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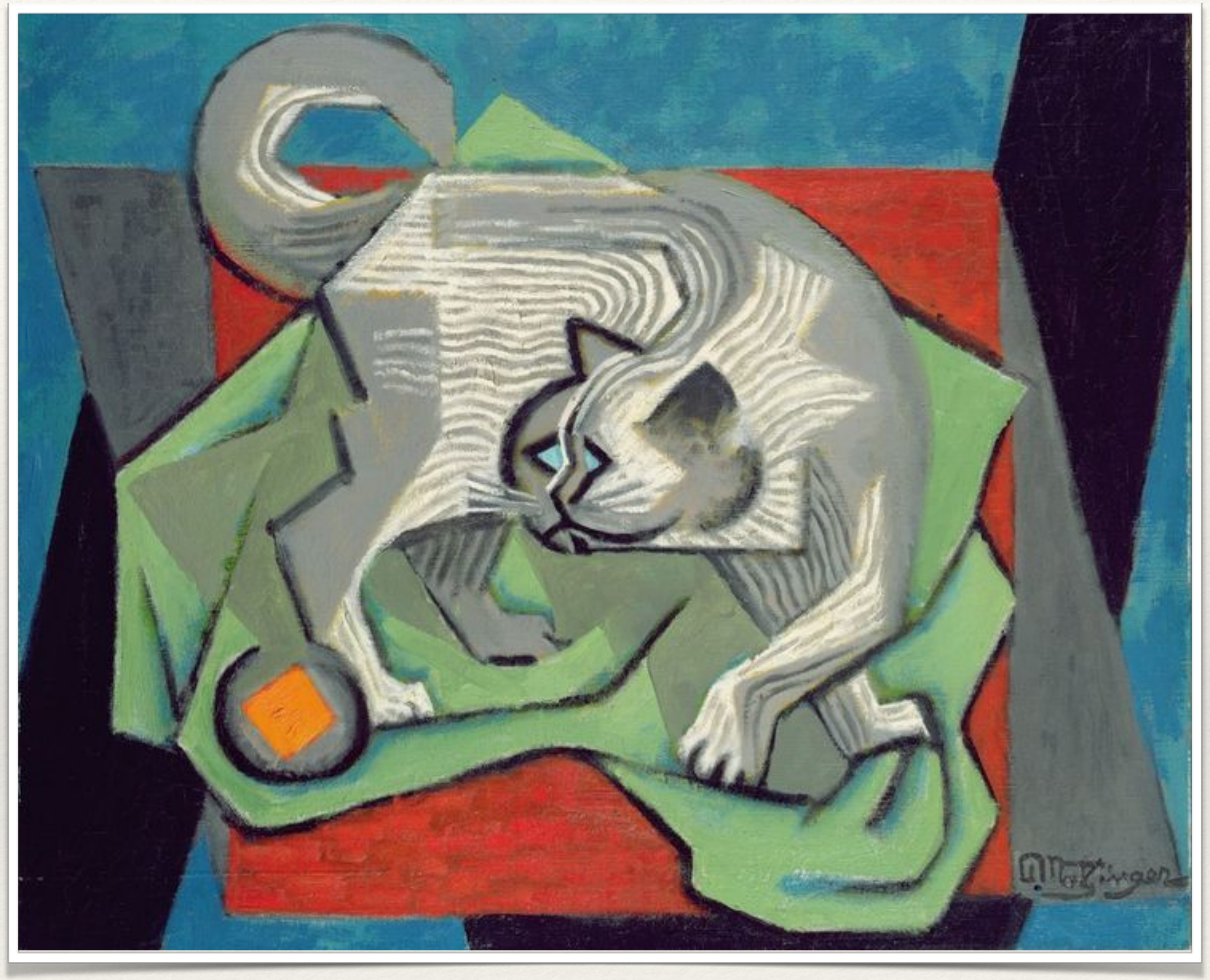
Quantum Mechanics

Lecture 4

Particle in a box;
Wave mechanics in 3D;
The generator of rotations;
Angular momentum.



