YESHIVA UNIVERSITY

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March 16, 2012

Kressel Research Scholarship
Committee Members
Yeshiva University

Dear Committee Members,

My research project is entitled “Using entropy to detect quantum phase transitions.” Enclosed please find the following:

1. Title page
2. Description of research
3. Budget
4. Timeline

This proposal is countersigned by my faculty mentor Dr. Lea F. Santos.

Thank you for considering me for this incredible opportunity.

Sincerely,

Davida Kollmar

Davida Kollmar
Undergraduate Student
Stern College for Women
Yeshiva University

Mentor:

Léa F. Santos

Lea Ferreira dos Santos
Assistant Professor of Physics

(1) Title Page

Using entropy to detect quantum phase transitions

Application for the Kressel Research Scholarship

Stern College for Women

Yeshiva University

March 16, 2012

Davida Kollmar

Mentor: Lea Ferreira dos Santos, physics

(2) Description of Research

Contents

(i) Introduction
(ii) Importance and scope of the research
(iii) Research plan, my role, and my background/skills/previous experience
(iv) Expected results
(v) References

(2.i) INTRODUCTION

In classical physics, a thermal phase transition occurs when the temperature of a material reaches a critical point. As an example, take water/ice. When water is in the liquid phase, the molecules can move around freely, although there are still intermolecular forces between them. Because of the free movement, there is a high level of entropy, or disorder, within the system. As the water is cooled, however, the molecules slow down and their kinetic energy is therefore lowered. The molecules begin to arrange themselves into a lattice structure and the water turns into ice. This highly organized arrangement results in lower entropy. In thermodynamics, phase transitions are understood as a desire of the system to minimize its free energy $F=E-TS$, where E is energy, T is temperature, and S is entropy. As the temperature goes down, the entropy decreases. The only way to guarantee that F will be minimized is if the energy also decreases, as in the crystal structure. Similarly, as heat is added to the system and its energy increases, the entropy also increases, keeping F small. Thermal phase changes are common phenomena and are easy to detect because they usually involve visible changes, such as the transition from water to ice.

At absolute zero temperature ($T = 0$ Kelvin), according to classical physics, we would expect the water molecules to stop moving and the phase to be stable. However, at low temperatures, the classical laws break down and quantum physics takes over [1]. In the quantum domain, the so-called uncertainty principle states that it is not possible to simultaneously specify both the position (potential energy) and the momentum (kinetic energy) of each molecule. The delicate balance between the two energies, similar to the balance between energy and entropy in the case of thermal phase transitions described above, implies the existence of more than one phase even at $T = 0$ K [2]. Remarkably, these phases have different macroscopic properties which can be experimentally detected.

From preliminary readings, I have learned that there are in fact several types of quantum phase transitions [2,3].

One type relates to the magnetic properties of the system. Spin is an intrinsic property of elementary particles associated with their angular momentum. The constituents of matter, electrons, protons, and neutrons, have spin-1/2, which implies that in a strong magnetic field, they can align either parallel or antiparallel to this field. In a spin-1/2 system, when all spins are pointing in the same direction, the material is said to be ferromagnetic. When the spins point in random directions, the material is said to be paramagnetic. At 0 K, a quantum phase transition can occur when a material switches from being paramagnetic to being ferromagnetic.

Another type of quantum phase transition is the switch from a superfluid to an insulator. A boson is an atom that has an even number of electrons, protons, and neutrons. At very low temperatures, a bosonic system becomes a superfluid, a state in which the particles flow past each other with no viscosity. However, it is possible to use optical lattices to organize the supercool atoms into a crystal. Optical lattices are formed by standing waves made of lasers [4]. As the periodic potential of these waves increase, the bosons become locked in to the areas with the lowest potential. Eventually, the bosons become an insulator because they are no longer free to flow.

The purpose of this project is to learn more about quantum phase transitions and verify whether they may be detected by observing the system's entropy. There are many different definitions of entropy [5,6] and I will study many of them. One of the most popular definitions is that entropy is the amount of disorder within a system. Some argue that a better definition is the amount of information that must be learned in order to determine the value of something in the system. The definition of entropy that I am particularly interested in is called invariant correlational entropy, which has already been used to detect quantum phase transitions in nuclear systems [7].

(2.ii) IMPORTANCE AND SCOPE OF THE RESEARCH

The study of entropy and quantum phase transitions is important for several reasons. First, it will shed light on concepts which are fundamental to physics but which little is already known. Entropy is important because it is used to explain the notion of irreversibility in nature, the idea that there is a preferential direction in time, the so-called "time's arrow," From the second law of thermodynamics, systems prefer to go from states of less entropy to states of more entropy. Additionally, phase changes surround us daily on the macroscopic level. It is important to understand how these macroscopic changes are caused by microscopic fluctuations.

Another reason why this research is important is because there have been many recent experiments in the field, such as those with optical lattices mentioned earlier [8]. These experiments are being conducted to study quantum phase transitions, but theory is needed to explain the experimental results. My project will focus more on the theory and the computational aspect of the ongoing research.

