecules can be aligned

closely. The two structurally aligned molecules can be used to develop a more reliable sequence alignment. The human μ -OR sequence is then aligned with the two structurally aligned rhodopsin sequences. Based on the aligned sequences, the homology model of the human mu-OR (shown in Figure 1) is developed using the structures of the rhodopsin. The view of the molecule shows the extra-cellular side of the receptor on the top and the intra-cellular side of the receptor on the bottom.

Fig. 1. Homology model of the μ opioid receptor. This image was generated by Autodock Tools.

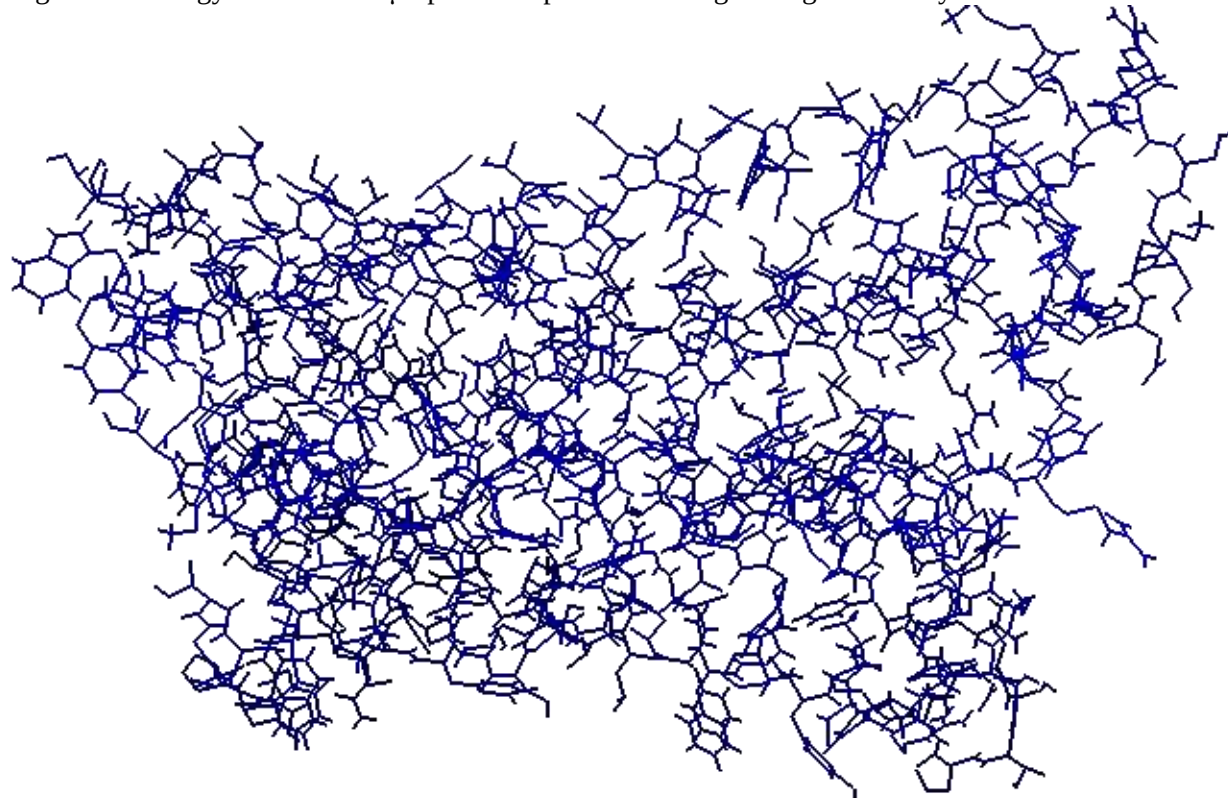


Figure 1 is a side view of this approximately conical structure. The cell membrane would pass vertically through the middle of the receptor. To the left is the binding area of the receptor which catches ligands passing outside the cell. The right side of the cell stretches into the cytoplasm, holding cellular components in place and ready for phosphorelation.

Ligand-Receptor Docking

With a good model of the receptor in hand, candidates for strongly bound ligands can be evaluated. To block a harmful drug from doing its damage through the μ opioid receptor, a stronger-binding ligand has to be found. The agonists bind very tightly, so we turned to

a database of known antagonists for the μ opioid receptor. Not all of them bind tightly enough to be useful, but they can be used to test Autodock's finesse at binding. Accordingly, 155 ligands with experimentally measured affinity binding to the μ -receptor were taken from BindingDB and docked to the receiving surface, on the left in Fig. 1. Default settings were used for Autodock's search algorithms,

with one exception. To speed along docking, 250,000 evaluations were used in place of 2,500,000. With these inputs and a grid area over the whole left face of the μ opioid receptor, docking scores for all 155 ligands were obtained. Table 1 displays the ligands, their K_i , and the docking score of their first docked

conformation. It is obvious from Table 1 that experimentally measured ligand-receptor binding affinity (K_i values) and Autodock's docking scores are uncorrelated. Since docking score is proposed to be a measurement of the binding affinity, the results indicate that the problem is with the docking scores.

Table 1

	Ligand	K_i	Docking Score (kcal/mol)
1	4-anilidopiperidine	0.38	-8.42
2	H-Tyr-c	0.55	-6.66
3	C-terminal modified bifunctional peptideinal	0.65	-4.69
4	4-anilidopiperidine, 12	1.1	-3.77
5	4-anilidopiperidine, 11	1.2	-4.92
6	tDADA	1.3	-6.16
7	cDADA	1.35	-6.99
8	Biphalin	1.4	-3.09
9	YDAGF	2.8	-5.81
10	Bifunctional peptide ligand	5.5	1
11	4-anilidopiperidine, 17	5.7	-5.6
12	CCK-opioid peptide-opioid peptide-Op, 10	5.9	-2.66
13	C-terminal modified bifunctional peptideinal, 6	6.8	-1.42
14	DALEA	7.7	-3.56
15	CCK-opioid peptide-opioid peptide-Op, 8	7.8	0.43
16	C-terminal modified bifunctional peptideinal, 5	9.5	-2.27
17	Bifunctional peptide ligand, 7	9.7	0.6
18	spiropiperidine 52	14	-7.6
19	4-anilidopiperidine 10	14	-4.9
20	DADLE	15	-4.91
21	CCK-opioid peptide-opioid peptide 11	22	-2.24
22	4-anilidopiperidine 14	23	-6.67
23	Bifunctional peptide ligand 4	23	0.14
24	CCK-opioid peptide-opioid peptide 3	25	-1.23
25	spiropiperidine 47	26	-6.72
26	CCK-opioid peptide-opioid peptide 9	26	-2.34
27	Bifunctional peptide ligand 3	27	-1.56
28	spiropiperidine 46	28	-6.51
29	Bifunctional peptide ligand 1	28	0.04
30	spiropiperidine 40	29	-7.19
31	C-terminal modified bifunctional peptideinal	29	-3.27
32	CCK-opioid peptide-opioid peptide 7	34	-2.1
33	spiropiperidine 54	35	-7.28
34	Bifunctional peptide ligand 5	36	-0.69
35	spiropiperidine 48	36	-6.44
36	spiropiperidine 50	37	-6.87
37	spiropiperidine 55	37	-7.21
38	CCK-opioid peptide-opioid peptide 2	39	-3.23
39	4-anilidopiperidine 15	40	-6.91
40	spiropiperidine 59	43	-6.73
41	C-terminal modified bifunctional peptideinal 4	46	-3.36
42	Ro 64-6198	47	-7.49
43	spiropiperidine 3	48	-6.79
44	spiropiperidine 72	50	-6.71
45	RDADA 11	56.9	-7.73
46	spiropiperidine 53	59	-6.27
47	4-aminoguanazoline derivativeno 9d	60	-8.53
48	spiropiperidine 63	61	-6.81
49	spiropiperidine 61	64	-6.52
50	IDADA 13	64.5	-4.1

Investigation of Autodock Free Energy Function

We investigated the inconsistency of the docking scores with the experimental protein-ligand affinity. Autodock 4 estimated its docking scores based on the terms for van der Waals force, dispersion/repulsion, hydrogen bonding, electrostatics, and desolvation energy. The van der Waals force involves the attraction or repulsion of molecules based on their geometries. Induced dipoles in neutral molecules constitute the dispersion/repulsion force, and electrostatic interactions are determined by the interaction of electron charges. The desolvation energy is the energy it would take to return a bound complex to its original two molecules. The electrostatic force climbs steeply below 1 Angstrom, with a full range from about 10^3 to -10^3 kcal/mol. A hydrogen bond is the attractive interaction of a hydrogen atom with an electronegative atom, like nitrogen or oxygen.

The contributions of these terms are handled using semiempirical equations. Averages of large groups of molecules with known force values have been collected and integrated into a few governing equations, and these are used to calculate the free energy of the user's particular molecule. The greatly simplified free energy estimation challenged the accuracy of the docking scores. The averages and approximations at work in the free energy function are responsible for the breakdown in docking score accuracy. These generalizations affect the contribution of each force to the docking score. When molecules are closer than 1 Angstrom, dispersion/repulsion and desolvation become less consequential, and the hyperbolic energies of hydrogen bonding and electrostatics mostly cancel out. The AMBER field, used to calculate the bound complex geometry, assigns distances between the atoms, and the approximations it makes can change the docking score by many kilocalories per mole. This explains the discrepancy between K_i and docking score in Table 1.

While docking scores are less reliable, Autodock is far better at determining the structure of the bound complexes.

Autodock is able to assemble complexes with an RMS error of 2 angstroms. The difference in accuracy between the two tasks springs, once again, from Autodock's use of averages. This approach is far more useful for obtaining a correct shape. Even if two atoms are connected with an error of a small fraction of an angstrom, the overall structure of the complex will still be approximately correct. The same error could virtually destroy a calculation of binding energy, since the hyperbolic nature of several binding forces could mean an error of multiple kilocalories.

Patterns of Docking Structure

Autodock's structural accuracy is supported by the different conformations of the ligands during docking. The docking area of the μ opioid receptor is an elliptical space marked with a few small pits, grooves, and hills. Ligands tended to couch themselves in the depressions of the surface, giving them more surface area for bonding. Table 2 describes the most common locations, which are explained in the graphics that follow. In addition to landscape, the surface is also peppered with several colors in the figure to represent different zones of attraction. A yellow hydrogen-donating sulfur occupies the bottom right, while a blue nitrogen sits in the top center. The most attractive of all these features, however, is the pit below and to the left of the surface center. All ligands had at least one of their conformations docked here, scattering around the rest of the surface according to their size and shape.

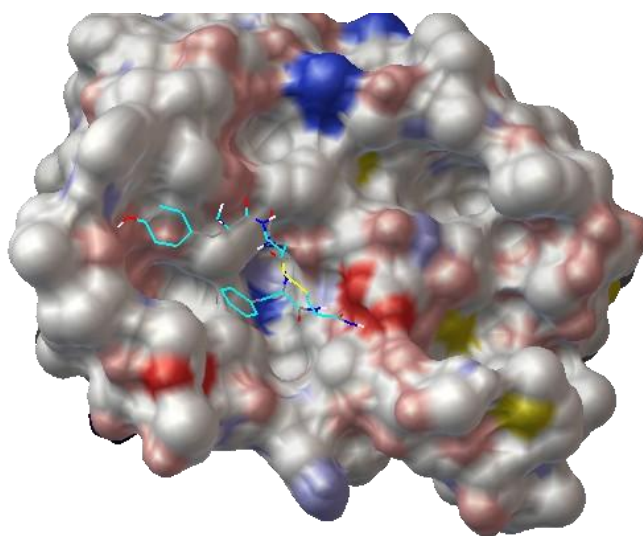
It is tempting to think, based on the similar docking patterns among ligands of the same type, that Autodock's generalizations could be mitigated by altering its semiempirical formulas based on data from experiments similar to that of interest. Barbault et. al. used this approach to better parameterize Autodock's free energy function for RNA complexes. Although it did marginally increase the accuracy of the free energy function, the task was labor intensive, impractical for the general user of Autodock. Here, only a cursory treatment is given to the relevance of docked location to ligand structure. Simple, functional names are given to a few docking sites in order to keep the analysis clear.

Table 2

Pit	South	West	Above Sulfur
4-anilidopiperidine	C-terminal modified bifunctional peptide	Spiropiperidine analogue	tDADAE
H-Tyr-c	CCK-Opioid Peptide	4-aminoguinazoline derivative	Spiropiperidine analogue
cDADAE	Bifunctional Peptide Ligand	Piperidine Derivative	Ro 64-6198
DALEA	Spiropiperidine analogue	2-benzoylquinazoline analogue	4-aminoguinazoline derivative
DADLE			YDAGF-NH2
IDADAE			rDADAE
			Piperidine Derivative
			2-benzoylquinazoline analogue
			benzo[g]quinazoline derivative

99 different ligands were sampled to compile this chart. They represent the 99 lowest-Ki ligands which bind to the μ opioid receptor, as listed in the Binding Database. Names given above refer to the different chemical families represented by the 99 ligands. Area designations and denizens are described below. Some ligand families occur in more than one location, and this is because a ligand's conformations often bind, in significant numbers, to more than one site on the cup.

Fig. 2: Pit



This 4-anilidopiperidine, 16 demonstrates the meaning of the meaning of the Pit location. The middle of this ligand rests within a depression of the binding surface, here referred to as the Pit. The lowest energy

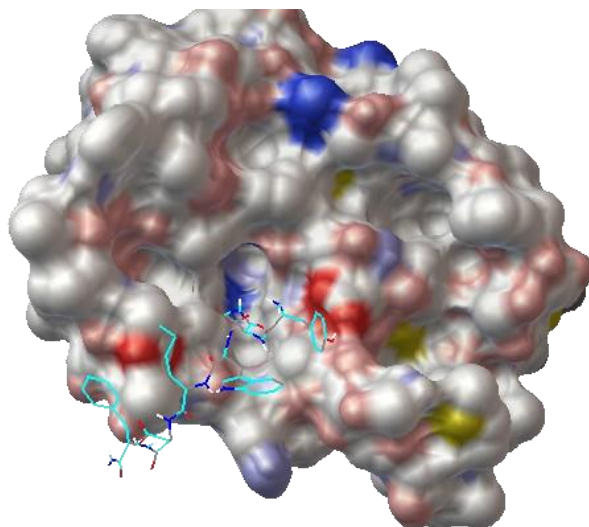
conformation of nearly every ligand that was examined can be found either within the Pit or bordering it. A very few ligands find their lowest binding energies elsewhere on the binding surface, but in these cases,

the Pit always presents a close second conformation, if not always a first.

Because of the universality of this area, only those

ligands with all conformations in the Pit are placed in this category. The members of Pit do not occur in any other site category.

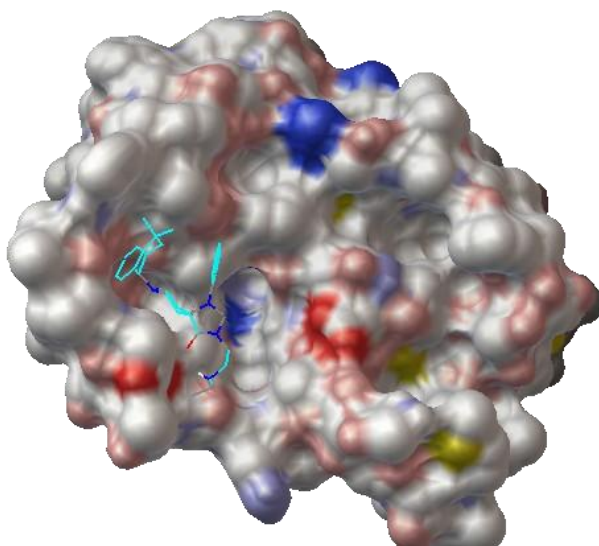
Fig. 3: South



This zone refers to the area south of the pit. As is shown in the above graphic by CCK-Opioid Peptide, 8, a ligand can be both in the pit and south of it in this category. Far from an exception, this circumstance dominates the 'South' grouping. It is separated from the 'Pit' group by the lopsided crawl south of the pit exhibited by the ligand.

'South' ligands generally consist of long carbon chains with varying numbers of carbon rings. With the exception of the spiropiperidine analogues, South has no ligand overlap with either the West or Above Sulfur groups.

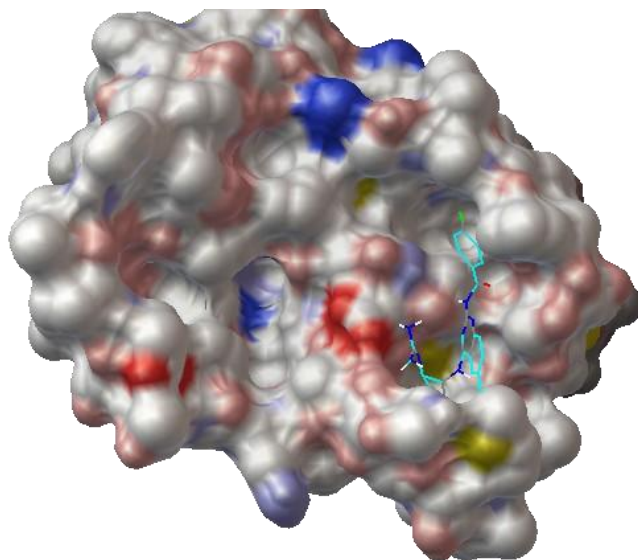
Fig. 4: West



Spiropiperidine analogue, 55 belongs to the West group. Members of this group lie just to the west of

the depression called the pit. Like members of Above Sulfur, members of West tend to be smaller, having

almost no crossover with South members, which are much larger on average.
Fig. 5: Above Sulfur



Here, ligand 2-benzoylquinazoline analogue, (1S, 2R)-17 sits atop a yellow sulfur atom, demonstrating the positioning of atoms in the Above Sulfur group. Here, ligands can stretch vertically up from the sulfur, as 2-benzoylquinazoline has done, or they may float horizontally above it near the upper rim of the receptor. 2-benzoylquinazoline is a good

representative of ligand size for this group. Above Sulfur ligands tend to be much smaller than those in South. With the exception of spiropiperidine analogues, Above Sulfur has no crossover with South.

Conclusion

Autodock is most useful as a screening tool, allowing one to cull 100 promising ligands from databases of thousands. Once this smaller group of potentially useful ligands has been assembled, docking programs like Autodock are exchanged for experimental investigations. Decades of practice have refined the experimental determination of protein-ligand binding affinity, however, the convenience of docking simulations have yet to exceed their limitations.

Because Autodock is unable to handle docking scores for molecules of ordinary complexity, such as those for which crystal structures exist, dealing with GPCRs are far beyond the software's capabilities. Computerized methods are useful for preliminary screening of ligand binding ability, but summing the effects of multiple forces acting in three dimensions on hundreds or thousands of atoms is still far beyond the capabilities of a program such as Autodock. Before such a goal can be realized, both desktop computer power and understanding of the binding process must surpass by far their current incarnations.

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Exploration of Convective Structures in Rotating Fluids with Simple Equipment

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Abstract

The convective behavior of rotating water has fundamental significance in geophysical applications. Here we describe a series of laboratory experiments to study convective structures in rotating fluids in ranges of Rayleigh flux number Ra_f from 6×10^4 to 10^7 and of Taylor number Ta from 5×10^6 to 10^7 . A transitional convective ring pattern, corresponding to a preconditioning phase, is seen to form from interactions between the fluid spin-up, for which we determine the times of complete formation and destruction and minimum ring diameter of the centermost ring in terms of Ra_f and Ta . The ring structure evolves into an irregular vortex grid, corresponding to a semi-stationary mixing phase, with the number density of vortices $N \propto h^{-2} Ta^{1/2} Ra_f^{-1/6}$, where h is the fluid depth. Using basic equipment, such as a record player, a digital camera, a dish of water, and color dye we are able to see these relationships with some degree of accuracy.

I. INTRODUCTION

An inviscid fluid rotating sufficiently fast inhibits motion in the direction of the axis of rotation due to the Taylor-Proudman theorem, essentially restricting fluid flow to two dimensions. However, convective instabilities caused by heat or mass flux at the fluid boundaries drive vertical motions. This makes vertical motion possible in narrow sheets or small vortices where competition between vertical stratification and convective instabilities lifts away the Taylor-Proudman constraint. This behavior results in interesting convective structures that can be observed in the laboratory.

The study of convective structures in rotating fluids is of interest for various applications, including the dynamics of open-ocean deep convection at the Gulf of Lions. Here, ocean currents produce a large cyclonic background circulation. Continual heat loss at the surface of the ocean, caused by the colder air, then causes isopycnals, constant-density surfaces, to dome up near the surface. This convective instability can then initiate stage of violent mixing, wherein the entire fluid column overturns and ascending and descending currents can penetrate the whole depth of the ocean (Jones and Marshall 1993).

Open-ocean deep convection is characterized by three successive phases: *preconditioning*, occurring on the large scale (of order 100 km); *violent mixing* occurring in localized, intense plumes (with scale of order 1 km); and *sinking and spreading* of the convectively tainted water, on a scale of 5–10 km (Jones and Marshall 1993; and references therein). In the preconditioning phase, the water is rotating on a large scale and a wave of cold air comes in causing buoyancy forcing due to surface cooling, making the system predisposed to overturn. This initiates the violent mixing phase, wherein the fluid column overturns and cold water flows downward in multiple cells with diameters of order 1 km, depths sometimes as large as the depth of the ocean, and downward velocities on the order of 10 cm s^{-1} . These plumes rapidly mix the properties of the system, forming a chimney of homogeneous fluid which, under the influence of gravity and rotation,

deforms and spreads out at middle depths. Additional fluid from outside the system enters to replace lost fluid near the surface of the water, leading to restratification at layers near the surface and the eventual breakup of the chimney on the timescale of days.

We can create a similar situation in the home laboratory using a basic setup, such as a dish of water rotating on a record player. If the temperature of the water T_w is less than or comparable to the temperature of the air in the room T_a , then there is a heat flux through the surface of the water caused by evaporation, sensible heat transfer, and thermal radiation. The heat flux causes the surface temperature of the water T_s to become cooler and denser than the temperature of the water, creating a convective instability. By turning on the record player, we cause the fluid to push toward a stratified arrangement that competes with the convection driven by the heat flux. Using dye, we can see convective structures formed during the process as the water spins up to reach the angular velocity of the record player and after as the system approaches a steady state. In doing so, we see a transient stage of convective ring formation similar to the preconditioning described in open ocean deep convection. We also see a final state wherein a large distribution of vortices form with depths as large as the water depth in the dish, similar to the plumes in the violent mixing stage previously described.

II. EXPERIMENTAL METHOD

In our experiment, we take a large plastic dish 34 cm in diameter and fill it with water to a depth h , usually around 2.5 cm. The dish is then set on an old record player with an angular velocity adjustable to 16 (1.68), 32 (3.35), and 48 (5.03) rpm (rad/s). Since the latter higher rotation rates introduces a noticeable free-surface slope and makes the water dish more likely to fly off of the record player, most experiments are conducted at 16 rpm. The dish is centered on the record player so that the system will be symmetric about the axis of rota-

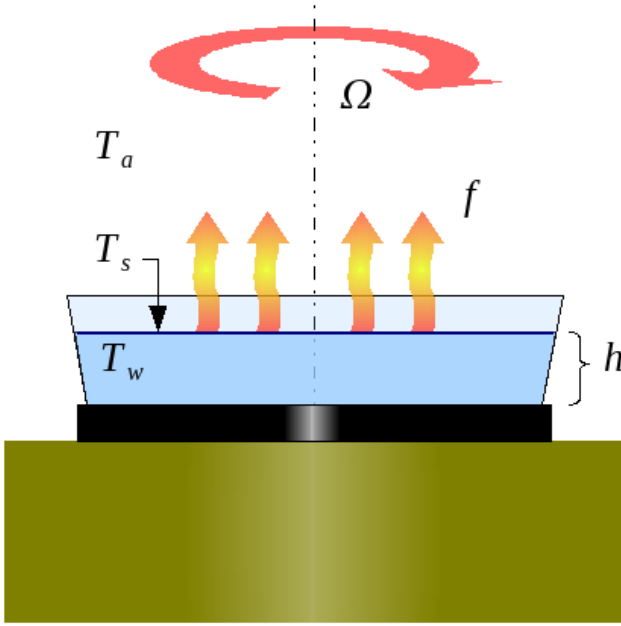


FIG. 1: Dish filled with water at temperature T_w to depth h rotates on a record player at constant angular frequency Ω in air at a temperature T_a . For $T_a \lesssim T_w$, heat flux f through the surface of the water lowers the water surface temperature T_s , creating a convective instability.

tion. After placing the water dish on the record player, a small quantity of dye is sprinkled into the water and the record player is turned on. The experimental apparatus is shown in FIG. 1. Heat flux exits the fluid through the surface by evaporation (latent heat), sensible heat flux, and thermal radiation. The temperature of the water T_w is kept larger than or close to the temperature of the air T_a so that the total heat flux through the water's surface f is positive. A positive heat flux at the water's surface creates a cooling effect making the surface temperature T_s less than T_w . The resultant buoyancy forcing (convective instability) combined with the stratification due to rotation forms convective patterns that the dye allows us to see.

All experiments were conducted using tap water because it is readily available and its properties would likely be close enough to those of distilled water for the measurement accuracy of our experimental setup. Assuming that the main determining characteristics of our experiment are the heat flux f and the stratification caused by the angular velocity of the record player Ω , all quantitative data for our experiment should be able to be classified using the similarity criteria given by the Rayleigh flux number

$$Ra_f = \frac{\alpha g f h^4}{\rho c_p k^2 \nu} = \frac{B h^4}{k^2 \nu}, \quad (1)$$

and the Taylor number

$$Ta = \frac{4\Omega^2 h^4}{\nu^4} = \frac{\omega^2 h^4}{\nu^4}, \quad (2)$$

where

$$B = \frac{\alpha g f}{\rho c_p} \quad (3)$$

is the surface buoyancy loss (ie. rate of kinetic energy dissipation) and $\omega = 2\Omega$ is the Coriolis parameter. Here g is the gravitational acceleration and the definitions of the thermodynamic properties α , ρ , c_p , k , and ν are given in the table in FIG. 2.

Boubnov and Golitsyn were the first to experimentally study convective structures in rotating fluids for a wide range of determining parameters (Boubnov and Golitsyn 1986). In their experiment, a square or cylindrical jar with an open top, insulated sides and an aluminum bottom is filled with distilled water. The water in the container is heated from below by circulating water at temperature T_T (called the thermostat) through a basin in contact with the container's aluminum bottom. The water in the container is cooled via the contact of the uncovered surface of the water with the colder air. After some time, the temperature of the water in the vessel reaches an approximately constant value T_w (to an accuracy of the order of a tenth of a degree) which is slightly cooler than the water in the thermostat. At this time, additional particles are introduced to the water, for purposes of visualization. The flows are visualized by aluminum powder at the surface, or by bromium-thymol blue dye, or by permanganate particles. The turn table is then switched on, rotating the container at a constant angular velocity. The spin-up of the water causes the dye to immediately form a spiral on the surface. After a time, ring structures and vortices appear.

A. Calculating the Heat Flux

Assuming that the the heat flux through the plastic container is negligible, the total heat flux through the water is equal to the sum of the sensible, latent (evaporative), and radiative heat flux through the surface of the water, denoted f_{sens} , f_{lat} , and f_{rad} respectively. The sensible heat flux can be calculated using the semiempirical formula

$$f_{sens} = 0.14 \rho c_p \Delta T_{sa}^{4/3} \left[\alpha k^2 g \nu^{-1} \left(1 + \frac{m}{Bo} \right) \right]^{1/3}. \quad (4)$$

Here $\Delta T_{sa} = T_s - T_a$ is the difference between the temperature of the water surface and the temperature of the air, and the rest of the symbols in the above equation are defined in the table in FIG. 2. The unitless factor m is given by $m = 0.61 c_p T_a / \ell$, and all the molecular coefficients in the above equations are for air (not water) at a temperature of $\frac{1}{2}(T_s + T_a)$. Also, Bo is the Bowen ratio,

which relates the sensible and latent heat flux, and is given by

$$Bo = \frac{f_{sens}}{f_{lat}} = \left(\frac{k}{k_e} \right)^{1/2} \frac{c_p \Delta T_{sa}}{\ell \Delta q}. \quad (5)$$

In this equation Δq is the difference of specific absolute humidities at the surface of the water and in the room:

$$\Delta q = \frac{\xi e_s}{p - (1 - \xi)e_s} - \frac{\xi e_a}{p - (1 - \xi)e_a} \approx \frac{\xi(e_s - e_a)}{p}, \quad (6)$$

where e_s and e_a are the saturation vapor pressures of water vapor at temperatures T_s and T_a respectively, and $\xi = 0.62197$ is the ratio of specific gas constants, of water vapour to dry air. In practice, the calculated value of the partial saturation pressure varies greatly based on the value of the relative humidity at that point in the room. At the surface of the water, we assume that the humidity is 100%, but the relative humidity of the air in the room needs to be calculated specifically at the time of the experiment. This can be done by calculating the wet and dry bulb temperatures in the room, as explained in Section (A 2) of the appendix. The thermal radiation flux is given by

$$f_{rad} = \sigma(T_s^4 - T_a^4), \quad (7)$$

where $\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ is the Stefan constant. Thus the total heat flux f is given by

$$f = (1 + Bo^{-1}) f_{sens} + f_{rad}. \quad (8)$$

In our experiments, the radiative heat flux never exceeds 10% of the total heat flux, and the Bowen ratio $Bo \ll 1$ so that the latent heat flux is the dominant contribution to the total heat flux. This also explains why vortical structures do not appear when the top of the dish is covered by a plastic sheet: in this case evaporation is prevented and sensible heat flux is also hindered, resulting in a significantly smaller total heat flux.

The primary problem with using these equations to calculate the heat flux through the surface of the water is that it requires a measurement of the temperature at the surface of the water. We can get around this by recursively approximating the temperature at the water surface. We begin by using the approximation $T_s \approx T_w$, and calculating f based on this using the above equations. Then we apply the equation

$$\Delta T_{sw} = 2.82 \left(\frac{f}{\rho c_p} \right)^{3/4} \left(\frac{\nu}{\alpha g k^2} \right)^{1/4} \quad (9)$$

where $\Delta T_{sw} = T_s - T_w$ is the temperature drop across the surface of the water and, unlike before, all the molecular coefficients are for water at a temperature T_w . We can then calculate a new approximation for T_s using $T_s = \Delta T_{sw} + T_w$ and use this to calculate a new value of f . If we wished to, we could continue this process to obtain successively good approximations, but normally one such iteration is enough to obtain a precision of with about 1% (Boubnov and Golitsyn 1986).

Symbol	Definition
α	Coefficient of thermal expansion
g	Gravitational acceleration
f	Total heat flux through the fluid
h	Depth of the rotating fluid layer
ρ	Density
c_p	Specific heat capacity at constant pressure
k	Thermodiffusivity
k_c	Thermal conductivity
ν	Kinematic viscosity
Ω	Angular velocity of water dish
ℓ	Latent heat of water vapor formation
T_a	Temperature of the air
T_w	Temperature of the water
T_s	Temperature of the water surface
k_e	Coefficient of water vapor diffusion in air
p	Air pressure in room
B	Surface buoyancy loss

FIG. 2: Table of symbols.

III. RESULTS

In our experiment, we varied the heat flux through the surface of the water by changing the temperature of the water for a constant height of $h = 2.5 \text{ cm}$ and a constant angular frequency $\Omega = 1.68 \text{ rad/s}$. Before each experiment, we measured both the water temperature T_w and the air temperature T_a and wet bulb temperature T_{wet} in the room. These values are presented in the table in FIG. 3.

A. Convective Rings

When dye is introduced to the water dish and the record player is turned on, a pattern of concentric convective rings forms. The rings are of varying radius about the axis of rotation with the innermost ring having a diameter d_{min} . Inside the centermost ring some vortices may immediately form. After a time τ_r , the rings become fully formed and begin to transform into vortices. This starts as wavy perturbations on the rings, starting with the innermost ring, which grow and roll-up into vortices, as in a Kelvin-Helmholtz instability. This is the mechanism for vortex formation, but it is cannot be the only mechanism, since vortices may form inside the inner ring almost immediately. After a time τ_v , the rings are fully deformed and only vortices remain. Our measurements of these quantities are presented in the table in FIG. 3.

