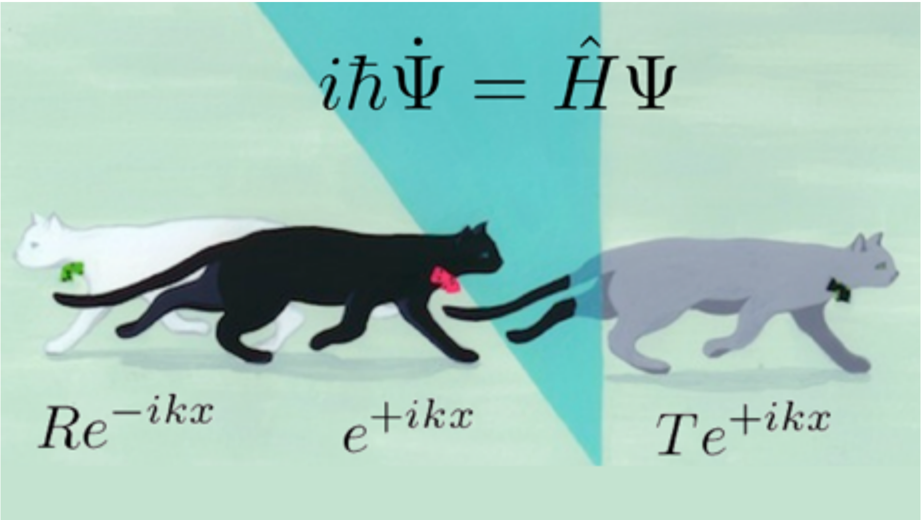
Exploring Quantum Physics

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

Solving the Schrödinger Equation

Part I. Simple constructive techniques



Solving the Schrödinger Equation

Wikimedia Public Domain

Erwin Schrödinger
1887-1961
1933 Nobel Prize in Physics
"for the discovery of new productive forms of atomic theory".

The Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

All accessible information is contained in the wavefunction $\Psi(t)$

Treat the Schrödinger equation as an initial value problem: given $\Psi(t)$, we integrate this equation to find $\Psi(t+\tau)$

What could possibly go wrong?

Solving the Schrödinger Equation

Wikimedia Public Domain

Erwin Schrödinger
1887-1961
1933 Nobel Prize in Physics
"for the discovery of new productive forms of atomic theory".

PRL 109, 230802 (2012) PHYSICAL REVIEW LETTERS week ending 7 DECEMBER 2012

Ytterbium in Quantum Gases and Atomic Clocks: van der Waals Interactions and Blackbody Shifts

M. S. Safronova,[1] S. G. Porsev,[1,2] and Charles W. Clark[3]

[1]*Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA*
[2]*Petersburg Nuclear Physics Institute, Gatchina, Leningrad District 188300, Russia*
[3]*Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland, Gaithersburg, Maryland 20899-8410, USA*

(Received 22 August 2012; published 5 December 2012)

We evaluated the C_6 coefficients of Yb-Yb, Yb-alkali, and Yb-group II van der Waals interactions with 2% uncertainty. The only existing experimental result for such quantities is for the Yb-Yb dimer. Our value, $C_6 = 1929(39)$ a.u., is in excellent agreement with the recent experimental determination of 1932(35) a.u. We have also developed a new approach for the calculation of the dynamic correction to the blackbody radiation shift. We have calculated this quantity for the Yb $6s^2\,{}^1S_0 - 6s6p\,{}^3P_0^o$ clock transition with 3.5% uncertainty. This reduces the fractional uncertainty due to the blackbody radiation shift in the Yb optical clock at 300 K to the 10^{-18} level.

