YESHIVA UNIVERSITY

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March 15, 2012

Kressel Research Scholarship
Committee Members
Yeshiva University

Dear Committee Members,

My research project is entitled "Dynamics of quantum systems with many interacting particles." You will find in the following pages:

(1) A title page;
(2) The description of this project;
(3) A one-page research "time-line" in bullet-point form.
(4) A one-page spreadsheet of my proposed budget;

This project is countersigned below by my mentor Dr. Lea F. Santos.

I thank you for your consideration and look forward to hearing from you.

Sincerely,

Kira Joel

Kira Joel
Undergraduate Student
Stern College for Women
Yeshiva University

Mentor:

Léa F. Santos

Lea Ferreira dos Santos
Assistant Professor of Physics

(1) Title page:

Dynamics of quantum systems with many interacting particles

Application for the Kressel Research Scholarship

Stern College for Women

Yeshiva University

March 15, 2012

Kira Joel

Mentor: Professor Lea Ferreira dos Santos, Physics

(2) Project Description:

Dynamics of quantum systems with many interacting particles

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Contents:

1. INTRODUCTION

In classical physics we have tools that allow us to predict the dynamics of a system. Using Newton's Laws we have a firm understanding of the interplay between forces, and we can understand how an object's position, velocity, or acceleration may change. Newton's Laws help us understand many different types of motion, including both linear and rotational movement. These laws are very versatile and correctly describe the behavior of macroscopic objects such as planes, cars, and people. However, these laws do not correctly predict the behavior of tiny objects. In order describe the dynamics of objects that are microscopic in size we must use quantum mechanics [1].

In order to evolve quantum systems in time I will first need a deeper understanding of quantum mechanics. As opposed to simply studying one particle I will be working with many particles interacting with one another, which further complicates the picture. I am interested in understanding how these interactions, as well as other aspects such as the presence of impurities and the geometry of the system, may affect the dynamics of the particles. In particular, I want to understand what determines a good conductor or an insulator. Furthermore, in the case of a conductor, I would like to see what kind of transport behavior it has. Does it transfer particles without dissipation or diffusely? [2,3]

In the classical domain, it is widely accepted that chaotic systems should show diffusive transport behavior, while integrable systems should be associated with ballistic (dissipationless) transport behavior. Before we continue, I should tell you more about what chaotic and integrable systems are. We use models to describe real systems in nature. When the model can be analytically solved, it is called integrable. Chaotic systems, on the other hand, are unpredictable. We can find approximate numerical solutions to them, but we are unable to describe them in the long term. Most systems found in nature are in fact chaotic. Examples include weather, population growth, and the spread of diseases [4].

Formally, classical chaos is related to the extreme sensitivity of the dynamics of a system to its initial conditions. To better explain this, we need to introduce the concept of phase-space. Phase-space consists of all values of position and momentum that a particle can have. Each point in phase-space corresponds to a particular value of position and momentum of the particle. In a chaotic system the trajectories in phase-space of two particles that have very close initial conditions diverge exponentially in time.

In the quantum domain the notion of trajectories in phase space can no longer be applied. In the quantum limit we can never know the exact position and exact momentum of the particle at the same time. This is known as the uncertainty principle [1]. However, it has been observed that the spectrum of the quantum system shows different properties depending on whether or not its classical counterpart is chaotic. From the spectrum we determine whether a quantum system is chaotic or not [5].

There is still much debate regarding the conditions that determine the specific transport behavior of a system in the quantum domain. There have also been attempts made to establish a correspondence between integrable and ballistic, and chaotic and diffusive, but it is far from well established. By studying the transport behavior of different models in both chaotic and non-chaotic domains, I plan to contribute to this ongoing discussion.

This project will be numerical. I will start by studying models that describe isolated (chaotic and non-chaotic) quantum many-body systems and will analyze their static and dynamic properties. Once I get a clear picture, time permitting, I will then couple the system to two baths of different temperatures, one hot and one cold, so that I can study how heat is transferred from one to the other. My goal is to better understand the microscopic origins of the Fourier law [5,6]. This law states that the flux of heat is proportional to the gradient of temperature. This is, however, an empirical law that is based on observations. Nobody has yet managed to derive it from truly fundamental principles. My research project aims at making advances in this direction.

