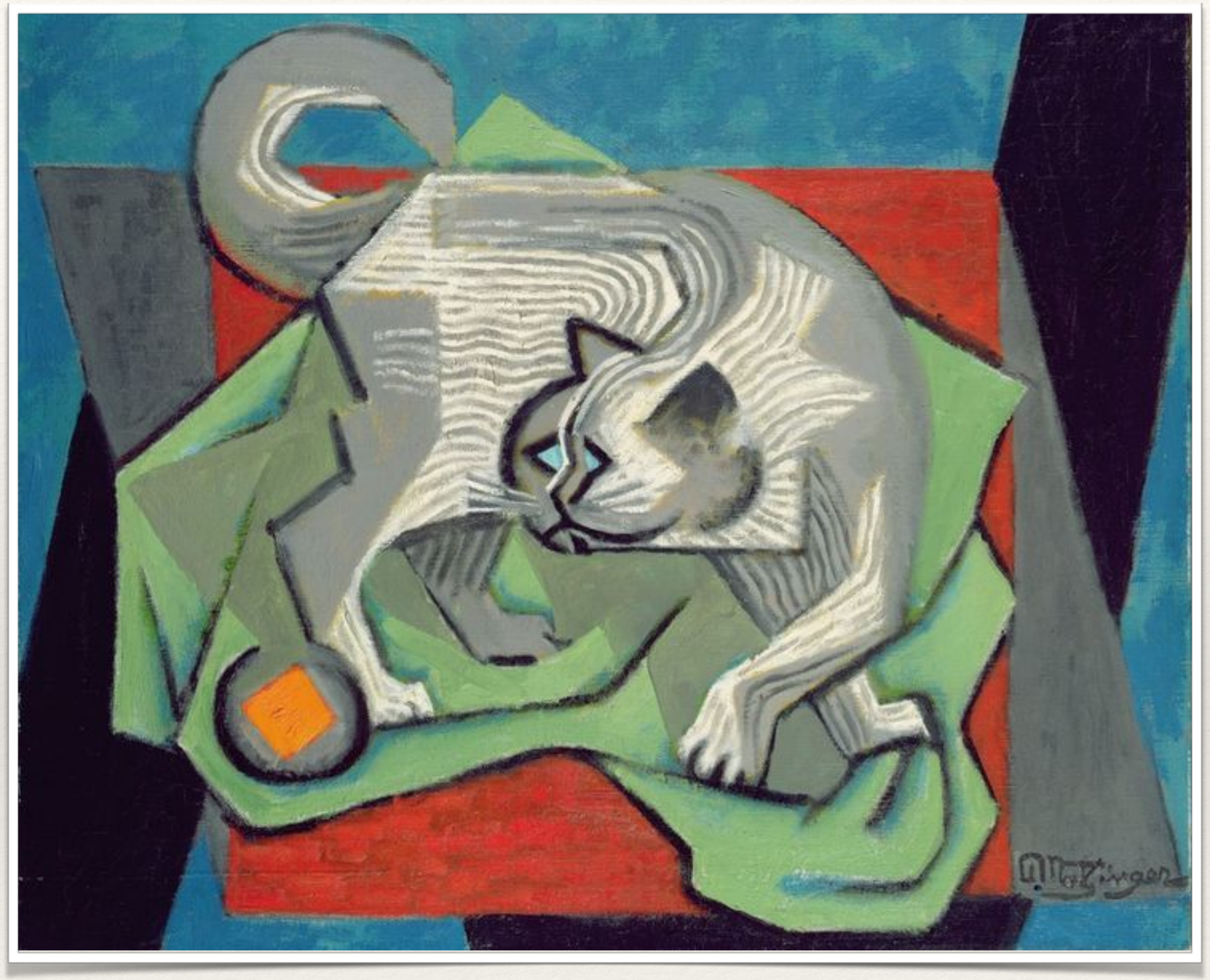
Prof. Steven Flammia

Quantum Mechanics

Lecture 7

Spherical coordinates;
Separation of variables;
Angular quantum numbers;
Intrinsic vs. orbital AM;
Spherical harmonics.



A quick recap

A two-body interacting Hamiltonian can be transformed to relative coordinates:

$$H = \frac{\hat{\mathbf{p}}_1^2}{2m_1} + \frac{\hat{\mathbf{p}}_2^2}{2m_2} + V(|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|) \qquad \Rightarrow \qquad H = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(|\hat{\mathbf{r}}|)$$

Angular momentum commutes with *H*, so simultaneous eigenstates exist:

$$[L_z, H] = [L^2, H] = [L_z, L^2] = 0$$

$$H|E, l, m\rangle = E|E, l, m\rangle$$

$$L^2|E, l, m\rangle = l(l+1)\hbar^2|E, l, m\rangle$$

$$L_z|E, l, m\rangle = m\hbar|E, l, m\rangle$$

$$\mathbf{L} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} \qquad L_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

(+ cyclic)

Spherical coordinates

To exploit the symmetry of the reduced *H*, transform to spherical coordinates:

In cartesian coordinates $\mathbf{x} = (x, y, z)$

In spherical coordinates $\mathbf{r} = (r, \theta, \phi)$

Spherical coordinates

Recall our expression for **L**:

Now use the gradient formula:

Compare with the previous expression:

$$\nabla^2\psi(\mathbf{r}) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

Spherical coordinates

We therefore have: In spherical coordinates $\mathbf{r} = (r, \theta, \phi)$

For the simultaneous eigenstates:

The time-independent Schrödinger eq. in radial coordinates becomes:

Separation of variables

The L.H.S. is independent of (θ,ϕ), so solve via separation of variables.