A quick recap

Translation is generated by momentum:

$$T(\delta x) = 1 - \frac{i}{\hbar}\hat{p}\delta x \qquad T(a) = \mathrm{e}^{-i\hat{p}a/\hbar}$$

Momentum obeys the relations:

$$[\hat{x}, \hat{p}] = i\hbar \qquad \hat{p} = \hat{p}^\dagger \qquad \hat{p} \xrightarrow[\text{x basis}]{} \frac{\hbar}{i}\frac{\partial}{\partial x}$$

The time-independent Schrödinger equation for a 1D particle with potential is:

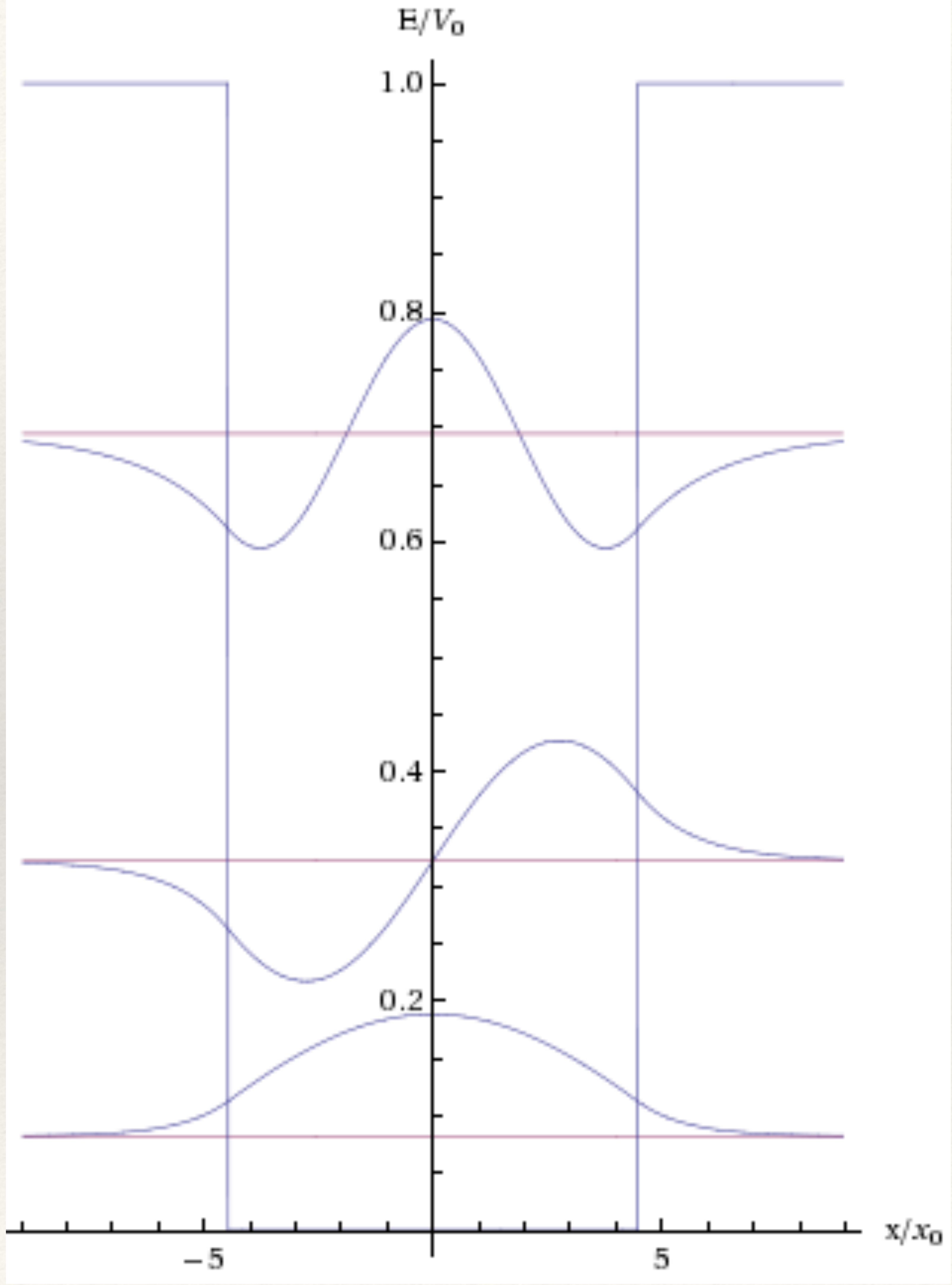
$$-\frac{2m\left(E - V(x)\right)}{\hbar^2}\psi_E(x) = \frac{\partial^2}{\partial x^2}\psi_E(x)$$

