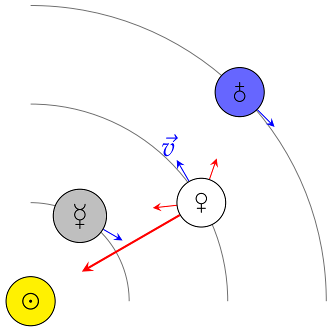
The Minimizing Game

David Gustavsson

There is a notoriously difficult problem in quantum mechanics called the quantum mechanical many-body problem: what happens to a collection of particles which interact with each other? One method to get approximative solutions is to use an object called a Slater determinant, and minimizing its energy with gradient descent.

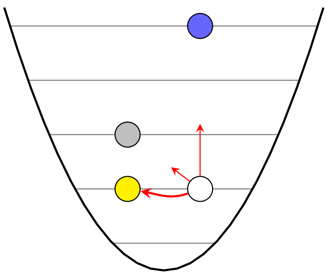
A classical problem

When Sir Isaac Newton had proposed his law of gravity in the 17th century, he tried to apply it to the movements of astronomical objects. Unfortunately, some of his calculations turned out to match reality poorly, and the reason turned out to be quite simple: Venus is moving in a circular orbit because it is affected by a force pulling it towards the Sun, but once in a while Mars or Earth passes by near enough that Venus' orbit is affected. Of course when that happens, Earth's orbit is also slightly changed, and so the position of every planet depends to some degree on the position of every other – they form a combined N-body system, and the positions of each of them quickly becomes impossible to predict analytically. The only way forward was to make approximations and simulations; if the planets' positions and velocities are known at a certain moment in time, and if you make a small enough step forward in time, then you can make a reasonably accurate prediction of where they will be and how fast they will be moving. The difference to an analytical description is that you need to make the calculation for each of the tiny time steps between now and the time you're interested in, and the accuracy of your prediction will depend not only on the accuracy of your initial measurement but on the accuracy of each of those calculations.



Classical 4 body problem: forces (in red) acting on Venus. Not to scale.

The quantum parallel

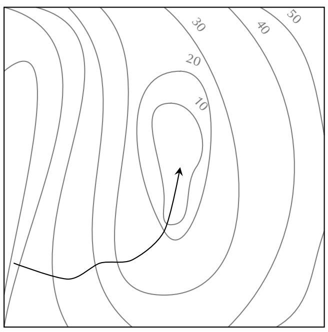


Quantum mechanical 4 body problem.

Keeping track of the eight planets and the sun in our solar system using classical mechanics is difficult, but quantum mechanics is – as usual – on another level. The quantum mechanical N-body problem is the question of where particles in a potential are likely to be found and what energies they are allowed to have, if they are interacting with a certain force. The protons and neutrons in an atomic nucleus are one such system, which means good approximative solutions to the quantum mechanical N-body problem is important to nuclear physics.

One often used approximation for fermions (like neutrons, protons and electrons) is an object called a *Slater determinant*, which uses a number of basis states given by how a single particle would have acted in the same potential, and a set of coordinates in that basis for each of the N particles. If care is taken when choosing these coordinates, the Slater determinant will be an approximation to the solution, and we are guaranteed that its energy is higher than the actual energy of the real system. This last point sounds like a problem, but is in fact a strength: If we can find a set of coordinates which result in a lower energy, we know that it will be a better approximation. This means that we can start from a Slater determinant, and then alter the coordinates in any way that leads to lower energy – until it cannot go any lower.

This alteration is done through *gradient descent*, and can be likened to looking for the bottom of a valley by walking along the steepest downhill path until you reach the lowest point. Such terrestrial gradient descent would be 2-dimensional, varying your latitude and longitude to find the minimum. A Slater determinant is represented by $M \times N$ coordinates – 40 of them for the figure to the left – but the general idea is the same. In my thesis, *Excited States in Variational Many-Body Approaches*, I implemented this method to find both ground and excited states for the quantum mechanical many-body problem using this idea. Several Slater determinants were found one after another to add up to a high accuracy solution, and more determinants were added to describe additional excited states.



Gradient descent in 2D.

Supervisor: **Gillis Carlsson**
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Department of Physics, Faculty of Engineering, Lund University