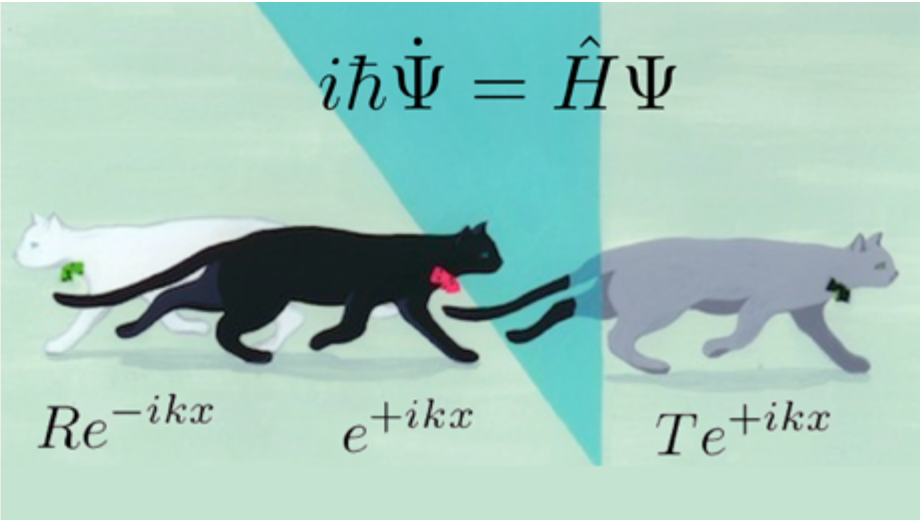
# Exploring Quantum Physics

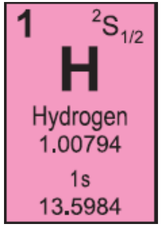
Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

# Atomic Structure and Spectra

## Part III. Cracking the hydrogen code



# Atomic Structure and Spectra



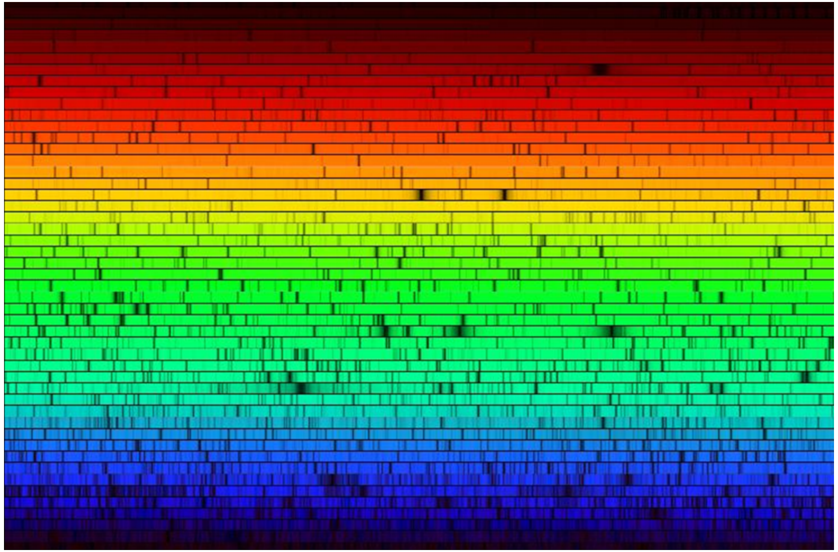

656 nm

410 nm


λ = 650 nm R

λ = 532 nm G

λ = 405 nm V

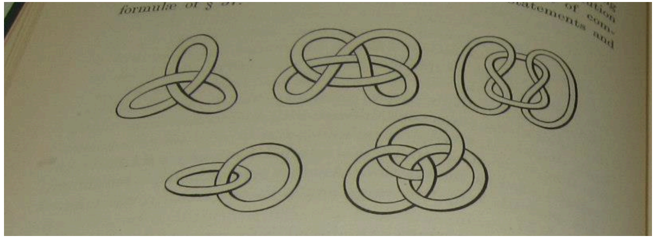


# Atomic Structure and Spectra

**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 . . .

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**Vortex knots in a Bose-Einstein condensate**