Particle in a box / finite square well

These tools give us insight into interesting physics!

$$-\frac{2m\left(E - V(x)\right)}{\hbar^2}\psi_E(x) = \frac{\partial^2}{\partial x^2}\psi_E(x) \qquad V(x) = \begin{cases} 0 & |x| < L/2 \\ V_0 & \text{otherwise} \end{cases}$$

- Fixed number of bound states
- Quantized energy levels, $E_n \propto n^2/mL^2$ when $V_0 \to \infty$
- Particles "exist" in classically forbidden regions
- Energy eigenstates with $E > V_0$ cannot be normalized
- Scattering states must form wave packets
- States can scatter *back* off a potential well



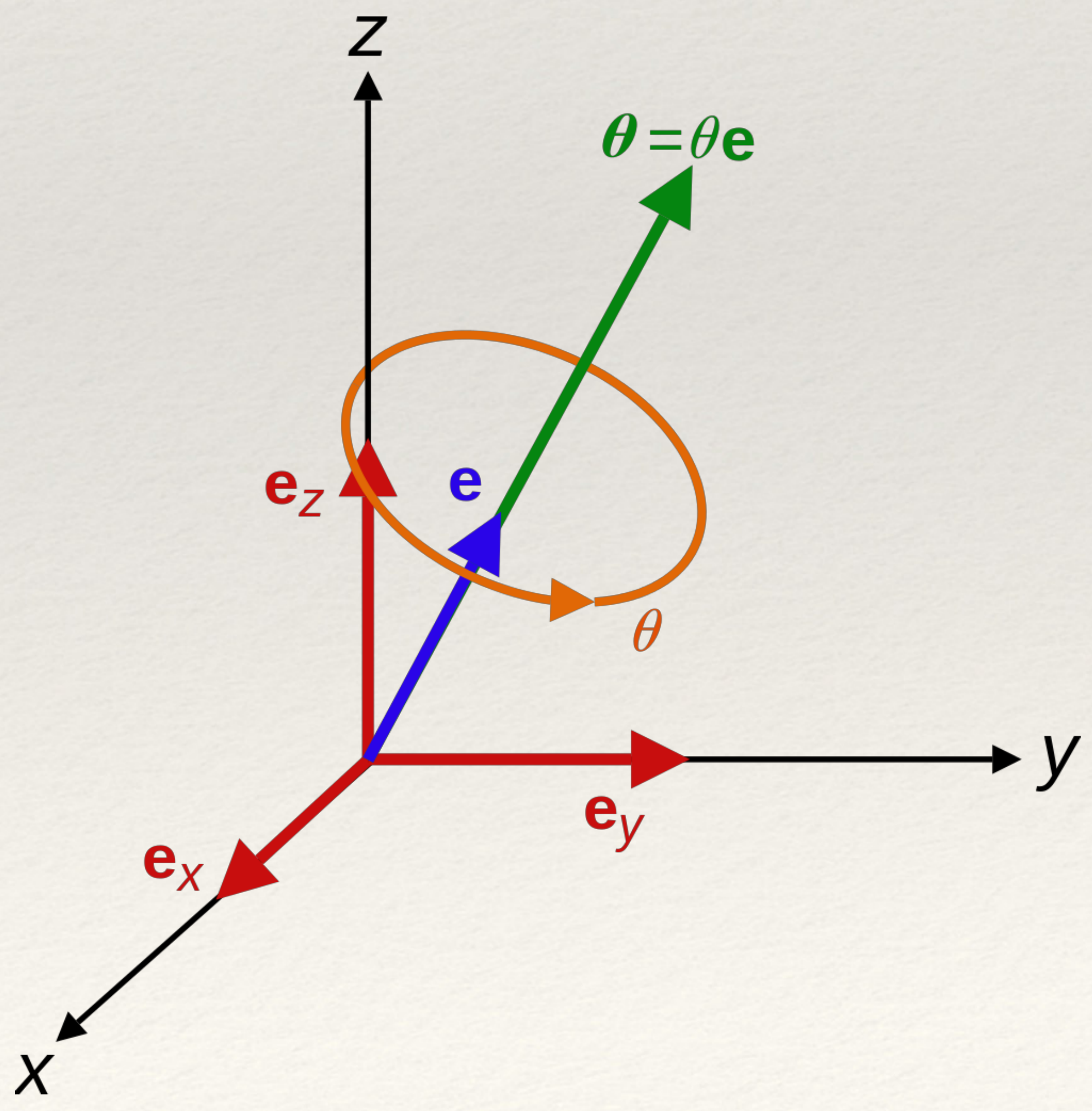
Towards 3D wave mechanics: rotations

Our eventual goal is to get a quantitative understanding of the physics of atoms. "Particle in a box" is too simple to give predictions that match experiment.