Regarding the scope of the research, I will be working with quantum systems. The laws of quantum mechanics apply to very small particles, and are often counterintuitive. In my research I will be studying systems consisting of many interacting quantum particles, known as quantum many-body systems. I will consider one-dimensional systems, where quantum effects are enhanced. These systems are computationally more approachable than multi-dimensional systems, but are still very complex. I will study particular models of complex systems that have been used to describe current experiments about quantum phase transitions.

(2.iii) RESEARCH PLAN, MY ROLE, AND MY BACKGROUND

As part of my research project, I will read articles and books about entropy and quantum phase transitions, as recommended to me by my mentor. I will use *Mathematica* to write computer programs for a particular quantum system and will compute its entropies. I will gather data and analyze the results for indication of quantum phase transitions. I will separate and identify phases based on results from the entropies. After I am reasonably certain of my results, I will study other systems to try to generalize my findings. Once I have obtained my results, I will write them up. If they are sufficiently novel and interesting, I will prepare them for publication. I will also present my findings at the APS March Meeting.

My personal role in the research program will be to write all of the computer programs, analyze the data, make plots, and write the results.

I am qualified to pursue this project because I have already begun to research many of the concepts involved. I have read chapters in a book about entropy and have read articles about quantum phase transitions. Additionally, I have learned how to use the software *Mathematica*, which I will use to write my computer programs. I have many basic skills in that software, such as manipulating matrices and graphing.

I am a physics major and plan on attending graduate school in a physics related field. As a physics major, my coursework gives me background in the topics being researched. I am currently taking Modern Physics, which provides an introduction to quantum mechanics. I will be taking courses in Quantum Mechanics and in Thermodynamics in Fall 2012, which will give me an even deeper understanding of quantum systems and the concept of entropy. I have taken a course in Mathematical Physics, which may prove helpful for some of the calculations I will be doing. I also plan on taking Computer Science next fall, which will teach me new computer programs so that I could learn how to approach the same problem in different ways.

Finally, I have previous research experience. This past summer, I participated in the inaugural YU-Bar Ilan Summer Science Research Internship Program. The experience gave me valuable skills in the different stages of research. Some of those skills were particular to the project I was involved in. I worked in the biomedical engineering lab of Dr. Orit Shefi, using a computer program called Neuron J to measure the axons and dendrites of leech neurons. I then used Excel to average my measurements and to make graphs based on my results. This experience taught me how to take computer programs that I was already familiar with and figure out how to use them in new and more complicated ways. Some other skills I learned apply to any type of research. Since I was in the lab all day, I learned how to focus on my research and to be dedicated to the task at hand. Also, I learned how to prepare my findings for dissemination. I presented a slideshow presentation at the end of the summer, and will be presenting an updated slideshow based on some new measurements that I made at SURGE, Stern's undergraduate research exchange. I have written abstracts of my research for the group, for Stern's Women in Science, and will soon be submitting a similarly updated abstract to YU's Undergraduate Research Abstract Publication. Additionally, my lab has submitted a paper for publication which is partially based on the research I did for them. I was included in the editing process, and I am a co-author of the paper.

(2.iv) EXPECTED RESULTS

At this point I do not know what my results will be. There have been works that examined quantum phase transitions in a nuclear system with the invariant correlational entropy, and my results might match up to those results. In particular, there are some well known critical points in spin-1/2 systems, so I expect the invariant correlational entropy to be able to detect them. However, so little is known about this area of study that it is hard to predict what I will find.

(2.v) REFERENCES

[1] D. J. Griffiths, *Introduction to Quantum Mechanics*. (Prentice Hall, Second edition.)

[2] S. Sachdev, Quantum phase transitions. *The New Physics*, G. Fraser, Ed. http://qpt.physics.harvard.edu/newphysics_sachdev.pdf.

[3] S. Sachdev, *Quantum Phase Transitions*. (Cambridge University Press, ed. 2)

[4] M. Greiner, S. Frolig, Optical lattices. *Nature* **453,** p. 736-738 (2008).

[5] A. Ben-Naim. *Entropy Demystified*, (World Scientific, New Jersey, Revised ed., 2008).

[6] L. F. Santos, A. Polkovnikov, M. Rigol, Entropy of isolated quantum systems after a quench. *Physical Review Letters* **107,** p.040601 (2011).

[7] A. Volya, V. Zelevinsky, Invariant correlational entropy as a signature of quantum phase transitions in nuclei. *Physics Letters B* **574**, p. 27-34 (2003).

[8] M. Greiner, O. Mandel, T. Esslinger, T. Hänsch, I. Bloch, Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. *Nature* **415,** p. 39-44 (2002).

(3) Budget

I would like to request partial support to attend the 2013 American Physical Society March Meeting, which will be held in Baltimore from March 18-22. At that meeting I will be presenting the results of my research.

$250.00

(4) Timeline

Spring 2012:

- Begin learning *Mathematica*
- Read articles and books about entropy and quantum phase transitions
- Start writing the computer program for the particular system I will be studying

Summer 2012:

- Finish writing the computer program
- Diagonalize matrix to get the system's energy spectrum
- Compute entropies
- Gather data and analyze the results
- Examine results for indication of quantum phase transitions
- Advise a high school student in her project and teach her *Mathematica*

Fall 2012:

- Separate and identify phases based on results from the entropies
- Study other systems to try to generalize results

Spring 2013:

- Write up results to prepare for publication
- Present findings at the APS March Meeting