A picture of a typical ring formation pattern is included in FIG. 4. The ring formation shown has a minimum ring diameter, and the distance between concentric rings tends to decrease with increasing radius. Also, the rings

T_a (°C)	T_{wet} (°C)	T_w (°C)	f (W/m ²)	τ_v (s)	τ_r (s)	d_{min} (cm)
31.6	18.7	24.0	5.4494	107	266	2.4978
32.9	19.9	29.0	26.549	75	130	3.5455
31.3	19.5	26.8	26.745	66	124	3.2951
32.4	19.5	27.0	28.802	82	152	2.8488
26.7	18.0	26.5	59.428	58	112	3.2821
26.4	17.8	26.7	70.421	70	132	3.4385
31.0	19.8	30.0	75.636	48	106	4.5295
31.1	19.5	31.0	108.03	69	124	4.1581
32.2	19.6	32.1	125.01	62	122	4.3221
28.2	18.5	31.0	158.50	50	109	4.1312
26.8	18.0	30.7	172.23	57	96	5.2604
30.9	19.3	33.1	179.97	59	124	5.4928
26.7	18.0	31.8	206.78	58	113	5.1572
31.9	19.5	34.9	225.54	65	102	6.6491
28.1	18.3	34.7	282.81	56	104	5.3903
31.0	19.5	37.3	327.85	59	92	6.4474
32.0	19.6	38.0	341.22	51	86	5.7978
27.8	18.4	37.8	403.82	54	75	6.1256
27.6	18.4	38.2	422.88	56	99	6.1134
32.3	19.4	41.0	476.26	60	93	4.8290
26.4	17.6	41.2	584.36	50	100	7.0739

FIG. 3: Measured results for 21 different heat fluxes.

in the picture close to the center ring are beginning to roll up and form vortices.

We now consider some quantitative characteristics of convective rings, beginning with studying the behavior of τ_r . Convection creates a vertical velocity dependence on the spatial coordinate z as

$$w(z) = a(Bz)^{1/3}, \quad (10)$$

with $a \approx 0.4$ for $\Omega = 0$ (Boubnov and Golitsyn 1986). This gives us an average vertical velocity of

$$\bar{w} = \frac{1}{h} \int_0^h w(z) dz = \frac{3}{4} a (Bh)^{1/3}. \quad (11)$$

The ring formation is a preconditioning phase resulting from a complicated interplay between the spin-up of water and convection. This leads us to expect the ring formation time to be on the order of the convective time scale $h/\bar{w}$. We can express this timescale in terms of the timescale of a viscous fluid h^2/ν as

$$h/\bar{w} = \frac{4}{3a} \left(\frac{h^2 \rho c_p}{\alpha g f} \right)^{1/3} = \frac{4}{3a} \frac{h^2}{\nu} Gr_f^{-1/3}, \quad (12)$$

where Gr_f is the Grasshof flux number:

$$Gr_f = \frac{\alpha g f h^4}{\rho c_p \nu^3} = Ra_f Pr^{-2}, \quad (13)$$

and $Pr = \nu/k$ is the Prandtl number.

The dependence of τ_r on $(h^2/\nu) Gr_f^{-1/3}$ is presented in FIG. 6. The 21 measured times τ_r presented in the figure give a linear curve fit

$$\tau_r = c_0 h^2 \nu^{-1} Gr_f^{-1/3} + c_1$$

in seconds with $c_0 = 1.04151$ and $c_1 = 40.9232$. Here the determination coefficient of $r^2 = 0.75674$ and a correlation coefficient of $r = 0.86991$. A determination coefficient close to 1 is indicative of a well-determined statistical relationship.

There is a minimum diameter d_{min} of the central ring which Boubnov and Golitsyn found to depend on the angular velocity ($d_m \propto \Omega^{-1}$), water depth, and heat flux. Using the Ekman length scale $l_E = (\nu/\Omega)^{1/2}$, this hints to a scaing of the form

$$d_{min} = c_2 l_E Ta^{-1/4} Ra_f^\alpha = \frac{c_2}{\sqrt{2}} \left(\frac{l_E^2}{h} \right) Ra_f^\alpha. \quad (14)$$

We treated the data from 21 measurements presented in FIG. 7 with the above equation and found $c_2 = 57.0727 \pm 24.75$ and $\alpha = 0.282867 \pm 0.02812$ with a determination coefficient of $r^2 = 0.87596$ and a correlation coefficient of $r = 0.93593$. Here the $\pm$ error factors represent the standard error, and the value of $\alpha = 0.4$ originally obtained by Boubnov and Golitsyn is within error. For $\alpha = 1/3$, also within error, we have a simpler, but hard to understand, interpretation of Equation (14). In this case

$$d_{min} = \frac{c_2}{\sqrt{2}} \left(\frac{l_E^2}{h} \right) \left(\frac{\epsilon h^4}{k^2 \nu} \right)^{1/3} = \frac{c_2}{\sqrt{2}} (\epsilon h)^{1/3} \Omega^{-1} Pr^{2/3} = \frac{4c_2}{3a\sqrt{2}} \frac{\bar{w}}{\Omega} Pr^{2/3}. \quad (15)$$

This points to an interplay between convection and rotation.

After existing for some time, the rings begin to roll up into vortices. The time of vortex formation τ_v , taken from switching on the record player to the disappearance of the last ring, was found by Boubnov and Golitsyn to depend on the heat flux f , the depth h , and the angular velocity. Again using the viscous time scale h^2/ν , the equation for this dependence can be expressed as

$$\tau_v = c_3 h^2 \nu^{-1} Ra_f^{-2/3} Ta^{1/4} + c_4, \quad (16)$$

where $c_3 = 8.50231 \pm 0.6562$ and $c_4 = 86.4816 \pm 3.627$ with determination coefficient $r^2 = 0.89834$ ($r = 0.94781$) for 21 points. The dependence of τ_v on $(h^2/\nu) Ra_f^{-2/3} Ta^{1/4}$ is presented in FIG. 8.

B. Convective Vortex Pattern Structure

When the rings break up into vortices, they spread out into something resembling a semi-regular hexagonal



FIG. 4: Picture of the typical structure of convective rings formed during the preconditioning phase. The rings have a minimum ring diameter d_{min} , and the distance between concentric rings decreases away from the center of the dish. Rings close to the center of the dish are beginning to roll up and form vortices due to shear instability.

grid of vortices such that if the mean distance between the centers of neighboring vortices is d , an approximate vortex density for the system is $N = \frac{\sqrt{3}}{2}d^{-2}$. A typical picture of a vortex pattern is shown in FIG. 5. For a large enough ratio of Taylor number to Rayleigh flux number Ta/Ra_f , we enter a linear regime wherein the vortex distribution is very close to a regular hexagonal grid (Boubnov and Golitsyn 1986). In this regime, linear theory predicts

$$\frac{h}{d} \frac{\sqrt{3}a_{cr}}{4\pi} \approx 0.18Ta^{1/6} \quad (17)$$

where a_{cr} is the critical spatial wave length, given by

$$a_{cr} = \left(\frac{1}{2}\pi^2Ta \right)^{1/6} \approx 1.3Ta^{1/6} \quad (18)$$

with accuracy greater than 1% for Prandtl number $Pr = \nu/k > 0.677$ and Taylor numbers $Ta > 10^6$. When

Ta/Ra_f becomes too small, however, the linear behavior no longer applies. This threshold was found to occur for values $Ta/Ra_f < 24.5$, and the mean spacing d was then found to vary as

$$d = c_5 l_E Ra_f^{1/12}. \quad (19)$$

We obtained results for 17 values of d in the nonlinear regime. The results are included in the table in FIG. (9). The value of d is measured averaging the nearest-neighbor distance between every vortex at a single instant in time. This is done by taking a picture of the system at some time after all the vortices are formed and opening it in an image manipulation program, such as GIMP. At the location of every vortex, we place a single black pixel. Then we remove the original image so that we are left with a collection of black pixels on a white background. This new image is then processed by another program written with the ImageMagick MagickWand C API that

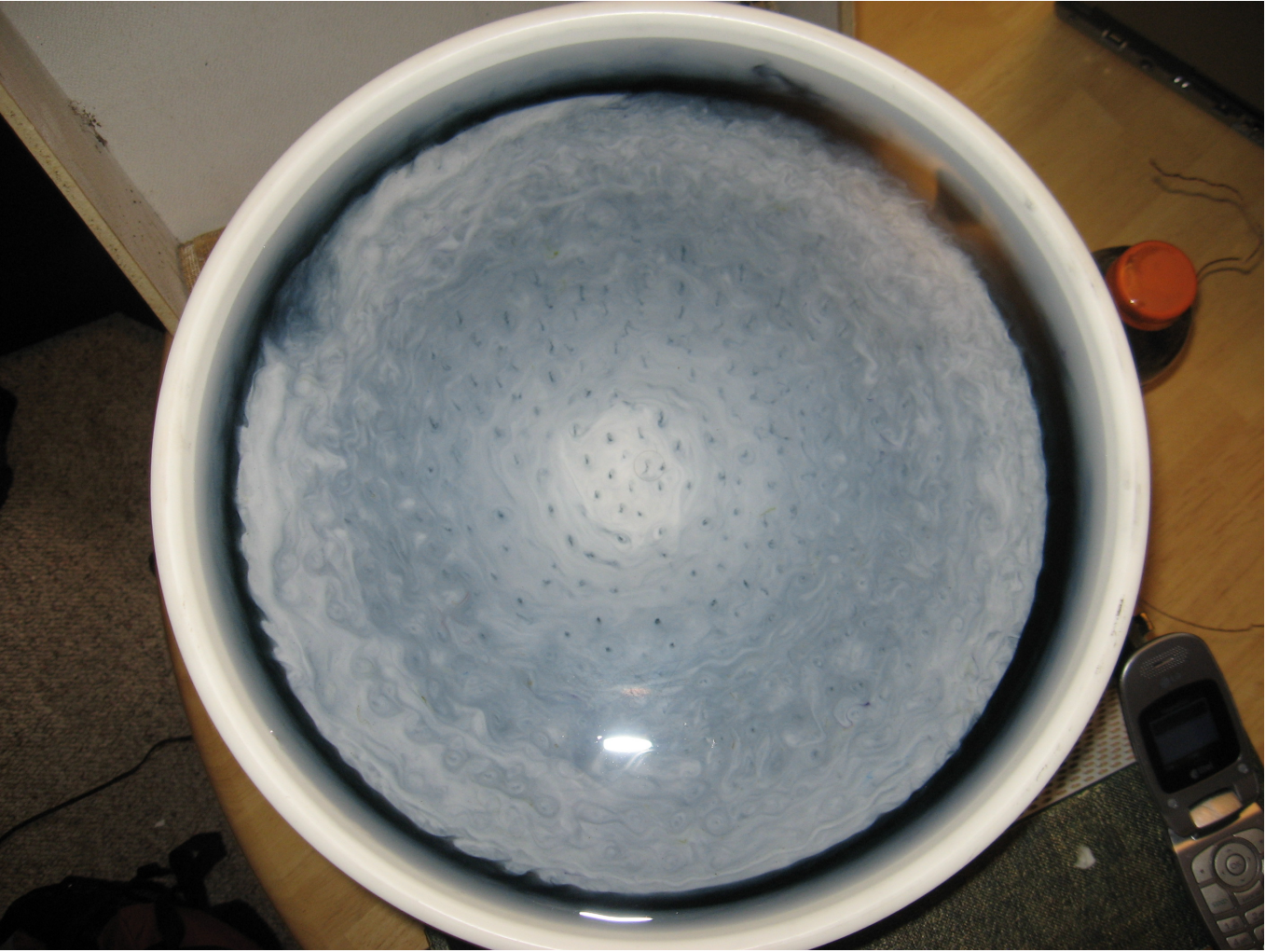


FIG. 5: Picture of the typical structure of convective vortices formed during the violent mixing phase. The vortices have an average nearest-neighbor spacing d , corresponding to an approximate vortex density of $N = (\sqrt{3}/2)d^{-2}$.

outputs a file of the positions of every pixel. This new file is then read with another program that calculates the average distance between nodes. This process is time consuming, but it results in a value of d with the level of accuracy necessary to see the very weak dependence of d on Ra_f .

We obtained $c_5 = 508.005$ (for d in centimeters) with the determination coefficient $r^2 = 0.91567$ ($r = 0.95691$). This agrees well with the value of 510 obtained by Boubnov and Golitsyn. A plot of d with respect to $l_E Ra_f^{1/12}$ is included in FIG. 10 below.

IV. CONCLUSIONS

We have performed experiments on convection in rotating water with a free surface and analysed the results for a wide range of the similarity criteria Ra_f and Ta . The experiments have shown that competition between convec-

tion caused by heat flux and stratification caused by fluid rotation generate various convective vortex patterns, and that each of these patterns is preceded by an intermediate stage of convective rings caused by the interaction of fluid spin-up with the buoyancy forcing due to the surface cooling. The ring formation time τ_r was found to depend linearly on the convective time scale $h/\bar{w}$. The ring patterns were found to have an innermost ring whose size was the result of a complex interplay between convection and rotation, and was proportional to $\bar{w}/\Omega Pr^{2/3}$. In deep ocean convection simulations, such as the ones performed by (Jones and Marshall 1993), the Prandtl number is generally set to 1, so this simply predicts a proportionality to $\bar{w}/\Omega$. The vortex formation time (ring destruction time) τ_v was found to vary linearly with $(h^2/\nu)Ra_f^{-2/3}Ta^{1/4}$, though no simple interpretation of this is currently available. Lastly the average spacing between vortices d was found to vary as $d \propto l_E Ra_f^{1/12}$ in the nonlinear regime $Ta/Ra_f < 24.5$, corresponding to a vortex number den-

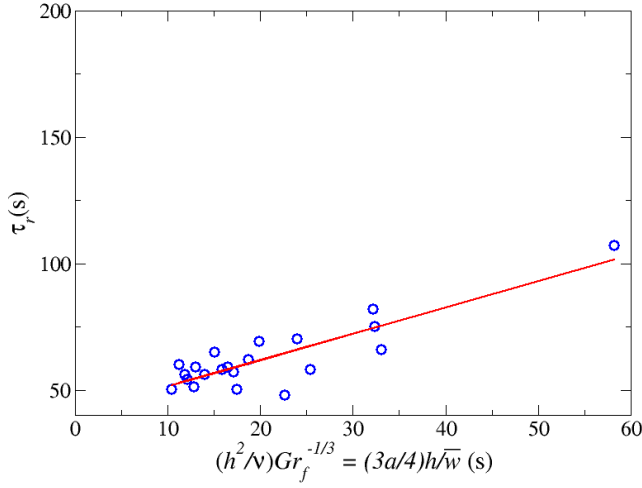


FIG. 6: Time of complete formation of ring pattern (and start of wavy ring perturbations) τ_r in seconds with respect to the viscous timescale h^2/ν scaled by the inverse cubic root of the Grasshov number.

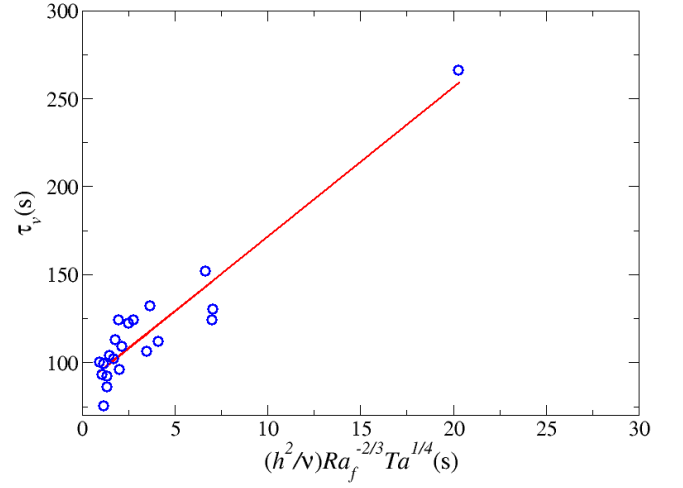


FIG. 8: Time from starting the record player to the complete disappearance of the rings and the formation of the vortices τ_r in seconds with respect to the viscous timescale h^2/ν scaled by $Ra_f^{-2/3}Ta^{1/4}$.

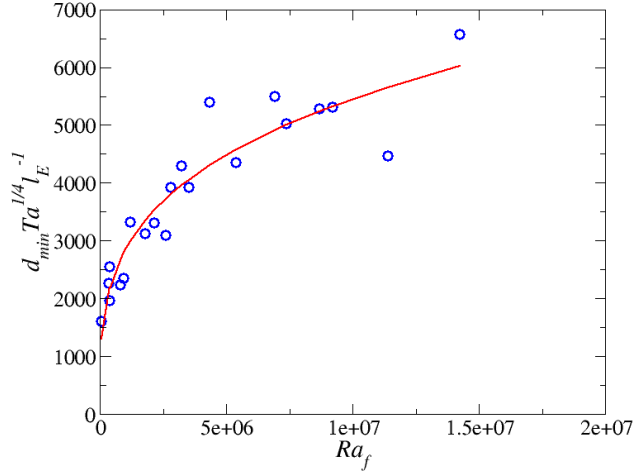


FIG. 7: Dependence of the minimum ring diameter d_{min} in centimeters scaled by the Ekman length $l_E = (\nu/\Omega)^{1/2}$ on the Taylor and Rayleigh flux numbers.

sity $N \propto h^{-2}Ta^{1/2}Ra_f^{-1/6} \propto \Omega$.

Some of the problems with the current results are that they are for only a narrow range of values, averaged over a limited quantity of points. Future studies could consider a wider range of Rayleigh flux and Taylor numbers concerned, and average over more trials to obtain even more accurate results. Also, the preconditioning phase in deep ocean convection is caused by the onset of convection caused by heat flux on an already rotating system, while our preconditioning phase is caused by rotation induced on an already convectively unstable system. This makes it more difficult to draw conclusions about sim-

$l_E Ra_f$ (mm)	d (cm)	std. dev. (cm)
1.86281088	1.2726	0.2830
2.09758481	1.0462	0.1996
2.05563238	1.0311	0.2044
2.35987391	1.1631	0.2724
2.38858970	1.1886	0.2705
2.39677758	1.2344	0.2562
2.08746731	1.0848	0.2349
2.27973777	1.1945	0.2615
2.22799608	1.1321	0.2405
2.39303605	1.2202	0.2933
2.35374107	1.1877	0.2593
2.40816554	1.2357	0.2934
2.42803885	1.2446	0.2775
2.37489717	1.2134	0.2295
2.23556625	1.1907	0.2560
2.26437832	1.1412	0.2184
2.39345452	1.1554	0.2405

FIG. 9: Measured results of d for 17 different heat fluxes with corresponding standard deviation.

ilarity of the phases. Future experiments could therefore look into inducing a heat flux on an already rotating system, thereby making the connections between the preconditioning phases immediately obvious. Lastly future research could employ a high resolution digital video recorder to measure such things as the vortex circulation, ring and vortex formation time as a function of the radius, as well as quantities concerned with vortex interac-

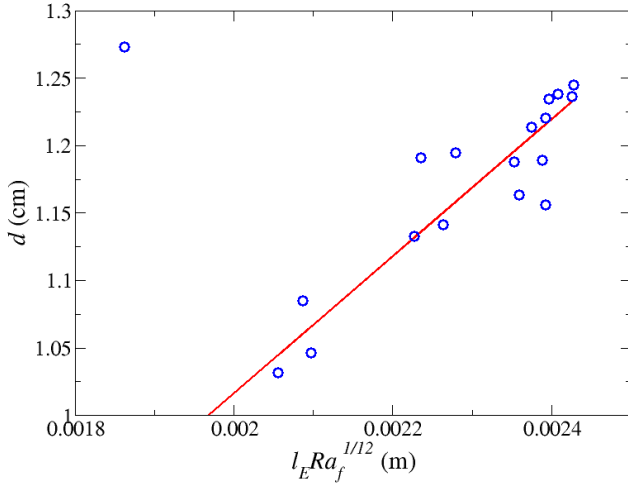


FIG. 10: Average spacing between adjacent vortices d in centimeters scaled by the Eckman length $l_E = (\Omega/\nu)^{1/2}$ with respect to the Rayleigh flux number Ra_f in the nonlinear regime ($Ta/Ra_f < 24.5$). The value in the upper left corner of the graph is for d evaluated in the linear regime ($Ta/Ra_f = 81.28$) and is included for comparison.

tions.

Acknowledgments

I would like to thank my mentor Dr. Balasubramanya Nadiga of CCS-2 for his help, invaluable advice, and record player. He also provided several to help explain the necessary geophysical fluid dynamics concepts, including (Pedlosky 1979), (Cushman-Roisin 1994), and (McWilliams 2006). I would also like to thank James Colegan and Norm Magee for their unebbing efforts in coordinating the Los Alamos Summer School program. The Los Alamos Summer School students are also deserving of thanks for allowing me to borrow various articles of equipment, such as a digital camera, and for making such a fun and unique experience. I need to thank my room mate as well for putting up with having a precariously full spinning dish of water positioned in various places about the apartment, including but not limited to the dinner table, for days on end. Finally, I would like to thank the Los Alamos National Laboratory and the National Science Foundation for funding this project.

APPENDIX A: CALCULATION OF THERMODYNAMIC PROPERTIES

1. Saturation Vapor Pressure

The saturation vapor pressure of water p_w is the pressure exerted by water at a specific temperature. It can

be approximated in a variety of ways. The Arden Buck equation relates the saturation vapor pressure to temperature for moist air, and is more accurate than other methods in the temperature range of -80 to 50°C . It is given by

$$p_w = 611.21 \exp\left(\frac{(18.678 - T/234.5)T}{257.14 + T}\right) \quad (\text{A1})$$

where T is the temperature of the air in degrees Celsius and p_w is in Pascals.

To calculate the water vapor pressure in the air of the room e_a , we can then use the relative humidity RH , defined as:

$$RH = e_a/p_w. \quad (\text{A2})$$

If the relative humidity in the room is not known, then it is possible to instead use the dry and wet bulb temperatures of the room along with Equation (A3), as explained below.

2. Relative Humidity

If one measures the temperature of the room with two different thermometers, one of which is wet, they may notice a significant difference in the temperature readings. This is because the water on the wet thermometer is evaporating, transferring heat and causing the temperature reading to be less. This fact is useful in that it allows one to measure the relative humidity in the room using the different temperatures.

If T is the temperature of the dry thermometer, and T_{wb} is the temperature of the wet thermometer, called the dry and wet bulb temperatures respectively, then the water vapor pressure in the air e_a is approximated by the equation

$$e_a = p_w - p(T - T_{wb})0.00066(1.0 + 0.00115T_{wb}). \quad (\text{A3})$$

This is the same equation used by the National Oceanic and Atmospheric Administration to calculate water vapor pressure. Here p_w is as defined in Equation (A1), and p is the atmospheric pressure in the room. The relative humidity can then be calculated using Equation (A2).

In practice, the temperature of a wet thermometer may fall for several minutes before reaching a steady value. After this, it may begin to increase again, as it becomes dry again. To keep the thermometer from drying too quickly, it is helpful to wrap it in a damp paper towel or wet piece of cloth. Of course, for this to work well, the water used to wet the thermometer should be about room temperature. To decrease the amount of time it takes for the temperature reading to stabilize, one can use a fan to blow on the thermometer. This drastically decreases the time it takes the thermometer to reach its minimum value and does not affect the measured temperature.

Symbol ($aT^3 + bT^2 + cT + d$)	a	b	c	d
c_p air (10^3 J/kg K)	-7.4×10^{-10}	7.04×10^{-7}	-6.6×10^{-6}	1.00423
c_p water (10^3 J/kg K)	-1.006×10^{-6}	$9.995 \times 10^{-5} \pm$	-0.003409	4.21858
ν air (10^{-6} m ² /s)	-4.86×10^{-8}	0.0001111	0.08616	13.389
ν water (10^{-4} m ² /s)	-9.13×10^{-8}	1.072×10^{-5}	-0.0005647	0.017838
k_c air (W/m K)	1.78×10^{-11}	-2.84×10^{-8}	7.746×10^{-5}	0.024064
α water (1/K)	1.825×10^{-9}	-2.304×10^{-7}	1.7572×10^{-5}	-6.680×10^{-5}
k_e (10^{-4} m ² /s)	-1.79×10^{-7}	1.31×10^{-5}	0.001448	0.20928

FIG. 11: Expansion coefficients for some useful thermodynamic properties.

3. Air Density

The density of moist air in general will be different from that of dry air. In particular, one has to take into considerations contributions to the air pressure caused by water vapor: the total pressure p is equal to the sum of the partial pressure of dry air p_d and the water vapor pressure in the air e_a . The total density of the air will be the sum of the densities of the water vapor in the air and dry air. Using the ideal gas approximation $p = \rho RT$, where T is the temperature in Kelvin and R is the gas constant, we find

$$\rho = \frac{e_a}{R_w T} + \frac{p_d}{R_a T} = \frac{e_a}{R_w T} + \frac{p - e_a}{R_a T} \quad (\text{A4})$$

where R_w and R_a are the gas constants for water and air respectively.

4. Water Thermal Diffusivity

The thermal diffusivity of water k is related to the thermal conductivity of water k_c via the relation

$$k = \frac{k_c}{\rho c_p} \quad (\text{A5})$$

where ρ is the density of water and c_p is the heat capacity of water at constant pressure. The thermal conductivity can be calculated very accurately as follows. The calculation is based on the interpolation equations released by the International Association for the Properties of Water and Steam in Berlin, Germany in September 1998 in an article entitled ‘‘Revised Release on the IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substance’’ (Cooper and Dooley 2008). Define

a_0	0.0102811	C_1	0.642857
a_1	0.0299621	C_2	-4.11717
a_2	0.0156146	C_3	-6.17937
a_3	-0.00422464	C_4	0.00308976
b_0	-0.397070	C_5	0.0822994
b_1	0.400302	C_6	10.0932
b_2	1.060000	d_1	0.0701309
B_1	-0.171587	d_2	0.0118520
B_2	2.392190	d_3	0.00166937
		d_4	-1.0200

Then

$$k_c = \sqrt{T_r} (a_0 + a_1 T_r + a_2 T_r^2 + a_3 T_r^3) + b_0 + b_1 \rho_r + b_2 \exp(B_1(\rho_r + B_2)^2) + \left(\frac{d_1}{T_r^{10}} + d_2 \right) \rho_r^{9/5} \exp(C_1(1 - \rho_r^{14/5})) + d_3 S \rho_r \exp\left(\frac{Q}{1+Q} (1 - \rho_r^{1+Q}) \right) + d_4 \exp\left(C_2 T_r^{3/2} + \frac{C_3}{\rho_r^5} \right) \quad (\text{A6})$$

where T_r is $T/647.26$, $\rho_r = \rho/317.7$, T is the temperature in Kelvin, and ρ is the density in kg/m³. The values of Q and S are given in terms of $\delta_T = |T_r - 1| + C_4$ with

$$Q = 2 + \frac{C_5}{\delta_T^{3/5}},$$

and

$$S = \begin{cases} 1/\delta_T, & \delta_T > 1 \\ C_6/\delta_T^{3/5}, & \delta_T \leq 1 \end{cases}.$$

5. Temperature Dependence of Thermodynamic Properties

While the values of various thermodynamic quantities change with the temperature, often the quantity of

change is not very significant over the temperature ranges we have considered in the above experiment (24 – 40 degrees Celsius). When the change is significant, a third-order expansion with respect to the temperature is generally sufficient to accurately detail its variation. For sake of completeness, in the table in FIG. (11) we have listed the expansion coefficients of several thermodynamic properties required in the above experimental calculations.

The expansions assume T is in degrees Celsius and are found by curve fits on standard temperature tables of the given thermodynamic properties. Additionally, the temperature dependence of other thermodynamic variables are given by the following equations:

$$\ell = -0.0614342T^3 + 1.58927T^2 - 2364.18T + 2500790; \quad (\text{A7})$$

$$\alpha_{\text{air}} = \frac{1.01133}{T + 273} - 0.0237018 \times 10^{-3}; \quad (\text{A8})$$

$$\rho_{\text{water}} = \frac{998.0}{(1 + \beta(T - 20))(1 - (p - 101352)/E)}. \quad (\text{A9})$$

Here T is the temperature in degrees Celsius, p is the pressure in Pascals, ℓ has units of J/kg, α has units of 1/K, and ρ has units of kg/m³. The constants $\beta = 0.88 \times 10^{-4}$ (1/K) and $E = 2.15 \times 10^9$ (N/m²) are the volumetric temperature coefficient and bulk modulus of fluid elasticity respectively for water.

APPENDIX B: SCALING TERMS

Symbol	Name	Definition
Ra_f	Rayleigh flux number	$\frac{\alpha g f h^4}{\rho c_p k^2 \nu}$
Ta	Taylor number	$\frac{4\Omega^2 h^4}{\nu^2}$
Nu	Nusselt number	$\frac{f h}{\rho c_p k \Delta T}$
Pr	Prandtl number	ν/k
Gr_f	Grasshof flux number	$\frac{\alpha g f h^4}{\rho c_p \nu^3}$
l_E	Ekman length	$(\nu/\Omega)^{1/2}$
l_K	Kolmogorov microscale	$\nu^{3/4} \epsilon^{-1/4}$

FIG. 12: Table of symbols.

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Charge Optimization for Geometrically Asymmetric Water Molecule

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Concepts from empirical valence bond and density functional theories are used to construct a new charge-dependent potential energy surface for a water molecule. The model is derived from a variational energy based on three charge resonances. Thus, constructing a variable-charge potential requires the mixing of valence-bond states. The mixing parameters are related to the atomic charges. We deduce state-mixing from constrained density functional theory with fractional charges by a standard fitting procedure. Calculations by Brenman and Valone provided the necessary energies [1]. We interpolate the known values for the symmetric stretch to predict the off-diagonal hamiltonian elements for a water molecule in the asymmetric stretch vibrational mode. The asymmetric stretch hamiltonian is diagonalized to predict optimal charges and energies. The results indicate that our model has some qualitative accuracy but also suggest that a fourth charge resonance is necessary to construct the potential energy surface.

I. INTRODUCTION

Molecular Dynamics (MD) is a simulation method that treats molecules as classical particles that follow the laws of Newtonian dynamics. To use an MD simulation, there are three requirements: First, we need to specify the initial position and velocity of each molecule in the system. Second, we need to designate boundary conditions for the system. Last, we need to know the force field that will govern each molecule. According to Newtonian dynamics, the force on each particle in the system is given by

$$F_i = m_i a_i = -\nabla_i V, \quad (1)$$

where F_i is the force that acts upon the i th particle due to the interactions between itself and every other particle in the system, m_i is the mass and a_i is the acceleration of the i th particle, ∇_i is the gradient operator, and V is the potential energy of the system. By finding the functional form of the potential energy for the entire system, we can predict the total force acting upon each atom in a molecule or material.

We start by finding the form of the potential energy for just one water molecule. We know from other calculations and experiments that charges can and sometimes should be distributed fractionally between subsystems of a system that is overall neutral. Our potential energy surface (PES) must accommodate any distribution of charge within an overall neutral water molecule. The subsystems in question are the three atoms. The total number of electrons in the molecule must equal the number of protons, but the electrons can reside anywhere in the molecule. The protons, on the other hand, remain fixed in their respective nuclei. The charge on atom A is given by

$$q_A = Z_A - N_A, \quad (2)$$

where Z_A is the number of protons and N_A is the number

of electrons in the atom. Z_A is always an integer, but N_A can be fractional, so the charge q_A can be fractional.

Fractional charge implies quantum-mechanical averaging over two or more charge states of an atom. Consider a diatomic molecule and suppose that there are only two important valence bond (VB) states. In one state, denoted as ψ_0 , both of the atoms in the molecule are neutral. In the other state, ψ_+ , one atom has a charge $+1$ and the other atom has a charge -1 . In both states, the molecule is overall neutral. A state in which both atoms have fractional charges results from mixing the two states with some mixing coefficient λ :

$$\Psi = \psi_0 + \lambda\psi_+. \quad (3)$$

We want to be able to write the variational energy $\bar{E}$ of this state in terms of the charge q .

