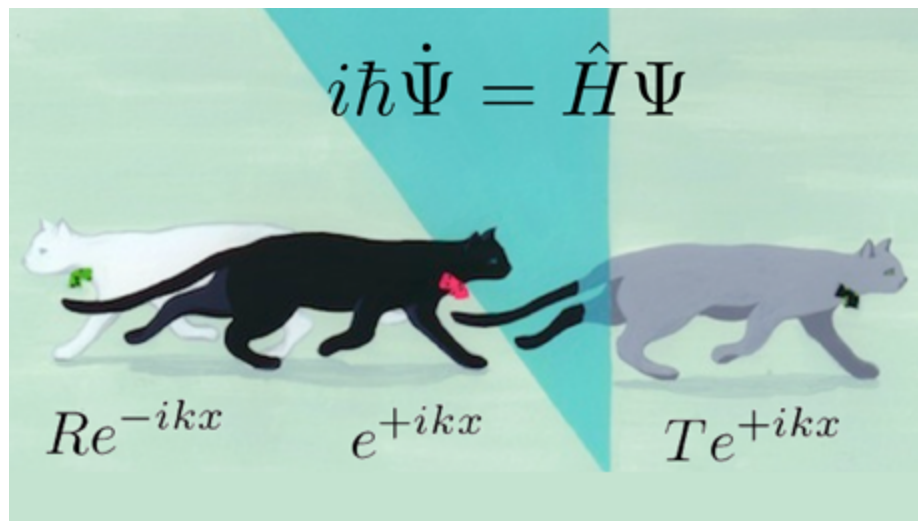


## Solving the Schrödinger Equation

### Part III. Variational Estimates and Applications



# Solving the Schrödinger Equation

## **Don't Leave Home Without It**

Our canonical one-dimensional Gaussian function:

$$\Psi(x) = \frac{1}{\pi^{1/4} d^{1/2}} \exp \left[ -\frac{x^2}{2d^2} \right]$$

This is the ground-state wavefunction for a particle of mass  $m$  and frequency  $\omega$ , in which case

$$d = \sqrt{\frac{\hbar}{m\omega}}$$

Do this **once!** : What is

$$\langle \Psi(x) | T | \Psi(x) \rangle = \langle \Psi(x) | \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} | \Psi(x) \rangle \quad ?$$

# Solving the Schrödinger Equation

## **Remember the Virial Theorem**

Recall that for the harmonic oscillator:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 = T + V(x)$$

the virial theorem states:

$$\langle \Psi(x) | T | \Psi(x) \rangle = \langle \Psi(x) | V(x) | \Psi(x) \rangle$$

# Solving the Schrödinger Equation

## **Remember the Virial Theorem**

Recall that for the harmonic oscillator:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 = T + V(x)$$

the virial theorem states:

$$\langle \Psi(x) | T | \Psi(x) \rangle = \langle \Psi(x) | V(x) | \Psi(x) \rangle$$

Applies to any state,  
even time-dependent  
wavepacket

$$\langle \Psi(x) | T | \Psi(x) \rangle = \frac{1}{2} \langle \Psi(x) | \hat{H} | \Psi(x) \rangle$$

Valid in any number of  
dimensions

# Solving the Schrödinger Equation

## Universal Average Kinetic Energy of Gaussian

Our canonical one-dimensional Gaussian function:

$$\Psi(x) = \frac{1}{\pi^{1/4} d^{1/2}} \exp \left[ -\frac{x^2}{2d^2} \right]$$

This is the ground-state wavefunction for a particle of mass  $m$  and frequency  $\omega$ , in which case

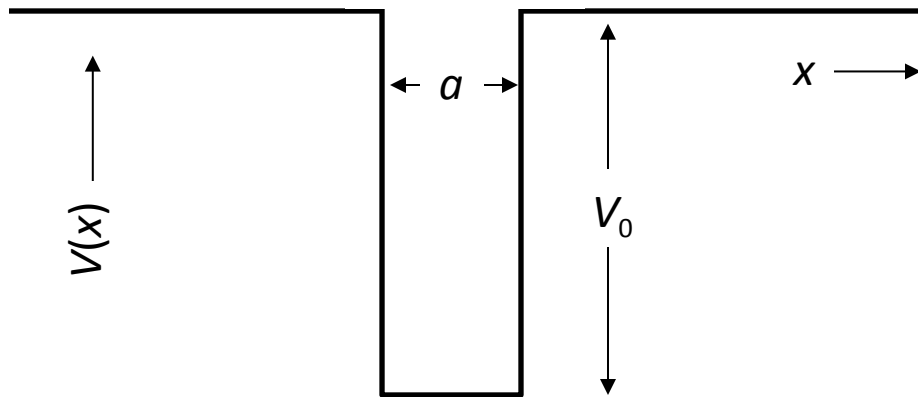
$$d = \sqrt{\frac{\hbar}{m\omega}}$$

$$\langle \Psi(x) | T | \Psi(x) \rangle = \frac{1}{2} \langle \Psi(x) | \hat{H} | \Psi(x) \rangle = \frac{1}{2} \frac{\hbar\omega}{2} = \frac{1}{2} \frac{\hbar^2}{2md^2}$$

Remember the correspondence of the Gaussian with the harmonic oscillator ground state, and you will never need to do this integral again!

