(1) PROJECT DESCRIPTION:

Microscopic origins of irreversibility

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1. INTRODUCTION

If one were to place a collection of atoms in the corner of a box in a vacuum, and then release the atoms, what would happen? The atoms would spread uniformly throughout the box. One would not expect these atoms to then suddenly rearrange themselves back in their original corner, leaving the rest of the box empty. This second situation would be in conflict with what we know from the Second Law of Thermodynamics, which states that entropy always increases. Entropy, introduced in the 1860s, is a function of the state of a system, in the same way that temperature is a function of state. Another general way to phrase the Second Law of Thermodynamics is that natural processes tend towards greater disorder. Entropy is also called "time's arrow", since it allows us to find which direction time is going (always towards states of greater disorder). Ludwig Boltzmann clarified the concept of entropy further by applying a statistical approach. He defined the "macrostate" of a system as the macroscopic properties (such as volume and temperature), and the "microstate" as the velocity and position of every particle in the system. Generally, we cannot determine every single microstate in a system; there are far too many particles to allow this. However, we do know that many different microstates can correspond to the same macrostate. This statistical approach assumes that each microstate itself has an equal probability to any other microstate. But the macrostate with the highest probability will be the one in which the particles move randomly throughout the whole space.

A system in which the particles move entirely at random is called ergodic. This means that particles are moving at all speeds, in all places in space. This is the type of system which can be described by the statistical approach.

Classical physics explains the behavior of macroscopic systems, such as how fast a rock is falling, or what the heat increase in a given fluid is. But we know that all macroscopic systems are in fact made up of many, many microscopic systems – each individual particle is a microscopic system. Microscopic systems are described by quantum physics – the theory which describes the behavior of very small objects, such as electrons. Thus, we should be able to explain any macroscopic behavior by describing the microscopic behavior of the system's particles. However, to do this, we need to understand what makes a quantum system ergodic. Because of the difference in nature between classical physics and quantum physics, ergodicity (or chaos) must be defined differently.

I want to understand what ergodicity is at the quantum level. To do this, it is important to understand what the best quantities are to indicate whether a quantum system is ergodic or not. I would also like to understand whether ergodicity in quantum systems enables those systems to be described by the same statistical approach as we use in classical physics with macroscopic systems.

2. INTELLECTUAL MERIT

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

The subject of quantum systems' ability to be described by statistical mechanics has been a challenge for physicists since the 1920s, when it was addressed by Schrodinger and von Neumann.

Interest in this subject has been renewed in modern times with the rapid miniaturization of technology. Moore's Law states that every eighteen months, the number of transistors per unit area etched onto a silicon chip doubles. However, there is a limit as to how many transistors can put on any one silicon chip. To enable the continuation of the miniaturization of technology, it may be possible to create a "quantum computer", which operates using quantum systems. A quantum computer would be able to store vast amounts of information on very small chips, and thus could be used for much more powerful computations than any we can do using today's computers. The more we understand how these quantum systems can be described, the closer we are to being able to manipulate them and use them to store data.

2.2 How well qualified is the proposer to conduct the project?

- I am a double-major in physics and computer science, intending to continue my education in Mechanical Engineering at the graduate level.
- From computer science courses: This project is numerical, so my background in C++ programming will be helpful. In particular, the class I am taking now in Spring 2011 in *Numerical Analysis* will be useful, as will be *Computational Methods in Science and Research*, which I plan to take in Fall 2011.
- From physics courses: This project requires both knowledge in quantum mechanics and statistical mechanics: I had a first introduction to quantum mechanics in the *Introduction to Modern Physics* course in the Fall of 2010. I am learning about statistical mechanics in the course *Thermodynamics and Statistical Mechanics*. I will apply to my research what I learned in these courses and at the same time will further extend my understanding of these subjects in the more challenging context of the real and unexplored research environment.
- In order to study a system numerically we need a model to describe it. During the summer 2010, I studied one-dimensional models of particles, determining (by using mathematical models) whether a system was a metal or an insulator. The systems were made of a one-dimensional chain of particles, in which each location could be occupied by a maximum of one particle. I studied how the energies of each particle and the interactions between them can enable or inhibit their "hopping", that is, their ability to move along the lattice. Defects along the lattice changed the energy levels of the sites, thus inhibiting hopping. Additionally, strong interaction between adjacent particles would also prevent hopping.