Classical electrostatic potentials have long been used to describe interactions among atoms in a molecule. The usual structure of an electrostatic interaction between a neutral pair of atoms looks like

$$\begin{aligned} \bar{E}_{AB}(q, R_{AB}) = & E_0(R) + E_A^{(0)} + \mu_A q + \frac{1}{2}\eta_A q^2 \\ & + E_B^{(0)} - \mu_B q + \frac{1}{2}\eta_B q^2 - \frac{q^2}{R_{AB}}, \end{aligned} \quad (4)$$

for charge q not an integer. Here, E_0 represents short-range potential functions, such as exponential, Morse, Leonard-Jones, or Rose potentials. μ is the chemical potential and η is the hardness of each atom. The last term in Eq. (4) is the pairwise coulombic interaction. However, this functional form becomes unphysical at dissociation (that is, for large R). When optimizing q from $\frac{\partial E_{AB}}{\partial q} = 0$, the optimal charge q is

$$q = -\frac{\mu_A - \mu_B}{\eta_A + \eta_B - \frac{2}{R_{AB}}}. \quad (5)$$

At dissociation, $\frac{2}{R_{AB}} = 0$, but the other terms are physical properties of the atoms and do not disappear. Ac-

cording to this model, the atoms are not neutral at dissociation, but they should be. Thus, we need to find a different form for the PES.

For the water molecule, we assume a model wave function constructed from three basis VB states. We write the variational energy in terms of the state-mixing coefficients and hamiltonian matrix elements. The matrix elements are obtained from constrained density functional theory (C-DFT) [2] calculations performed for a geometrically symmetric molecule. We approximate the matrix elements for a geometrically asymmetric molecule and estimate the ground-state energy. We use Mathematica [3] to solve for the mixing coefficients that give the lowest energy for specified bond lengths, and from those coefficients we predict the optimal charges on each atom and the ground-state energy. Our estimates imply at least a qualitatively correct charge asymmetry. However, the energies predicted by C-DFT are lower than those found using the Becke3-Lee-Yang-Parr (B3LYP) exchange correlation [4, 5]. This discrepancy leads us to suppose that we need to add another basis state to our model.

II. METHODS

A. Deriving the Variational Energy

Theoretically, quantum mechanics tells us that the general Schrödinger equation,

$$\hat{H}\Psi = E\Psi, \quad (6)$$

can be used to find the potential energy of any system. However, the Schrödinger equation can only be analytically solved for one system, the hydrogen atom. To solve the Schrödinger equation for a water molecule, which has ten electrons and three nuclei, we need to simplify it. The full molecular hamiltonian is

$$\begin{aligned} \hat{H} = & -\frac{\hbar^2}{2} \sum_{\alpha} \frac{1}{m_{\alpha}} \nabla_{\alpha}^2 - \frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{\alpha} \sum_{\beta > \alpha} \frac{Z_{\alpha} Z_{\beta} e^2}{r_{\alpha\beta}} \\ & - \sum_{\alpha} \sum_i \frac{Z_{\alpha} e^2}{r_{i\alpha}} + \sum_j \sum_{i > j} \frac{e^2}{r_{ij}}, \end{aligned} \quad (7)$$

where α and β represent nuclei and i and j represent electrons. We use the Born-Oppenheimer approximation to break down the hamiltonian into the electronic and nuclear parts, on the assumption that because the electrons are so much lighter and hence move so much faster than the nuclei, the nuclei can be regarded as stationary. The first term of Eq. (7), the kinetic energy of the nuclei, is thus zero. We can also isolate the nuclear repulsion potential,

$$\hat{V}_{NN} = \sum_{\alpha} \sum_{\beta > \alpha} \frac{Z_{\alpha} Z_{\beta} e^2}{r_{\alpha\beta}}. \quad (8)$$

The electronic hamiltonian is then

$$\begin{aligned} \hat{H}_{el} = & -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 - \sum_{\alpha} \sum_i \frac{Z_{\alpha} e^2}{r_{i\alpha}} \\ & + \sum_j \sum_{i > j} \frac{e^2}{r_{ij}} + \hat{V}_{NN}. \end{aligned} \quad (9)$$

We use Eq. (9) to state the electronic Schrödinger equation,

$$\hat{H}_{el}\psi_{el} = E_{el}\psi_{el}. \quad (10)$$

To solve this equation, we specify the nuclear coordinates. Eq. (10) must be re-solved for every different geometry. The total electronic energy of the system has contributions from the electronic kinetic energy, external potential due to the nuclei, and the electron-electron repulsion potentials. Because the internuclear distance $r_{\alpha\beta}$ in Eq. (8) is constant for each geometry, V_{NN} is also constant and does not affect E_{el} . Thus, for a given configuration of nuclei, E_{el} represents the effective PES for atoms moving in an averaged distribution of electrons.

Because we want a variable-charge potential, it makes sense to write E_{el} in terms of the charges on each atom. We start to do this by transforming the electronic Schrodinger equation into its variational form. We multiply both sides of Eq. (10) by ψ_{el}^* , the complex conjugate of the electronic wave function, and we integrate over all of space, notated by $\int_0^{\infty} \dots d\tau$. This gives us

$$\int_0^{\infty} \psi_{el}^* \hat{H}_{el} \psi_{el} d\tau = \int_0^{\infty} \psi_{el}^* E_{el} \psi_{el} d\tau. \quad (11)$$

Since E_{el} is a constant, we can isolate it by dividing both sides of Eq. (11) by $\int_0^{\infty} \psi_{el}^* \psi_{el} d\tau$. Eq. (11) then becomes

$$E_{el} = \frac{\int_0^{\infty} \psi_{el}^* \hat{H}_{el} \psi_{el} d\tau}{\int_0^{\infty} \psi_{el}^* \psi_{el} d\tau}, \quad (12)$$

the variational form of the potential energy. A more concise way to write this is

$$E_{el} = \frac{\langle \psi_{el} | \hat{H}_{el} | \psi_{el} \rangle}{\langle \psi_{el} | \psi_{el} \rangle}. \quad (13)$$

E_{el} yields the effective variational PES V needed in Eq. (1).

If we write ψ_{el} as a linear combination of basis functions,

$$\psi_{el} \equiv \psi^{\dagger} c, \quad (14)$$

where ψ is a vector of N-electron basis states and the c are variational coefficients, then the hamiltonian matrix is

$$H = \langle \psi | \hat{H} | \psi^{\dagger} \rangle. \quad (15)$$

For ψ_{el} normalized, Eq. (13) becomes

$$\begin{aligned} E_{el} &= c^{\dagger} H c \\ &= \text{tr } c^{\dagger} H c = \text{tr } H c c^{\dagger} \\ &\equiv \text{tr } H \rho. \end{aligned} \quad (16)$$

B. Three-State Model for Water Molecule

In order to use Eq. (13), we need to know the electronic wave function ψ_{el} . There is simply no way to find the real wave function, so we use an approximation. We consider the electronic wave function to be a linear combination of three basis charge distributions. The three atoms in the water molecule are labeled as L, O, and R.

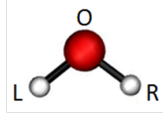


FIG. 1: The three atoms of a water molecule: H-O-H.

We assume that the overall water molecule is neutral, but charges can be distributed in different ways among the three atoms. In the first arrangement, each atom is neutral, denoted as $\psi_{000} \equiv \psi_0$. The second arrangement places a charge of +1 on the left hydrogen (atom L), a charge of -1 on the oxygen (atom O), and no net charge on the right hydrogen (atom R). This arrangement is denoted by $\psi_{+-0} \equiv \psi_\lambda$. The third arrangement is the mirror image of the second: the left hydrogen is neutral, the oxygen has a charge of -1, and the right hydrogen has a charge of +1. This arrangement is denoted by $\psi_{0-+} \equiv \psi_\gamma$. The total electronic wave function is a linear combination of these three charge distributions:

$$\psi_{el} = C_{000}\psi_{000} + C_{+-0}\psi_{+-0} + C_{0-+}\psi_{0-+}. \quad (17)$$

For conciseness, we will write Eq. (17) as

$$\psi_{el} = \psi_0 + \lambda\psi_\lambda + \gamma\psi_\gamma, \quad (18)$$

where λ and γ are the state-mixing coefficients.

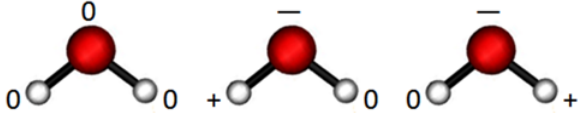


FIG. 2: Charge resonances ψ_0 , ψ_λ , and ψ_γ , respectively.

In order to express E_{el} as a function of charge, we need to express the mixing coefficients in terms of the charges on each atom.

$$\begin{aligned} q_L &= Z_L \frac{\lambda^2}{1 + \lambda^2 + \gamma^2} \\ q_O &= Z_O \frac{\lambda^2 + \gamma^2}{1 + \lambda^2 + \gamma^2} \\ q_R &= -(q_L - q_O) \end{aligned} \quad (19)$$

Solving Eq. (19) for the mixing coefficients, we find that

$$\begin{aligned} \lambda^2 &= \frac{\frac{q_L}{Z_L}}{1 - \frac{q_O}{Z_O}} \\ \gamma^2 &= \frac{\frac{q_R}{Z_R}}{1 - \frac{q_O}{Z_O}} \end{aligned} \quad (20)$$

where Z_L , Z_O , and Z_R are the respective integer charges for the resonances.

C. Constrained Density Functional Theory

Our method of approximating the hamiltonian elements requires information about certain excited states, and most electronic structure methods do not provide this information directly. We use C-DFT [2] to estimate E_{el} , adding a constraint x as a source of excitation. That is, the ground-state energy of the constrained system will be above the ground-state of the unconstrained system. Then, by relating the charges used in the constraint to the mixing coefficients in Eq. (20), we can estimate the hamiltonian matrix elements needed to construct our variational PES. Instead of depending on the electronic wave function ψ_{el} , the energy becomes a functional of the electron number n_{el} . As a result, the hamiltonian also becomes a functional of the electron number. If we can find n_{el} , the Hohenberg-Kohn theorem of DFT says that we will then be able to find the ground-state energy and hamiltonian.

We write n_{el} as a summation of single-particle electron orbitals:

$$n_{el} = \sum_{i\sigma} \phi_{i\sigma}^2(r). \quad (21)$$

In unconstrained DFT, we find n_{el} by solving the Kohn-Sham equations, a set of coupled equations which describe energy in terms of $\phi_{i\sigma}$:

$$\begin{aligned} \left(-\frac{1}{2}\nabla^2 + V_{ext}(r) + \int \frac{n(r')}{|r-r'|} dr' + V_{xc\sigma}(r', n) \right) \phi_{i\sigma} \\ = \epsilon_{i\sigma} \phi_{i\sigma}. \end{aligned} \quad (22)$$

C-DFT adds a constraint term to the regular electronic energy in the Kohn-Sham equation:

$$\begin{aligned} W[n, V_c] &= E[\phi, N_c] + V_c \left(\sum_{\sigma} \int w_c^{\sigma} n^{\sigma}(r) dr - N_c \right) \\ N_c &= \sum_{\sigma} \int w_c^{\sigma}(r) n^{\sigma}(r) dr. \end{aligned} \quad (23)$$

N_c specifies the number of electrons to be found around each atom. We can vary N_c to solve the constrained Kohn-Sham equation for fractional numbers of electrons.

D. Asymmetric Optimization

Brenman and Valone calculated the optimal energies and charges for the geometrically symmetric water molecule from the C-DFT method [1]. The left and right bond lengths, d_{OL} and d_{OR} , range from 0.7 Å to 1.6 Å, and they are always equal. The charges on the hydrogen atoms, q_L and q_R , are also equal. These calculations

were used to determine the hamiltonian elements for the symmetric stretch.

Our current work dealt with the asymmetric stretch vibrational mode of a water molecule, when $d_{LO} \neq d_{OR}$. We interpolated the data from the symmetric stretch to predict the off-diagonal hamiltonian elements for the specified bond lengths for a geometrically asymmetric water molecule, utilizing the following approximations:

$$\begin{aligned}\bar{H}_{00} &\approx \frac{H_{00}(d_{LO}) + H_{00}(d_{OR})}{2} \\ \bar{H}_{\lambda\gamma} &\approx \frac{H_{\lambda\gamma}(d_{LO}) + H_{\lambda\gamma}(d_{OR})}{2} \\ H_{0\lambda} &= H_{0\lambda}(d_{LO}) \\ H_{\lambda\lambda} &= H_{\lambda\lambda}(d_{LO}) \\ H_{0\gamma} &= H_{0\gamma}(d_{OR}) \\ H_{\gamma\gamma} &= H_{\gamma\gamma}(d_{OR}).\end{aligned}\quad (24)$$

We diagonalized the hamiltonian matrix using Mathematica to predict optimal charges and energies for every pair of bond lengths in intervals of 0.1 Å between 0.7 Å and 1.6 Å, inclusive. The energies are eigenvalues of the hamiltonian matrix, and the desired mixing coefficients are related to the eigenvector for the lowest energy. Using Eq. (20), we can obtain the optimal charges on each atom from the mixing coefficients.

III. RESULTS

Our findings show that although we have not yet fully constructed a variable-charge PES for the water molecule, our model of charge resonances is headed in a promising direction.

Fig. (3) displays the energies predicted by C-DFT and those obtained from the B3LYP exchange correlation. We find that the C-DFT energies are significantly lower. This results from our making independent estimates of the off-diagonal hamiltonian elements, as in Eq. (24). It indicates that we did not make the correct assumptions

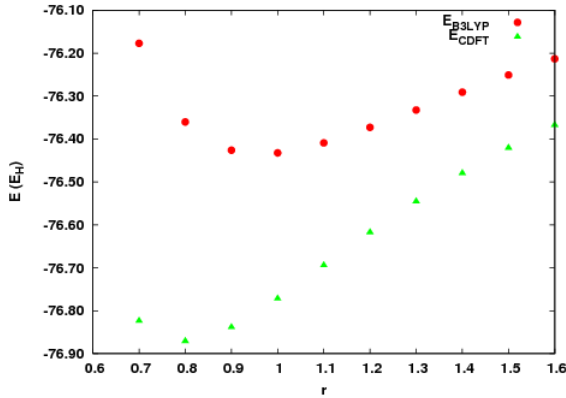


FIG. 3: Comparison of energy fits for B3LYP exchange correlation and C-DFT.

about which resonances are operating in the C-DFT calculations.

However, when approaching dissociation, the hamiltonian predictions still follow qualitatively accurate trends. Fig. (4) shows that as R increases, the off-diagonal elements $H_{0\lambda}$ and $H_{\lambda\gamma}$ approach zero, while the diagonal elements H_{00} and $H_{\lambda\lambda}$ approach some constant.

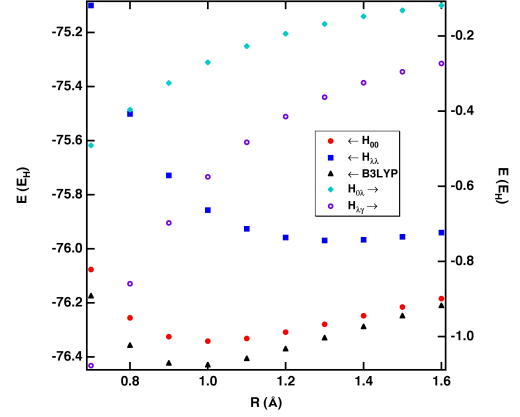


FIG. 4: Hamiltonian predictions from C-DFT using the B3LYP functional.

Physically, this makes sense. Consider a geometrically asymmetric molecule with a large d_{OR} . As d_{OR} increases, atom R gets closer to dissociation, so its charge q_R decreases. To maintain the overall neutrality of the molecule, q_L must increase. Eq. (18), the molecule's wave function, becomes dominated by ψ_λ and ψ_0 . Likewise, E_{el} becomes dominated by $H_{\lambda\lambda}$ and H_{00} , both of which approach constant values as atom R approaches dissociation. The other contributions to E_{el} , namely the off-diagonal elements $H_{0\lambda}$ and $H_{\lambda\gamma}$, go to zero.

The results of our asymmetric charge optimization follow a similar trend. Fig. (5) demonstrates that the greatest difference $q_L - q_R$ occurs when one bond is around its normal optimized length, about 0.96 Å, and the other bond is significantly stretched or compressed. Thus, with a greater geometric asymmetry comes a greater charge asymmetry in the molecule.

Qualitatively, our model seems to be performing as

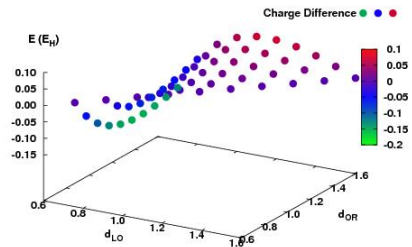


FIG. 5: Charge asymmetries for geometrically asymmetric molecule.

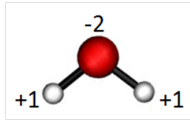


FIG. 6: The new charge resonance, ψ_δ .

desired. As a possible solution to the discrepancy in energy fits, we postulate a fourth charge resonance for our model. We place a charge of +1 on each hydrogen and -2 on the oxygen. This state is denoted as ψ_δ .

ψ_δ looks like the sum $\psi_\lambda + \psi_\gamma$. However, ψ_δ does not replace ψ_λ and ψ_γ . Charge asymmetries would not be obtainable without ψ_λ and ψ_γ , and without charge asymmetries, optimization for the asymmetric stretch would not be possible. Fig. (7) displays the optimal charge q as a function of the bond length. A water molecule with

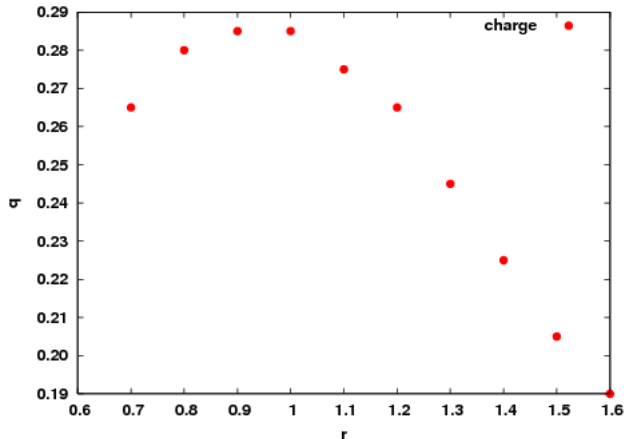


FIG. 7: Optimal charge as a function of bond length.

two different bond lengths would necessarily have different optimal charges on each hydrogen atom—which would not be possible without including ψ_λ and/or ψ_γ .

Notice that the addition of a fourth resonance creates a problem. Under the condition that the four mixing coefficients are normalized, there are three free parameters—we call them λ , γ , and δ . However, there are still only three possible charges, and under the condition of overall neutrality, only two of those charges are free parameters. A resolution to this problem is discussed by Valone and Jindal [6].

IV. CONCLUSIONS AND FUTURE WORK

The initial three-state model of charge resonances for the water molecule turned out to be incomplete. To fix this, we postulated the existence of a fourth, symmetric charge resonance. We also need to rework the approximations used for the asymmetric hamiltonian elements in Eq. (24).

We can test our model by comparing the charge asymmetry with that found by solving the Kohn-Sham equations using an asymmetric geometry instead of a fractional constraint.

We eventually hope that the variable-charge PES for a single water molecule can be used to model the behavior of liquid water: In liquid water, the bonds are different lengths. Additionally, the structure of a water molecule, H_2O , is similar to that of many metal dioxides, such as SiO_2 , so we hope that the PES may shed more light on those materials as well.

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VI. APPENDIX

A side project this summer was working with Scalable Parallel Short-range Molecular Dynamics (SPaSM). SPaSM is a three-dimensional MD simulation code. The issue that we are concerned with is that the current integrator does not perform well when dealing with particles of disparate masses [7].

MD simulations work by integrating the hamiltonian equations of motion to update each and every particle's position and velocity. Each particle in the system experiences a force related to the potential energy of the system, as described in Eq. (1). At every timestep in the simulation, the force acting on each particle, along with each particle's position and velocity, is plugged into Newton's equations to find each particle's new position and velocity. However, when a particle's position changes, the inter-particle interactions also change, so the forces acting on each particle need to be recalculated at every timestep.

Many numerical integration methods exist. SPaSM used Störmer Verlet integration, in which the equations of motion for particle i are expressed as

$$\begin{aligned}\vec{x}_i(t + \Delta t) &= \vec{x}_i(t) + \vec{v}_i\left(t + \frac{\Delta t}{2}\right)\Delta t \\ \vec{v}_i\left(t + \frac{\Delta t}{2}\right) &= \vec{v}_i\left(t - \frac{\Delta t}{2}\right) + \frac{\vec{F}_i}{m_i}\Delta t,\end{aligned}\quad (25)$$

where F_i is the force acting on and m_i is the mass of particle i .

The new method is Runge-Kutta integration. The

equations of motion for particle i are

$$\begin{aligned}\vec{x}_i(t + \Delta t) &= \vec{x}_i(t) + (\vec{g}_{0i} + 2\vec{g}_{1i} + 2\vec{g}_{2i} + \vec{g}_{3i})\frac{\Delta t}{6} \\ \vec{v}_i(t + \Delta t) &= \vec{v}_i(t) + (\vec{f}_{0i} + 2\vec{f}_{1i} + 2\vec{f}_{2i} + \vec{f}_{3i})\frac{\Delta t}{6},\end{aligned}\quad (26)$$

where the subquantities used in the integration are

$$\begin{aligned}\vec{g}_{0i} &= \vec{v}_i(t) \\ \vec{f}_{0i} &= \frac{\vec{F}(\vec{x}_i(t))}{m_i} \\ \vec{g}_{1i} &= \vec{v}_i(t) + \frac{\vec{f}_{0i}}{2}\Delta t \\ \vec{f}_{1i} &= \frac{\vec{F}(\vec{x}_i(t) + \frac{\vec{g}_{0i}\Delta t}{2})}{m_i} + \frac{\vec{g}_{0i}}{2}\Delta t \\ \vec{g}_{2i} &= \vec{v}_i(t) + \frac{\vec{f}_{1i}}{2}\Delta t \\ \vec{f}_{2i} &= \frac{\vec{F}(\vec{x}_i(t) + \frac{\vec{g}_{1i}\Delta t}{2})}{m_i} + \frac{\vec{g}_{1i}}{2}\Delta t \\ \vec{g}_{3i} &= \vec{v}_i(t) + \vec{f}_{2i}\Delta t \\ \vec{f}_{3i} &= \frac{\vec{F}(\vec{x}_i(t) + \vec{g}_{2i}\Delta t)}{m_i} + \vec{g}_{2i}\Delta t.\end{aligned}\quad (27)$$

Calculating each $\vec{f}_{ni}$ requires advancing the particle's coordinates and calculating the force at that position. As a result, each timestep contains four force recalculations and three intermediate position updates, as well as the final updates to $\vec{x}_i$ and $\vec{v}_i$. Runge-Kutta integration is therefore more computationally expensive, but it maintains better conservation of energy than does Verlet.

Modeling two boson systems in an optical lattice

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The dynamics of two bosonic particles interacting via contact and/or long-range forces in two sites of an optical lattice are analyzed using the Bose-Hubbard model. The Hilbert space of the problem is reduced from three to two allowing for representation of the model in the Landau-Zener form. The Landau-Zener system was solved numerically in Maple and the results were compared to the exact solution. Two cases were considered: the evolution in the time interval $t=[-\infty, \infty]$ and $t=[0, \infty]$. Implications of these results on dynamics of bosonic particles were considered.

I. INTRODUCTION

Recently, optical lattices have been used to trap ultracold atoms [1]. This development has exciting prospects in many different areas, including molecular, atomic, optical, and condensed matter physics. Moreover, it shows promise in the field of quantum information processing for contributing to the development of a quantum computer [2].

Optical lattices are created by the interference of laser beams. The lattice can be one, two, or three dimensional, and can be engineered in different shapes, i.e. rectangular, triangular, etc. [3]. The versatility of the lattice is part of the attraction to this new field. The structure that holds the atoms can be rigorously controlled and adjusted in real time.

The atoms are held in the potential wells having the structure of $\cos(\mathbf{k}\mathbf{r})^2$. Atom-laser field interaction restricts the motion of the atoms confining them to the vicinity of potential minima [4].

The energy of the atoms in a potential well determines which quantum phase they are in. A high ratio of kinetic to interaction energy indicates superfluidity, where atoms tunnel between lattice sites easily. Conversely, a low ratio of kinetic to interaction energy causes the system to approach the Mott insulating phase where on-site atom number fluctuations are suppressed and correlations between atoms are short-ranged [5].

This research has been mainly focused on modeling dynamics of two bosons trapped in two lattice sites. In the first calculations, the long-range (e.g., dipole-dipole) interaction was ignored, and then added into the Hamiltonian later.

II. BOSE-HUBBARD MODEL

The Hamiltonian for atoms in an optical lattice can be described as

$$\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{a}_i \hat{a}_j^\dagger + \hat{a}_j \hat{a}_i^\dagger) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad (1)$$

where the sum goes over nearest-neighboring sites. The variable J is the kinetic energy, U is the interaction energy of the particles, and $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators, respectively. They operate as follows

$$\begin{aligned} \hat{a}_i |m_1, m_2, \dots, m_i, \dots\rangle &= \sqrt{m_i} |m_1, m_2, \dots, m_i - 1, \dots\rangle \\ \hat{a}_i^\dagger |m_1, m_2, \dots, m_i, \dots\rangle &= \sqrt{m_i + 1} |m_1, m_2, \dots, m_i + 1, \dots\rangle \\ \hat{n}_i |m_1, m_2, \dots, m_i, \dots\rangle &= m_i |m_1, m_2, \dots, m_i, \dots\rangle \end{aligned} \quad (2)$$

where $|m_1, m_2, \dots, m_i, \dots\rangle$ is a state with m_i atoms at the i^{th} lattice site [6]. The operators follow the commutation relations

$$\begin{aligned} [\hat{a}_i, \hat{a}_j^\dagger] &= \delta_{ij} \\ [\hat{a}_i, \hat{a}_j] &= [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0. \end{aligned} \quad (3)$$

III. TWO-BODY PROBLEM

A. Time-Independent System

In this research, we were concerned with two particles distributed over two lattice sites. The Hilbert space is defined by the three vectors $|1\rangle = |1, 1\rangle$, $|2\rangle = |2, 0\rangle$, $|3\rangle = |0, 2\rangle$. After rescaling by U , the Hamiltonian for this system is given by

$$\hat{H} = -\frac{J}{U} (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{1}{2} [\hat{n}_1 (\hat{n}_1 - 1) + \hat{n}_2 (\hat{n}_2 - 1)]. \quad (4)$$

When applied to the basis, the Hamiltonian can be represented by the matrix

$$\hat{H} = \begin{pmatrix} 0 & -\sqrt{2} J/U & -\sqrt{2} J/U \\ -\sqrt{2} J/U & 1 & 0 \\ -\sqrt{2} J/U & 0 & 1 \end{pmatrix}. \quad (5)$$

having eigenenergies

$$\epsilon_1 = \frac{1}{2} - \frac{1}{2} \sqrt{1 + 16 \frac{J^2}{U^2}}, \epsilon_2 = 1, \epsilon_3 = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 16 \frac{J^2}{U^2}}. \quad (6)$$

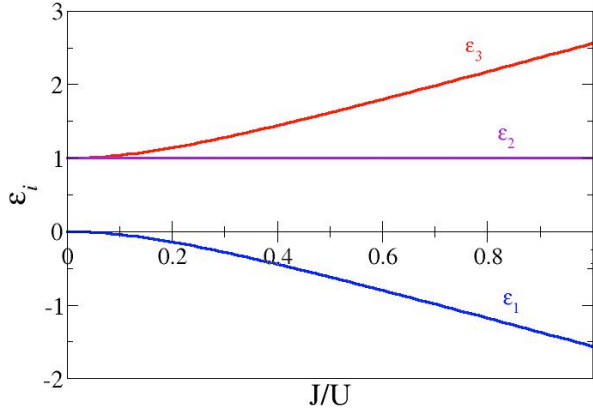


Figure 1: Plot of the three eigenenergies of $\hat{H}$ (5). The blue line represents the ground state energy, and the purple and red lines represent the excited state energies.

The eigenvectors of this Hamiltonian are

$$\begin{aligned} \mathbf{v}_1^T &= \frac{2J/U}{\sqrt{\alpha^2 + \alpha}} \left(\frac{1+\alpha}{2\sqrt{2}J/U}, 1, 1 \right), \quad \mathbf{v}_2^T = \frac{1}{\sqrt{2}} (0, 1, -1) \\ \mathbf{v}_3^T &= \frac{2J/U}{\sqrt{\alpha^2 - \alpha}} \left(\frac{1-\alpha}{2\sqrt{2}J/U}, 1, 1 \right) \end{aligned} \quad (7)$$

where $\alpha = \sqrt{1 + (4J/U)^2}$.

As discussed before, the ratio of kinetic to interaction energy, J/U , determines the quantum phase occupied by the atoms. In the superfluid limit, $J/U \rightarrow \infty$, the system is found to be in a linear combination of all three states: $\mathbf{v}_1^T = \left(\frac{1}{\sqrt{2}}, \frac{1}{2}, \frac{1}{2} \right)$ and the state is described as $\frac{1}{\sqrt{2}}|1,1\rangle + \frac{1}{2}|2,0\rangle + \frac{1}{2}|0,2\rangle$. This is to be expected as the probabilities represent a simple system with two particles and two possible locations, and no other imposed limits. Conversely, in the insulator limit, $J/U \rightarrow 0$, the system is found in $\mathbf{v}_1^T = (1, 0, 0)$, so the atoms are in the state $|1,1\rangle$. Due to finite size effects we do not see a many-body quantum phase of our system in these two limits. Our ground state, however, resembles closely the superfluid and Mott insulator ground states of a large system in the limit of $U=0$ and $J=0$, respectively. They are defined as

$$|\text{SF}\rangle = \sqrt{\frac{N!}{M^N}} \sum_{\{n_i\}} \frac{|n_1, \dots, n_M\rangle}{\sqrt{n_1! \dots n_M!}}, \quad |\text{MI}\rangle = |1, 1, 1, \dots\rangle, \quad (8)$$

for an N particle system over M sites.

B. Time-Dependent System

In order to simplify the results, the Hamiltonian was applied to a different Hilbert space, given by $|1,1\rangle$, $\frac{1}{\sqrt{2}}(|2,0\rangle + |0,2\rangle)$, and $\frac{1}{\sqrt{2}}(|2,0\rangle - |0,2\rangle)$ [3]. We define $a(t)$, $b(t)$, and $c(t)$ as the coefficients for the vectors defined above, respectively. The time-dependent Schrödinger equation is presented below:

$$i \frac{\partial}{\partial t} \begin{pmatrix} a(t) \\ b(t) \\ c(t) \end{pmatrix} = \begin{pmatrix} 0 & -2\frac{J}{U} & 0 \\ -2\frac{J}{U} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a(t) \\ b(t) \\ c(t) \end{pmatrix}. \quad (9)$$

In this case, $\hbar$ has been omitted as we are working with dimensionless theory. This equation shows that the third vector, $\frac{1}{\sqrt{2}}(|2,0\rangle - |0,2\rangle)$ is dynamically decoupled from the first and second vectors, and as we will start the evolution from the $|1,1\rangle$ state, it can be omitted. The wavefunction can now be simplified as

$$|\psi(t)\rangle = a(t)|1,1\rangle + b(t) \frac{|2,0\rangle + |0,2\rangle}{\sqrt{2}}, \quad (10)$$

where $|a|^2 + |b|^2 = 1$. The Schrödinger equation can be reduced to a 2×2 system given by

$$i \frac{\partial}{\partial t} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} 0 & -2\frac{J}{U} \\ -2\frac{J}{U} & 1 \end{pmatrix} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}. \quad (11)$$

Applying the rotation

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{e^{it/2}}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}, \quad (12)$$

and defining $|\psi(t)\rangle = e^{-it/2} (a'(t)|1'\rangle + b'(t)|2'\rangle)$, where

$$\begin{aligned} |1'\rangle &= \frac{1}{\sqrt{2}}|1,1\rangle - \frac{1}{2}(|2,0\rangle + |0,2\rangle) \\ |2'\rangle &= -\frac{1}{\sqrt{2}}|1,1\rangle - \frac{1}{2}(|2,0\rangle + |0,2\rangle), \end{aligned} \quad (13)$$

the time-dependent Schrödinger equation is reduced to the Landau-Zener (LZ) model [8]:

$$i \frac{\partial}{\partial t} \begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \frac{t}{\tau} & 1 \\ 1 & -\frac{t}{\tau} \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix} = \hat{H}_{\text{LZ}} \begin{pmatrix} a' \\ b' \end{pmatrix}, \quad (14)$$

where $|a'|^2 + |b'|^2 = 1$ and $t/\tau = 4J/U$. In Section VI, we will explain the time-dependent J/U ratio driving the system. The quench timescale, τ , determines how quickly the system evolves through time. The instantaneous eigenenergies of $\hat{H}_{\text{LZ}}$ (14) are:

$$\epsilon_1 = -\frac{1}{2}\sqrt{1 + (t/\tau)^2}, \quad \epsilon_2 = \frac{1}{2}\sqrt{1 + (t/\tau)^2}. \quad (15)$$

Figure 2 shows them graphically. Qualitatively, it shows that far from the anti-crossing, the energy gap is large, and the evolution will be adiabatic. The highest probability of exciting the system is at the anti-crossing, when $t=0$.