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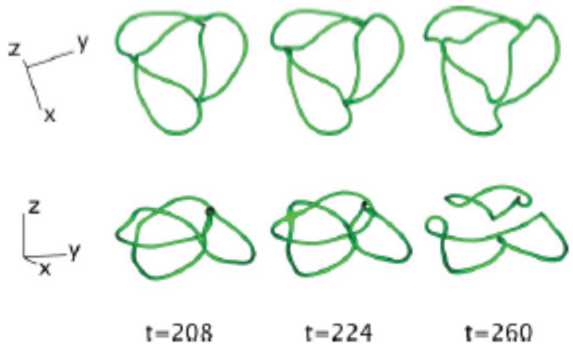
We present a method for numerically building a vortex knot state in the superfluid wave function of a Bose-Einstein condensate. We integrate in time the governing Gross-Pitaevskii equation to determine evolution and shape preservation of the two (topologically) simplest vortex knots which can be wrapped 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.

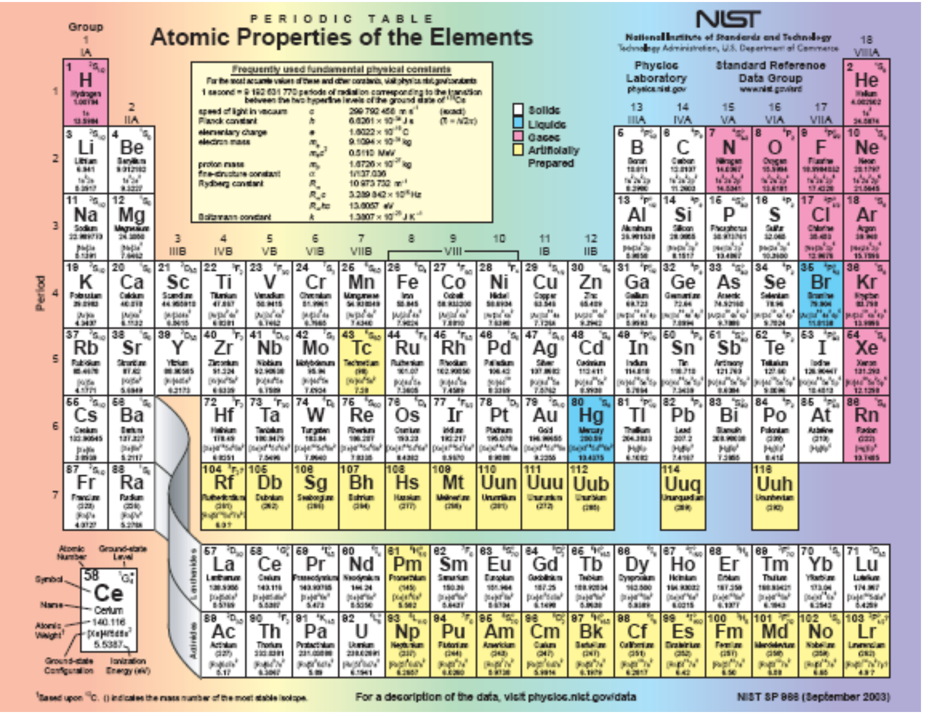
**1911:** Rutherford's shocking discovery that 99.9% of the mass of the atom is concentrated in a $10^{-15}$ of its volume.

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, $He^{+}$, $Li^{2+}$, . . ., $U^{91+}$ Ps He $\bar{p}$

# Atomic Structure and Spectra

## NIST Periodic Table: Atomic Properties of the Elements




High-resolution image at

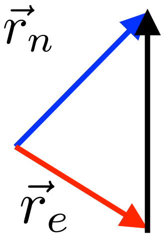
**`http://j.mp/NISTPT`**

# 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* + δ*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:

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

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