Applying the Correspondence Principle to the Three-Dimensional Rigid Rotor

David Keeports
Mills College
dave@mills.edu

Quantum Mechanical Correspondence Principle

No system strictly obeys classical mechanics

Instead, all systems are quantum systems, but …

“Quantum systems *appear* to be classical when their quantum numbers are very large.”

The Instructional Challenge in Presenting the Correspondence Principle

Consider “obviously classical” systems and show that they are really quantum systems

Correspondence Principle Applied to Fundamental Quantum Systems

Particle in 1-Dimensional Box

Particle in 3-Dimensional Box

Harmonic Oscillator

2-Dimensional Rigid Rotor

3-Dimensional Rigid Rotor

Hydrogen Atom

Particle in 1-Dimensional Box

$$\psi(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$$

$$\text{if } n \to \infty$$

uniform probability distribution

from $x = 0$ to $x = L$

Particle in 3-Dimensional Box

$$\psi(x,y,z)=\left(\frac{8}{abc}\right)^{\frac{1}{2}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)\sin\left(\frac{n_z\pi z}{c}\right)$$

if $n_x,\ n_y,\ n_z \rightarrow \infty$

uniform probability distribution
within 3-dimensional box

Harmonic Oscillator

$$\psi_v(x) = N_v H_v(\alpha x) e^{-(\alpha x)^2/2}$$

$$\text{as } v \rightarrow \infty$$

probability is enhanced at turning points

2-Dimensional Rigid Rotor

$$\psi(\phi) = \frac{1}{\sqrt{\pi}}\sin(m\phi) \qquad \psi(\phi) = \frac{1}{\sqrt{\pi}}\cos(m\phi)$$

$$\text{if } m \rightarrow \infty \text{ all angles become equally probable}$$

In each case as a quantum number increases by 1,

$$\Delta E / E \simeq 0$$

System energy appears to be a continuous function, *i.e.*, quantization *not* evident

A Classical Three-Dimensional Rigid Rotor

Consider a rigid rotor of binary star dimensions rotating in *xy*-plane

Assume both masses are solar masses *M* and separation is constant at r = 10 AU

$$\mu = \frac{M^2}{M+M} = \frac{M}{2}$$

$$I = \mu r^2 = 2.226 \text{ x } 10^{54} \text{ kg m}^2$$

$$\text{From } F = \frac{Gm^2}{r^2} = \frac{mv^2}{(r/2)} = \frac{m(r/2)^2\omega^2}{(r/2)},$$

$$\omega = 2.815 \text{ x } 10^{-7} \text{/s}$$

$$L = I\omega = \ 6.266 \text{ x } 10^{47} \text{ kg m}^2/\text{s}$$

$$K = K_{rot} = \frac{1}{2} I\omega^2 = \frac{L^2}{2I} = \ 8.820 \text{ x } 10^{40} \text{ J}$$

$$U = \text{ constant } \equiv 0 \text{ during rotation}$$

$$E = K + U = \ 8.820 \text{ x } 10^{40} \text{ J}$$

But does this 3-D rotor really obey classical mechanics?

No, it is a quantum system that only appears to obey classical mechanics because its quantum numbers are very large!

Why Are Quantum Numbers Large?

Eigen-Operators for 3-D Rigid Rotors

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

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

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

Spherical Harmonics Are Eigenfunctions

Eigenvalues of Operators

$$\hat{H}Y_{J,M_J}(\theta,\phi)=\frac{J(J+1)\hbar^2}{2I}Y_{J,M_J}(\theta,\phi)$$

$$\hat{L}^2Y_{J,M_J}(\theta,\phi)=J(J+1)\hbar^2Y_{J,M_J}(\theta,\phi)$$

$$\hat{L}_zY_{J,M_J}(\theta,\phi)=M_J\hbar\ Y_{J,M_J}(\theta,\phi)$$

$$J=\ 0,\ 1,\ 2,\ \ldots$$

$$M_J=\ -J,\ -J+1,\ \ldots,\ +J$$

For assumed orbit in the *xy*-plane, angular momentum and its *z*-component are virtually indistinguishable, so …

$$L \cong L_z$$

$$\frac{L_z}{L} = \frac{M_J \hbar}{\sqrt{J(J+1)}\hbar} \cong 1$$

$$\boxed{J = M_J \to \infty}$$

The Size of $J = M_J$

$$E = \frac{J(J+1)\hbar^2}{2I} = 8.820 \text{ x } 10^{40} \text{ J}$$

$$J = 5.94 \text{ x } 10^{81}$$

Large!