Up to the normalization factor, the eigenvectors for the LZ model are

$$\mathbf{v}_1 = \begin{pmatrix} \frac{1}{-\sqrt{1 + (t/\tau)^2} - t/\tau} \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} \frac{1}{\sqrt{1 + (t/\tau)^2} - t/\tau} \\ 1 \end{pmatrix} \quad (16)$$

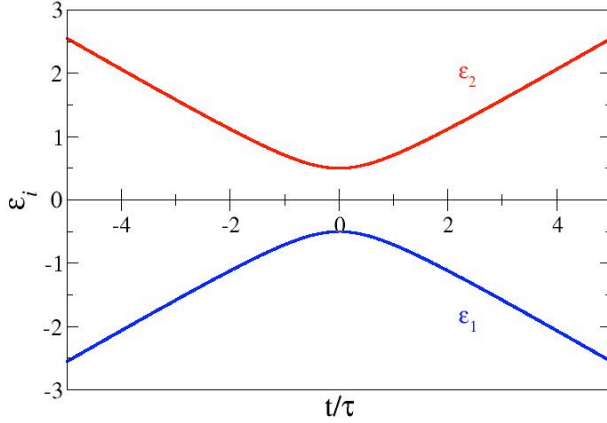


Figure 2: Plot of the eigenenergies of $\hat{H}$ (14) as a function of t/τ . The red line indicates the excited state, while the blue line indicates the ground state of the system.

where v_1 is the instantaneous ground state eigenvector, and v_2 is the excited state instantaneous eigenvector.

To check this result qualitatively, the limit of $t \rightarrow \pm\infty$ is considered. As $t \rightarrow -\infty$ we see that $v_1^T = (1, 0)$ and $v_2^T = (0, 1)$, while when $t \rightarrow +\infty$ we get $v_1^T = (0, 1)$ and $v_2^T = (1, 0)$. This can be immediately obtained by skipping the off diagonal terms in the Landau-Zener Hamiltonian.

For future convenience, these eigenstates in a normalized form can be parameterized by

$$v_1 = \begin{pmatrix} -\sin\left(\frac{\theta}{2}\right) \\ \cos\left(\frac{\theta}{2}\right) \end{pmatrix}, \quad v_2 = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix}, \quad (17)$$

where $\cos(\theta) = \varepsilon / \sqrt{1 + \varepsilon^2}$, $\varepsilon = t/\tau$, and $\theta \in [0, \pi]$ [9].

IV. DYNAMICS OF LZ MODEL

In this section, the LZ model was solved numerically. We obtained the probability that the system is in the excited state as a function of τ . In subsection A, the system evolves in the time interval $t = [-\infty, \infty]$. In subsection B, the system evolves in the time interval $t = [0, \infty]$. The former case corresponds to an evolution that starts far away from the anti-crossing, evolves past it and ends far away from it. The latter evolution starts at the anti-crossing center and then takes the system far away from it. In both cases the evolution starts from the instantaneous ground state of the Landau-Zener Hamiltonian at the initial time of the evolution.

These numerical solutions were performed using Maple. The default mode used for solving this LZ system does not produce results to the desired accuracy. Therefore, we have added a numerical routine called *dverk78* in the *dsolve* command in Maple. This setting finds a numerical solution using a seventh-eighth order continuous Runge-Kutta method [10]. This reduces the error in keeping the normalization of the wave function to

$\left| |a'|^2 + |b'|^2 - 1 \right| = O(10^{-8})$, which is sufficient for our purposes.

A. Time Interval $t = [-\infty, \infty]$

This is the classic Landau-Zener problem well known in physics. We consider it here for purely educational purposes. We evolve the system numerically from $t_0 = -10 \cdot \tau$, and $t_f = t_0$ and plot the excitation value as a function of τ . Using (17), the initial conditions for these simulations are given by

$$a' = -\sin\left(\frac{\theta(t_0)}{2}\right), \quad b' = \cos\left(\frac{\theta(t_0)}{2}\right), \quad (18)$$

where $\theta(t_0) \approx \pi$, i.e. the system starts in the ground state.

A loop was created for $\tau = [0.1, 10]$. Again using (17), the final excitation probability was calculated as $\rho_{ex} = \left| \langle \psi | v_2 \rangle \right|^2$. This can be written in a compact form as

$$\rho_{ex} = \left| a'(t_f) \cdot \cos\left(\frac{\theta(t_f)}{2}\right) + b'(t_f) \cdot \sin\left(\frac{\theta(t_f)}{2}\right) \right|^2. \quad (19)$$

Using these methods, the excitation probability was determined by a fit to numerical data in the range $\tau = [0.1, 10]$. The equation derived from the data is the linear fit

$$\ln(\rho_{ex}) = 0.002 - 1.5708 \cdot \tau,$$

obtaining

$$\rho_{ex} = 1.002 \cdot \exp(-1.5708 \cdot \tau).$$

Allowing small discrepancies due to numerical errors, this matches the celebrated Landau-Zener [8] solution,

$$\rho_{ex} = \exp\left(-\frac{\pi}{2} \tau\right). \quad (20)$$

This is the exact result for all τ 's. It is used in various fields of physics. Figure 3 shows the data matched with this formula.

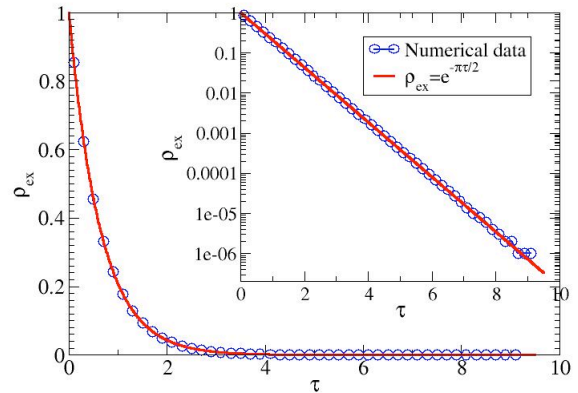


Figure 3: Plot of the excitation probability of the Landau-Zener system. The blue circles show the numerical data from Maple, and the red line represents the exact expression (20).

B. Time Interval $t=[0,\infty]$

This problem can be regarded as the modified Landau-Zener problem as the initial condition for this evolution differs from the classic Landau-Zener problem. It turns out, however, that this version of the Landau-Zener evolution is relevant for studies of cold atom dynamics in an optical lattice (see Section VI).

The numerical calculations were repeated with the initial conditions set at $t=0$ instead of $t=t_0$, i.e., with

$$a' = -\sin\left(\frac{\theta(0)}{2}\right), b' = \cos\left(\frac{\theta(0)}{2}\right), \quad (21)$$

where $\theta(0)=\pi/2$. In this case, the excitation probability does not converge to a simple equation quickly. It is necessary to do the calculations for $\tau=[0,75]$, again with $t_f=10\cdot\tau$, to determine the solution. For $\tau\gg 1$, we obtained a linear fit of

$$\ln(\rho_{ex}) = -1.354 - 2.0075 \cdot \ln(\tau),$$

$$\text{or } \rho_{ex} = 0.2582 \cdot \tau^{-2.0075}.$$

The results are shown in Figure 4.

According to [3], the exact solution here is

$$\rho_{ex}(\infty) = 1 - \frac{2}{\pi\tau} \sinh\left(\frac{\pi\tau}{4}\right) e^{-\pi\tau/8} \left| \Gamma\left(1 + \frac{i\tau}{8}\right) + e^{i\pi/4} \sqrt{\frac{\tau}{8}} \Gamma\left(\frac{1}{2} + \frac{i\tau}{8}\right) \right|^2. \quad (22)$$

Expanding equation (22) for large τ ,

$$\rho_{ex}(\infty) = \frac{1}{4\tau^2} + O(\tau^{-4}). \quad (23)$$

This formula matches well with the one found from the data shown in Figure 4.

This result is strikingly different from the previous solution for $t=[-\infty,\infty]$. Most surprising is that the excitation probability does not decay exponentially anymore

For future calculations, it is useful to expand (22) for small τ as well [3]. In this limit we get

$$\rho_{ex} = \frac{1}{2} - \frac{\sqrt{\pi}}{4} \sqrt{\tau} + O(\tau^{3/2}). \quad (24)$$

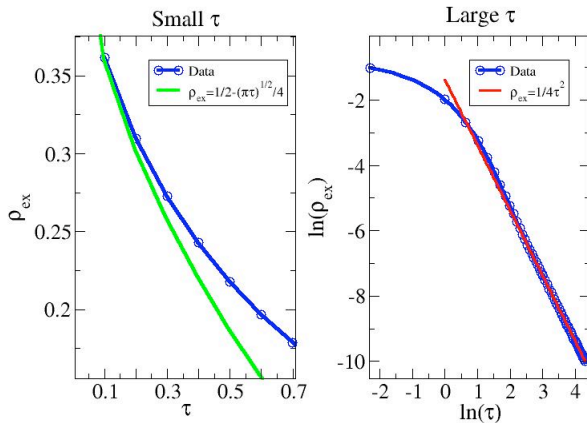


Figure 4: Plot of ρ_{ex} vs τ for $\tau=[0.1,100]$. The left plot depicts the limit $\tau\ll 1$ where (24) holds [3]. The right plot represents $\tau\gg 1$ where we expect (23) to be the solution.

We have checked numerically that this expansion is accurate for $\tau<0.2$. See the left plot of Figure 4.

V. MODEL WITH LONG-RANGE INTERACTION

A. Time-Independent System

In the previous sections, the long-range interaction between bosons has been ignored. One example of such interaction may result from dipolar forces between bosons, and has been shown to lead to interesting quantum phases [5]. For the two-particle, two-lattice site system, the Bose-Hubbard model with the long-range interaction term reads

$$\hat{H} = -\frac{J}{U}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{1}{2} \sum_{i=1}^2 \hat{n}_i(\hat{n}_i - 1) + \frac{1}{2} \frac{V}{U} \hat{n}_1 \hat{n}_2. \quad (25)$$

where V is the potential energy from the long-range interactions.

In the basis $|1,1\rangle, |2,0\rangle, |0,2\rangle$, the Hamiltonian becomes

$$\hat{H} = \begin{pmatrix} \frac{1}{2} \frac{V}{U} & -\sqrt{2} \frac{J}{U} & -\sqrt{2} \frac{J}{U} \\ -\sqrt{2} \frac{J}{U} & 1 & 0 \\ -\sqrt{2} \frac{J}{U} & 0 & 1 \end{pmatrix} \quad (26)$$

with eigenenergies

$$\begin{aligned} \varepsilon_1 &= \frac{1}{2} + \frac{1}{4} \frac{V}{U} - \frac{1}{2} \sqrt{\left(1 - \frac{1}{2} \frac{V}{U}\right)^2 + \left(4 \frac{J}{U}\right)^2} \\ \varepsilon_2 &= 1, \\ \varepsilon_3 &= \frac{1}{2} + \frac{1}{4} \frac{V}{U} + \frac{1}{2} \sqrt{\left(1 - \frac{1}{2} \frac{V}{U}\right)^2 + \left(4 \frac{J}{U}\right)^2}. \end{aligned} \quad (27)$$

and (unnormalized) eigenvectors

$$\begin{aligned} v_1^T &= \left(\frac{-4\sqrt{2} \frac{J}{U}}{\left(1 - \frac{1}{2} \frac{V}{U}\right) - \sqrt{\left(1 - \frac{1}{2} \frac{V}{U}\right)^2 + \left(4 \frac{J}{U}\right)^2}}, 1, 1 \right) \\ v_2^T &= (0, 1, -1) \\ v_3^T &= \left(\frac{-4\sqrt{2} \frac{J}{U}}{\left(1 - \frac{1}{2} \frac{V}{U}\right) + \sqrt{\left(1 - \frac{1}{2} \frac{V}{U}\right)^2 + \left(4 \frac{J}{U}\right)^2}}, 1, 1 \right) \end{aligned} \quad (28)$$

When V/U is set equal to zero, (26), (27), and (28) are equal to (5), (6), and (7), up to normalization, as is to be expected.

B. Time-dependent System

The Hamiltonian in (26) can be simplified in the same way as before by rewriting the Hamiltonian in the basis

$|1,1\rangle, 1/\sqrt{2}(|2,0\rangle+|0,2\rangle), 1/\sqrt{2}(|2,0\rangle-|0,2\rangle)$. In this basis,

$$\hat{H} = \begin{pmatrix} \frac{1}{2}\frac{V}{U} & -2\frac{J}{U} & 0 \\ -2\frac{J}{U} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (29)$$

If the time evolution is started with zero overlap on the third vector, it is dynamically decoupled, and can thus be ignored. Therefore, the time-dependent Schrödinger equation is

$$i\frac{\partial}{\partial t}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\frac{V}{U} & -2\frac{J}{U} \\ -2\frac{J}{U} & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}, \quad (30)$$

where a and b are described by (10).

The next step in this calculation is transforming the Schrödinger equation presented in (30) into the Landau-Zener format. The rotation described by (12) is used for the transformation, except the time dependent factor, $e^{it/2}$ is replaced by $e^{[t/2+V/4U]}$, obtaining

$$i\frac{\partial}{\partial t}\begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4\frac{J}{U} & -\frac{1}{2}\frac{V}{U}+1 \\ -\frac{1}{2}\frac{V}{U}+1 & -4\frac{J}{U} \end{pmatrix}\begin{pmatrix} a' \\ b' \end{pmatrix}. \quad (31)$$

The wave function is

$$|\psi(t)\rangle = e^{-i[t/2+V/4U]}\left(a'(t)|1'\rangle + b'(t)|2'\rangle\right). \quad (32)$$

Quite surprisingly we observe two distinct dynamical regimes. First, when $V/U=2$, the two states $|1'\rangle$ and $|2'\rangle$ evolve independently even when J/U is time-dependent (as before, we assume $4J/U=t/\tau$). This is contrast to the $V=0$ case where the two levels were coupled and evolved in a non-trivial way. In other words, the addition of the long-range interaction term to the Hamiltonian can switch off level coupling, which is a novel and unexpected feature.

Second, when $V/U \neq 2$ we can reduce (31) to a traditional Landau-Zener system by the following rescalings

$$t' = t \cdot \delta, \quad \tau' = \tau \cdot \delta^2, \quad \delta = -\frac{1}{2}\frac{V}{U} + 1, \quad (33)$$

where we assume that $\delta > 0$ for simplicity. After that we end up with

$$i\frac{\partial}{\partial t'}\begin{pmatrix} a' \\ b' \end{pmatrix} = \frac{1}{2}\begin{pmatrix} t'/\tau' & 1 \\ 1 & -t'/\tau' \end{pmatrix}\begin{pmatrix} a' \\ b' \end{pmatrix}, \quad (34)$$

which reduces in the limit of $V \rightarrow 0$ to (14). The difference is that we have a new quench time scale once $V \neq 0$, and $V \neq 2U$. Indeed,

$$\tau' = \tau \cdot \left(-\frac{1}{2}\frac{V}{U} + 1\right)^2. \quad (35)$$

This is again surprising as it shows that we can slow down or speed up the quench by adjusting the strength of long-range interactions, while keeping the time dependence of J/U completely unchanged.

VI. QUENCH DYNAMICS

Our system can be driven by the change of the lattice height. Initially we assume $J/U=0$, which can be easily achieved by considering deep lattice limit as J/U decreases exponentially with lattice depth. By lowering the lattice depth, atoms will start to jump between the sites and $J/U > 0$. In a real system, the change of the lattice height will change both J and U . Here we simplify the problem by assuming that U is constant, while J is linearly ramped up. As evident from former sections, the convenient choice for time dependence of J is

$$\frac{J}{U} = \frac{1}{4}\frac{t}{\tau}, \quad (36)$$

as it guarantees that we will end up with Landau-Zener-like evolutions. The quench factor, τ , defines the rate at which J/U changes. Here $\tau=0$ implies infinitely fast quench that would produce no change in the state of the system. Conversely, large τ indicates a slow transition, where the system stays close to its instantaneous ground state (if the evolution has started from a ground state as well). In other words, the evolution is near adiabatic.

The evolution starts at $t=0$ and goes to $t \rightarrow \infty$. The initial state is $|1,1\rangle$ which is the ground state of the Bose-Hubbard Hamiltonian (4) for $J/U=0$. In terms of the eigenstates of the Landau-Zener system (34), the evolution starts from the ground state right at the anti-crossing center as $|1,1\rangle$ equals $(|1'\rangle - |2'\rangle)/\sqrt{2}$: see (17). This is why we end up with the modified Landau-Zener problem and need to use (23) and (24) instead of (20).

As the system evolves through time, we are interested in the correlation function

$$C_1(t) = \frac{1}{2}\langle\psi(t)|\hat{a}_1^\dagger\hat{a}_2 + \hat{a}_2^\dagger\hat{a}_1|\psi(t)\rangle, \quad (37)$$

which describes how well the atoms are correlated to each other as a function of time [3]. This is also interesting as it can be determined experimentally by measurement of the interference pattern after releasing the atoms from the lattice. Initially this correlation function is zero, as we start from the uncorrelated Mott state. It attains the value of unity when the system is driven adiabatically to $J/U \rightarrow \infty$, i.e., to a two-level analog of deep superfluid limit.

Using (32), we have verified that

$$C_1(t) = 1 - 2|a'(t)|^2, \quad (38)$$

where $|a'(t \rightarrow \infty)|^2 = \rho_{ex}$, the excitation probability. As determined in sections III and IV, ρ_{ex} can be represented as a function of τ . This relationship between C_1 and τ makes it possible to achieve a desired correlation factor based on the time quench factor in an experimental setting.

Using the expressions for excitation probabilities (23-24) and formula (38), we obtain the correlation function by the end of time evolution for the problem with long-range interactions:

$$C_1(t \rightarrow \infty) = 1 - \frac{1}{2\tau^2 \left(-\frac{1}{2}\frac{V}{U} + 1\right)^4} + O\left(\tau^{-4} \left(-\frac{1}{2}\frac{V}{U} + 1\right)^{-8}\right) \quad (39)$$

for large τ , and

$$C_1(t \rightarrow \infty) = \frac{\sqrt{\pi}}{4} \sqrt{\tau} \left(-\frac{1}{2}\frac{V}{U} + 1\right) + O\left(\tau^{3/2} \left(-\frac{1}{2}\frac{V}{U} + 1\right)^3\right) \quad (40)$$

for small τ . Both cases can be experimentally verified in a setup similar to the one from [11].

VII. SUMMARY

We have considered two bosonic particles interacting in an optical lattice via both short-range and long-range interactions using the Bose-Hubbard model. The problem was reduced to the Landau-Zener form and analyzed in two time intervals, $t \in [-\infty, \infty]$, and $t \in [0, \infty]$. We calculated the excitation probability as a function of the time quench factor, τ . We have applied these results to the model involving long-range interactions. We have found that system dynamics strongly depends on the strength of these interactions. In particular, we have found that when long-range interactions are twice stronger than on-site interactions ($V/U=2$), the two levels of the 2×2 Hamiltonian become uncoupled. In all other cases, the quench time scale depends on the strength of long-range interactions leading to an interesting new effect. Namely, we have shown that depending on the ratio of V/U , the quench can be accelerated or decelerated. It would be interesting to understand this new effect better in the future as well as study the atom number fluctuations in this system to fully characterize all non-trivial observables.

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Vetting Proposed Models for Intermediate Levels of the Visual Cortex

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ABSTRACT

While there have been numerous attempts in the field of computational neuroscience to map the pathways of the visual cortex, there is still a great deal of uncertainty regarding the optimal stimuli for the neurons found in the intermediate layers of the cortex V2 and V4. A recently proposed model theorizes that complex three-dimensional shape representation may evoke a strong response in the inferotemporal cortex (IT), suggesting that neurons in V2 and V4 may encode parameters applying to multiple surface fragments, such as local curvature and object-relative orientation and position. We hypothesize that the use and manipulation of 3d modeling and rendering software will provide insight into whether such a model of V2 and V4 is a sufficient representation for object detection and recognition in IT.

I. Introduction

The field of computational neuroscience has made great strides in providing a structured method for understanding the workings of the mind and in creating algorithms for helping computers to operate in more human-like tasks, particularly in the area of visual cognition, performing functions such as object detection and recognition. Through efforts to observe the workings of visual cognition, it has been observed that object recognition in the cortex is regulated by a hierarchical pathway running from the primary visual cortex (V1) through the intermediate visual areas II (V2) and IV (V4), to the inferotemporal cortex (IT). There are certain key features to note about this ventral pathway, regarding the hierarchical fashion in which it operates. As information travels from V1 to IT, its representation in each sequential layer becomes increasingly complex, as the optimal stimuli for the neurons in each layer become increasingly specific. In addition, there is an observed increase in invariance to position and scaling of objects in more complex layers. It is in the highest layers of complexity where tasks such as object detection and recognition appear to occur. There has been an enormous amount of effort put into modeling the transitions between the layers of the cortex, though as of yet, researchers have not been able to agree upon a universally accepted mapping.

It has been established through experiment that the neurons in the retina and in V1 function as “edge detectors,” reacting to sharp contrasts in shade present within the visual field. What puzzles researchers at this point is the pathway that information takes through the intermediate visual areas V2

and V4, where visual data is processed and represented in a format that can be used by IT for object recognition. A recent paper published discusses the possibility that, rather than focusing on two-dimensional pattern representation, V2 and V4 encode information regarding complex three-dimensional shape representation. In such a case, neurons would encode information about curvature, orientation, and object-relative position of two-dimensional surface fragments that compose whole three-dimensional objects. The convenience of such a model lies in the fact that curvature and object-relative values are largely viewpoint invariant and unaffected by translations or scaling.

What we propose to do is vet this hypothesis, that neurons do indeed encode information regarding these three-dimensional variables. If we could somehow prove that feeding this information into IT is a sufficient representation for accurate object recognition, then it suddenly becomes worthwhile to find methods for extracting information regarding curvature and object-relative variables from raw pixel data. For this reason, our proposed project works with analyzing three-dimensional models and rendered scenes in which these variables are implicitly stored within the vertex data of the objects. By using these models, we are able to bypass the difficult step of determining how to extract the information from the rendered scene and go straight to the output data.

At our current state, neural network models such as PetANNNet (PANN), when applying learning algorithms to raw pixel data, often fail at even simple binary classification tasks (animal/no animal) when provided with a set of scenes, performing no better than pure chance. It has been demonstrated time and time again that such methods ultimately fail and that a representation analyzing huge multi-dimensional pixel spaces utilizes far more neurons than are present in IT. If we could instead create a multi-dimensional vector space carrying variables such as relative and absolute x-y position, slant, tilt, and local curvature of surface patches, with each neuron corresponding to a particular surface patch, it seems much more reasonable to assume that the inferotemporal cortex could work with such a model.

II. Methods

In order to test our hypothesis, we plan to create a simple binary classification task, aiming to generate a large number of three-dimensionally rendered scenes, 50% of which contain a target object and 50% of which do not. The scenes will be rendered under various lighting angles from random camera viewpoints and the raw pixel data would be fed into a conventional machine learning algorithm, such as PANN, asking it to determine whether or not each of the scenes contains the target object. We imagine that varying the sizes, locations, and orientations of objects would cause sufficient variations in the representations of the scenes that PANN would struggle with such a task.

The alternative method for performing this task is the method we are most interested in testing, which involves going past the visual rendering of the scenes and delving straight into the vertex/face data. With each randomly generated scene, not only do we have a visual representation of the scene, we also create a file coded in some sort of 3d file format, which carries the vertex coordinates of the modeled scene and the corresponding faces. From this data, it is left to a series of calculations to determine the varying parameters, such as relative/absolute position, orientation, and local surface curvature of each of the boundary patches specified in the modeling format.

This leaves a number of tasks that have to be accomplished by the program that will process the scenes. It is first necessary for the program to discern which faces are visible and which faces are occluded from

the camera viewpoint. Once this has been established, we can easily determine the orientation of each face by calculating its normal vector, determining its slant and tilt in the x and y directions, respectively. From these values, it becomes possible to also calculate local surface curvatures by observing the difference in the normal vector over a surface, relative to the neighboring faces.

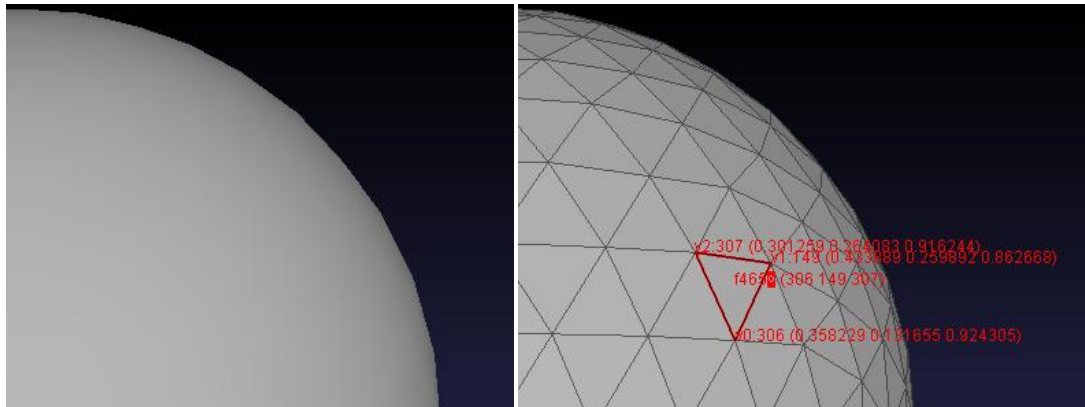


Figure 1: The above picture depicts a curved surface, which appears smooth and uniform from a rendered standpoint but can be broken down into an array of triangular surface patches and vertices, from which implicit data regarding curvature and object-relative position can be extracted. We feed the image on the left to PANN, containing only the raw pixel data from the rendered surface, whereas we plan to feed the data represented in the image on the right to an SVM and compare the success rates of the two methods.

To calculate relative positioning of faces, it becomes necessary to first establish a center from which faces can be relatively measured. This can be roughly calculated by calculating the center of mass of the triangular faces that compose the object, assigning each face with an equal value for surface density. Once this center is calculated and its absolute position determined, the relative position of each face can be determined from the difference between its absolute position and the absolute position of the object's center.

Once the three-dimensional object file has been run through our program and these parameters have been specified and calculated, we can use these values to flood a multi-dimensional vector space, which can then be fed into a support vector machine, where a learning algorithm can be specified and the simple binary classification task can be performed by the SVM, hopefully with results close to the rate of accuracy of a human. If this is indeed the case, we have evidence that it is worthwhile to further study this model for the intermediate levels of the visual cortex.

III. Results

Before even testing this hypothesis, it is necessary to understand the basics of three-dimensional modeling. After extensive misdirection, we were able to determine that the Wavefront .obj format worked as a basic, universally accepted file format with vertex and face data explicitly written in ASCII

format within the file structure. This makes the format very easy to read and work with, as there is no file compression or conversion processes to deal with when running the files through the program.

Another problem we faced was determining how to randomize, render, and output the scene files for the machine learning algorithms to process. First we worked with OpenGL, creating very basic scenes with simple objects such as blocks, pyramids, and cones, whose dimensions, positions, and orientations could be parameterized and randomly placed throughout the scene. We were able to export these scenes to .obj format by using GLIntercept and OGLE. As our understanding of rendering progressed, we progressed to finding more complex models online of more complex models, such as animals, cars, and planes, and were able to arrange them about a scene using Blender and other free-source rendering software.

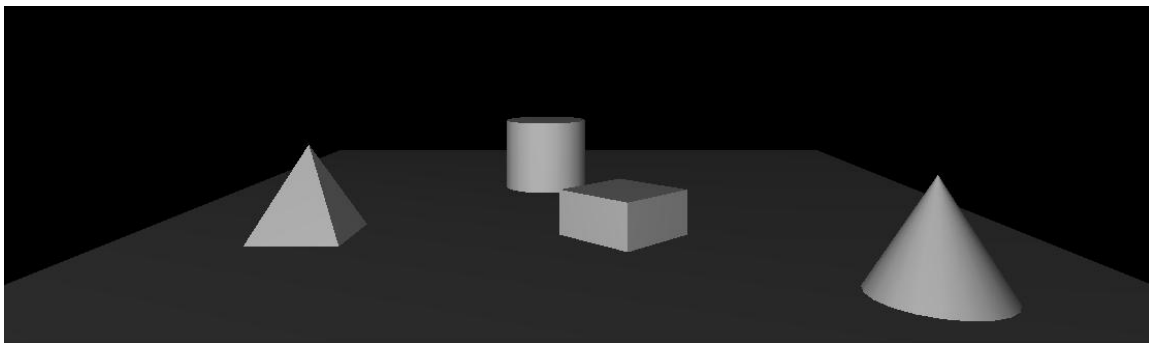


Figure 2: Example of a very basic scene rendered in OpenGL and exported to .obj format using GLIntercept and OGLE. Such a scene can be randomized to have objects placed throughout the viewing plane from varying viewpoints and fed to machine learning algorithms to perform simple binary classification tasks. (e.g. whether or not the scene contains a pyramid) Varying parameters and adding textures to the scene would likely cause PANN to struggle with even such a basic task.

IV. Conclusion and Future Work

Many of the key problems have been solved in determining the structures and layouts of three-dimensional file formats and how the vertices and faces are explicitly encoded within these formats. Our methods for vetting our hypothesis have been modified countless times due to misdirection, and only now do we have a clear vision of which direction the project should be headed. We now have a firm set of objectives which we need to complete in order to continue with the research and produce concrete results.

While we were able to solve a good deal of the problems regarding the generation and rendering of the three-dimensional scenes, we have not yet implemented the code that will act upon the .obj file formats, extracting the vertex/face data and performing calculations on them to obtain the variables that are proposed to be determined in the intermediate levels of V2 and V4. Once the code is written, the project becomes a matter of feeding its output into an SVM learning classifier and determining the accuracy of the model.

V. Acknowledgements

Many thanks go to James Colgan, Sally Seidel, and Norm Magee and their efforts in administering, organizing, and providing for the Los Alamos Summer School. Additional thanks are given to UNM for hosting the program and to the NSF for providing the funding to make it possible. A special note of appreciation goes to my mentor, Gar Kenyon, who managed to be an inspiring source of motivation for me even through my prolonged periods of stress and frustration.

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Electric Field-Driven Stacking of Red Blood Cells: Environmental Implications

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Abstract

Understanding potential biological effects of electromagnetic fields is of ever-growing importance in this increasingly electronic age. Knowing the underlying mechanisms of any biological effects of such fields would be an important step in determining whether health hazards will be a concern and at what exposures they might be triggered. In this study, we model how an external electric field can cause formation or stabilization of rouleaux, or coin-stack-like structures of red blood cells, suspended in plasma. Rouleaux formation occurs naturally, particularly in connection with infections or certain cancers, but it has also been shown that exposure to electromagnetic fields can intensify the effect via dielectrophoresis. The analogous phenomenon using colloidal particles in place of red blood cells is called “pearl chain formation”. We show that pairwise calculations of cell energies are insufficient to accurately predict the energetics of long rouleaux. Additionally, observed changes in dielectric properties as a function of configuration imply that an electric field, if strong enough, will drive aggregation and sedimentation. Our approach involves modeling a stack of cells as an ellipsoid and calculating the energies of various configurations of multiple red blood cells in a dielectric medium. Comparing energy formations of an extended prolate ellipsoid to that of a slightly shorter one plus an oblate ellipsoid in its lowest energy orientation allows estimation of a field threshold for the thermodynamically significant rouleaux stabilization. The resulting field is below the safety threshold derived based only on thermal heating.

Introduction

Rouleaux formation is the stacking of red blood cells into what resemble rolls of coins. It occurs naturally, and was first observed back in 1827 [1]. Although the phenomenon is seen in healthy people, excessive rouleaux are associated with certain conditions, such as infections, anemia, diabetes, and cancers like multiple melanoma [2]. Cell aggregation is also thought to be a major component of blood viscosity in veins [3].

