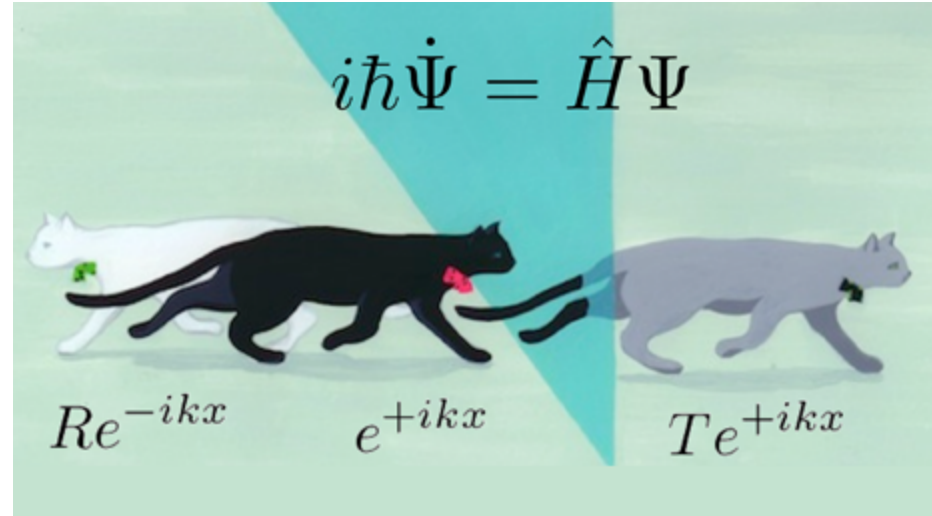


Atomic Structure and Spectra

Part II. Cracking the hydrogen code



Atomic Structure and Spectra

Tools for controlled dispersion of light: refraction and **diffraction**

$\lambda = 650 \text{ nm}$

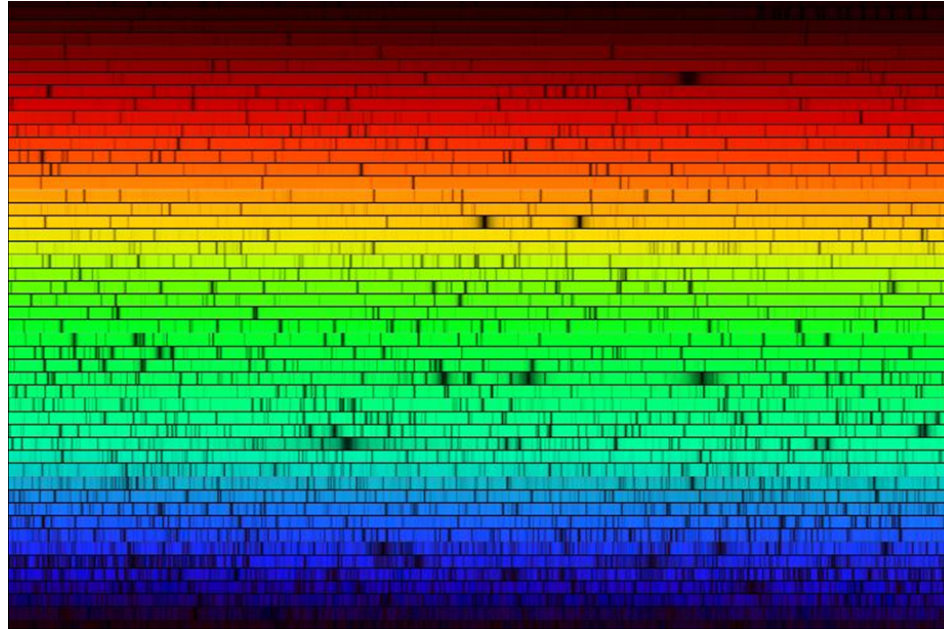
R

$\lambda = 532 \text{ nm}$

G

$\lambda = 405 \text{ nm}$

V



Nigel Sharp, National Optical
Astronomical Observatories

When seen under high resolution, there are numerous **dark lines** in the spectrum of the Sun. This pattern was decoded using the techniques we discuss this week.

Atomic Structure and Spectra

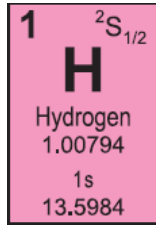
Nick Ares, Wikimedia Commons



Gases of atoms and simple molecules often produce light of vivid appearance when they are excited in electric discharges.

The neon marquee sign of the 1937 State Theater in Auburn, California.