# Solving the Schrödinger Equation

## Variational Estimate of Energy of Attractive Dirac Delta



Dirac delta widely used as “pseudopotential” that encodes information about a complex potential- e.g. in description of collisions between ultracold gas atoms (Bose-Einstein condensates).

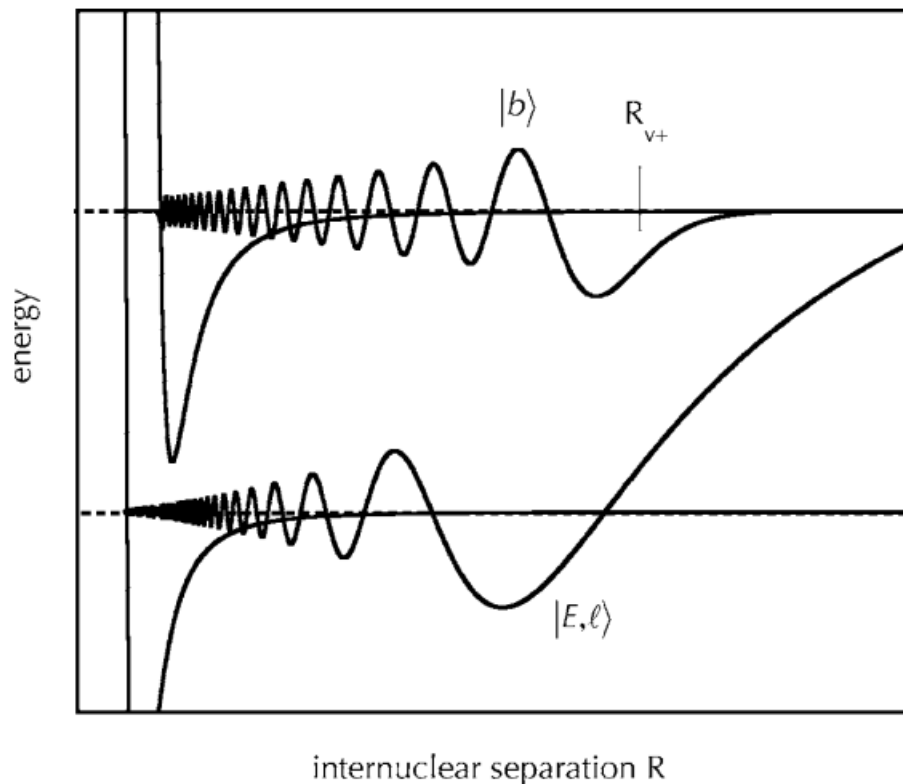
Useful when deBroglie wavelength

$$\lambda_{\text{dB}} = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \gg a$$

$$V(x) \approx -V_0 a \delta(x) \text{ since } \int_{-\infty}^{\infty} dx V(x) = -V_0 a$$

# Solving the Schrödinger Equation

## Variational Estimate of Energy of Attractive Dirac Delta



Schematic wavefunction describing collisions of two cold atoms . Note highly oscillatory behavior at small internuclear separation  $R$ , where the potential is strong. If one is concerned with processes that occur at large  $R$ , one may often use a *pseudopotential* at small  $R$  that yields the right large- $R$  wavefunction.

K. M. Jones, E. Tiesinga, P. D. Lett and P. S. Julienne,  
Rev. Mod Phys. **78**, 483 (2006)

# Solving the Schrödinger Equation

## Variational Estimate of Energy of Attractive Dirac Delta

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - V_0 a \delta(x) \quad \Psi(x) = \frac{1}{\pi^{1/4} d^{1/2}} \exp \left[ -\frac{x^2}{2d^2} \right]$$

$$\langle \Psi(x) | T | \Psi(x) \rangle = \frac{1}{2} \frac{\hbar^2}{2m d^2}$$

$$\langle \Psi(x) | V(x) | \Psi(x) \rangle = -\frac{V_0 a}{d \sqrt{\pi}}$$

$$\langle \hat{H} \rangle$$

$d$

**Same minimization condition  
as for hydrogen atom**