3. RESEARCH PLAN AND MY ROLE

The first step in this research is to select appropriate models to describe our system of interest. I will begin with the models I studied during the summer 2010, but I will further extend these models to include more terms describing the interactions between the particles. I want to have many way to introduce randomness into my systems, thus enabling me to make more general statements.

I will write computer programs to use the Hamiltonian matrix (a matrix which describes these systems) to compute chaos indicators. I will begin by using Mathematica, which is a software with which I am already familiar from my summer research. However, Mathematica is limited to matrices of dimensions of around 3000. Therefore, to study larger quantum systems, I will learn Fortran (which can deal with matrices of dimensions of around 15000) and rewrite the codes in that language. I will then be able to use my mentors Linux workstation to run my codes. I am interested in large systems, called quantum many-body systems, since they will allow me to have good statistics and reliable results for chaos indicators.

Chaos indicators are those quantities which are used to determine whether a quantum system can be considered to be chaotic. These quantities cannot be measured experimentally; they are computed in accordance with quantum theory. I will read the references regarding this topic suggested by my mentor, and also search for more references to understand chaos indicators and their computation further. I will try to reproduce some of the results from these articles, and then to compute the chaos indicators for my systems. There are various chaos indicators, some of which fail under certain conditions. There may even be indicators which have not yet been studies.

After identifying the conditions under which a quantum system becomes chaotic, I will then study quantities which can be measured experimentally, such as kinetic energy or interaction energy. I will then check whether these results agree with the predictions of statistical mechanics and whether this only occurs in chaotic systems. If indeed it is the case that these values agree only in cases where the system is chaotic, I will be able to say that quantum chaos is a requirement for the system to be described by the same statistical methods used to describe macroscopic systems.

The analysis above is based only on static properties of the systems. To further support my results, I can study the time evolution of these systems and whether their behavior in time is also in accordance with statistical mechanics.

I will be completely in charge of writing the codes, collecting the data, and computations. My mentor will assist me with references, the questions I will have during the project, and the interpretation of my results. I will also prepare a slide presentation to present my findings at the America Physical Society March Meeting 2012. My mentor and I also hope to write a scientific paper together about my results.

4. EXPECTED RESULTS

I cannot say definitely what I will find in this research. Research is different than coursework, in that with research, we never really know with certainty what the results will be. If we did, there would be no need for the research.

I expect to find results which show that quantum chaos is indeed a requirement for the ability for the quantum system to be described by statistical mechanics. However, if I find results to the contrary, these results would be equally, if not more, interesting. The beauty of research is that one never quite knows what one will obtain, and surprising results can lead to new and improved ways of thinking.

5. REFERENCES

(2) PROPOSED BUDGET

(a) I would like to request funding to present the outcome of my research findings at the American Physical Society (APS) March Meeting in 2012. This conference will take place in Boston, MA, from February 27 to March 2, 2012.

US $900.00

(b) I would also like to request funding to download the student version of Mathematica to my computer.

US $80.00

Total: US $980.00

(3) RESEARCH TIME-LINE:

Summer 2011:

- Review models that I studied during my summer research in 2010 and extend them to include further interacting terms in the Hamiltonian.
- Run my old programs and write new ones to find eigenvalues and eigenvectors of the system models considered.
- Search for references and study about quantum chaos.

Fall 2011:

- Use the data for eigenvalues and eigenvectors to identify the conditions under which the models studied become chaotic.
- Analyze the advantages and disadvantages of various chaos indicators.
- Study observables and verify whether a one to one correspondence between quantum chaos and statistical description exists.

Spring 2011:

- Compare the static results for the observables obtained in the fall with their time dynamics. Verify whether predictions for correspondence between quantum chaos and a statistical description are confirmed by the dynamics.
- Prepare to show my results at the American Physical Society March Meeting 2012. Submit abstract, prepare slides, and rehearse the oral presentation.
- Organize my results to write a paper and send it to a scientific journal. Be involved in the whole process of an article submission.