Some experiments have observed rouleaux formation in response to radio-frequency (RF) electromagnetic fields, and also strong DC magnetic field gradients [4]. The case of RF-driven rouleaux is an example of pearl chain formation, in which particles align minimizing

the energy of the induced electric dipoles (see figure 1(c) and (d)). Whether pearl chain formation can affect biological systems at RF intensities below the safety thresholds established to prevent dangerous elevation of body temperature is a question that has been considered from the point of view of RF and microwave safety [4].

In the current study, we use a simple model to approximate the energies of different simple configurations of red blood cells. We show that the formation of rouleaux is energetically favored for a stack of five cells or more. We consider whether previous energy estimates, based solely on pairwise calculations of cell energies [5], is insufficient to aptly model the point at which electric stabilization overcomes thermal fluctuations.

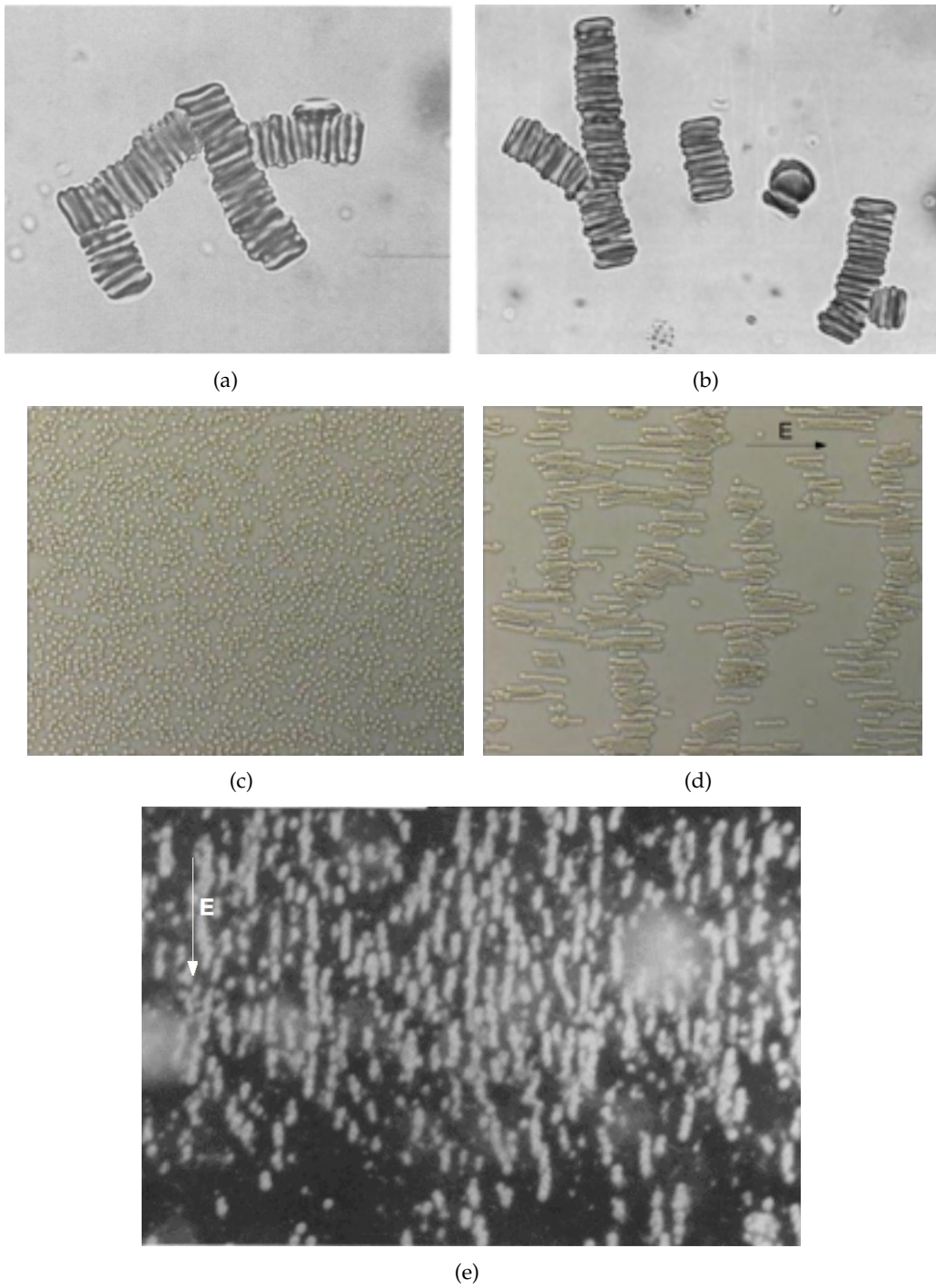


Figure 1: (a) and (b): Examples of naturally occurring rouleaux formation, i.e. with no electric field [1] and [6]. (c) and (d): Example of pearl chain formation of colloidal particles (c) without and (d) with an applied electric field [7]. (e): The chaining of red blood cells under an electric field of 50 V/cm [4].

Model

In order to calculate exact energies, we use a simple model. We approximate a single red blood cell as an oblate ellipsoid, with dimensions of $8 \mu\text{m}$ in diameter and $2 \mu\text{m}$ in thickness, and a prolate ellipsoid to model a rouleau of cells. We calculate the energies of various orientations and sizes of ellipsoids using standard equations [8].

The potential energy of a dielectric ellipsoid under an applied electric field is given in terms of the relative permittivity within the ellipsoid, ϵ_1 , and that of the surrounding fluid, ϵ_2 , as well as the resulting field within the body, $\mathbf{E}^-$, and the applied field, $\mathbf{E}_0$. A theorem in Stratton relates the total electrical energy of a dielectric in space to the integral over the volume of just the dielectric:

$$U = \frac{\epsilon_2 - \epsilon_1}{2} \int_V \mathbf{E}^- \cdot \mathbf{E}_0 dv ,$$

where

$$\mathbf{E}^- \cdot \mathbf{E}_0 = \frac{E_{0x}^2}{1 + \frac{abc}{2} \left(\frac{\kappa_1 - \kappa_2}{\kappa_2} \right) A_1} + \frac{E_{0y}^2}{1 + \frac{abc}{2} \left(\frac{\kappa_1 - \kappa_2}{\kappa_2} \right) A_2} + \frac{E_{0z}^2}{1 + \frac{abc}{2} \left(\frac{\kappa_1 - \kappa_2}{\kappa_2} \right) A_3} .$$

Here, $\kappa_i = \frac{\epsilon_i}{\epsilon_0}$, where ϵ_0 is the permittivity of free space. The values a, b , and c are the radii of the ellipsoid, while A_i is called the depolarization factor along either the x, y , or z axis. For an oblate ellipsoid, $a = b > c$. For the orientation shown in figure 2(a), the field is applied in the direction of c , and thus the only relevant depolarization factor is A_3 .

$$A_3 = \int_0^\infty \frac{ds}{(s + a^2)(s + c^2)^{\frac{3}{2}}} = \frac{2}{(a^2 + c^2)^{\frac{3}{2}}} \left(\frac{\sqrt{a^2 - c^2}}{c} - \tan^{-1} \frac{\sqrt{a^2 - c^2}}{c} \right) .$$

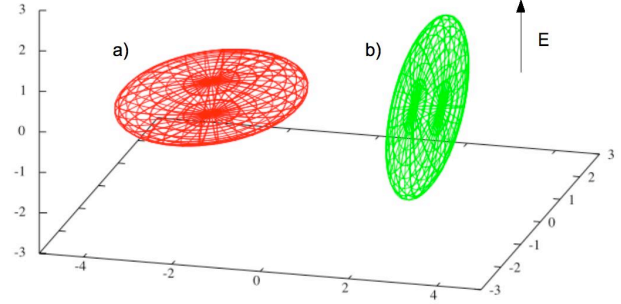


Figure 2: Oblate ellipsoids modeling single red blood cells.

In figure 2(b), the field is applied along the longer axis (radius = $a = b$), and so the only depolarization factor needed is A_1 , which can be calculated from

$$A_1 + A_2 + A_3 = \frac{2}{abc} ,$$

knowing $A_1 = A_2$.

In the case of a prolate ellipsoid (see figure 3), $a > b = c$ and the depolarization factors take a different form. The external electric field is applied along the major axis a , and so A_2 and A_3 are not needed. $\mathbf{E}^- \cdot \mathbf{E}_0$ depends only on A_1 , which is given by

$$A_1 = \int_0^\infty \frac{ds}{(s + b^2)(s + a^2)^{\frac{3}{2}}} = -\frac{1}{a^3 e^3} \left(2e - \ln \frac{1 + e}{1 - e} \right) , *$$

where

$$e = \sqrt{1 - \frac{b^2}{a^2}} .$$

*Note: We have corrected a sign error from Stratton in the equation for A_1 .

The only frequency dependence stems from ϵ_1 and ϵ_2 (and κ_1 and κ_2). These values we estimated from experimental data by A. Irimajiri et al. [9] for the blood plasma, which surrounds

the blood cells, and turbulent blood. We considered a frequency of 0.1 kHz, which corresponds to a permittivity of roughly 300 for the blood plasma and 3,000 for the turbulent blood. We chose the given frequency, because the permittivity inside the cells is significantly higher than in the surrounding plasma. This is important, for it increases the electric field intensity, and thus lowers the potential energy of the cell formations.

It is important to note, here, that we approximate the permittivity values inside a cell to be that of turbulent blood. Because the latter also includes blood plasma, which has a lower permittivity, the value we used is an underestimate for the true permittivity of the red blood cells themselves. This correction would lead to a larger energy value and thus lower the estimated field threshold.

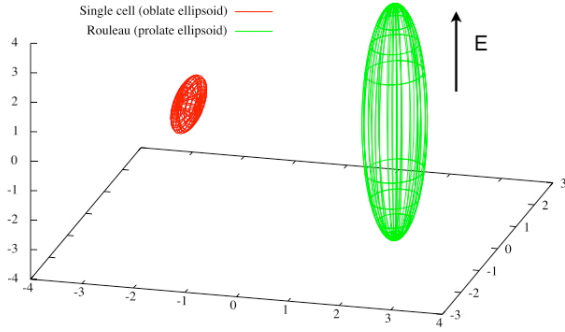


Figure 3: An oblate and a prolate ellipsoid, modeling a single cell and a rouleau of cells.

Results

We first calculated the energy of a single red blood cell in two different orientations with respect to an applied electric field. We found that the orientation pictured in figure 2(b) is of lower energy than that of 2(a), and is thus the favored orientation.

Next, we evaluated the above potential energy equation for two different formations. The first involved adding the energy of a rouleau of length $n - 1$ cells with one single cell in its minimum energy orientation. This was compared to the energy of a single rouleau of length n cells. In effect, we looked at the energy of keep-

ing a cell separate from the rouleau compared to adding that cell to the end of the rouleau chain.

In figure 4, the red bars mark the energy of a prolate ellipsoid of length $n - 1$ cells, which corresponds to $2(n - 1) \mu\text{m}$, plus that of a single oblate ellipsoid in its lower energy orientation. The green bars indicate the energy of a single rouleau of n cells, or $2n \mu\text{m}$. For up to five cells, it is unfavorable for the cells to chain together; however, for $n \geq 5$ the growing of the chain is favored. (In our model, 4 cells is a sphere.) As n increases, the difference between the green and red bars gets larger, and it becomes increasingly more favorable to extend the rouleau (and hence more costly to remove a cell).

Figure 5 demonstrates the difference between the energies shown in figure 4. The pairwise calculations performed previously [5] assumed a constant energy of extending a rouleau. Figure 5 shows that this assumption was false for $n < 50$, since the graph is not constant. In fact, the graph drops off quickly as $n \rightarrow 44$, indicating a significant margin of error in the pairwise calculations. Therefore, the field needed for rouleaux formation to occur is lower than earlier estimates.

Also, there is a minimum energy difference for a rouleau of around 44 cells. Beyond this value, it is still favorable for the cell to attach onto the rouleau; however, the favorability ceases to increase, and actually decreases very slightly to a constant value with each added cell.

To provide an estimate for the minimum electric field strength required for rouleaux formation to occur, we compared the energy difference to the thermal energy $k_B T$ at body temperature. As $n \rightarrow \infty$, the energy difference approaches the constant -807.9 . For fields as low as 96 V/m , the energy of extending a rouleau exceeds the thermal energy. This implies the contribution of the electric field to the thermal stability of the rouleau cannot be neglected at fields of this order of magnitude.

Discussion

Our first goal in this study was to determine how stable a long chain of red blood cells is compared to single cells dispersed

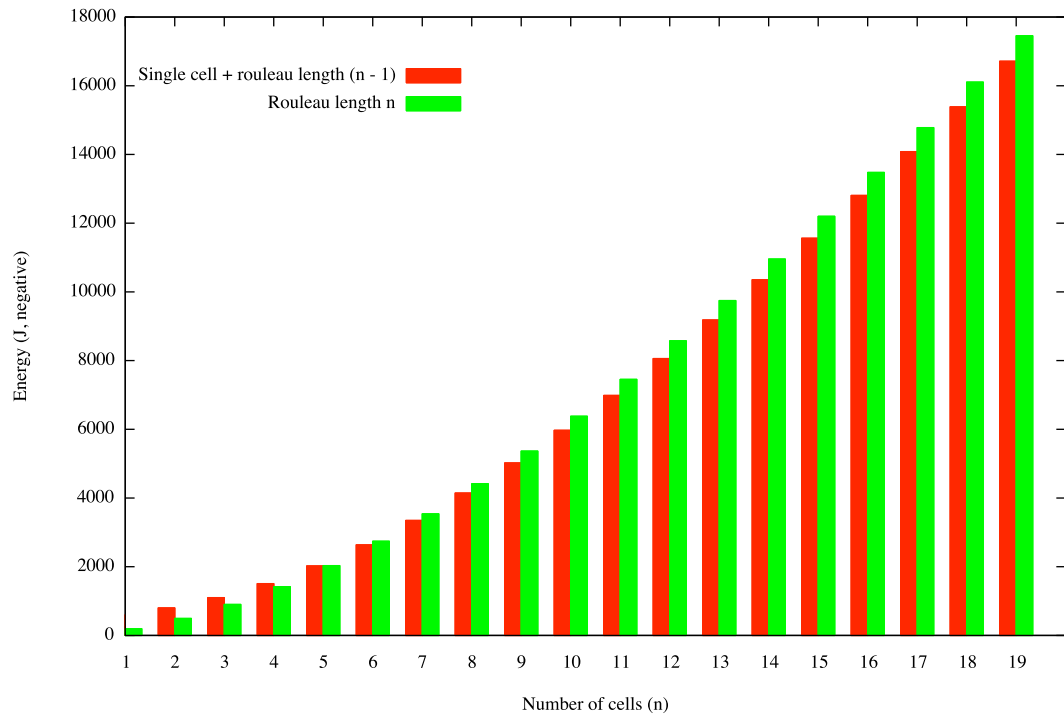


Figure 4: Comparing the energy of extending a rouleau by one cell (green) vs. keeping the cell separate (red).

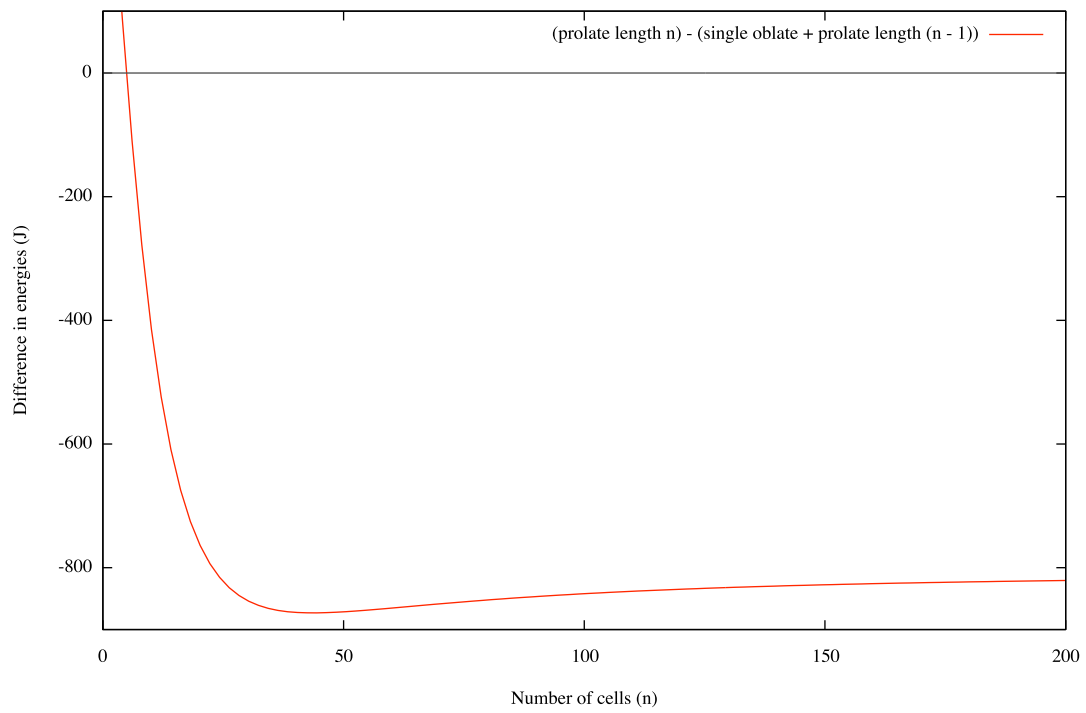


Figure 5: The difference in energy between adding the n th cell to a rouleau vs. keeping the n th cell separate.

throughout the plasma. We found that longer rouleaux become increasingly more energetically favorable, and thus the energy does not initially scale linearly as previously thought. The energy of stability increases faster than linearly for slightly prolate ellipsoids, because longer ellipsoids attract the electric field when $\epsilon_1 > \epsilon_2$. Experiments indicate $\epsilon_1 > \epsilon_2$ for blood cells in the frequency range of 30 kHz to 1 MHz. This range of frequencies is used by many switch mode power supplies, compact fluorescent lamps, and AM radio.

Additionally, from our results we were able to compare the potential energy of a rouleau with the thermal energy, and calculate the electric field threshold for forming rouleaux. The American National Standards Institute's current human safety threshold for electric field exposure for frequencies from 10 kHz to 1 MHz is 614 V/m [10]. This greatly exceeds the field needed to cause rouleaux formation, according to our model. This indicates that the current safety standards may be overlooking potential biological hazards. Future experiments should consider cases of high concentration of plasma proteins that can seed rouleaux formation in unhealthy humans, and determine effects on blood viscosity.

Acknowledgements

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Determining Optimal Cuts for 120 GeV $p+p$ Collisions at Fermilab e906 Experiment

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August 20, 2009

Abstract

The e906 experiment at Fermilab was simulated to determine optimal cuts and geometry. Products from $p+p$ 120 GeV events were produced by a Monte Carlo generator and run through the detector assembly. Drell-Yan events were also run exclusively to allow di-muon behavior in particular to be analyzed. Various opening angle cuts were run with 10000 events, and compared. This found that the di-muons energy distribution and spatial center was affected by opening angle cuts, but not overwhelmingly. The energy difference in the mean was found to be 7.26% for an angle cut of .5 and 1.23% for an angle cut of $\pi/2$. The spatial hit distribution mean center was shifted by 98.03 cm in the x direction for a .5 opening angle cut, and 90.4 cm for an opening angle cut of $\pi/2$: a significant change.

1 Introduction

The e906 experiment will collide protons at 120 GeV. The resulting particles can be used to determine properties of the proton. Specifically of interest is the Drell-Yan cross section, as this may be used to calculate the ratio of anti up to anti down virtual quarks. Previous experiments such as e866 have established that this flavor ratio is larger than 1/2 instead of being 1/2 as initially expected [1][3]. This ratio depends upon the momentum fraction: the fraction of the momentum carried by the virtual particles. The momentum fraction range over which this ratio is known will be significantly expanded by e906 [5]. The e906 experiment must balance hit rates with background ratios. Properties such as absorption medium, distance from impact point, and energy cuts all must be set to maximize useful information. The events of interest at e906 are Drell-Yan, which produce lepton pairs by annihilating a virtual quark in one proton with the virtual quark in the other proton. This produces a virtual proton which decays into a pair of leptons [1][2]. Specifically of interest to e906 are the di-muons produced by this process, because they are longer lived and more penetrating, and thus can be separated from the large number of other particles produced by the collisions. Detector station four is the last detector, which allows it to recognize the di-muons with reasonable certainty as other particles have been filtered out. Di-muon hits on the other detectors can thus be identified.

The particular cut that was investigated for this example was the opening angle. The beam is only partly filtered out by the target and beam stop, potentially causing the detector to be overwhelmed. Particularly of interest therefore are opening angle cuts because they can remove these unimportant particles and focus on the di-muons, but the effect of this cut on di-muon distribution needs to be determined.

2 Methods

Ultimately the largest effort was spent setting up the environment, and simulation package. The problems run into were many in number, both complex and mundane. Most of these issues are too in depth for this overview, and thus will not be included in this description. A separate technical note is planned to assist others with the e906 simulation and environment setup. Those issues will be detailed there. The simulation was installed and run on a Dell T3400 with four cores running Scientific Linux 5.3 and on an i686 architecture. The e906 simulation is based on Geant 4. Geant is a package intended for collider simulations. It combines physics process

libraries with detector geometry to create Monte-Carlo simulations of specified physics events. The process libraries come from multiple sources. For this program *Geant 4.9.2.p01* was used. Installing this version of Geant required the following tools and libraries. *CLHEP*, *cernlib*, *pythia6*, *GDML*, *xercesc*, *gcc* (with *gfortran* enabled) and running the simulation requires these additional tools and libraries: *openGL*, *root*, *G4EMLOW.6.2*, *G4ABLA.3.0*, *G4RadioactiveDecay.3.2*, *PhotonEvaporation.2.0*, *G4NDL3.12*.

2.1 GCC

Installing *cernlib* requires *gfortran*. The *gfortran* on GCC was used for this installation. GCC came pre-installed on the SL5.3 distribution used for this install. The current version of GCC as of this writing is 4.0.1, which requires *GLIBC 2.4*.

2.1.1 GLIBC

GLIBC 2.4 requires *mpfr-2.4.1* and *gmp-4.2.4*. MPFR is a multiple precision floating point operations c library. It is based on GMP, a multiple precision library. Theoretically *mpfr* and *gmp* can be installed along with *glibc* by simply extracting the libraries, and placing the contents of each in folders named *gmp* and *mpfr* in the *glibc* directory. This failed, however, on the SL4.3 being used originally for this install. Separately installing these libraries before *glibc* also did not work. As this seemed to be a problem with this Scientific Linux install, a scratch installation of SL5.3 was performed instead.

2.2 CLHEP

CLHEP, short for *A Class Library for High Energy Physics* provides C++ classes for various mathematical tools useful to high energy physics simulations.

2.3 cernlib

Cernlib has appropriate binaries for most installs of scientific linux. In this case the binary used was *i686-slc5-gcc41-opt* which comes as three files: *cernlib.tar.gz*, *cernbin.tar.gz*, *include.tar.gz*. Unpacking these produced the directory: *2006b*. This contains *686-slc5-gcc41-opt* and *include*. *i686-slc5-gcc41-opt* also contains *bin* and *lib*. A symlink named *pro* to the *686-slc5-gcc41-opt* was created in the Cernlib root directory. Symlinks named *lib*, *include*, and *bin* were likewise created to their respective folders

2.4 pythia6

Pythia simulates high energy physics events, primarily collisions. *Pythia 6.4*, the version used for this installation, is based upon Fortran 77 while the version soon to supplant it, 8.1 is based upon C++.

2.5 GDML

GDML stands for Geometry Description Markup Language. The experiment geometry is encoded in *GDML*. This allows for the position and material of the structure and of the detectors to realistically interact with the particles. *GDML* requires *xercesc*.

2.6 xercesc

Xerces-C++ is an XML parser that allows other applications to read and write in XML.

2.7 OpenGL

OpenGL is required for many of the visualization options *geant* allows. OpenGL was included with the SL5.3 distribution used.

2.8 Geant 4 installation

In the Geant4.9.2.p01 source directory the following was done to build geant:

```
./Configure -build
```

and then

```
./Configure
```

was used to create the env.sh and env.csh configure files. Environment variables for geant and the other packages were also set.

2.9 e906 compiling and running

The most recent version of the simulation used was GMC revision 217. The env.sh was run before the e906 simulation make. Also the e906 work directory was set using the G4WORKDIR environment variable. Various other environment variables such as GMCROOT for the source home, GMC_FLAT for flat root output, and E906_SHARE for geometry files and miscellaneous add ons, as well as adding \$GMCROOT/lib to the LD_LIBRARY_PATH. once the dictMakefile was run, and the libRunStructure.so found and added to .rootlogon as:

then:

```
make clean
```

and

```
make
```

to execute:

```
$G4WORKDIR/bin/Linux-g++/GMC
```

and finally ran events with:

```
/run/beamOn xxx
```

for xxx events.

2.10 ROOT

Root is a data analysis framework specifically designed for working with the large data sets typical of high energy physics. Analysis and visualization of e906 output was done primarily through root. Root uses X windows for displaying graphics produced, so the xterm config file was set to output to the display being used.

3 Results

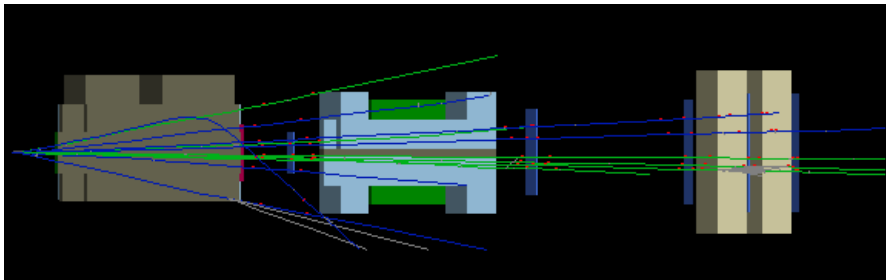


Figure 1: Ten di-muon events overhead view

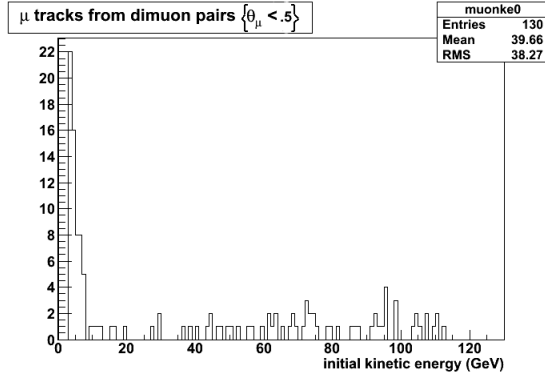


Figure 2: Opening angle less than $1/2$

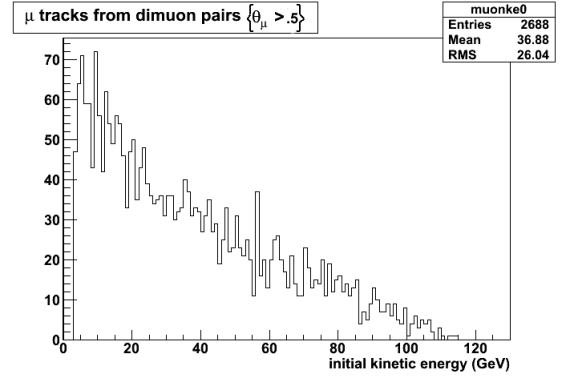


Figure 3: Opening angle greater than $1/2$

Compare to the energy distributions with $\theta_\pi > \frac{\pi}{2}$ or $\theta_\pi < \frac{\pi}{2}$:

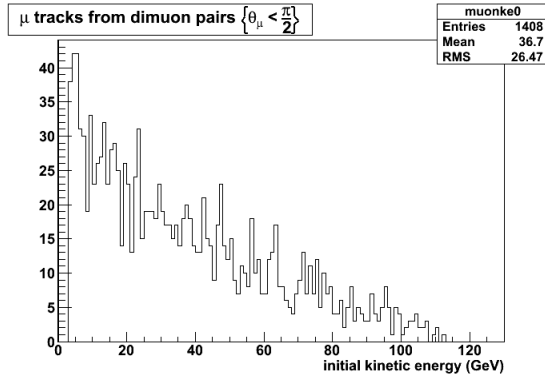


Figure 4: Opening angle less than $\pi/2$

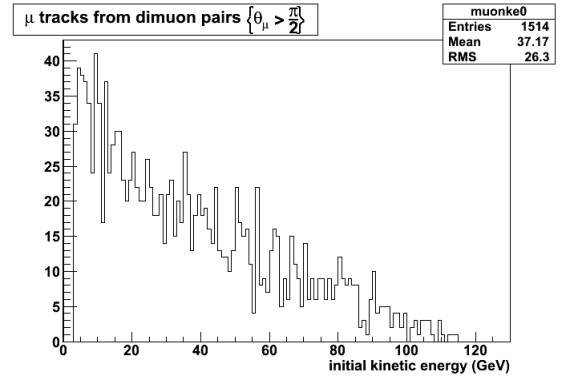


Figure 5: Opening angle greater than $\pi/2$

The density of tracks with opening angles less than $.5$ peaks strongly at the low energies, whereas the $\frac{\pi}{2}$ cut fairly evenly divides the tracks, with neither having significant difference over the energy scale. The mean for the $\theta_\pi < \frac{\pi}{2}$ cut is larger than the $\theta_\pi > \frac{\pi}{2}$ whereas the $\theta_\pi < .5$ is smaller than the $\theta_\pi > .5$. The difference in means of $.47$ for $\frac{\pi}{2}$ and -2.78 for the $.5$ cut. This means that the $.5$ angle cut changes the di-muon energy distribution by only $\frac{2 \times 2.78}{36.88 + 39.66} = 7.26\%$ difference for the opening angle cut of $.5$ and $\frac{2 \times .47}{36.88 + 39.66} = 1.23\%$ difference for an opening angle cut of $\pi/2$.

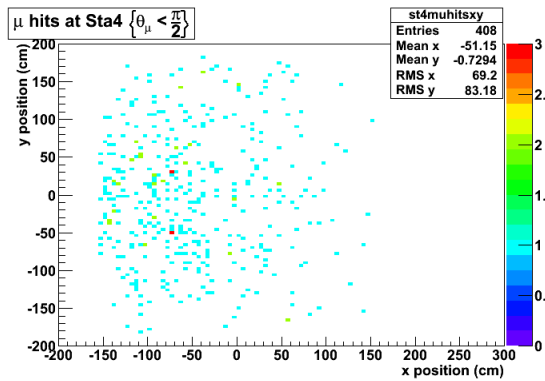


Figure 6: Opening angle less than $\pi/2$

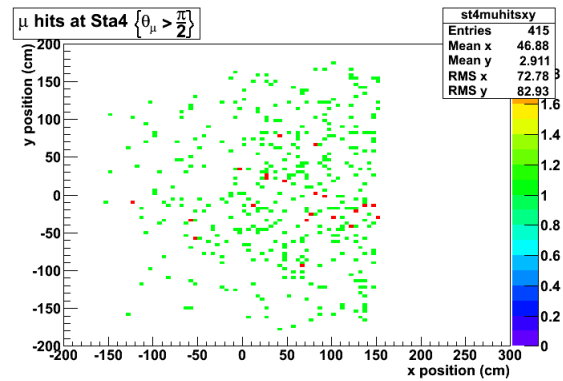


Figure 7: Opening angle greater than $\pi/2$

The difference in the x mean hit position is much greater than the y change. The x difference was a full 98.03 cm. This is a very large change on a detector only four meters across.

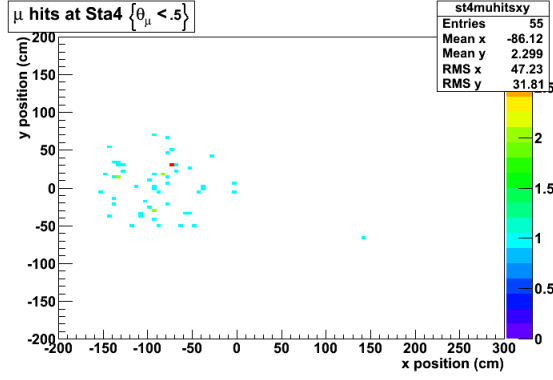


Figure 8: Opening angle less than .5

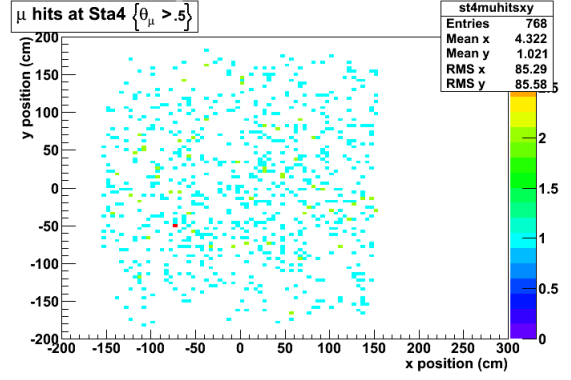


Figure 9: Opening angle greater than .5

The x mean hit position difference for an angle cut of .5 is 90.4 cm. The x position difference is thus concentrated on the lowest end of the angle distribution.