To achieve that, we'll need to build on our toolkit from 1D and incorporate one more phenomenon that doesn't exist in only one dimension: **rotations**.

Introduce the rotation operator:

$$R(\theta\mathbf{e})$$ Rotate with right-hand orientation around axis **e** by angle θ.



How do rotation operators act on spin states?
Example: spin-1/2

$$R\left(\frac{\pi}{2}\mathbf{e}_y\right)|\mathbf{z}_+\rangle = |\mathbf{x}_+\rangle \qquad R\left(\frac{\pi}{2}\mathbf{e}_y\right)|\mathbf{z}_-\rangle = |\mathbf{x}_-\rangle$$

Makes sense… but what about a possible overall phase? Because a global phase won't change physical observables, we might need to add it to consistently define rotation operators.

Rotation operators

Let's be more systematic and recycle the recipe for time and space translations. Introduce a generator for infinitesimal rotations around each axis:

$$R(\delta\theta\mathbf{e}_z) = \left(1 - \frac{i}{\hbar}J_z\delta\theta\right) \qquad R(\theta\mathbf{e}_z) = \mathrm{e}^{-iJ_z\theta/\hbar}$$

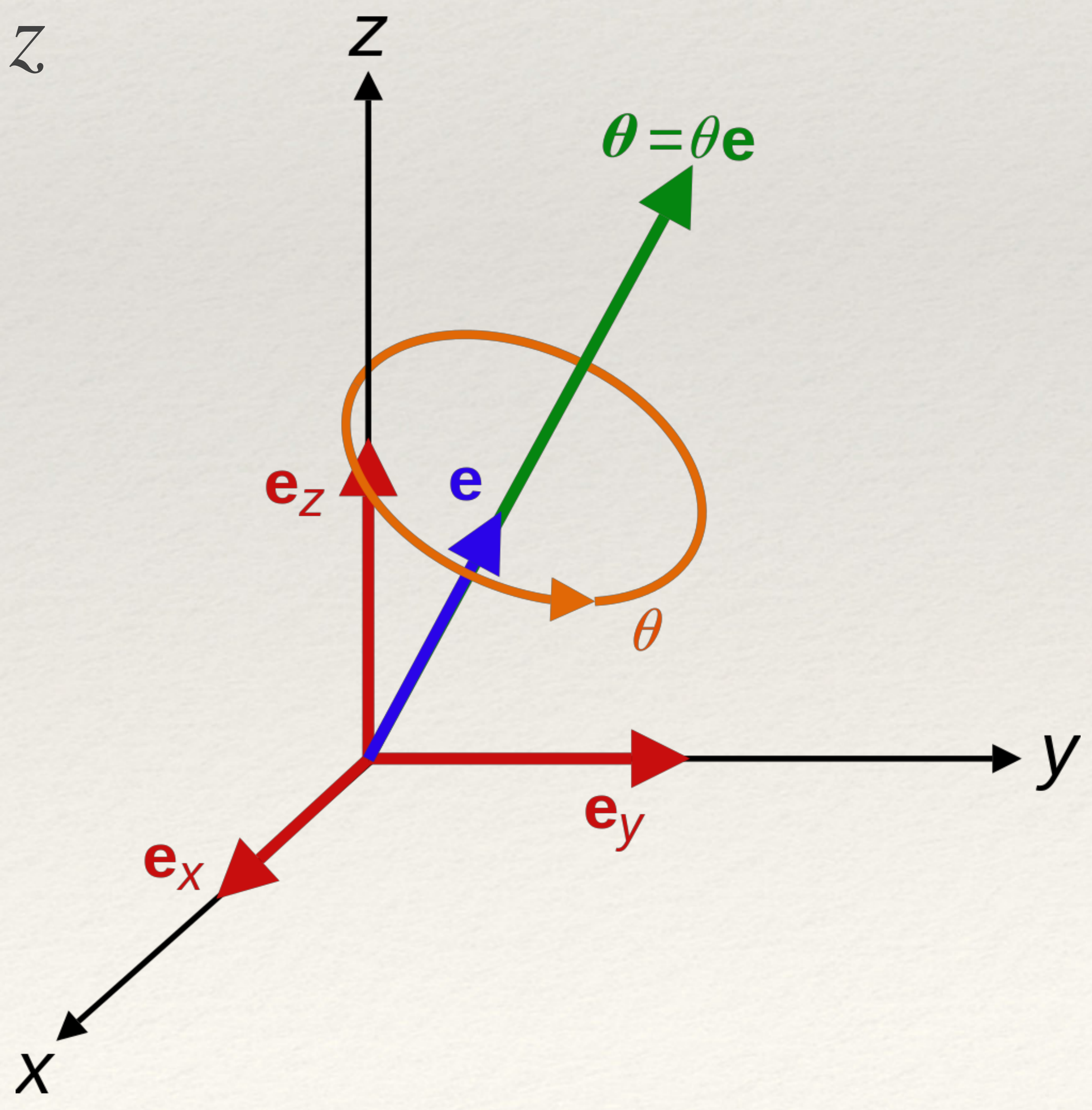
It must be unitary, so J_z is Hermitian. $\quad R^\dagger R = 1 \;\Rightarrow\; J_z^\dagger = J_z$