Atomic Structure and Spectra

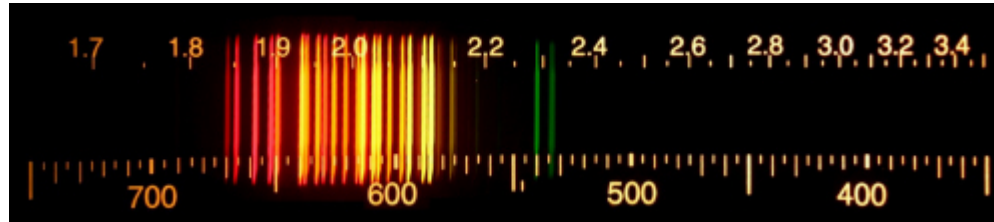
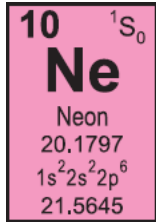


Wavelength

R

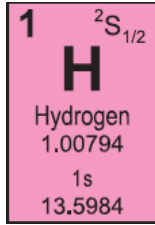
G

V



Emission spectra of gases often show sparse line structure – atoms only emit particular colors – evidence for “quantum” physics.

Atomic Structure and Spectra



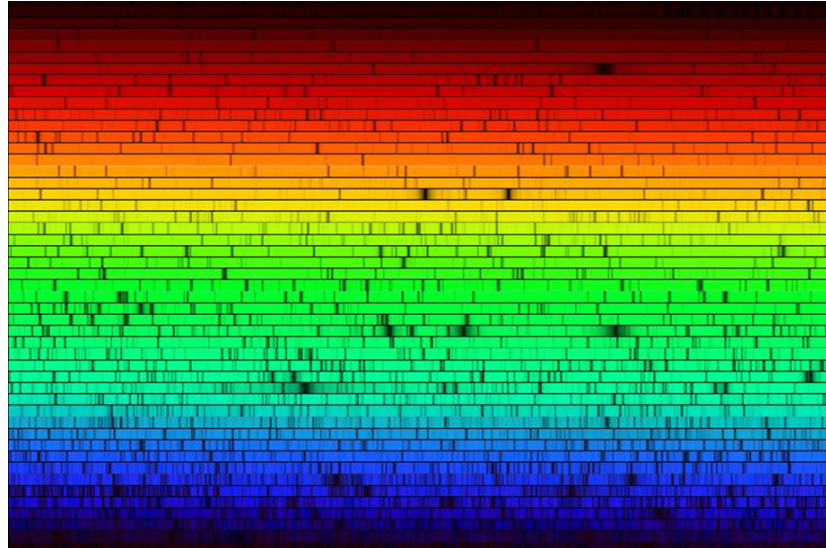
$\lambda = 650 \text{ nm}$



$\lambda = 532 \text{ nm}$



$\lambda = 405 \text{ nm}$

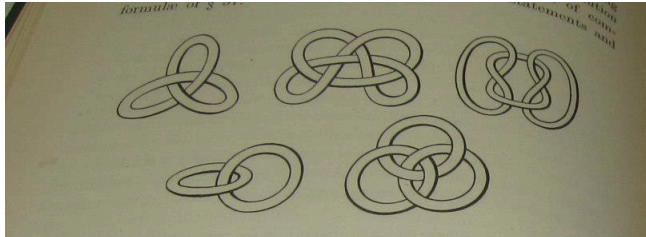


Atomic Structure and Spectra

How does one account for the invariable properties of atoms?

In Newtonian mechanics, a system of particles can have any initial values of positions and velocities, which then determine the course of its evolution. How then can there be atoms with invariable properties?

Perhaps atoms are vortex rings in some kind of pervasive fluid?



W. Thomson 1869

1. ON VORTEX ATOMS.

[*Proceedings of the Royal Society of Edinburgh*, Vol. vi, pp. 94—105;
reprinted in *Phil. Mag.* Vol. xxxiv, 1867, pp. 15—24.]

AFTER noticing Helmholtz's admirable discovery of the law of vortex motion in a perfect liquid—that is, in a fluid perfectly destitute of viscosity (or fluid friction)—the author said that this discovery inevitably suggests the idea that Helmholtz's rings are the only true atoms. For the only pretext seeming to justify the monstrous assumption of infinitely strong and infinitely rigid pieces of matter, the existence of which is asserted as a probable hypothesis by some of the greatest modern chemists in their rashly-worded introductory statements, is that urged by Lucretius and adopted by Newton—that it seems necessary to account for the unalterable distinguishing qualities of different kinds of matter. But Helmholtz has proved an absolutely unalterable

Atomic Structure and Spectra

How does one account for the invariable properties of atoms?

Vortex knot structures are now returning to interest in atomic physics – for rather different reasons – but they aren't the source of atomic structure . . .

PHYSICAL REVIEW E 85, 036306 (2012)

Vortex knots in a Bose-Einstein condensate

Davide Proment,^{1,2,*} Miguel Onorato,^{1,2} and Carlo F. Barenghi³

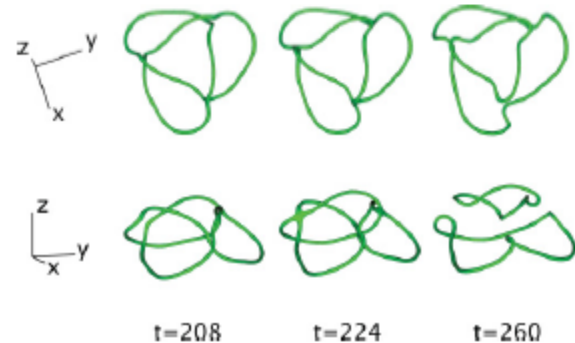
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We present a method for numerically building a vortex knot state in the superfluid wave function of a Bose-Einstein condensate. We integrate in time the governing Gross-Pitaevskii equation to determine evolution and shape preservation of the two (topologically) simplest vortex knots which can be wrapped over a torus. We find that the velocity of a vortex knot depends on the ratio of poloidal and toroidal radius: for smaller ratio, the knot travels faster. Finally, we show how vortex knots break up into vortex rings.



