# Quantum Chaos and Atoms

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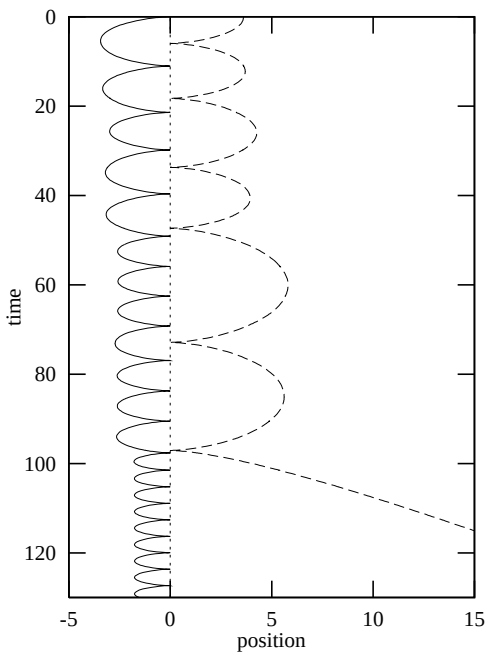
With the concept "quantum chaos" we usually understand a quantum mechanical system where the corresponding classical system is chaotic. A classical system is called chaotic if a small change in the starting position gives a large change in the final position after some time; the so called "butterfly effect". A quantum mechanical system is typically described by energy states, and what we measure may be the energy of the light emitted as the electron jumps from one state to another. These states are independent of time and there is no sense in talking about chaos directly for the energy states. However, the fixed energy states may be a result of chaotic classical motion of the electrons.

The motion which is completely non-chaotic is called integrable. There are few, but important, examples of integrable systems: a point particle inside a rectangular box, the harmonic oscillator, and two particles interacting with a Coulomb force as the hydrogen atom. Most other things may have more or less chaotic motion. When we investigate atomic systems we find that the isolated hydrogen atom is integrable. All other atoms and hydrogen interacting with some particles or field may be chaotic. The "old quantum mechanic", invented by Niels Bohr, did only work for hydrogen atom and not for other atoms. But using the fact that the motion is chaotic we can use a modern version of Bohr's theory and find the energy levels of atoms. This 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. Poincaré showed hundred years ago that the "three body problem" could not be solved analytically as for example a two body problem like hydrogen. We can simplify this three body problem by starting out with all three particles on a line. The particles will then continue to move along the line, and this configuration has a low energy because the distance between the electrons is as large as possible.

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 dashed 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 side kicks the electron on the right side out such that 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 disappears is an unstable chaotic trajectory. By closer examination one find that there is a fractal set of starting points which do not escape, and this fractal set of unstable orbits can be used in a Bohr-like quantum theory (Gutzwiller trace formula theory) which give us the energies for the helium atom with only a few percents error. We actually get most of the bounded states (Rydberg series) and also most of the excited states, using these chaotic orbits.




An other system which can be described in a very 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. Also for this system we can calculate energy states from the chaotic motion.

You may 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.