2. INTELLECTUAL MERIT

How important is the proposed activity to advancing knowledge and understanding within its own field or across different fields?

This research has several significant purposes. Firstly, this project aims at determining the conditions for a system to behave as a metal, meaning a good conductor, or as an insulator. Secondly, in a world and an age in which the rate of technological advancement is rapidly increasing, understanding the transport behavior of particles, heat, magnetization, and information in quantum many-body systems is vital. One of the most challenging aspects in the development of new electronic devices, such as microchips and hard disks, for instance, is the mitigation of local heating. A clear picture of heat transfer can provide important information in order to best create devices that quickly remove heat.

How well qualified is the proposer to conduct the project?

- I am majoring in physics and plan to continue on to receive a degree in Mechanical Engineering.
- I have two previous experiences doing physics research. Although I did not know much about the topics before beginning, through readings, discussions, and hard work I was able to get a good handle on the information and make significant contributions to the research projects.
- Both of my previous research experiences involved computational aspects. I took a course in Stern College, Introduction to Computer Science, in which I learned C++ programming, as well as the concepts of computer programming in general. My previous research experiences included learning languages such as *Fortran* and *Matlab*.
- I am currently in the middle of learning *Mathematica* which is the software that will be used for this project.
- I am currently in a class called Modern Physics which addresses many aspects of quantum mechanics. This will give me a basis on which I can further my studies of quantum mechanics.
- In Fall 2012 I plan to take the course Introduction to Quantum Mechanics.
- For the section of this research program involving the transport of heat, my background from the course in Thermodynamics and Statistical Mechanics, which I took in Spring 2011, will be very helpful.

3. EXPECTED RESULTS

One of the most exciting aspects of doing research is that we do not know what the results will yield. However, there are several goals for this research program. This project will include an in depth study of quantum mechanics in order to better understand how microscopic objects behave. This study is quite fascinating since quantum particles behave differently than larger objects that behave according to the laws of classical physics. In order to set up the project I will learn how to write computer codes in *Mathematica* that will describe our situation. I will then, hopefully, be able to see if the system behaves in accordance with Fourier's Law of heat transfer.

While we do not know exactly how the system of particles will behave, we do expect the interaction between the particles to affect its dynamics. Additionally, we expect that the initial state of the particles may affect the outcome as well. This means that the system may behave differently if we begin with all of the particles condensed in one area than when we begin with the particles spread out. When the particles are very spread out, the effects of the interactions may not be so strong.

4. REFERENCES

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

[2] L. F. Santos, *Transport Control in Low-Dimensional Spin-1/2 Heisenberg Systems,* Phys. Rev. E **78**, 031125 (2008).

[3] S. Langer, F. Heidrich-Meisner, J. Gemmer, I. P. McCulloch, and U. Schollwock, *A real-time study of diffusive and ballistic transport in spin-1/2 chains using the adaptive time-dependent density matrix renormalization group method,* Phys. Rev. B **79,** 214409 (2009).

[4] J. Gleick, *Chaos: Making a New Science* (Viking, New York, 1987).

[5] A. Gubin and L. F. Santos, *Quantum chaos: An introduction via chains of interacting spins 1/2*, Am. J. Phys. **80**, 246 (2012).

[6] M. Buchanan, *Heated debate in different dimensions*, Nature Phys. **1**, 71 (2005).

[7] C. Mejia-Monasterio, T. Prosen, and G. Casati, *Fourier's law in a quantum spin chain and the onset of quantum chaos,* Europhys. Lett. **72**, 520 (2005).

(3) Research Timeline

Summer:

- Read literature and articles on the topics of quantum mechanics and heat transfer.
- Using *Mathematica* I will write computer codes to describe our quantum system of interacting particles.
- Learn how to diagonalize the Hamiltonian describing the system and obtain information about the system spectrum.
- The next step is to evolve the system in time and analyze its behavior.

Fall:

- I will then extend the system to include two baths of different temperatures interacting with the system. This will allow us to study how the heat is transferred from the hot bath to the cold bath.

Spring:

- I will analyze the data on the transfer of heat.
- If the data is inconclusive, and time permitting, I will use a different program called *Fortran* to study larger systems.
- Write a long report about my results.

(4) Proposed 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