And J_z clearly has units of angular momentum.

Moreover, **z**-aligned states must be eigenstates for every θ!

Example: spin-1/2

$$R(\theta\mathbf{e}_z)\,|\,\mathbf{z}_\pm\rangle = \mathrm{e}^{i\phi_\pm(\theta)}\,|\,\mathbf{z}_\pm\rangle$$



Rotation operators

How does the phase depend on the angle? To remain consistent with interpretation as angular momentum, we must have for spin-1/2:

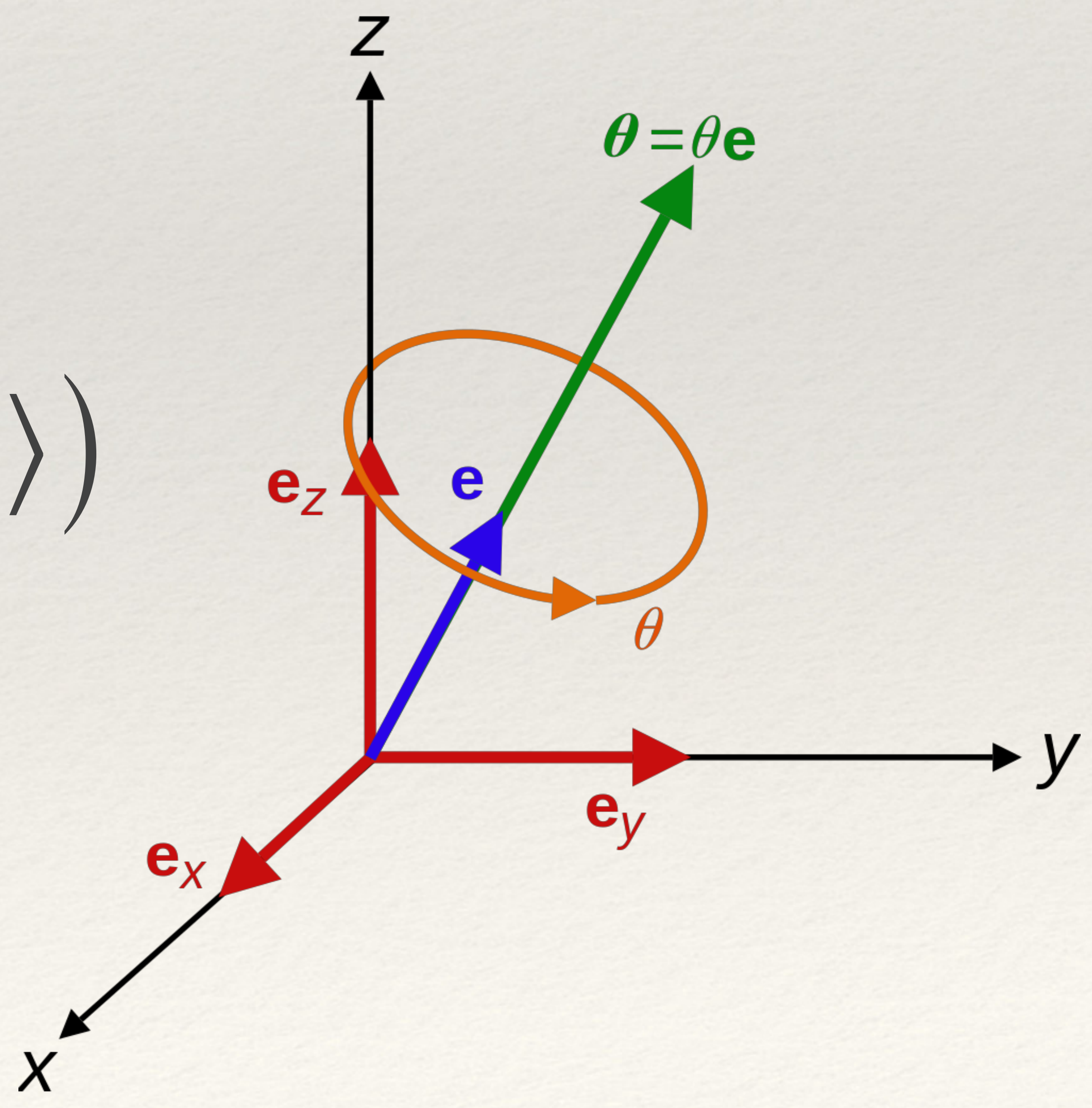
$$J_z |\mathbf{z}_+\rangle = \pm \frac{\hbar}{2} |\mathbf{z}_+\rangle \qquad\qquad R(\theta \mathbf{e}_z) |\mathbf{z}_\pm\rangle = \mathrm{e}^{\mp i\theta/2} |\mathbf{z}_\pm\rangle$$