Energy and the Correspondence Principle

Suppose that J increases by 1:

$$\frac{\Delta E}{E} = \frac{E(J+1) - E(J)}{E(J)} = \frac{2}{J} = 3.37 \text{ x } 10^{-82}$$

Energy quantization unnoticed

Rotor Orientation From Spherical Harmonic Wavefunctions

$$Y_{J,M_J}(\theta,\phi) = \Theta_{J,M_J}(\theta)\Phi_{M_J}(\phi)$$

$$\Theta_{J,M_J}(\theta) = N_{J,M_J} P_{J,M_J}(\theta)$$

$$\Phi_0(\phi) = \frac{1}{\sqrt{2\pi}}$$

$$\Phi_{M_J,c}(\phi) = \frac{1}{\sqrt{\pi}}\cos(M_J\phi)$$

$$\Phi_{M_J,s}(\phi) = \frac{1}{\sqrt{\pi}}\sin(M_J\phi)$$

$\Theta_{J,M_J}(\theta)$ can be complex

$$\Theta_{J,M_J}(\theta) = \frac{(-1)^J}{2^J J!}\sqrt{\frac{2J+1}{2}\frac{(J-|M_J|)!}{(J+|M_J|)!}}\sin^{|M_J|}\theta\frac{d^{J+|M_J|}(\sin^{2J}\theta)}{[d(\cos\theta)]^{J+|M_J|}}$$

But when $J = M_J$, $\Theta_{J,M_J}(\theta)$ is very simple:

$$\boxed{\Theta_{J,M_J}(\theta) = N_J \sin^J\theta}$$

Because $\Theta_{J,M_J}(\theta) = N_J \sin^J \theta$

If $J \to \infty$,

probability $\to 0$ unless $\theta = \dfrac{\pi}{2}$

probability $\to 0$ outside *xy*-plane

$$\Phi_{M_J,c}(\phi) = \frac{1}{\sqrt{\pi}} \cos(M_J \phi)$$

$2M_J$ angular nodes and

$2M_J$ angular antinodes

If $M_J \to \infty$, probability is proportional to $\Delta\phi$

No ϕ is favored

Localization of axis at a particular ϕ requires superposition of wavefunctions with a range of angular momentum values

Uncertainty principle: Angular certainty comes at the expense of angular momentum certainty

The Hydrogen Atom Problem in the Large Quantum Number Limit: Consider Earth-Sun System

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{Gm_S m}{r}\psi = E\psi$$

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi - \frac{e^2}{4\pi\varepsilon_0}\frac{\psi}{r} = E\psi$$

Results for Quantum Earth

$$n = 1, 2, 3, \ldots$$

$$l = 0, 1, 2, \ldots, n-1$$

$$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$$

$$E = -\frac{G^2 m^3 m_S^2}{2\hbar^2} \frac{1}{n^2}$$

$$L = \sqrt{l(l+1)}\hbar$$

$$L_z = m_l \hbar$$

Assumed circular orbit implies

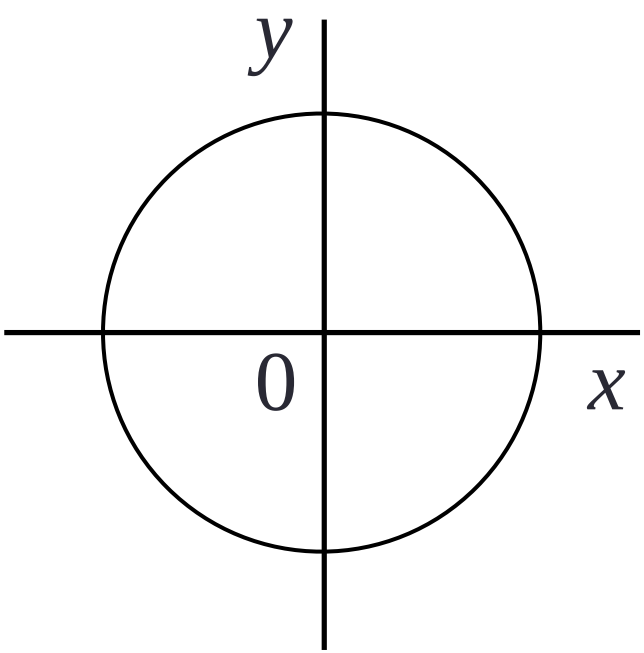
$$n \cong l = m_l \rightarrow \infty$$

consistent with correspondence principle

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)\Theta_{lm_l}(\theta)\Phi_{m_l}(\phi)$$

With $n \cong l = m_l \to \infty$,

$\psi_{nlm_l}(r,\theta,\phi)$ implies that Earth's spatial probability distribution is



Earth is in a hydrogen-like orbital characterized by huge quantum numbers

Quantum Mechanical Earth: Where Orbitals Become Orbits. *European Journal of Physics*, Vol. 33, pp. 1587-98 (2012)

End