4 Conclusions

The e906 simulation can be used to calculate many useful parameters for planning the experiment. An opening angle cut does not appear to significantly bias the di-muon distribution. Specifically a cut of .5 changes the mean by approximately 2.78 - a 7.26% difference, while a cut of $\pi/2$ makes a 1.23% difference. More significantly the x mean hit position change for a cut of $\pi/2$ is 98.03 cm and for a cut of .5 is 90.4 cm. Future work includes determining σ_z : the distance between reconstructed impact point and the actual impact point. Multiple targets may be used in e906. The σ_z distribution is important to determining minimum distance between targets. Using multiple targets allows multiple experiments to be run simultaneously. Unfortunately the track reconstruction is imperfect and the source of a given event could be mistaken if targets are too close. This imperfection is what σ_z is measuring. Another important measurement that e906 will allow is the energy loss of quarks traveling through the nuclear medium. This is done by comparing Drell-Yan di-muons from proton impacts with targets of varying nuclear mass [2]. Thus multiple targets will allow the comparison of these different nucleons quickly. Other examples of information obtained from old e-series experiments that e906 may improve on are measuring the gluon distributions in the neutron and proton. The gluon distribution is identical in neutrons and protons to the limit of current measurements [4]. More work is needed, and is being undertaken to produce more simulation results, as well as understand the current results, and apply them to planning the e906 experiment.

5 Acknowledgments

Shon Watson for assistance in understanding the e906 simulation.
Zhengyun You for help installing Geant 4. 



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Correction of the Near Threshold Behavior of Collisional Excitation Cross-Sections in the Plane-Wave Born Approximation

Simone Brookes and David P. Kilcrease

Abstract

Plasmas that are not in thermal equilibrium are important in stellar atmospheres such as our Sun's and magnetic fusion reactors like the planned ITER device. The modeling of these plasmas requires the solution of population rate equations that employ many collision excitation, de-excitation, ionization, and recombination cross-sections. A simple and fast way to calculate these cross-sections is to use the high-energy Born approximation. Although easy and fast to calculate, the Born approximation for collisional excitation suffers from a serious flaw at low energy; it goes to zero. The more accurate but more time-consuming calculation using the Distorted Wave method does not have this problem and compares well with experiment. In this project, we will use a simple method to correct these Born cross-sections to have more accurate low energy behavior and compare the results with more accurate cross-sections. We will also compare our "fix" with other proposed methods to correct the low energy behavior of the cross-section to show that the data obtained using our fix is often in the closest agreement to those obtained using the Distorted Wave calculation.

Introduction

In striving for greater accuracy of excitation cross-sections at low energy, numerous modifications have been made to the Plane-Wave Born approximation. These modifications have been made to correct the inaccurate cross-section dimensions calculated using the original Born approximation at and near the threshold energy levels for given excitations and ionizations. The original Elwert modification to the Born approximation generated greatly improved results at low energies where both the Plane-Wave Born and Cowan-corrected Plane-Wave Born calculation methods were highly inaccurate.

However, the results obtained using the Elwert-corrected Plane-Wave Born calculations were less accurate than other methods at high energies; the original Elwert formula yields cross-sections that do not decrease rapidly enough to agree with Distorted Wave results at high energies. Thus, our modification to the Elwert correction was made in order that Elwert's formula decrease more rapidly as energy increases. We compared the two correction methods; the Cowan and Elwert corrections to the Born approximation; with the original Born approximation as well as with our Modified-Elwert correction. The effectiveness of each method of correction can be judged according to its agreement with the results of the Distorted Wave calculation for excitation cross-sections. For this project, we focused on the electron excitation cross-sections for four prominent solar elements: carbon, iron, nitrogen, and oxygen.

Methods

Our Modified-Elwert Correction:

$\sigma_{PWB}(E_i)$ is the Plane Wave Born cross-section for collisional excitation.
 $\sigma_C(E_i)$ is the corrected cross-section;

$$\sigma_C(E_i) = f(E_i)\sigma_{PWB}(E_i), \text{ and}$$

$$f(E_i) = \frac{\omega_f}{\omega_i} \cdot \frac{1 - e^{-\omega_i}}{1 - e^{-\omega_f}}, \text{ where}$$

$$\omega_{i,f} = \frac{2\pi Z_{i,f}}{k_{i,f} a_0}$$

and for collisional excitation we take $Z_i = Z_f = Z$. Energies are expressed in terms of Rydbergs; $\hbar = 1$, $2m = 1$, $\frac{e^2}{2} = 1$, and $a_0 = 1$, so that $E_f = E_i - \Delta\omega$ and $k_f^2 = k_i^2 - \Delta\omega$, where k is the free electron momentum, Z is the effective charge of the ion, and $\Delta\omega$ is the excitation energy for the collisional excitation. Then,

$$\begin{aligned} f(E_i) &= \frac{k_i}{k_f} \cdot \frac{1 - e^{-\frac{2\pi Z}{k_i}}}{1 - e^{-\frac{2\pi Z}{k_f}}} \\ &= \frac{\sqrt{E_i}}{\sqrt{E_i - \Delta\omega}} \cdot \frac{1 - e^{-\frac{2\pi Z}{\sqrt{E_i}}}}{1 - e^{-\frac{2\pi Z}{\sqrt{E_i - \Delta\omega}}}}. \end{aligned}$$

In terms of threshold units, $X = \frac{E}{\Delta\omega}$.

$$\text{Thus, } f(X) = \sqrt{\frac{X}{X-1}} \cdot \frac{1 - e^{-\frac{2\pi Z}{\sqrt{X\Delta\omega}}}}{1 - e^{-\frac{2\pi Z}{\sqrt{\Delta\omega(X-1)}}}}.$$

Near threshold, $X \rightarrow 1$, and $f(X) \approx \sqrt{\frac{X}{X-1}} \cdot (1 - e^{-\frac{2\pi Z}{\sqrt{X\Delta\omega}}})$.

$$\text{For large } X, \text{ however, } f(X) \approx \frac{1 - \frac{\pi Z}{\sqrt{\Delta\omega X}}}{1 - \frac{\pi Z}{\sqrt{\Delta\omega(X-1)}}} \approx 1 + \frac{\pi Z}{2X\sqrt{\Delta\omega X}}, \text{ where } \frac{\pi Z}{2X\sqrt{\Delta\omega X}} \ll 1.$$

Consider a function $Z'(X)$;

$$Z'(X) = \frac{Z}{X}.$$

At $X=1$ (the excitation energy threshold), $Z'(1) = Z$, while as $X \rightarrow \infty$ (high energy), $Z'(X \rightarrow \infty) \rightarrow 0$. So $f(X)$ now smoothly goes to one and the Plane-Wave Born approximation becomes more accurate. In addition, our Modified-Elwert-correction falls off faster to better agree with the Distorted Wave results at high energies.

Using, in order, the CATS, ACE and TAPS codes (from the Los Alamos National Laboratory's suite of atomic physics codes) we produced data which, we then plotted to display the area of excitation cross-sections versus the energy of the transition in threshold units. For each electron transition we examined, we produced data sets using the Plane-Wave Born, Cowan-corrected Plane-Wave Born, Elwert-corrected Plane-Wave Born, Modified-Elwert-corrected Plane-Wave Born, and Distorted Wave methods of calculation. Each of our graphs displays the data obtained using all five methods of calculation for a given excitation.

There are innumerable possible transitions to choose from, particularly when considering the number of possible excitation and ionization states in heavier stellar elements such as iron. We set distinct parameters in choosing which transitions we would examine in order to assemble and present a consistent body of results from which, we would be able to draw cogent conclusions. In the electron excitations we studied, the change in spin, Δs , we allowed was always zero and the allowed dipole moment, Δl , was always one. Again, for the sake of consistency and simplification, we collected data only for those transitions whose change in angular momentum, Δj , was either zero or one. Furthermore, in selecting transitions to include in our results we chose to present graphs showing excitations with a Δj value of one, exclusively.

Results

In all of the following excitation cases, the transitions shown have an allowed spin value of $\Delta s = 0$, an allowed dipole moment of $\Delta l = 1$, and a change in angular momentum of $\Delta j = 1$. Each graph shows a Cross-section vs. Energy plot for an electron excitation which, includes data obtained using the Cowan (PWB Cowan) and Elwert (PWB Elwert) corrections to the Plane-Wave Born approximation as well as our fix (PWB Elwert MOD), the original Born Approximation (PWB), and the Distorted Wave (DW) calculation methods. In all except the excitation of lithium-like oxygen (Figure 4.3) where our correction was no more effective than the other correction methods we used, the results of our Modified-Elwert-correction are the closest to the Distorted Wave results.

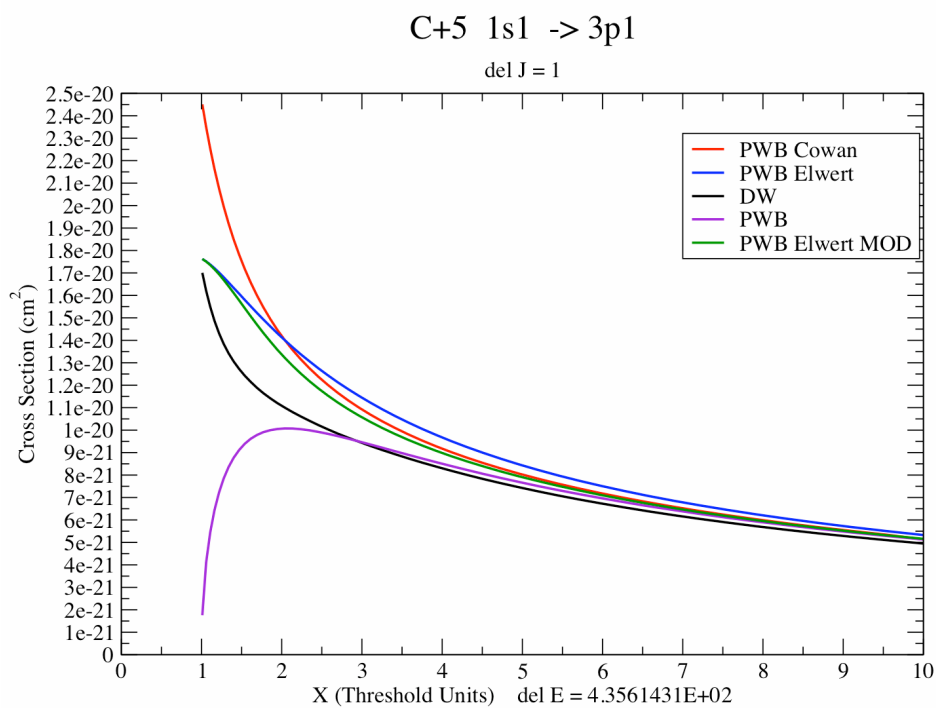
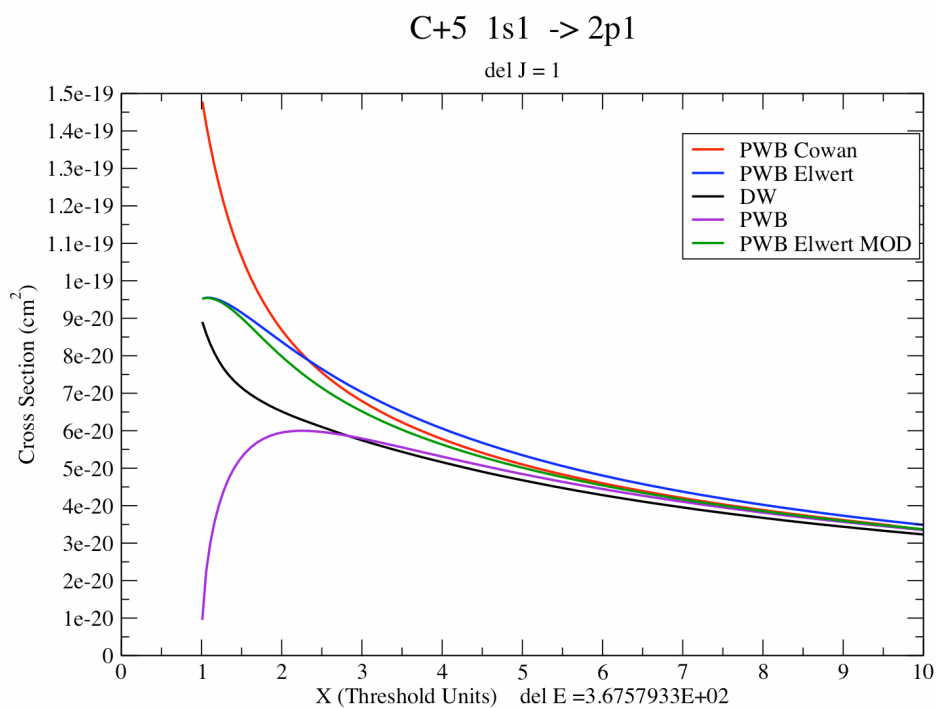


Figure 1.1-2: Hydrogen-like Carbon

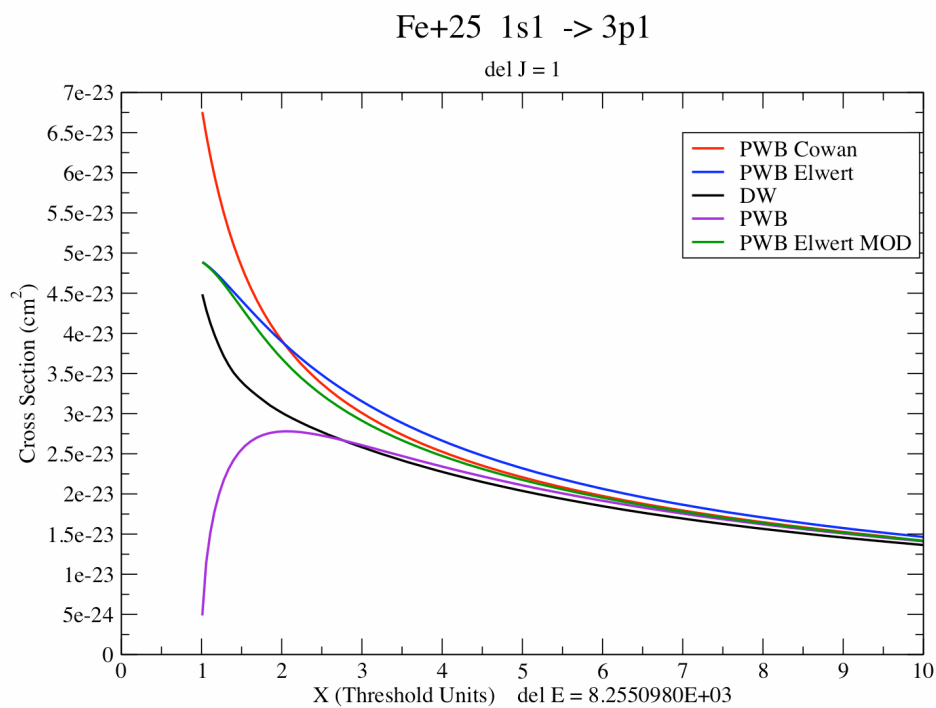
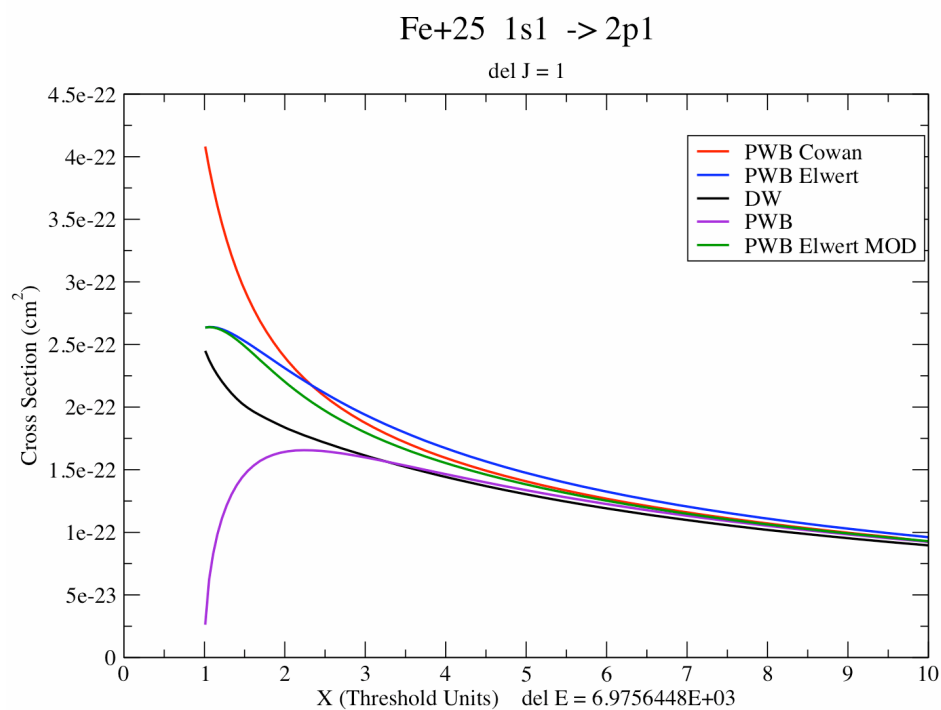


Figure 2.1-2: Hydrogen-like Iron

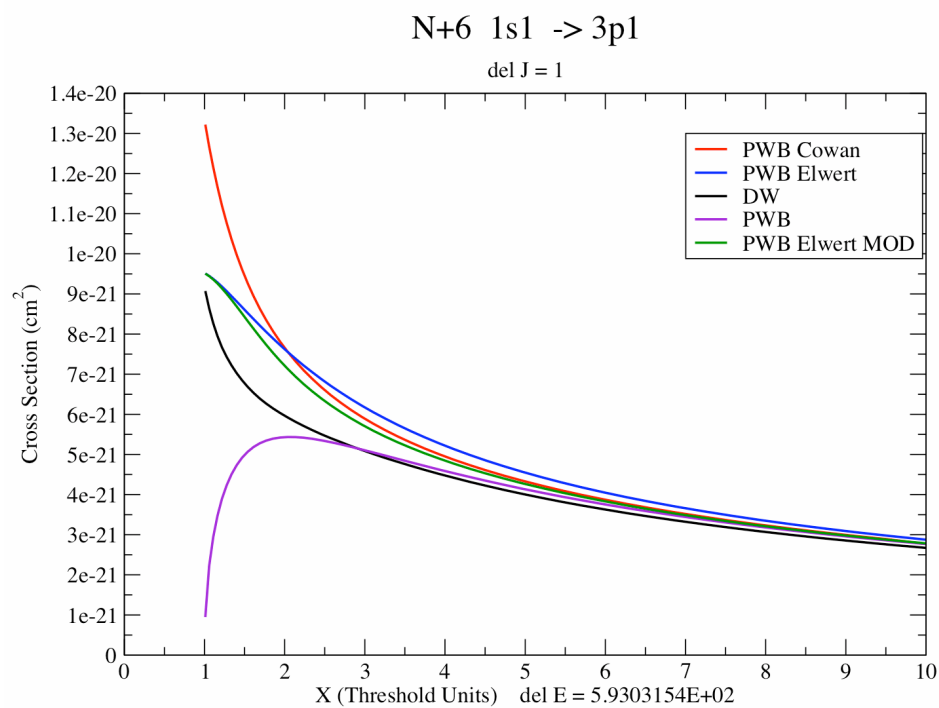
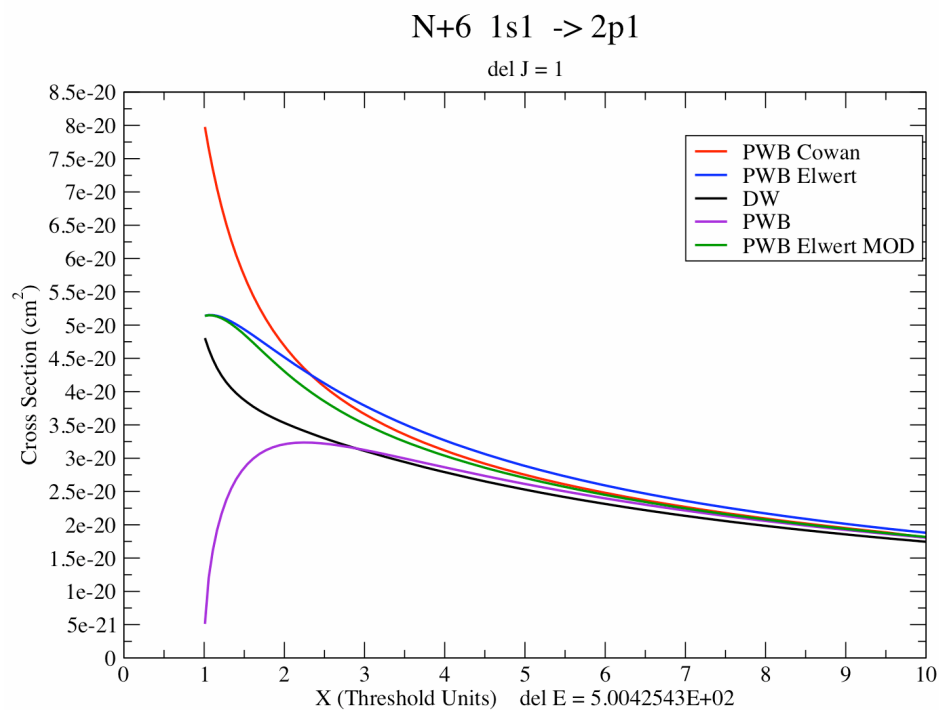
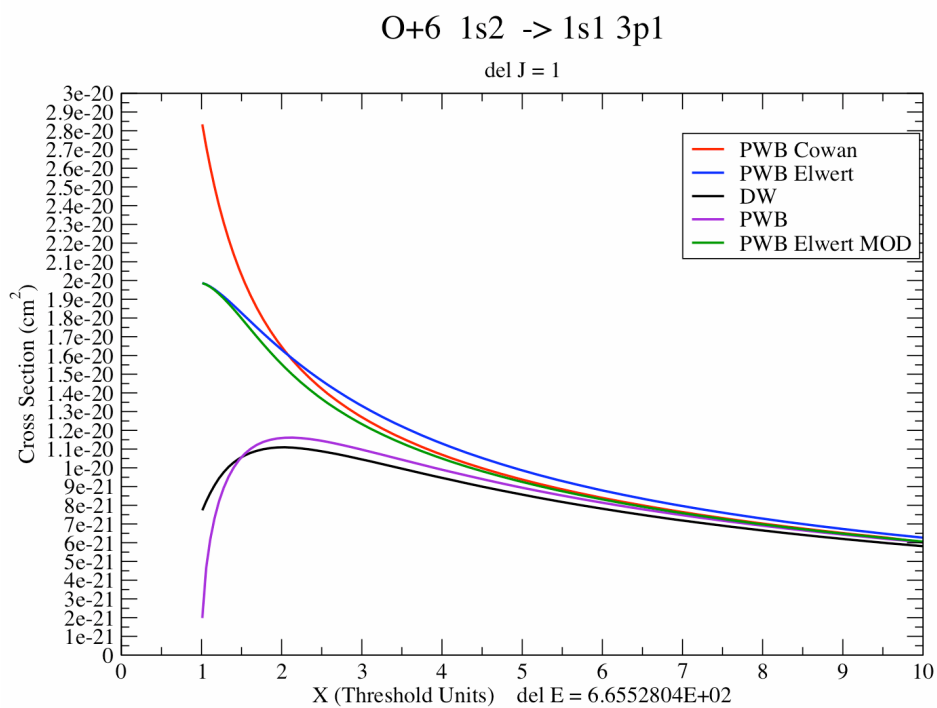
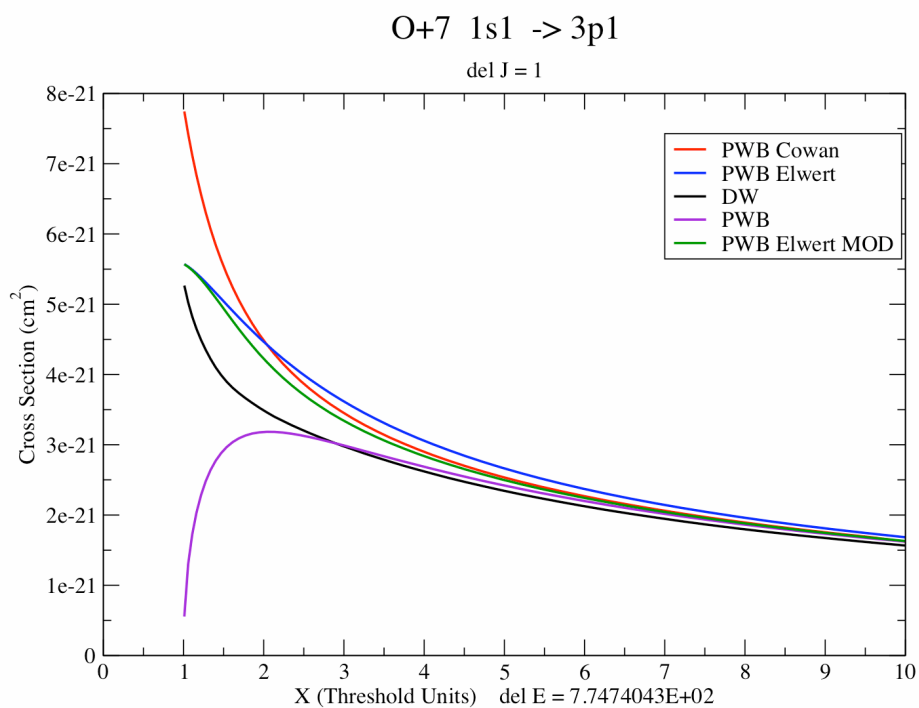


Figure 3.1-2: Hydrogen-like Nitrogen



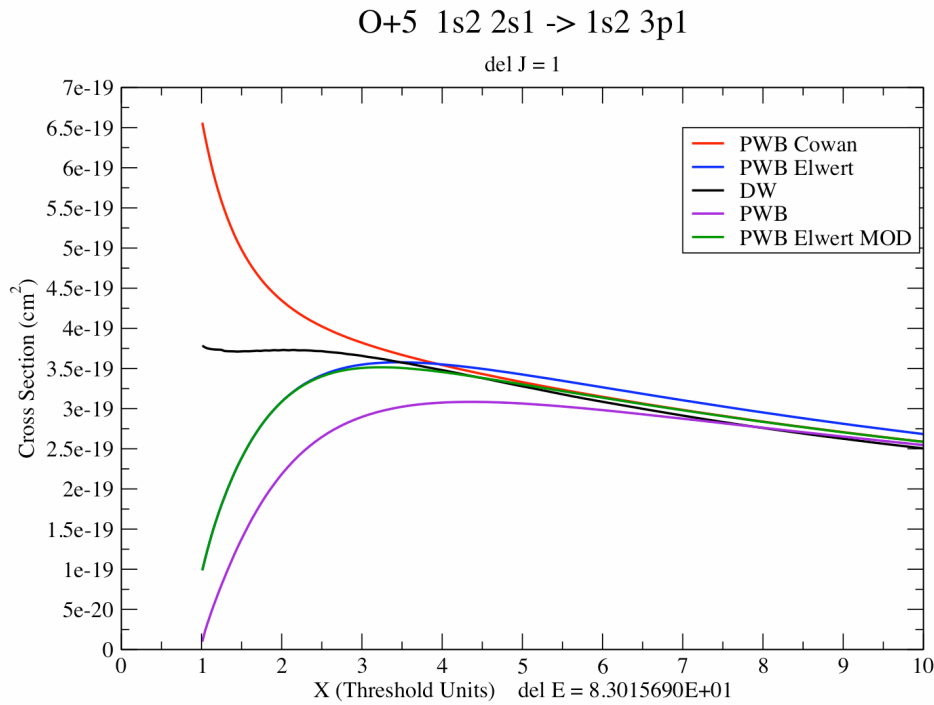


Figure 4.1-3: Hydrogen-like, Helium-like, and Lithium-like Oxygen

Conclusions

Our results demonstrate that the results of our "fix," the Modified-Elwert-corrected approximation, are the closest to the standard Distorted Wave approximation results at and near threshold energy levels in most of the electron excitations we examined. As such, we were able to improve upon the accuracy of Cowan's and Elwert's corrections to the Born approximation near threshold energies where better agreement with experiment was needed. Again, our Modified-Elwert-correction yielded the best results in most cases. In addition to its relevance to the study of non-equilibrium plasmas and the planning and operation of magnetic fusion reactors, calculation methods that result in more accurate projections of electron excitation and ionization cross-sections at lower energies would also be useful to the fields of astrophysics and atmospheric physics.

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Agent-based Analysis of Malware Propagation

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August 14, 2009

Abstract

The need for Internet security has increased alongside the Internet's usefulness as a tool for businesses, homeowners, and the government alike. Protecting its infrastructure and knowing its vulnerabilities is vital in the face of future malicious attacks. Being able to identify the weakest points in the networks will improve security and allow us to set well-informed priorities on security threats. In this study, we plan to model malware propagation using agent based simulation while taking into account the social and communal characteristics of the interaction networks. The main obstacles lay in determining what kinds of computers were vulnerable to what types of malware, which we resolved by gathering statistical data on the distribution of operating systems, software, and their CVEs (Common Vulnerabilities and Exposures). Also, the challenge of modeling a communications network of such large scale and complexity as the Internet was using addressed by using SimCore to build and simulate social networks, of the kind most often found in email networks, modeling attacks that are spread through phishing, attachments, or malicious links. Using this knowledge, we sought to develop software that could simulate virus attacks on large-scale communication networks.

1 Introduction

Our ultimate goal in this project is to develop a suite of software that can be used to realistically simulate cyber incidents in large scale communications networks. We will incorporate an accurate representation of the distribution of software in the United States by collecting statistical information on the market share of different types of software and populate 100 million end devices, mostly computers, using these statistics. Our simulation will incorporate a socially-based means of propagation, where malware is spread mostly through links and attachments sent through email networks.

2 Populate End Devices with Software

We collected statistical information as to the distribution of software around the country. Some software information is easily available, such as operating system or browser market share statistics from sites such as StatOwl or Fingerprint, who gather information from visitors to theirs' and others' websites. We also had to take into account the different distributions of software between users of different operating systems or browsers. For example, Internet Explorer is far more likely to be found on a Windows operating system than Safari, which is far more prevalent on Macs.

We then populated over 100 million end devices with software that reflected the market share statistics, while taking into account these dependencies. Because of the assumptions we made regarding the prevalence of programs depending on things such as the operating system, we compared the statistics we collected to the statistics of our simulated end devices. For example, in comparing email client market share data with our own distribution of email clients, we found that they closely agreed:

Email Client	Market Share	Simulation	Percent error
Yahoo! Mail	29.3	29.46	0.55
Outlook 2003	14.1	14.02	0.57
Outlook 2007	13.1	13.04	0.46
Hotmail	25.3	25.32	0.08
Apple Mail	4	3.96	1
Gmail	4	4.01	0.25
Comcast	3	3.05	1.67
AOL Mail	3	3.05	1.67
Thunderbird	2	2.05	2.5
Windows Live Mail	2	2.03	1.5

Figure 1: Home Computers

Email Client	Market Share	Simulation	Percent error
Outlook 2003	29.4	29.26	0.48
Outlook 2007	7.1	7.07	0.42
Hotmail	33.4	33.28	0.36
Yahoo! Mail	14.2	14.07	0.92
Gmail	6.1	6.02	1.31
Apple Mail	4.1	4.54	10.73
Windows Live Mail	3	2.99	0.33
Thunderbird	2.4	2.45	2.08
Lotus Notes	0.2	0.21	5
AOL Mail	0.1	0.09	10

Figure 2: Business Computers

2.1 Format of Statistical Distributions

Having collected software distribution information, we needed to put it in a format that could be easily read and changed if new or different information was discovered in the future. The format must also be able to reflect the inherent dependencies between different software. For example, the probability of an end device containing the OpenOffice office suite is different depending on the type of Operating System the end device has.

