Quantum Monte Carlo calculation of the Hydrogen molecule ground state energy

Pablo Ximenez de Olaso Coronado

School of Physics and Astronomy. University of Southampton

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Monte Carlo simulations are a popular tool used to solve complex problems using random numbers. To help explain how they work, let's imagine you're planning a road trip to a new city.

Before setting off, you want to estimate how long it will take to get there. However, numerous factors influence travel time, such as traffic, weather, and road conditions. So, predicting the exact time is difficult.

This is where Monte Carlo simulations come in. By inputting different variables like distance, traffic, speed limit, and rest stops, and then running the simulation many times with different random numbers, you can estimate travel time. When rolling a dice, each random number produces a different outcome. Running the simulation multiple times generates a range of possible travel times, rather than one definitive answer.

Using the average of all the simulation results, you can estimate travel time more effectively and plan for unexpected delays. Monte Carlo simulations are useful in finance, engineering, and science for dealing with uncertainty and variability by analyzing a range of results. This principle can be applied in a number of different areas used by physics, mathematics, engineering and finance. It is used, for example, to solve integrals and, the topic of this project, finding the ground state energy of a hydrogen molecule.

In quantum mechanics, the ground state energy is the lowest possible energy that an atom or molecule can have. Just like a ball rolling down a valley, electrons tend towards the lowest potential energy that they can. In this state, the electrons are as close to the nucleus as possible and are in their lowest energy levels. If energy is added to the atom or molecule, the electrons can move to higher energy levels, but when they release energy, they will return to the ground state.

A hydrogen molecule H_2, is made up of two electrons and two protons. The protons will repel each other and the protons will attract the electrons. A common simplification that is done in Quantum Physics is the Born-Oppenheimer approximation. Imagine the electrons in a molecule as planets orbiting the atomic nuclei, which are like the sun. The planets move very fast around the sun, while the sun remains relatively stationary. Just like we treat the sun to be stationary and the planets move around it, we treat the protons to be at fixed positions, and the electrons will orbit it.

By writing equations that are physically reasonable for the movement of electrons (making use of something called the Metropolis method) and making a trial wavefunction, we estimate an upper boundary for the energy of the system. Shifting the proton positions, we find at which separation the energy will be at its lowest.

The second step is more complex. The Schrödinger equation allows us to calculate the probability of finding a particle at a certain location and time, based on its initial state and the forces

acting on it. By doing a mathematical trick involving imaginary time, we can treat the Schrödinger equation like a diffusion equation, which is the equation that explains how heat spreads through a metal rod. We then evolve the energy value that we had calculated from our trial wavefunction to the ground state energy. With the ground state energy, we calculate the energy that would be needed to break apart a nucleus into its individual protons and neutrons. This is called the binding energy. The binding energy is an important concept in nuclear physics because it determines the stability and properties of atoms. For example, atoms with a high binding energy are more stable and less likely to undergo radioactive decay.

We find in this computational experiment a proton separation of $S = 0.77\mathring{A}$ (compared to the experimental $S \approx 0.74\mathring{A}$) where an angstrom ($\mathring{A}$) is equivalent to 10^{-10} meters (or 10 billionth of a meter). We find a binding energy of $E_b = 4.171$ eV (compared to the experimental $E_b \approx 4.75$ eV). Other papers implementing the Born-Oppenheimer approximation have found a binding energy of $E_b \approx 4.25$ eV.

A helium atom is structurally very similar to a hydrogen molecule. It has two protons and two electrons, but it also has two neutrons. The two neutrons and protons are held very tightly together by something called the strong force. Because of this, there is no separation between the protons. So, we use our model, with a proton separation of $S = 0\mathring{A}$, to find the energy of a helium atom. We find an energy (called "local energy" in this case) of $E = -78.32$ (experimentally shown to be E = -78.9 eV).

Even though our findings, for both the hydrogen molecule and the helium atom, don't completely match the experimental results, they do show that the mathematical methods implemented do work as intended. However, these methods take a long time to run on the hardware available. We expect that, by more thoroughly calculating the different parameters and running the simulations for longer periods of time, the results would be improved. Furthermore, these methods could be implemented for atoms of higher electron compositions by adjusting the formulas to each particular case.