**Science Project Detailed Research Plan**

**Please complete the information/questions begun/seen below in red ink. Save this document to your computer, and add a printed hardcopy to your application.**

**Date: 10/13/2019**

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**Project Title:** : **(What is the effect of XXXX (changing variable) on YYYYY (your measured end point)?** Choose a title that identifies the content of your project. The title can include the nature of the study, the species used, and the place of field studies. It should reflect the principal objective of the investigation.

**My project Title is:** A comparison of Quantum Mechanical Path Integral approaches for Bose-Einstein Condensates (BEC) in a Harmonic Trap.

**Hypothesis:** Based on your reading and information research, organize everything you have discovered, and then make an estimate of what will happen.  Knowing certain things are true, you then predict what might happen if you change something. Your experiment, when successful, will allow you to determine if your hypothesis was correct or not.

**My project Hypothesis is:**

1. Performance and accuracy:
   1. PIGS will be the slowest algorithm due to its local path sampling and high rejection rate. Due to the high rejection rate, it forces us to use small displacements. As a result, it is the most accurate also since the best path is accepted.
   2. Levy Harmonic Path will be second in accuracy. It uses direct path sampling so that the path in any interval is a stochastic (random) interpolation of end points. It is a rejection-free algorithm and gives a stable distribution which is Gaussian.
   3. Tower Sampling also implements a rejection-free algorithm for sampling but is not optimal.
2. Density Matrix Localization
   1. More bosons in the density matrix of Feynman Path Integral Ground State (PIGS) algorithm will be localized around x=0 compared to Levy Harmonic Path which will be more accurate compared to Levy Harmonic Path with Tower Sampling.
3. Variability
   1. Levy Harmonic Path with Tower Sampling will have the highest variability. Levy Harmonic Path will be next followed by PIGS which will have the least variability.

**Materials:** List all necessary biological agents, chemicals, reagents, major instruments, and software which will be used.

**Softwares:**

* **PyCharm CE**
* **Python 2.7**
* **Github**
* **Matplotlib**
* **Scipy**

**States of Matter:**

* Bose-Einstein Condensates (BEC) in a Harmonic Trap
  + **Bose-Einstein Condensates (BEC):** This is a state of matter in which atoms are cooled to near absolute zero (fraction of microkelvins) and hence have no free energy to move. So, the atoms clump together and enter the same quantum ground state. This is observed with the superfluid properties of He-4.
  + **Harmonic Trap:** This is a harmonic potential containing a large number of particles that do not interact with one another (like in BEC). This enables experimental studies of Bose gases to be carried out.

**Algorithms / Concepts:**

* **Feynman Path Integrals:** It allows us to compute the quantum mechanical amplitude of a particle traveling from point A to point B by doing a sum or functional integral over the infinite quantum mechanically possible trajectories.
* **Path Integral Ground State Quantum Monte Carlo:**
  + Allows for the treatment of Quantum Mechanical system at zero temperature.
  + Solves the time-independent non-relativistic Schrodinger equation.
  + Works through imaginary time propagation. Evaluates the integral by discretization of time. This makes it applicable to large systems containing hundreds of particles.
  + Projects the trial wavefunction to the ground state and gives discrete imaginary worldlines constructed from products of short time propagator.
* **Levy Integrals:** It uses direct path sampling and is a rejection-free algorithm. The path is constructed from a stable Gaussian distribution.
* **Tower Sampling:** Tower Sampling also implements a rejection-free algorithm for sampling but is not optimal. It is based on determining the number based on probability which is proportional to the distribution weight.
* **Markov Chain Monte Carlo Metropolis Algorithm:** The Metropolis algorithm consists of two steps:
  + (i) the generation of a proposed configuration (or move)
  + (ii) the acceptance or rejection of the proposed configuration (or move).

**Methods**: Describe the **general methods** to be used, and why are you using the methods you have chosen? Why have you chosen the described controls? Examples would **be spectroscopy, photometric methods, direct measurement, volume displacement, voltage, energy output, etc. WHAT IS YOUR MEASURED END POINT(S)?**

**Independent Variables:**

* N: Number of Bosons
* Initial position (x,y,z) matrix of bosons

**Control Variables:**

* Wavefunction
* Imaginary time slice
* λ (hbar^2/2m kB) = 0.50
* T: Temperature
* Beta = 1/T
* δ for Center of Mass move = 0.50

**Dependent Variables:**

* Final position (x,y,z) matrix of bosons
* Density Matrix

**My general project methods are:**

* **Implement Path Integral algorithm simulation using Python.**
* **Run simulations of the algorithm varying the input varia**

**Detailed Experimental Procedure:** State your DETAILED methods, so that others could repeat your work **exactly**. Include details, giving exact specifications and quantities. [Your procedure will describe how you plan to do your experiment, changing only one variable at a time and keeping all the other parameters the same]. Describe your control so that you can compare results of your experiment with a standard for which the variable is unchanged. Make sure that you have three or more seeds/plants/animals in each of the control and experimental groups. Even better, have several experimental groups (e.g. more than one concentration of chemical you are testing, more than one time point, etc). Make measurements in metric units when possible.  Repeat the test more than once to see if your results are reproducible.

**My DETAILED project methods are:**

**Methods of Data Collection:** If you used a published method, reference the method, but describe any changes you made to it. If you used experimental organisms, identify them by genus and species. If you used a standard instrument, it suffices merely to name it, but if you devised a new or special method, describe it completely.

**My project uses the following method of data generation:**

**Bibliography:** List the authors and titles of five, (high school) or three (middle school) science or engineering books or articles that you have read and found useful for your research subject.

Example: Author ’s Name, Year of publication, “Quoted Title of Magazine Article (magazines only)”; Underlined *Title of Book or Magazine, date, volume, and number of magazine issue. Page numbers read. If you use a web site: www.urlname.ext, name of topic from the home page, author, and date read.*

**My bibliographic references are the following:**

**1.**

**2.**

**3.**

**4.**

**5.**