All information is stored in small text files. The files contain two columns, separated by tabs, with or without additional whitespace. The first column contains the names of the software or versions and the second column contains the probabilities, going from 0 to 100. A file named **OSys Possibilities** might contain the following contents:

Windows	89.1498544615076%
Mac	9.96687744655224%
Linux	0.873230954531768%
Other	0.0100371374084111%

All files are contained in one root directory, which is arbitrarily named **End-Device-Files/**. The root directory contains only subdirectories, which represent the different categories of software an end device can contain. The format of the category subdirectories is a number, followed by a dash, followed by the name of the category. For example, **2-OSys/** and **4-Plugin-m/**. The number indicates the order in which an end device should be populated with software, which is important when dealing with the dependencies and relationships between software. In this example, the operating system is more important because the types of plugins an end device has is very dependent on the type of operating system and should therefore be chosen first. The **-m** flag indicates that an end device can have multiple programs from this software category, and all probabilities will be interpreted as a chance of having having each program. For instance, a file named **Plugin Possibilities** might contain this:

Flash	94.87%
Java	79.62%
Windows Media Player	73.49%
Quicktime	61.57%
SilverLight	27.15%

In each of these subdirectories, there should be a text file that matches the name of category, like **Browser** or **OSys**. This file is used while populating an end device to choose software. When one is chosen, it searches in the same directory for a file that matches the name of the software, from which it picks an appropriate version. Within the **Browser** subdirectory, there might be files named **Browser probabilities**, **Firefox versions**, and **Firefox 1x**

versions. Depending on available information, there might be no version files at all.

Within each category subdirectory, there can be further subdirectories that indicate a dependency on other categories. The format for these directories should be the category name, followed by a colon, followed by the name of the software. For example, within **4-Plugin-m/**, there can be a directory called **System Type:Home/**, within which there might be a directory named **OSys:Mac/**. System Type is treated as a special type of category, which can only be Home or Business and is chosen by the user. When populating an end device, the script enters the applicable subdirectories, where there should be the files as described previously. If there are several applicable subdirectories, the one with the highest numbered priority is used.

2.2 EndDevice.pm

The EndDevice perl object provides an easy way to both generate new end devices and change the software associated with them. Both the input and output to EndDevice generally consists of a tab separated list on one line:

```
id [Home|Business] CategoryName:SoftwareName+VersionName
CategoryName:SoftwareName+VersionName |SoftwareName+VersionName ...
```

The methods of EndDevice are as follows:

- **setHome** - Should be used as a class method before creating any EndDevices to initialize the root directory as described in the previous section. Accepts one optional parameter, which should be the path to the directory. The default, set by the **\$home** variable, is **"/home/yparsons/End-Device-Files/"**. Returns void.
- **new** - Initializes a new EndDevice which will initially have no software. Accepts two optional parameters, the first of which is an id which is set to the **ID** variable. The second is the system type of the new EndDevice, and should be either "Home" or "Business". By default, the id is 100 and the system type is "Home". Returns a new EndDevice.
- **populate** - Populates the EndDevice with software, either randomly using the information in the directory described above, or with input in the format described above. Accepts one optional parameter, a tab separated list in the accepted format, and populates itself accordingly, including resetting the id and system type if necessary. If there is no parameter, it repopulates itself randomly, without resetting id or system type. Returns void.
- **setProgram** - Sets the software of a category according to parameters. Accepts 3 parameters, a category name, a program name, and an version name which may be an empty string. Resets the program and version associated with that category. Returns void.

- **addProgram** - Adds to the software of a category according to parameters. Accepts the same parameters as **setProgram**, only it is intended for categories which may have multiple programs installed.
- **clear** - Sets the programs and versions associated with a category to null. Accepts one parameter, a category name. Returns void.
- **pickANew** - Randomly picks new software for a category. Accepts one parameter, a category name. Clears the software of that category and picks a new one according to the information in the EndDevice's root directory. Caution should be exercised if, for instance, picking a new operating system because the probabilities of many other programs are dependent on it. Returns void.
- **getSoftware** - Returns the software associated with a category. Accepts one parameter, a category name. Returns a string of the software in the format described above. For example, `$foobar->getSoftware("OSys");` might return `"Windows+XP"`.
- **toString** - Returns a string describing the EndDevice, without an ending newline, in the accepted format. Accepts no parameters.

2.3 cyber-sim.pl

This script is the main software generator script. It generates a list of files which contain new end devices, and which are named **end-device-programs.prefix**. This script is run with 3 parameters. The first parameter should be a path to a FIPS file, which contains a list of ids for the new devices, and the second should be the path to a directory to place the new files. The third is optional, and is the EndDevice home directory described in the EndDevice section. The script might be run as follows:

```
[yparsons@minicow perl]\$ ./cyber-sim.pl FIPS.code ~/new-end-device/ ~/End-Device-Files/}
```

The FIPS file is a multi columned, tab-separated text file that describes the ids and system types that are to be used. For example:

"State"	"Prefix Code"	"Res Start"	"Res End"	"Co Start"	"Co End"
"AK "	"02 Alaska"				
"AL "	"01 Alabama"	100000000000	10001057628	10001057629	10001823033
"AR "	"05 Arkansas"	500000000000	50000554313	50000554314	50001003186

The first line is assumed to contain headers, and is thrown away. All extra columns, quotes and whitespace beyond the tabs are also ignored. The first column is the prefix which will be used as the extension to the finished file. The second column is ignored and is for the user's use. The next four columns are the beginning and ending ids for the Home and Business end devices respectively. If a line does not have any ids, as in the Alaskan line, it is ignored.

2.4 goThroughFiles.pl

If new information is discovered or something else needs to be changed about the end device files, then goThroughFiles is a template that can be used for this purpose. The script accepts one parameter, a directory which contains the files that need to be changed. When the script is run, for each file, the user is asked whether or not the file should be changed and is allowed to view the new file before the new changes are finalized. The user can change specific sections of the code to set up criteria for which files are to be changed and what is to be changed.

When changing a file, the original file is read in through the filehandle FILE and must be printed out through the filehandle NEWFILE. What is done in between can be changed depending on the situation. If new information was found concerning the distribution of office suites, and the user knew that these changes would only affect Linux machines, then this section could be rewritten as:

```
#####  
### make your changes to the file. print changes to NEWFILE #  
    while (<FILE>){  
        my $line = $_;  
        my $temp = EndDevice->new();  
  
        if (/Linux/){  
            $temp->populate($line);  
            $temp->pickANew(" Office Suite");  
            print NEWFILE $temp->toString()."\n";  
        }else{  
            print NEWFILE $line;  
        }  
    }  
#####
```

3 Extract Vulnerable End Devices Based on National Vulnerability Database

There are classes of software whose vulnerabilities are most often exploited by cyber attacks, such as browsers, e-mail clients, or the operating system itself. In order to accurately simulate the prorogation of a specific kind of malware throughout a network, we needed to be able to determine which computers are vulnerable. Lists of CVEs (Common Vulnerabilities and Exposures) were collected from the National Vulnerability Database. With this information, we could predict which and how many computers would become infected if a certain vulnerability was exploited. For example, malware that exploits a vulnerability in Linux will not be as widespread or as crippling to a network as malware

that attacks Windows. Linux comprises only about 1% of the market share, compared to Windows which has close to 90%.

3.1 CPE format

Common Platform Enumeration is a standard format used in CVEs by the National Vulnerability database to name software. It consists of a colon-separated list of descriptors for the software, from most to least importance:

cpe:/part:vendor:product:version:update:edition:language

part may be either **h**, **o**, or **a** to indicate hardware, operating system, or application. Other descriptors can be left blank if there is not enough information or if it is not applicable. All names are generally left in lower case. The leading **cpe:** is also generally left out because it is always present.

3.2 CPEMap.txt

This file contains a list of equivalences, in the form of two tab-separated columns, between the standard CPE format and the format that is used by EndDevice and other scripts. It may partially look like this:

Linux+SUSE	o:suse:suse_linux
Linux+Ubuntu Dapper	o:ubuntu:ubuntu_linux:6.06
Linux+Ubuntu Edgy	o:ubuntu:ubuntu_linux:6.10
Outlook+2007	a:microsoft:outlook:2007
Quicktime	a:apple:quicktime

Because there may be multiple ways to express one piece of software, multiple CPE formatted names may map to one of our names and vice versa. Future additions may simply added. This is used primarily by **read-cve3.pl**, which is described in a later section.

3.3 CVE.pm

The CVE object provides a container to hold information about different CVEs. By default it has only two variables, an ID and an array of **SOFTWARE**, containing a list of software that is affected by this vulnerability. Further variables may be added by the user. For example, if the user needs to keep track of the access level of a vulnerability, they may simply add this by saying '**\$cveobject->ACCESS = "NETWORK";**'.

The methods of CVE are as follows:

- **new** - Initializes a new CVE object with an ID and an empty array of software. Accept one parameter, an id. Returns a new CVE object.

- **addSoftware** - Adds a new vulnerable program to the software list. Accepts one parameter, a software name. Return void.
- **toString** - Returns a string with the contents of the object in an XML format. Accepts no parameters. All software will be tagged **SW** and all variables will be tagged with their variable name. One CVE may look like this:

```
<CVE=2008-1001>
    <SW>a:apple:safari:3.0.4</SW>
    <SW>a:apple:safari:3.0.3</SW>
    <SW>a:apple:safari:3.0.2</SW>
    <SW>a:apple:safari:3.0.1</SW>
    <SW>a:apple:safari:3.0</SW>
    <ACCESS>NETWORK</ACCESS>
    <AUTHENTICATION>NONE</AUTHENTICATION>
    <AVAILABILITY>NONE</AVAILABILITY>
    <COMPLEXITY>MEDIUM</COMPLEXITY>
    <CONFIDENTIALITY>NONE</CONFIDENTIALITY>
    <INTEGRITY>PARTIAL</INTEGRITY>
    <SCORE>4.3</SCORE>
</CVE>
```

3.4 read-cve3.pl

This script is an interactive program that accepts a CVE id and returns a list of affected end devices from a given file. The script accepts two parameters, the path of a file containing a list of CVEs and a path to a file containing a list of end devices. It also requires the CPEMap.txt file that was described earlier to be in the same file, and it uses the default root directory for the EndDevice objects.

```
[yparsons@minicow perl]\$ ./read-cve3.pl ~/perl/CVE.txt ~/end-device/end-device-programs.AL
```

When finished loading, the user is prompted to enter a CVE id, and will then display a list of software that is affected by that vulnerability, in both CPE format and in our format. The user is then prompted whether or not to save a list of ids that are affected. If the user responds yes, the script then searches through the file with the list of end devices for ids that contain that software. It then saves the list to a file named **CVE-*id*.txt**.

4 Future Work: Simulate Virus Propagation on Vulnerable End Devices

We are at this point implementing a method for simulating the propagation of malware through social networks, such as email. Malware such as this can spread

when someone clicks on a malicious link or downloads an infected attachment. An infected machine can then try to continue spreading the worm by emailing all other computers it knows about, such as through an address book. We will be using SimCore, a simulation engine, to follow the spread of a virus throughout the country and track its propagating speed. This will allow us to predict what kinds of response times will be needed for different viruses and how they will impact the structure of the Internet.

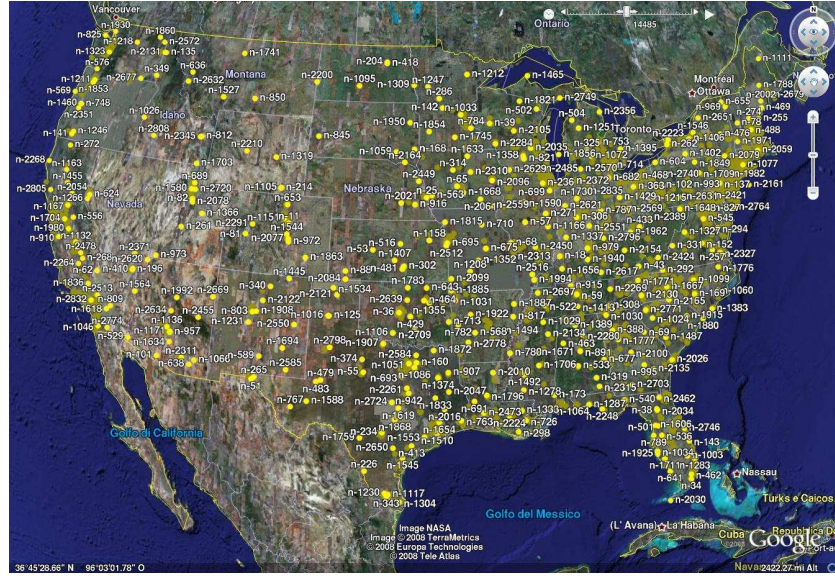


Figure 3: A snapshot of a prototype simulation, 3 hours and 21 minutes into the spread of a CodeRed-type worm.

5 Acknowledgements

I would like to thank my mentor, Hristo Djidjev, and Guanhua Yan for helping me and making my summer at Los Alamos such a wonderful experience. I would also like to thank my day-to-day heads of the Los Alamos Summer School, Norm Magee and Jame Colgan, who so willingly made sure we were comfortably sheltered and who patiently put up with needing to herd us like cats.

I would also like to thank the Los Alamos bus drivers, who are are very kind and who deserve some additional respect to the amount they already have.

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To Trap or Not to Trap? Electron behavior on elastic nanowires

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When do electrons on nanowires trap themselves – interact with the wire in such a way that they become localized? Electrons that are not self-trapped have wave functions substantially larger than the size of the cells on a nanotube (e.g. carbon), so in this case the discrete structure of the wire—that it is made up of cells—may be neglected. However, when an electron becomes self-trapped, its wave function is on the same order as the size of these cells, and so a model of the wire reflective of its discrete structure must be employed. The first model is known as the long polaron approximation, and the second as the atomistic approximation. However, there is scant data as to when each approximation is actually valid. In this work we determine for which parameter regimes the electron’s wave function undergoes finite-time collapse (i.e. the electron becomes localized), and thus when it is necessary to employ an atomistic approximation as opposed to a long polaron one. To model the system, we use equations similar in form to the non-linear Schrödinger equation and which incorporate coupling between the elastic field of the wire and the electron’s wave function. In some cases, analytical solution is possible, but in general it is not and numerical integration is used to solve.

PACS numbers: 61.46.-w, 65.80.+n, 68.35.Rh, 68.55.ag

INTRODUCTION

Nanotechnology, defined as manipulation of matter on the atomic or molecular scale [1], has been a subject of much contemporary interest. It has a wide variety of applications, from water purification to ultra-portable computing [2]. On the nanometer scale, quantum interactions become important to understanding the behavior of many possible nano-devices. In this work, we study the behavior of an electron on a nanowire by considering the elastic field of the wire as coupled to the electron’s wave function. We employ a Lagrangian deduced from considerations of the wire’s symmetry to find a set of coupled non-linear partial differential equations describing the time-evolution of the elastic field of the wire and the wave function of the electron. Because these equations are non-linear, and indeed the equation for the wave function is similar in form to the non-linear Schrödinger equation (NLSE), we suspect that for certain regions of parameter space and in certain dimensions finite-time collapse will occur [3]. This is a well-known phenomenon in the case of the non-linear Schrödinger equation, for which it occurs only in dimension 2 or higher and only for certain values of the potential term in the NLSE. Sulem and Sulem provide a detailed treatment [4], and Roberts and Newell derive, for N coupled NLSEs, a general set of conditions for which finite-time collapse occurs [5].

Finite-time collapse is defined formally as the case where the variance of the wave function goes to zero in finite time. It is important to note that the phrase finite-time is neither redundant nor superfluous: one might imagine a situation in which the variance tends to zero as time tends to infinity, but that this limit is never reached

(formally, that the infimum of the variance as a function of time is zero but that the set of all variances associated with the given wave function is not closed). Heuristically, finite-time collapse can be considered to mean that the particle represented by a given wave function has become localized. Should this happen, the scale of the wave function will be the same as that of the cells making up the nanowire, implying that an atomistic model of the nanowire—one that takes into account its honeycomb-like structure—must be employed. In contrast, if the electron’s wave function does not undergo finite-time collapse, the nanowire can be treated as a smooth strip with no finer structure, and the electron and its surrounding charge distribution as a long polaron (see Klinger [6] for a discussion of polarons and Nisoli for discussion of this approach [7]). We determine for which values of certain parameters, described below, finite-time collapse will occur, and therefore in which cases the atomistic or the long polaron viewpoint is appropriate. We treat here the case of a two dimensional wire, where the electron is considered to travel along the surface of the wire.

THE MODEL

i. Lagrangian and Equations of Motion

A nanowire has symmetry with respect to rotation about its long axis and also about an axis drawn perpendicularly through this axis. Using the most general form for the elastic energy that satisfies these constraints, we deduce the Lagrangian, with ψ as the electron’s wave function and $\mathbf{u} = (u_x, u_y) = \sum_k u_k \hat{k}$, $k = x, y$ as the

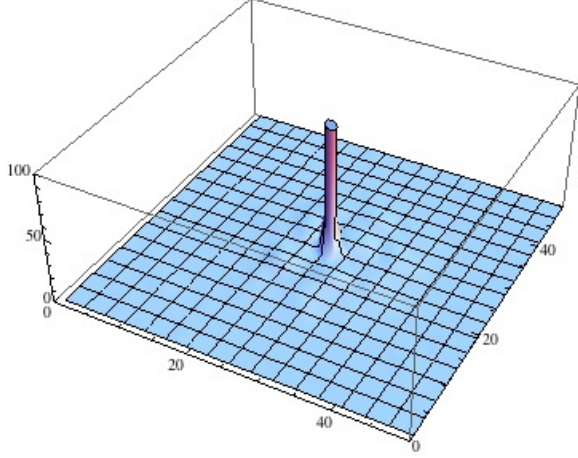


FIG. 1: A collapsed wave function $-|\psi|^2$ is on the z axis and the wire has been unrolled into the xy plane.

elastic field,

$$\mathcal{L} = -i\hbar\psi^*\frac{\partial\psi}{\partial t} + \frac{\sigma}{2}\dot{u}_i^2 - \frac{1}{2}\nabla u \mathbf{A} \nabla u + \frac{\hbar^2}{2m}\psi^*\Delta\psi - g_{ij}\nabla^{ij}u|\psi|^2. \quad (1)$$

For an isotropic medium, which our nanowire is assumed to be, $\mathbf{A}$ reduces to an appropriately symmetric tensor and $g_{ij}\nabla^{ij}$ becomes $\delta_{ij}g_{ij}$. g represents the coupling between the electron and the elastic field of the wire, and it is the primary parameter of interest for us,

as we expect that some values of g will result in finite-time collapse. Further, for an isotropic wire the equations of motion can be expressed in terms of Lamé symbols related to the physical properties of the material – their values are related by $K = \lambda + \frac{2}{3}\mu$, where K is the bulk modulus [8]. σ is the surface mass density of the wire. Varying with respect to ψ^* and $\mathbf{u}$ yields the equations for the time evolution of the system (2), (3):

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + g[\nabla \bullet \mathbf{u}]\psi \quad (2)$$

$$\sigma\ddot{u}_k = (\mu + \lambda)\nabla_k[\nabla \bullet \mathbf{u}] + \mu\Delta u_k + g\nabla_k|\psi|^2. \quad (3)$$

Notice that, if $g = 0$, our equation for u_k reduces to that for vibrations in an isotropic medium, as is physically reasonable considering that $g = 0$ implies no coupling between the electron and the wire. For comparison, we provide the nonlinear Schrödinger equation – χ is a parameter determining the strength of the focusing (negative χ) or defocusing (positive χ) potential:

$$i\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \chi|\psi|^2\psi. \quad (4)$$

In our problem, the potential proportional to $|\psi|^2$ in the NLSE (4) is simply replaced by a potential proportional to the strain tensor $\nabla \bullet \mathbf{u}$, and time is rescaled by $\hbar$. Thus, in our problem, g plays a role similar to that of χ in the NLSE. This will be of importance for how we study possible values of g . In one dimension, soliton solutions of the form

$$\psi(x, t) = \left(\frac{\zeta}{2}\right)^{\frac{1}{2}} \text{sech}(x\zeta) \exp[i(kx - \omega t)], \quad (5)$$

$$\text{with } \zeta = \frac{1}{2} \frac{m\lambda^2}{\sigma(v_s^2 - v^2)\hbar^2}, \quad (6)$$

$$v_s = \left(\frac{2\mu + \lambda}{\sigma}\right)^{\frac{1}{2}}, \quad (7)$$

where v_s is the longitudinal speed of sound in the wire, v is the soliton velocity, and λ and σ are the Lamé symbols, are possible, but in higher dimensions no analytical solutions exist, though Brizhik et al. [9] provide such solutions for slightly different forms of the coupling. We therefore use numerical methods to solve for the time evolution of arbitrary initial wave functions; at time zero the elastic field is uniformly zero because this corresponds to an initially unperturbed wire. Since we consider arbitrary initial wave functions, any situation in which the wire is initially perturbed and a given wave function exists on it will also be covered by this approach because at some later point in the time evolution of a different wave function with no initial deformation in the wire this set of conditions will be obtained. This argument may only hold if the evolutions through phase space of ψ and the elastic field are sufficiently ergodic, however – or, put another way, if the perturbed initial conditions we want to duplicate at a later time are not too pathological.

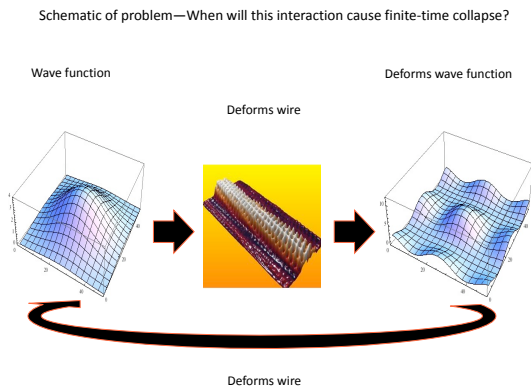


FIG. 2: Outline of the setup we study

ii. The Method

i. General Remarks

To solve, we discretize space by imposing a uniform mesh with boxes of width dx , and discretize time by advancing our solution by a small but finite time step dt . To solve the equation for ψ , we employ the symmetrized split-step Fourier method, described in more detail below (ii.). We assume that the elastic field remains constant and equal to its value at t_n over each time step from t_n to $t_n + dt$. This is a reasonable assumption because the minimum time in which the elastic field can respond to the wave function scales with $\tau_{Ch.} = \frac{dx}{v_s}$, where v_s is the speed of sound in the wire. Indeed, as long as the time step is smaller than this characteristic time, there will be negligible error introduced due to this approach. To solve the equation for the elastic field at each time step, we employ a simple explicit finite-differencing scheme, where we rewrite the equation for the elastic field as a difference equation (see (iii.)). Since this equation is second order in time, this approach results in error of order dt^3 , which is comparable to the error of the split-step Fourier method [10], [11]. Other methods might have been employed, but their disadvantages relative to the differencing we use will be discussed in (vi.) [12]. In this differencing, we consider the spatial derivatives of ψ to be constant and equal to their values at t_n for each time step from t_n to $t_n + dt$. In contrast to the approximation that the elastic field is constant over each time step, it is not so clear here that this approximation will not introduce significant error. Why it does not will be detailed in (iv.). For an overall picture of the solution method, see Fig. 3.

ii. The Symmetrized Split-Step Fourier Method

The wave equation for the electron can be written as

$$\frac{\partial \psi}{\partial t} = [\hat{D} + \hat{N}]\psi, \text{ with } \hat{D} = \frac{i\hbar}{2m}\Delta \text{ and } \hat{N} = -\frac{ig}{\hbar}[\nabla \bullet \mathbf{u}].$$

Formally, the solution is then obtained by re-arranging differentials and integrating, yielding

$$\psi(\mathbf{x}, t) = \exp[(\hat{D} + \hat{N})t]\psi(\mathbf{x}, 0). \quad (8)$$

Writing this in a form that admits of approximate numerical evaluation, we have

$$\psi(\mathbf{x}, t_0 + dt) = \exp[(\hat{D} + \hat{N})dt]\psi(\mathbf{x}, t_0). \quad (9)$$

Using the Baker-Hausdorff formula, we can write

$$\begin{aligned} \exp[\hat{D}]\exp[\hat{N}] &= \exp\left(\hat{D} + \hat{N} + \frac{1}{2}[\hat{D}, \hat{N}] \right. \\ &\quad \left. + \frac{1}{12}[\hat{D} - \hat{N}, [\hat{D}, \hat{N}]] + \dots\right), \end{aligned} \quad (10)$$

Schematic of Overall Solution Method

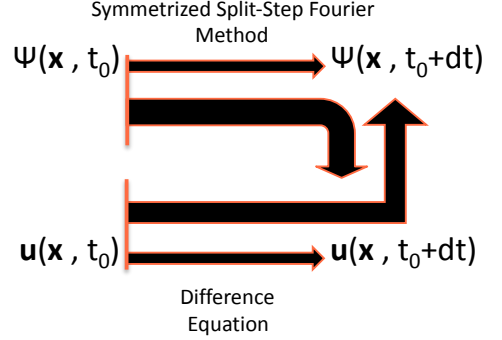


FIG. 3: See text for details on each part of solution method—horizontal arrows represent advancing in time, bent arrows represent dependencies of each solution on the other at an earlier time.

where $[\hat{D}, \hat{N}]$ denotes the commutator $\hat{D}\hat{N} - \hat{N}\hat{D}$. Thus, if we write

$$\psi(\mathbf{x}, t_0 + dt) = \exp[dt\hat{D}]\exp[dt\hat{N}]\psi(\mathbf{x}, t_0), \quad (11)$$

by comparison with (10), the error will be of order $\exp(\frac{dt^2}{2}[\hat{D}, \hat{N}])$. We now rewrite the previous approximate solution as

$$\psi(\mathbf{x}, t_0 + dt) = \exp[\frac{dt}{2}\hat{N}]\exp[dt\hat{D}]\exp[\frac{dt}{2}\hat{N}]\psi(\mathbf{x}, t_0) \quad (12)$$

and apply the Baker-Hausdorff formula twice to show that the error becomes of order $\exp(\frac{dt^3}{8}[\hat{D}, [\hat{N}, \hat{D}]])$. To compute the rightmost term in (12) above, we use

$$\begin{aligned} \exp[dt\hat{D}]\exp[\frac{dt}{2}\hat{N}]\psi(\mathbf{x}, t_0) &= \\ F^{-1}\{\exp[dt\hat{D}(ik)]F\{\exp[\frac{dt}{2}\hat{N}]\psi(\mathbf{x}, t_0)\}\}, \end{aligned} \quad (13)$$

where F and F^{-1} denote a Fourier and an inverse Fourier transform respectively. $\hat{D}(ik)$ is the expression for the diffusion term of the original wave equation with the differential operator itself replaced by ik , where k is the wave number associated with a given spatial point's Fourier transform (see **APPENDIX**).

Heuristically, this method takes a half time step using only the non-linearity, takes a Fourier transform of the

result, then turns on diffusion in frequency space (and goes a full time step with just diffusion), inverse Fourier transforms back to real space, and then takes a second half time step again using only the non-linearity. The method is symplectic, because complex exponentials are modulus-preserving, as are Fourier and inverse Fourier transforms by Parseval's theorem. This property renders it particularly appropriate for solving a quantum mechanical wave equation, as the solutions ought to have time-invariant norm. Conservation of the Hamiltonian is also tracked as a means of monitoring the accuracy of the numerical integration. We owe the symmetrization we employ to Tzeremes et al. [13], and the ideas for the proof above to Agrawal [10] and Banerjee [14].

iii. Finite-differencing the Elastic Field Equation

To simplify matters, we will show the differencing for one component of the elastic field, u_x . The equation for one component u_x of the elastic tensor $\mathbf{u}$ is

$$\sigma \ddot{u}_x = (\mu + \lambda) \partial_x [\partial_x u_x + \partial_y u_y] + \mu (\partial_{xx} u_x + \partial_{yy} u_x) + g \partial_x |\psi|^2, \quad (14)$$

Schematic of Symmetrized Split-Step Fourier Method

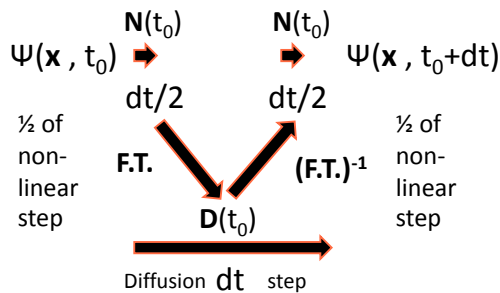


FIG. 4: Horizontal arrows mean advancing in time, diagonal arrows mean changing to frequency space and back. See text for definition of operators $N \equiv \hat{N}$ and $D \equiv \hat{D}$.

which written as a difference equation, defining $\alpha = \frac{\mu + \lambda}{\sigma}$ and $\beta = \frac{\mu}{\sigma}$, becomes

$$\frac{u_{x,j}^{n+1} + 2u_{x,j}^n - u_{x,j}^{n-1}}{dt^2} = \alpha \left[\frac{u_{x,j+1}^n + 2u_{x,j}^n - u_{x,j-1}^n}{dx^2} + \partial_x (\partial_y u_y) \right] + \beta \left(\frac{u_{x,j+1}^n + 2u_{x,j}^n - u_{x,j-1}^n}{dx^2} + \frac{u_{x,k+1}^n + 2u_{x,k}^n - u_{x,k-1}^n}{dy^2} \right) + \frac{g}{\sigma} \frac{|\psi|_{j+1}^2 - |\psi|_{j-1}^2}{2dx}. \quad (15)$$

$u_{x,j}^n$ indicates u_x at location (x_j, y_k) , $j = 1, 2, \dots, \frac{\text{wire length}}{dx} + 1$, $k = 1, 2, \dots, \frac{\text{wire circumference}}{dx} + 1$, time t_n , $n = 0, 1, \dots, \frac{t}{dt}$. $u_{x,k}^n$ indicates u_x at location (x_j, y_k) , with indices as above. The same conventions are employed for ψ . The 2nd term on the right hand side, which involves the mixed partial $\partial_x \partial_y u_y$, is differenced below in (16) for greater legibility, as well as because it is the only non-trivial term to difference. We compute the difference iteratively, first differencing $\partial_y u_y$ and then differencing this difference with respect to x .

$$\partial_x \partial_y u_y = \frac{(u_{y,k+1} - u_{y,k-1})|_{j+1} - (u_{y,k+1} - u_{y,k-1})|_{j-1}}{4dx^2} \quad (16)$$

To compute, we solve for u_j^{n+1} as a function of all of the other terms. A von Neumann stability analysis of this equation, assuming that all of the eigenmodes of the difference equation are of the form $u_{j,k}^n = \xi^n \exp[i(k_x j + k_y k)dx]$ and bounding the error due to the term proportional to ψ as $\frac{g}{\sigma} \frac{dt^2}{2dx}$ and thus negligible for $dt \ll dx$, yields

$$\xi = 2 \frac{dt^2}{dx^2} [\alpha (1 + i \sin(k_x dx) - \sin(k_x dx) \sin(k_y dx)) + \beta (i (\sin(k_x dx) + \sin(k_y dx)) + 2)] - 2 + \xi^{-1}. \quad (17)$$

We have by the triangle inequality that

$$|\xi| \leq (6\alpha + 8\beta) \frac{dt^2}{dx^2} + 2 + \left| \frac{1}{\xi} \right|. \quad (18)$$

Our concern is to show that $|\xi| \leq 1$, so we assume $|\xi| > 1$. In this case, $|\xi| - \frac{1}{|\xi|} > 0$, so we must simply show that when equality holds $|\xi| \leq 1$, which would contradict the assumption $|\xi| > 1$ and so show $|\xi| \leq 1$. When the equality in (18) holds, there are two possible values of $|\xi|$:

$$|\xi| = 1 + \frac{ML}{2} \pm (8 + 4ML + (ML)^2)^{\frac{1}{2}}, \quad M = 6\alpha + 8\beta, \quad L = \frac{dt^2}{dx^2}. \quad (19)$$

If the smaller value of $|\xi|$ is taken, it is possible to find L such that $|\xi| \leq 1$, but if the larger value is adopted, we have no contradiction. Unfortunately this seems to be the best that can be done with this stability analysis. See Press et al. [15] for discussion of finite differencing and von Neumann stability analysis.

iv. Proof error from taking ψ constant is small

As noted earlier, we assume ψ is constant as we advance $\mathbf{u}$ from time t_n to time t_{n+1} . It can be seen from taking a Taylor series centered at t_n for $\frac{\partial|\psi|^2}{\partial x_i}$ and writing a further Taylor series for the elastic field centered at t_n that the error from this assumption will be of order dt^3 . To leading order, we have, with $x_1 = x$ and $x_2 = y$,

$$\frac{\partial|\psi|^2}{\partial x_i} \approx \left(\frac{\partial|\psi|^2}{\partial x_i}\right)|_{t_n} + \left(\frac{\partial}{\partial t}\frac{\partial|\psi|^2}{\partial x_i}\right)|_{t_n}\Delta t \quad (20)$$

and to second order

$$\mathbf{u}(t_n + dt) \approx \mathbf{u}(t_n) + \dot{\mathbf{u}}(t_n)\Delta t + \frac{1}{2}\ddot{\mathbf{u}}(t_n)\Delta t^2. \quad (21)$$

Writing a further Taylor series for $\dot{\mathbf{u}}(t_n)$, we have

$$\dot{\mathbf{u}}(t_n) = \dot{\mathbf{u}}(t_{n-1}) + \ddot{\mathbf{u}}(t_{n-1})\Delta t. \quad (22)$$

Combining (20) and (21), it is evident that the error in $\mathbf{u}$ from $\ddot{\mathbf{u}}$ is of order Δt^3 , and combining (22), (21), and (20), the error in $\mathbf{u}$ from $\dot{\mathbf{u}}$ is of order Δt^3 as well.

v. Error due to Spatial Discretization

Since the equation for the elastic field involves $\frac{\partial|\psi|^2}{\partial x_i}$, the error of this equation due to spatial discretization will be of order dx^2 . The error in the equation for ψ due to this discretization will be of order dx^3 . Thus, the error due to spatial discretization will affect the evolution of the elastic field $\mathbf{u}$ more significantly than it will affect that of the wave function ψ . This problem can be mitigated in the following manner. To determine how fine to make the spatial mesh, we compute the value of the Hamiltonian as a function of successively increasing numbers of mesh points until it has converged to within some specified tolerance – i.e. the percentage difference between $H(n)$ and $H(n + \Delta n)$ is less than for instance 5%. Plots of $H(n)$ (Fig. 5) show that the Hamiltonian does have an asymptote as the number of mesh points $n \rightarrow \infty$, so it is justified to hope that increasing the number of mesh points will take us closer to the true value of H , and likewise to the true values of the other quantities of interest.