Canceling the angular parts yields an equation for the radial wave function:

Now make a substitution:

Radial wave function

The radial equation is thus equivalent to

This is the single-particle Schrödinger equation!

Note that this is independent of m, the L_z eigenvalue.

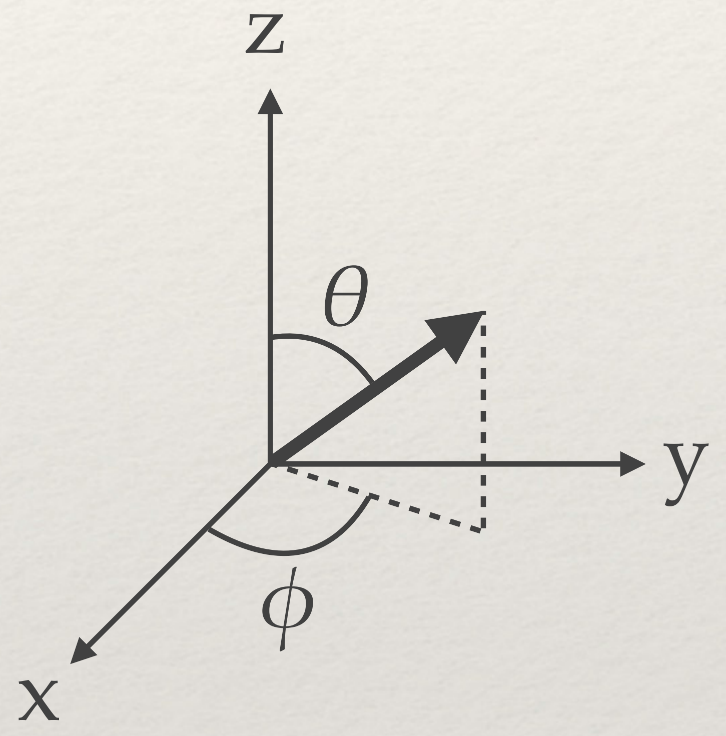
Angular quantum numbers

Recall our ansatz:

$$\psi_{E,l,m}(\mathbf{r}) = \langle \mathbf{r} \,|\, E, l, m \rangle = R(r)F(\theta, \phi) \qquad R(r) = \frac{u(r)}{r}$$

What about the angular part?

Recall, L_z is the generator of rotations around the z axis. Therefore:



Acting on the eigenstates we find:

Angular quantum numbers

Recall our ansatz:

$$\psi_{E,l,m}(\mathbf{r}) = \langle \mathbf{r} \,|\, E, l, m \rangle = R(r)\Theta(\theta)\Phi(\phi) \quad R(r) = \frac{u(r)}{r} \qquad \Phi(\phi) \propto \exp(im\phi)$$

However, m must be quantized:

But m still depends on l:

Angular quantum numbers

Recall our ansatz:

$$\psi_{E,l,m}(\mathbf{r}) = \langle \mathbf{r} \,|\, E, l, m \rangle = R(r)\Theta(\theta)\Phi(\phi) \qquad R(r) = \frac{u(r)}{r} \qquad \Phi(\phi) \propto \exp(im\phi)$$

$$\left(\frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_{\text{eff}}(r) \right) u(r) = E\, u(r) \qquad V_{\text{eff}}(r) = \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)$$

What about the polar angle?

They are the **associated Legendre polynomials**:

$$\Theta(\theta) \propto P_l^m(\cos\theta)$$

Where does this come from?
The equation has spherical symmetry; this is the analog of Fourier decomposition for periodic functions.

Spherical harmonics:

$$Y_l^m(\theta, \phi) = N_{l,m} \mathrm{e}^{im\phi} P_l^m(\cos\theta)$$

normalization

azimuthal component

polar component

Spherical harmonics

The form of the spherical harmonics can be found explicitly via ladder operators:

$$L_x = \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y = \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_\pm = L_x \pm iL_y$$

$$\Rightarrow \quad L_\pm = \frac{\hbar}{i}\mathrm{e}^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)$$

Now use on the highest/lowest weight states:

Spherical harmonics

This must be normalized:

Use lowering operator to obtain other solutions:

$$L_- | l, m \rangle = \sqrt{l(l+1) - m(m-1)} \, | l, m \rangle$$