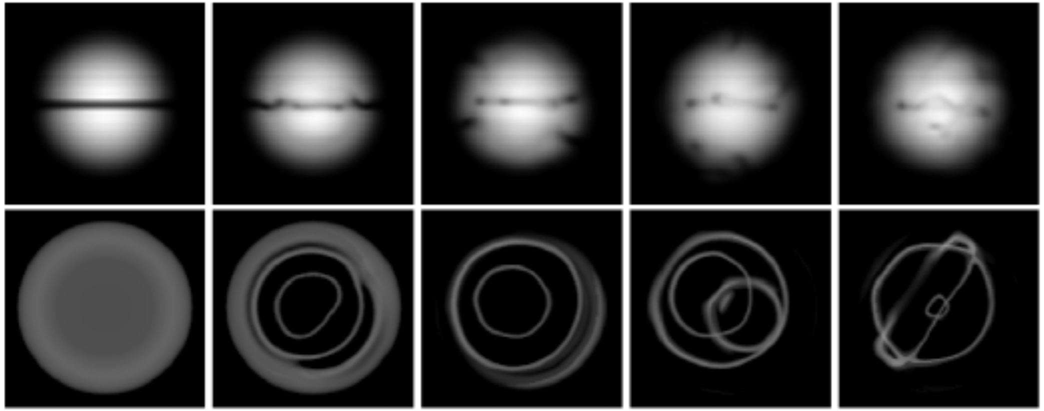
70 ${}^1S_0$
Yb
Ytterbium
173.054
$[Xe]4f^{14}6s^2$
6.2542

Ytterbium has 70 electrons. Suppose we Represent them on a 10 x 10 x 10 grid. Then Ψ is a vector of dimension $100^{70} = 10^{210}$
Completely infeasible!

Solving the Schrödinger Equation

Wikimedia Public Domain

Erwin Schrödinger
1887-1961
1933 Nobel Prize in Physics
"for the discovery of new productive forms of atomic theory".



B. P. Anderson, *et al.*, "Watching Dark Solitons Decay into Vortex Rings in a Bose-Einstein Condensate," *PRL* **86**, 2926 (2001)

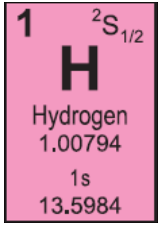
Sometimes we need to solve the full time-dependent Schrödinger equation e.g. when studying non-equilibrium quantum systems.

Solving the Schrödinger Equation

Wikimedia Public Domain

Erwin Schrödinger
1887-1961
1933 Nobel Prize in Physics
"for the discovery of new productive forms of atomic theory".

Stationary States



n_2 = 3 4 5 6

As we have seen, there are many interesting things that seem to be described by stationary quantum states. This is their story.

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi = E\Psi$$

Solving the Schrödinger Equation

Wikimedia Public Domain

Erwin Schrödinger
1887-1961
1933 Nobel Prize in Physics
"for the discovery of new productive forms of atomic theory".

Stationary States

$$\hat{H}\Psi = E\Psi$$

Ψ : "eigenfunction" or "eigenvector"

E : the energy, here an "eigenvalue"

What does it mean to "solve this equation" ?

Solving the Schrödinger Equation

Stationary States

$$\hat{H}\Psi = E\Psi$$

We will focus on systems of the following type, which describe electrons in simple atoms and molecules, motion of particles in periodic potentials, scattering of particles, etc. Here *M* designate the particle's mass and *V* is the potential energy function

$$\hat{H}\Psi(x,y,z) = \left[-\frac{\hbar^2}{2M}\nabla^2 + V(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z)$$

Usually we know *V* , and must solve for the unknown Ψ and *E.* But we start now with a constructive approach: we choose a function Ψ that we like, and find a *V* and *E* for which Ψ satisfies a Schrödinger equation!

Solving the Schrödinger Equation

Stationary States – a Constructive Approach

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z)$$

Implies

$$-\frac{1}{\Psi(x,y,z)}\left[\frac{\hbar^2}{2M}\nabla^2\Psi(x,y,z)\right] = E - V(x,y,z)$$

If you know how to differentiate Ψ, you can find *E* and *V* .

Let's go solve a Schrödinger equation!

Solving the Schrödinger Equation

Stationary States – a Constructive Approach

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z)$$

$$-\frac{1}{\Psi(x,y,z)}\left[\frac{\hbar^2}{2M}\nabla^2\Psi(x,y,z)\right] = E - V(x,y,z)$$

Any function will solve a Schrödinger equation, but not necessarily for a physically interesting potential.

We shall see in the next part that for any given *E and* V there are infinitely many solutions of the equations above.

Solving the Schrödinger Equation

Stationary States – a Constructive Approach

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z)$$

$$-\frac{1}{\Psi(x,y,z)}\left[\frac{\hbar^2}{2M}\nabla^2\Psi(x,y,z)\right] = E - V(x,y,z)$$

We conclude with a construction of *E and* V for one of the most widely-used functions in quantum mechanics.