Sanity check:

$$R\big(\theta \mathbf{e}_z\big) |\mathbf{x}_+\rangle = R\big(\theta \mathbf{e}_z\big) \frac{1}{\sqrt{2}} \big(|\mathbf{z}_+\rangle + |\mathbf{z}_-\rangle\big)$$

$$= \frac{1}{\sqrt{2}} \big(\mathrm{e}^{-i\theta/2} |\mathbf{z}_+\rangle + \mathrm{e}^{+i\theta/2} |\mathbf{z}_-\rangle\big) = \frac{\mathrm{e}^{-i\theta/2}}{\sqrt{2}} \big(|\mathbf{z}_+\rangle + \mathrm{e}^{+i\theta} |\mathbf{z}_-\rangle\big)$$

$$\theta = \frac{\pi}{2} \quad \longrightarrow \quad = \frac{\mathrm{e}^{-i\pi/4}}{\sqrt{2}} \big(|\mathbf{z}_+\rangle + i |\mathbf{z}_-\rangle\big) = \mathrm{e}^{-i\pi/4} |\mathbf{y}_+\rangle$$



Commutation relations for rotation operators

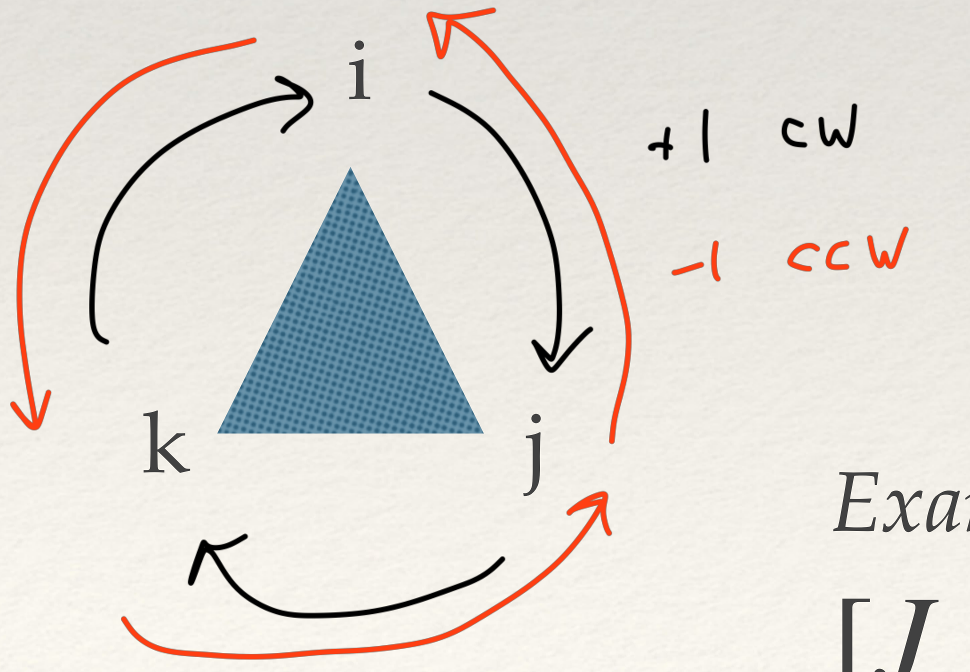
More generally, we can have a rotation about any axis:

