Quantum Chaos and Atoms

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A system of particles moving according to Newton's mechanic ("classical mechanics") is called chaotic if a small change in the starting position gives a large change in the final position after some time; the so called "butterfly effect". This is nowadays a much studied subject and chaos in classical systems is quite well understood. Quantum mechanical systems are described using a very different philosophy and it is not obvious how chaos appears in these systems. What we will sketch here is examples showing that chaos is very important for quantum mechanical systems, and to really understand atoms you have to understand that the electrons may have a chaotic motion inside the atom.

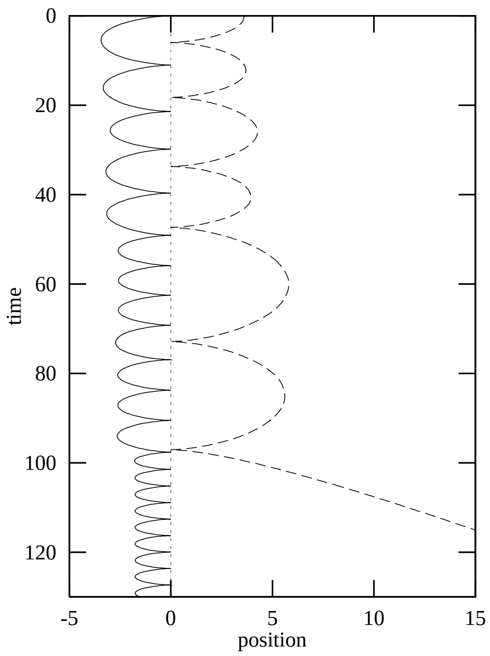
A quantum mechanical system is typically described by energy levels, and what we measure may be the energy of the light emitted as the electron jumps from one level to another. These levels are independent of time and there is no sense in talking about chaos directly for energy levels. However, an energy level may be the result of chaotic classical motion of the electrons.

The hydrogen atom (viewed as a Newton kind of system) is one electron moving around a nucleus in an elliptic orbit. There is no chaos for the hydrogen atom. All other atoms have more than one electron and may be chaotic. Niels Bohr discovered a quantum mechanical description which did work for the hydrogen atom, but not for any more complicated atoms. Using the fact that the motion is chaotic we can use a modern version of Bohr's theory and find the energy levels also of more complicated atoms. These "chaos calculations" has so far been done for the helium atom and for a hydrogen atom in a constant magnetic field.

The helium atom consists of three particles, and there is a Coulomb attraction between the positive nucleus and each of the two negative electrons and a Coulomb repulsion between the two negative electrons. We can simplify this problem by starting out with all three particles on a line. The particles will then continue to move along the line.

The helium atom on a line looks like this:

When we let the electrons move from the starting positions, we get a picture like the one shown in the next figure. The vertical axis is the time increasing downwards and the horizontal axis is the position of the two electrons; the left electron drawn with a whole line and the right electron drawn with a broken line. Each electron moves towards the nucleus, collides with it, and turns and moves away from the nucleus. We may view this special collision as a very narrow elliptic-like motion. When one electron is close to the nucleus it gives a "kick" to the other electron because of the electrical repulsion, and we find here that eventually the electron on the left hand side kicks the electron on the right hand side out, such that it moves away from the nucleus. The electron on the left side continues to oscillate while the right electron goes away. The interesting thing here is that the trajectory before one electron escapes is an unstable chaotic trajectory. We find that there is a so called "fractal set" of chaotic orbits and we use a modern version of Niels Bohr's quantum mechanics for these chaotic orbits and find the energy levels for the helium atom. We get a number of different energy levels using these chaotic orbits, and the levels are in agreement with observed atoms.



An other system which can be described in a similar way is the hydrogen atom in a magnetic field. Here, the electrical Coulomb force tries to force the electron to move in elliptic orbits while the magnetic field tries to make the electron move in a spiral, and the resulting motion is chaotic.

You can read more about this subject in the articles:

D. Wintgen, K. Richter, and G. Tanner, *Chaos*, **2**, 19 (1992).
G. Tanner and D. Wintgen, *Phys. Rev. Lett.* **75**, 2928 (1995).
H. Friedrich and D. Wintgen, *Phys. Rep.* **183**, 37 (1989).
G. Tanner, K.T. Hansen, and J. Main, *Nonlinearity*, (1996), to appear.