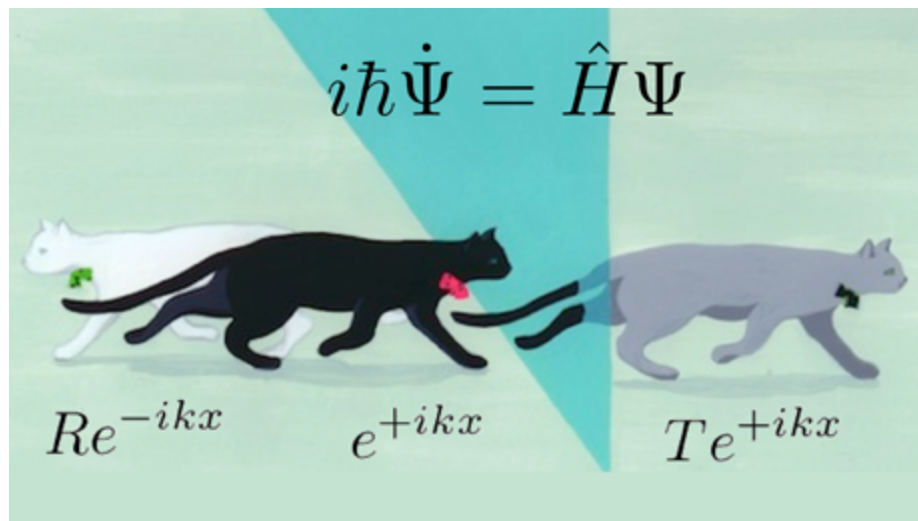


Solving the Schrödinger Equation

Part I. Simple constructive techniques



Solving the Schrödinger Equation

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The Schrödinger Equation

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

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

Erwin Schrödinger
1887-1961

1933 Nobel Prize in Physics
"for the discovery of new
productive forms of atomic
theory".

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



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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. Clark³

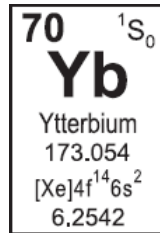
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We evaluated the C_6 coefficients of Yb-Yb, Yb-alkali, and Yb-group II van der Waals interactions with 2% uncertainty. The only existing experimental result for such quantities is for the Yb-Yb dimer. Our value, $C_6 = 1929(39)$ a.u., is in excellent 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.



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!

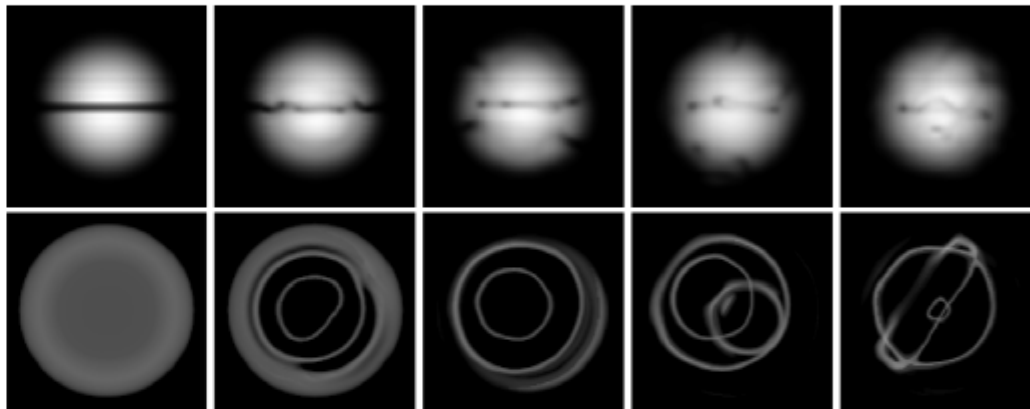
Solving the Schrödinger Equation

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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.

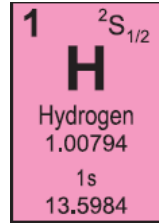


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Solving the Schrödinger Equation

Stationary States



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

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



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Solving the Schrödinger Equation

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.