$$R(\theta \mathbf{n}) = \mathrm{e}^{i\theta \mathbf{n}\cdot\mathbf{J}/\hbar} \qquad \mathbf{n}\cdot\mathbf{J} = n_x J_x + n_y J_y + n_z J_z$$

All the above insights can be generalized to any spin, not just spin 1/2.
To go beyond the spin-1/2, let us study the commutation relations

$$[J_i, J_j] = i\hbar \sum_k \epsilon_{ijk} J_k$$

Here ε is the Levi-Civita symbol, or totally antisymmetric tensor



Example:

$$[J_x, J_y] = i\hbar J_z$$

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i\ j\ k) \text{ is a cyclic permutation,} \\ -1 & \text{if } (i\ j\ k) \text{ is an anticyclic permutation,} \\ 0 & \text{if any index repeats.} \end{cases}$$

Total angular momentum: the Casimir operator

Rotations about different axes don't commute, but there is another invariant.

$$J^2 := J_x^2 + J_y^2 + J_z^2$$

Total angular momentum (squared), sometimes called Casimir operator

Recall: $[J_i, J_j] = i\hbar \sum_k \epsilon_{ijk} J_k$ $\qquad [A, BC] = B[A, C] + [A, B]C$

$$[J_z, J^2] = [J_z, J_x^2] + [J_z, J_y^2] + [J_z, J_z^2]$$

$$[J_z, J_x^2] = J_x[J_z, J_x] + [J_z, J_x]J_x = J_x(+i\hbar J_y) + (+i\hbar J_y)J_x$$

$$[J_z, J_y^2] = J_y[J_z, J_y] + [J_z, J_y]J_y = J_y(-i\hbar J_x) + (-i\hbar J_x)J_y$$

$$[J_z, J_z^2] = 0$$

$$\Rightarrow \quad [J_z, J^2] = 0$$

Simultaneous eigenstates, raising and lowering operators

Since J^2 and J_z are commuting and self-adjoint, they have a common eigenbasis.

$$J^2|\lambda, m\rangle = \lambda\hbar^2|\lambda, m\rangle$$

$$J_z|\lambda, m\rangle = m\hbar|\lambda, m\rangle$$

Here λ and m are labels for the eigenstates.
We sometimes call them "quantum numbers".

To be more explicit, we must define raising and lowering operators:

$$J_\pm = J_x \pm iJ_y$$

not self-adjoint!

Do these commute with J_z?

$$[J_z, J_\pm] = [J_z, J_x] \pm i[J_z, J_y] = (i\hbar J_y) \pm i(-i\hbar J_x) = \pm\,\hbar J_\pm$$

Doesn't commute!

Simultaneous eigenstates, raising and lowering operators

Although they don't commute, the mutual action on the basis is key:

$$J_z J_+ |\lambda, m\rangle = \big([J_z, J_+] + J_+ J_z\big)|\lambda, m\rangle = \big(\hbar J_+ + J_+ m\hbar\big)|\lambda, m\rangle = \hbar(m+1)J_+|\lambda, m\rangle$$

$$J_z\big(J_+|\lambda, m\rangle\big) = \hbar(m+1)\big(J_+|\lambda, m\rangle\big)$$

J_+ shifts the eigenvalue of J_z up by one

Similarly:

$$J_z\big(J_-|\lambda, m\rangle\big) = \hbar(m-1)\big(J_-|\lambda, m\rangle\big)$$

Note that raising and lowering commute with J^2, so λ is unchanged.

These operators add and subtract one quanta of angular momentum to the z-projection of the angular momentum eigenstates.