Atomic Structure and Spectra

How does one account for the invariable properties of atoms?

The trouble with continuum models – discovery of electrons and nuclei that certainly seemed to behave as particles.

1911: Rutherford's shocking discovery that 99.9% of the mass of the atom is concentrated in a 10^{-15} of its volume.

Atoms are *mostly empty space* with electrons orbiting the nucleus under the influence of long-range Coulomb interactions!

Let's see what classical mechanics says about the system of one electron and one nucleus: a hydrogen-like system $H, He^+, Li^{2+}, \dots, U^{91+}$ **Ps** **He $\bar{p}$**

Atomic Structure and Spectra

Wikimedia Public Domain



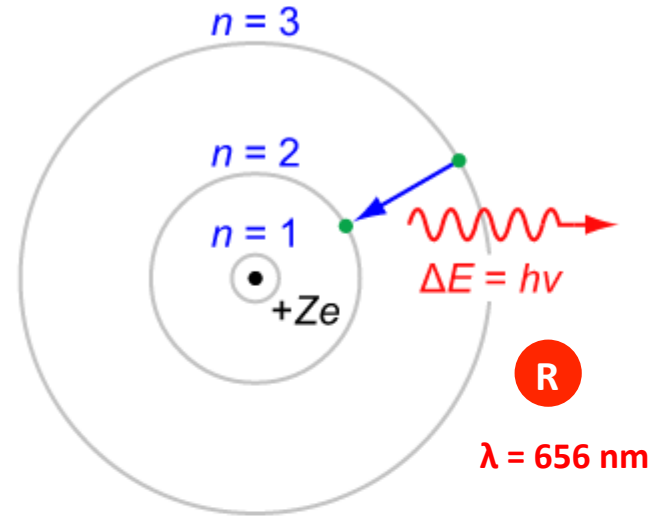
Niels Henrik David Bohr
1885-1962

1922 Nobel Prize in Physics
"for his services in the
investigation of the structure
of atoms and of the radiation
emanating from them".

Niels Bohr's great breakthrough

"On the Constitution of Atoms and Molecules," *Philosophical Magazine*,
Series 6, Vol. 26, No. 151, pp. 1-25 (July 1913).

**Key idea: the
stationary states
of hydrogen-like
atoms correspond
to certain
quantized circular
orbits described
by classical
equations of
motion.**



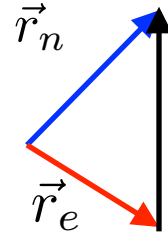
Wikipedia

Atomic Structure and Spectra

Classical equations of motion for hydrogen-like systems

Nucleus: position, mass, electric charge $\vec{r}_n; M; +Ze$

Electron: position, mass, electric charge $\vec{r}_e; m; -e$



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

$$M\ddot{\vec{r}}_n = -Ze^2\vec{r}/r^3$$

$$m\ddot{\vec{r}}_e = +Ze^2\vec{r}/r^3$$

$$\ddot{\vec{r}} = -\left[\frac{1}{M} + \frac{1}{m}\right]Ze^2\vec{r}/r^3$$

$$\mu\ddot{\vec{r}} = -Ze^2\vec{r}/r^3$$

$$\frac{1}{\mu} = \left[\frac{1}{M} + \frac{1}{m}\right]$$

$$\vec{p} = \mu\dot{\vec{r}}$$

First-order equations:

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$

Atomic Structure and Spectra

Why is it essential to have equations of motion that are first-order in time?

Understanding dynamics of a system S – whether classical or quantum – means that if you know the state of S at time t , you can calculate what it is at time $t + \delta t$:

$$S(t + \delta t) \approx S(t) + \delta t \dot{S}(t)$$

That's why Schrödinger's equation must be first-order in time! Given the wavefunction at time t , $\Psi(t)$, we find

$$\Psi(t + \delta t) \approx \left[1 - \frac{i\delta t \hat{H}}{\hbar} \right] \Psi(t)$$

Atomic Structure and Spectra

Why isn't Schrödinger's equation second-order in time like other wave equations?

Q: "Where does milk come from?"

A: "Milk comes from a bottle."

Q: "Silly! The bottle comes from a shop! When you consider first principles, milk comes from a shop!"

Those other equations (e.g. Maxwell's) were packaged "for your convenience" as second-order equations, but began life as first-order equations.

As is our classical mechanics of hydrogen-like systems, in Hamiltonian form:

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$
$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$