A particle in a simple harmonic oscillator (HO) potential energy well $V(x) = \frac{1}{2}kx^2$ has an initial wavefunction in the second excited state of the HO: $\Psi(x, t = 0) = \Psi_2(x)$.

Choose all of the statements that are correct.

A. The expectation value of the <u>position</u> of this particle depends on time t
B. The expectation value of the <u>momentum</u> of this particle depends on time t
C. The expectation value of the <u>energy</u> of this particle depends on time t
D. None of the above

CHM 305 The Quantum World Lecture 10: Angular Momentum

McQuarrie Ch. 6

Last time we discussed the quantum harmonic oscillator

- Briefly lay out what we know about the classical harmonic oscillator
- Introduce the quantum harmonic oscillator, and its relevance to molecular vibrations
- Write down the Schrödinger equation for this system, and examine the resulting wavefunctions and energy eigenvalues
- Learn about some nice properties of these wavefunctions





Road map for today: angular momentum

- Lay out definitions for classical circular motion and angular momentum
- Discuss rotations of classical and quantum mechanical rigid bodies
- Write down the Schrodinger equation and its solutions for the quantum rigid rotor in spherical coordinates
- Make connections to rotations of diatomic molecules and the hydrogen atom





 $\hat{H}\psi(\theta,\phi) = E\psi(\theta,\phi)$



Practice Problem #1:

The rigid rotor Hamiltonian has the form

$$\hat{H} = -\frac{\hbar^2}{2I} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial}{\partial \theta} \right] + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

and can also be written as

$$\hat{H} = \frac{\hat{\ell}^2}{2I}$$

Do \hat{H} and $\hat{\ell}^2$ commute? What does this tell you about their eigenfunctions?

Can you draw an analogy to the energy and linear momentum of a free particle?

Spherical Harmonics



Practice Problem #2:

Show that

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$



is a solution to the rigid rotor Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2I} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial}{\partial \theta} \right] + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

and find its energy eigenvalue.

Hydrogen atom orbitals

	s ($\ell = 0$)	$p(\ell = 0)$ p ($\ell = 1$)				d (ℓ = 2)					f (ℓ = 3)						
	m = 0	$m = 0$ $m = \pm 1$		m = 0	$m = \pm 1$		$m = \pm 2$		m = 0	$m = \pm 1$		$m = \pm 2$		$m = \pm 3$			
	S	pz	p _x	p _y	d _z 2	d _{xz}	dyz	d _{xy}	d _x z_yz	f _z 3	f _{xz} 2	fyz²	f _{xyz}	$f_{z(x^2-y^2)}$	$f_{x(x^2-3y^2)}$	$f_{y(3x^2-y^2)}$	
n = 1																	
<i>n</i> = 2	•	-															
n = 3	•	2			-	*	8										
n = 4	•	2	••		-	*	2			+	*	*	*	*			
n = 5	•	2	••	۲	÷	*	2		\$								
<i>n</i> = 6	0	3	••														
n = 7	0						•••	••••		•••							

https://en.wikipedia.org/wiki/Atomic_orbital