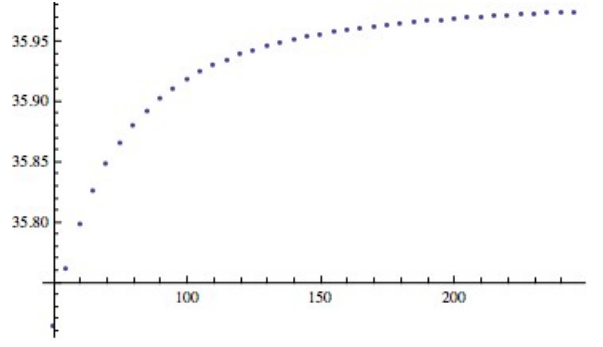


FIG. 5: The Hamiltonian plotted as a function of the number of boxes n in the mesh – note the asymptote as n grows.

vi. Disadvantages of Other Methods of Solution for Elastic Field Equation

There are several options available when confronted with a system of PDE's such as we solve in this work. The first is to find a formal solution for the coupled system in the form of a matrix mapping the system at time t to the system at time $t + dt$. One then finds a unitary transformation that diagonalizes this matrix, a transformation which always exists for small enough values of dt . Diagonalizing this matrix shows that the formal solution for the time evolution of the system is a matrix exponential. Thus, if the system of equations is written

$$\frac{d\mathbf{Y}}{dt} = \mathbf{G}\mathbf{Y}, \quad (23)$$

where $\mathbf{Y}$ is the state of the system at time t , the solution is

$$\mathbf{Y}(t + dt) = \exp[\mathbf{G}dt]\mathbf{Y}(t). \quad (24)$$

However, this method is disadvantageous because it may not be easily practicable to compute the necessary matrix exponential. A second option is to, along the same lines we have done, assume that ψ is constant while $\mathbf{u}$ evolves and visa versa, but to seek a formal solution for $\mathbf{u}$ as well as using the formal solution for ψ detailed in (ii.). This method may be effective, but the possibility of implementing it computationally depends strongly on the form of the formal solution for $\mathbf{u}$. The accuracy of this method also strongly depends on the specific form of this solution. For these reasons, then, we have avoided these methods of solution and instead used the explicit differencing for $\mathbf{u}$ detailed in (iii.).

RESULTS

i. NLSE

To test the accuracy of our integrator, we spent much time studying the non-linear Schrödinger equation, and

in so doing we obtained a surprising result we describe here. According to Roberts and Newell [5], in 2-d, if the Hamiltonian (and/or the variance) satisfies one of the below, then finite-time collapse will occur.

$$I. \ H < 0 \quad (25)$$

$$II. \ H = 0 \text{ and } V'(0) < 0 \quad (26)$$

$$III. \ H > 0 \text{ and } V'(0) < -4(HV(0))^{\frac{1}{2}}. \quad (27)$$

However, in our numerical work we determined that collapse occurs for $\chi = -12$, with a Hamiltonian of 1.33308. But it is clear from a plot of the variances of x and y that $V'(0)$ is non-negative, so it cannot satisfy condition *III*. Thus Roberts' and Newell's result evidently does not cover all possible cases where collapse occurs for the NLSE with periodic boundary conditions in x and y , which is what we have studied. It should further be noted that analytically, the possible region of values of χ for which collapse can occur is qualitatively different for $H = 0$ and $H \neq 0$. The upper plot is of the value of χ yielding collapse as a function of the standard deviation of the Gaussian which we set as the initial wave function, based on fixing the Hamiltonian as 1.33308, the value mentioned above at which we found the transition from collapse to non-collapse takes place. The lower plot is assuming this critical value of the Hamiltonian is zero, which given (27) appears not to be an upper bound. But it is the appropriate upper bound for systems in which the variance does not satisfy (26) or (27), which Fig. 7 gives us reason to suspect may be the case. With this in mind, then, it might be suggested that the region of collapse that can be predicted (at least using Roberts' and Newell's results) differs significantly in shape from the numerically obtained one. This might be because of the periodic boundary conditions we use, as Roberts and Newell prove the result only for wave functions that go to zero at positive and negative infinity. However, it seems that the only place their proof relies on this fact is in setting boundary terms in an integration by parts to zero, and with periodic boundary conditions it is easily observed that the same thing may be done, so their proof should generalize to the case we study. Therefore there must be some other reason we observe a larger region of collapse than can be proven to exist from an analytical standpoint.

ii. Electron-Wire Coupling

Unfortunately, due to the limited time available to us, we have not as of this writing obtained conclusive results determining the value of g for which finite-time collapse takes place in the system we study. However, a bit can be said analytically which provides fruitful seeds for future numerical studies we intend to make. While as we said earlier, g in our problem is similar to χ in the NLSE, the

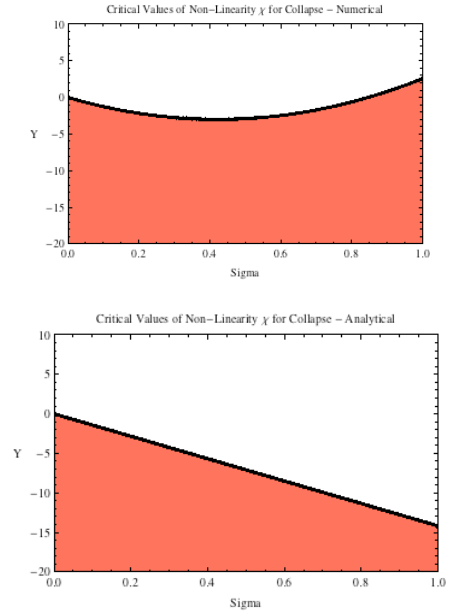


FIG. 6: Plots of results for study of NLSE—shaded area is region for which finite-time collapse occurs for a Gaussian with standard deviation σ ; $Y = \chi$ is as defined in (4). The equation governing the critical value of χ is $\chi_C = 4\pi H_C \sigma^2 - 8\pi^{\frac{1}{2}} \sigma$.

exact analog of χ in the NLSE is the quantity

$$\lambda' = \frac{g^2}{\sigma(v^2 - v_L^2)}, \quad (28)$$

where $v_L = v_s$ is the longitudinal speed of sound in the wire as before. With this equation in hand, there are two regimes to be studied. First, we set $v = 0$ and let the properties of the material determine v_L (recall it is given by $v_L^2 = \frac{2\mu+\lambda}{\sigma}$). We then look for g_C such that collapse occurs, and then compare the λ' corresponding to this g_C to the value of χ determined for the NLSE. We then look at the case where the velocity of the solution is non-zero, and fix g at g_C for which collapse took place when $v = 0$. We gradually scale up the velocity until the wave function goes from collapse to non-collapse—the physical intuition here is that by making v larger we are increasing the kinetic energy, and so making localization harder. But on the other hand, as $v \rightarrow v_L$, $\lambda' \rightarrow -\infty$, which corresponds to a more negative χ in the NLSE and therefore an increased chance of collapse. This is, in light of the physical intuition we would have had as above, a surprising result. Interpreted using the example of the Gaussian, though, it makes sense. Recalling the equation from Fig. 6, $\chi_C = 4\pi H_C \sigma^2 - 8\pi^{\frac{1}{2}} \sigma$, we note that as σ increases, so does χ , and of course as σ increases v must be decreasing. So as v decreases, the non-linearity

becomes more positive, meaning collapse is less likely, and therefore that in fact it seems that for $g = g_C$, all $v > 0$ will result in collapse. So we expect that all we need determine is the value of g_C for which collapse occurs with $v = 0$.

DISCUSSION

In this paper, we determined the value of χ , the factor multiplying the non-linearity, for which the NLSE transitions from non-collapse to collapse. We hoped to determine also the value of the coupling constant for which this transition occurs in the electron-wire system, but we have not yet been successful in so doing. This is our primary and next objective. We did, however, make analytical observations which will substantially simplify this calculation, as well as developing a coupled PDE solver which should allow us to achieve this objective in short order. We further observed that the region of collapse that can be proven analytically for the NLSE is noticeably smaller than the region numerically obtained, and observed that this cannot be because of the periodic boundary conditions we study as Roberts' and Newell's proof does generalize to this case. Finally, we showed that the solution method we intend to use to solve the coupled problem has error of second order or higher in both space and time, though we were unable to prove that it is unequivocally stable for some combination of dt and dx . Future

work will be directed towards establishing this, and in the longer term towards solving the coupled problem in 3 dimensions - i.e. the electron will be allowed to have any position on or within the nanowire. Finally, an additional direction of our future work will be to prove analytically when collapse will happen in this system, as well as possibly to develop an expansion of arbitrary initial wave functions in terms of eigenfunctions of the coupled system, at least where such eigenfunctions are available - they are known in 1-d, but unknown and possibly nonexistent in higher dimensions. ZS gratefully acknowledges Los Alamos Physics Summer School for financial support and Avadh Saxena for vehicular support.

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APPENDIX

Machine Implementation of the Split-Step Fourier Method

We use FFTW (Fastest Fourier Transform in the West) routines to compute the discrete Fourier transform of the appropriate term in (13). We must also recover the values of k associated with the Fourier transform it com-

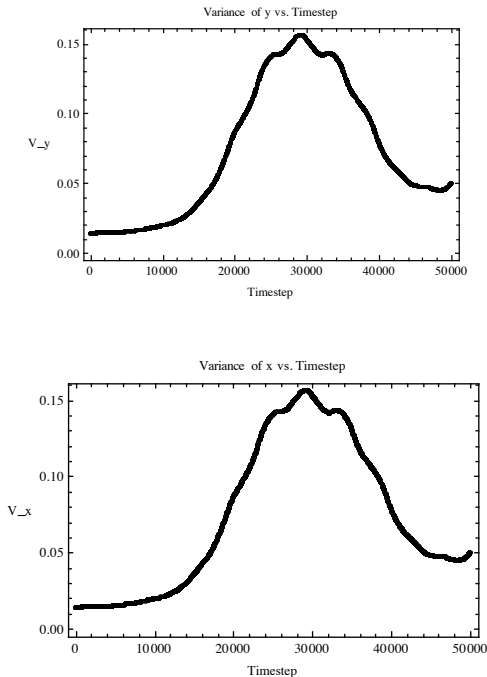


FIG. 7: Plots showing that $V'_x(0), V'_y(0) > 0$.

puts so we can take the diffusion step (recall that we replace $\frac{\partial}{\partial x}$ by ik). Recalling that the term being transformed was discretely sampled in space, with spacing dx , the Nyquist critical frequency (above and below which aliasing will take place – i.e. frequencies greater in absolute value will have their energy content folded over to frequencies that are less than the Nyquist critical frequency in absolute value) is given by $f_c = \frac{1}{2dx}$. Since we are transforming from position-space to frequency-space, it is logical that the position-space discretization implies a frequency-space discretization. We thus let the discretized frequency range from negative to positive the Nyquist frequency with uniform scaling. Thus $dk = \frac{1}{N \times dx}$ and $k_n = \frac{n}{N \times dx}$, $n = -\frac{N}{2}, \dots, \frac{N}{2}$, where N is the number of points in the mesh. Note that there are actually $n + 1$ frequencies here; it turns out that $k_{-\frac{N}{2}} = k_{\frac{N}{2}}$.

The discrete Fourier transform F_n of the appropriate term in (13) f_m is then given by

$$F_n = \sum_{m=0}^{N-1} f_m \exp\left[\frac{2\pi im}{N}\right]. \quad (29)$$

The exponential inside the summation is evidently periodic with period N , because adding N to its argument adds a factor of 2π which is equivalent to multiplying by

unity. Thus one can let m vary from zero to $N - 1$ as is done in (29) above. With this convention positive values of k have indices from unity to $\frac{N}{2} - 1$, $k = 0$ has index 0, and negative values of k have indices from $\frac{N}{2} + 1$ to $N - 1$. This amounts to adding N to all of the negative indices. Because FFTW employs this convention, it stores the transforms associated with the positive frequencies in the first half of the output and the transform values associated with the negative frequencies in backwards order in the second half. To associate the frequencies to the proper mesh points, we simply subtract $\frac{N}{2}$ from all of the frequencies with index greater than $\frac{N}{2}$. Note that we actually want to reorder the frequencies associated with the transform values rather than reordering the transform values themselves, because when we do the inverse Fourier transform next it will reverse things again and leave us with the term from (13) in the original order of discretization. To put the wave function into the code, we write it in row-major order: this is a specific way of creating a one-to-one mapping between a multi-dimensional space and a one-dimensional space which is presumably called row-major order because in a 2-D matrix, it is equivalent to reading along each row left to right. The reason to do this is that FFTW converts whatever input it receives into row-major order in any case, so it is more efficient to give it the input in this form in the first place.

Modeling Angiogenic Response to Tissue Dynamics

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Abstract

Angiogenesis, or new blood vessel growth, is critical to many debilitating ailments, including cardiovascular disease, macular degeneration and cancer. In the early stages of angiogenesis, vascular endothelial growth factor (VEGF) guides the development of new vascular sprouts by regulating vessel constituents – the endothelial cells. VEGF is a vital protein emitted by hypoxic tumors to induce angiogenic sprouting and obtain a blood supply. To explore new cancer therapies aimed at impeding tumor-induced angiogenesis, a 2D VEGF cell-based model with a collagen extracellular matrix is used. This model employs a Monte Carlo energy reduction algorithm to capture cellular and extracellular matrix interactions, including cell adhesion, migration, growth, and death. Using cell density and sprout length as metrics, simulations of sprout development using this spatio-temporal model are in close agreement with a recently conducted experiment showing vascular sprouting under different extracellular matrix concentrations.

Introduction

Angiogenesis is the process by which a new blood vessel sprouts from existing vasculature. Since tumors can induce angiogenesis, it is important to fully understand the mechanism by which this process occurs. A tumor, particularly when it becomes hypoxic, will secrete vascular endothelial growth factor (VEGF). VEGF is one of the most vital growth factors for the process of angiogenesis to occur. When the existing vasculature is stimulated by VEGF, it sprouts and

grows towards the tumor. Once a new vessel reaches the tumor, the vessel supplies oxygen and other nutrients to the tumor and enables further tumor growth. In order to develop novel cancer therapies, especially less harmful therapies, it is essential to understand the cellular processes involved in angiogenic sprouting.

The interior lining of blood vessels is composed of endothelial cells. These cells have surface receptors that enable them to receive signals from various biochemical agents, particularly those that stimulate growth and motility.^{1,3}

The extracellular matrix (ECM) is a component of the extravascular tissue region, or stroma. It is a molecular network mostly composed of fibrous collagen proteins.¹ The physical properties of the ECM, including density, heterogeneity, and stiffness all affect cell behavior. *In vitro* experiments of endothelial cells on collagen gels have shown that as density increases, so does matrix stiffness, which causes slower cell migration speeds. These results have been confirmed through simulations. Moreover, experiments demonstrate that directional sprouting, called branching, is induced by matrix tension. Endothelial cells attach to the ECM by way of $\beta 1$ integrin receptors that are sensitive to the collagen fibers. Once properly oriented, a focal adhesion anchors the cell to the ECM. These adhesions change dynamically to facilitate cell migration.² During new vessel growth, cells also adhere to each other through cell-cell junctions called cadherins.³ To actually develop and migrate, the cells must coordinate the focal adhesions with cell-cell bonds. In addition to managing these two factors simultaneously, the cells migrate due to chemotaxis, which is directed motility up chemical gradients.¹

During angiogenesis, the receptors for VEGF (tyrosine kinase), ECM (integrin), and cellular contact (cadherin) all play crucial roles. However, the signaling pathways within the cells are intricately connected and provide regulatory feedback to each other, called receptor crosstalk.³ The signaling network, despite the arrays of possible inputs, has a finite set of output states. These output states correspond to the following cell phenotypes: migratory, proliferating, quiescent, apoptotic, and a state in which the cell is both migrating and proliferating. To explore angiogenic sprouting, multi-scale cell-based model simulations are compared to an experiment recently conducted by Heilshorn and Shamloo⁴. In this experiment, microcarrier beads coated in endothelial cells were placed in a VEGF gradient and their growth was observed.

Methods

A two-dimensional multi-scale cell-based model is used to simulate angiogenesis. At the extracellular level, a partial differential equation describes the diffusion dynamics of tumor-secreted VEGF. At the cellular level, a lattice based model describes individual cellular interactions, including adhesion, growth, migration, and proliferation. The stroma incorporates matrix fibers and interstitial fluid, with the capability of including tissue-specific cells. The matrix fibers are assumed to be bundles of individual collagen fibrils, that are approximately 1.1 micron thick. These bundles are randomly placed at randomly chosen angles until the desired density is reached. As opposed to many previous models, each cell is not a single lattice point. Rather, in this model, each cell is composed of over 200 lattice points. This allows for more realistic modeling because each cell has a larger surface area that can interact with the environment. As Figure 1 shows, the simulations are initialized with a block of cells that represent a cell coated bead. Each cell is the equivalent of $\sim 10\mu\text{m}$ in diameter.⁴

The model employs the Metropolis algorithm in which changes are accepted probabilistically to reduce the total energy of the system in time. The probability of accepting a lattice update is:

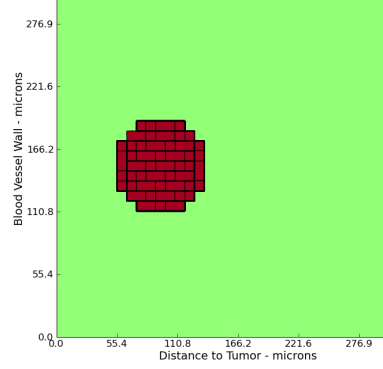


Figure 1: Initial configuration of cells to replicate cell coated microcarrier beads in Heilshorn and Shamloo experiment.

$$P_{acceptance} = \begin{cases} 1, & \text{if } \Delta E < 0 \\ e^{-\Delta E/kT}, & \text{if } \Delta E \geq 0 \end{cases} \quad (1)$$

where ΔE is the change in total energy and kT is the Boltzmann weighted temperature. The energy of the system is calculated by

$$E = \underbrace{\sum_{sites} J_{\tau,\tau'}(1 - \delta_{\sigma,\sigma'})}_{\text{adhesion}} + \underbrace{\sum_{cells} \gamma(a_{\sigma} - A_{\sigma}^T)^2}_{\text{growth constraint}} \quad (2)$$

$$+ \underbrace{\sum_{sites} \chi_{\sigma} \Delta V}_{\text{volume change}} + \underbrace{\sum_{cells} \alpha(1 - \delta_{a_{\sigma},a'_{\sigma}})}_{\text{cell-cell interaction}}$$

$J_{\tau,\tau'}$ represents the strength of adhesion between model constituents, where $\tau = \{F, M, T, E\}$ represents the constituents: interstitial **F**luid, **M**atrix fiber, **T**issue cell, and **E**ndothelial cell. δ is called the Kronecker delta function, and the term $(1 - \delta_{\sigma,\sigma'})$ serves to make sure that adhesion only occurs at the surface of the cells. The second term describes the growth constraint. γ is the membrane elasticity, a_{σ} is the current volume, and A_{σ}^T is the target volume.

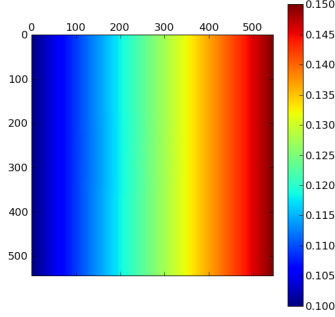


Figure 2: Steady-state solution to the equation gives initial VEGF concentration profile (pg/mL) commensurate with experimental profile.

The third term represents chemotaxis. The chemical potential χ varies by cell phenotype and is directly proportional to the VEGF gradient ΔV . V actually represents the concentration of VEGF in time $V(x,y,t)$. The last term ensures continuity, which is meant to prevent the cells from non-biological splitting. Exceeding the target volume or deforming unnaturally are costly in terms of energy which nearly eliminates such occurrences in the simulations.

The VEGF concentration profile is described by the diffusion equation

$$\frac{\partial V}{\partial t} = D\nabla^2 V - \lambda V - B(x, y, V) \quad (3)$$

where D is the diffusion constant, λ is the decay constant, and the function B represents the rate of cellular uptake. The concentration was set to match the gradient in the experimental set up.

The experiment performed by Heilshorn and Shamloo investigated the combination of biochemical gradients and matrix properties. Microcarrier beads, 100 μm in diameter, were cultured in a collagen gel matrix. Five different collagen matrix densities were used. The cells were then observed as they sprouted and developed.

Density (mg/mL)	0.7	1.2	1.9	2.7
Sprout Thickness (μm)				
Simulated	9 ± 5	16 ± 2	16 ± 3	22 ± 5
Observed		8 ± 4	18 ± 5	37 ± 11
Number of Cells				
Simulated	7	17	12	20
Observed	6	10	16	17

Table 1: Simulated versus observed results.

Results and Discussion

Table 1 summarizes a quantitative comparison between simulated and observed results. More work is being done to determine the validity and error of the results.

Figure 3 shows an example of a simulation of a block of cells in 1.2 pg/mL collagen matrix and can be compared to Figure 4, which is an image of the experiment with a microcarrier bead in a 1.2 pg/mL collagen matrix. The results of the experiment were captured with phase contrast and florescent microscopy. The simulations show promising results, that resemble the experiment, both with sprouting and branching.

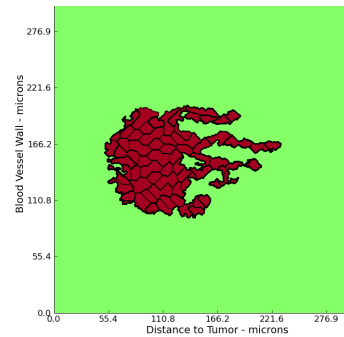


Figure 3: Simulation of a block of cells in 1.2 pg/mL collagen matrix

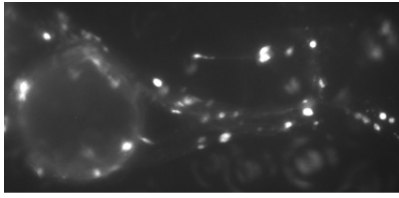


Figure 4: Experimental result from Heilshorn and Shamloo experiment showing sprout branching in 1.2 mg/mL matrix

Conclusion

This multi-scale mathematical model recapitulates the experimental results of Heilshorn and Shamloo. Perturbing the VEGF profile, matrix degradation and concentration leads to predictable sprout morphology. Based on these results, Heilshorn/Bauer groups will combine their theoretical and experimental techniques to explore novel anti-cancer therapies.

There are a significant number of ways in which this research can be furthered. Sprout turning can ideally be simulated. Tissue is not uniform throughout the body. Depending on the location, the density of the matrix and the variety of other cells that make up the stroma vary a great deal. Since it is accepted that cellular interactions with the ECM affects capillary sprout formation and morphology, fine tuning the environment and interactions of the model would allow more accurate predictability.

In this study, we focused on the changes in vessel development induced by changes in matrix density.

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Appendix

Parameter	Symbol	Model Value
VEGF diffusion	D	$3.6 \times 10^{-4}???$
VEGF Decay	λ	$.6498h^{-1}$
VEGF Uptake	β	.06 pg/EC/h
VEGF Source	S	.035 pg/pixel
Activation Threshold	v_a	.0001 pg
Adhesion		E/L
EC-EC	J_{ee}	31
EC-Fluid	J_{ef}	71??
EC-Matrix	J_{em}	76??
Fluid-Fluid	J_{ff}	71
Fluid-Matrix	J_{fm}	85
Matrix-Matrix	J_{mm}	85
Membrane Elasticity		E/L^4
EC	γ_e	0.8
Matrix	γ_m	0.5
Fluid	γ_f	0.5
Chemotactic Sensitivity	χ	1.11×10^6 E/conc
Tip Cell		1.42χ
Stalk Cell		1.5χ
Proliferating Cell		1.55χ
Intracellular Continuity	α	300 E/L
Bolzman Temperature	kT	2.5 E

Table 2: Parameters used

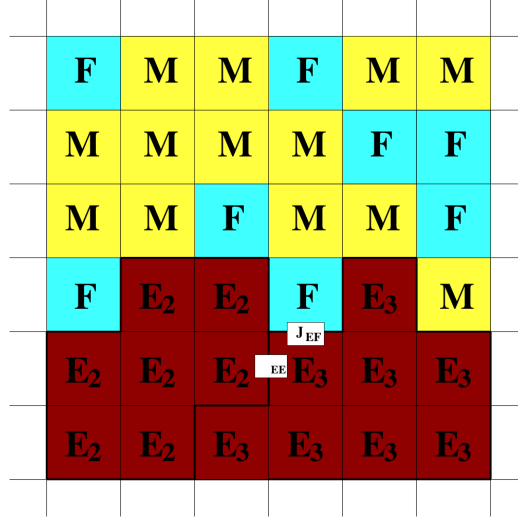


Figure 5: Magnification of the computational domain. Cells are red, fibers are yellow, and interstitial fluid is light blue

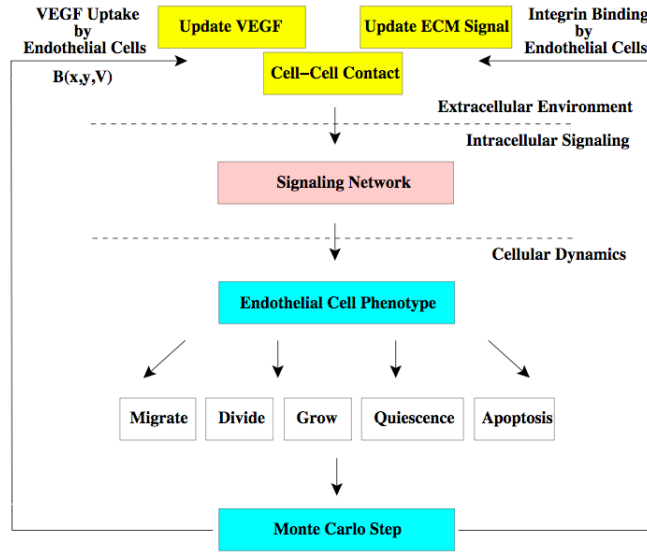


Figure 6: Bridging Multiple Scales

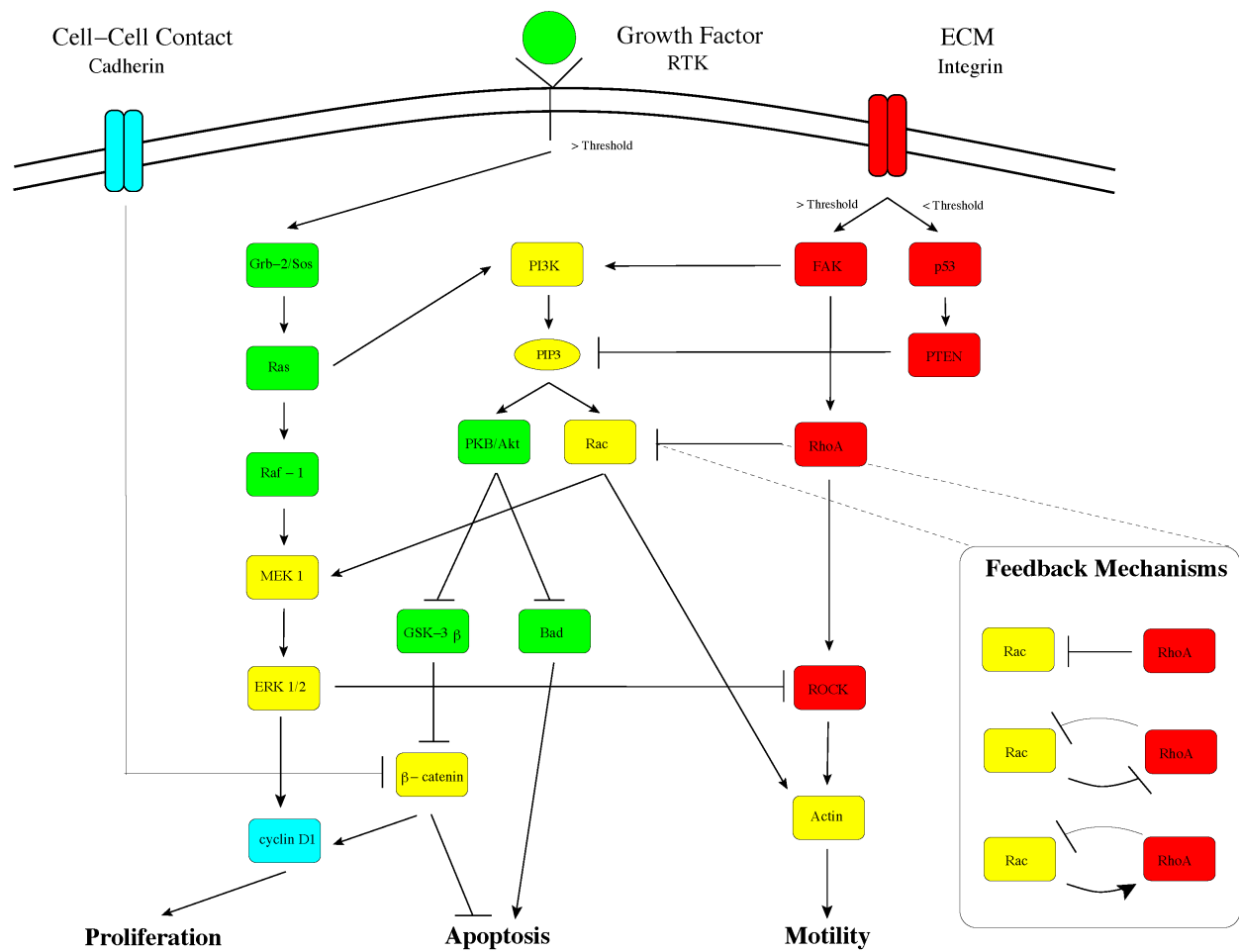


Figure 7: Cell Signal Transduction Network