Physics 438A – Lecture #8
Wave Mechanics for 3D Motion

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1 Position

The position eigenstate in three dimensions is given by

$$|\mathbf{r}\rangle = |x, y, z\rangle = |r, \theta, \phi\rangle$$

where any coordinate system that labels each point of space uniquely and smoothly is valid. The position operators for each of the three Cartesian coordinates act exactly as you would expect from the one-dimensional case:

$$\hat{x}|\mathbf{r}\rangle = x|\mathbf{r}\rangle, \quad \hat{y}|\mathbf{r}\rangle = y|\mathbf{r}\rangle, \quad \hat{z}|\mathbf{r}\rangle = z|\mathbf{r}\rangle$$

Note that the position operators commute with one another, i.e. $[\hat{r}_i, \hat{r}_j] = 0$. The position eigenstates are complete and orthonormal in the sense that

$$\int d^3r \; |\mathbf{r}\rangle\langle\mathbf{r}| = \iiint dx \; dy \; dz \; |x, y, z\rangle\langle x, y, z| = \mathbb{1}$$

and

$$\langle\mathbf{r}'|\mathbf{r}\rangle = \delta^3(\mathbf{r}' - \mathbf{r}) = \delta(x' - x)\delta(y' - y)\delta(z' - z)$$

Using the normalization condition, we see that

$$1 = \langle\psi|\psi\rangle = \int d^3r \; |\langle\mathbf{r}|\psi\rangle|^2 = \int d^3r \; |\psi(\mathbf{r})|^2$$

where $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle$ is the wave function describing a single particle in 3D Euclidean space, and the quantity $d^3r|\psi(\mathbf{r})|^2$ represents the probability of finding the particle in the state $|\psi\rangle$ in the volume d^3r around $\mathbf{r}$ if a measurement of position is carried out.

2 Linear Momentum

To determine the linear momentum operator, we start by introducing a three-dimensional translation operator that satisfies

$$T(\mathbf{a})|\mathbf{r}\rangle = |\mathbf{r}+\mathbf{a}\rangle$$

In knee-jerk fashion, consider an infinitesimal displacement $\delta\mathbf{r}$ and expand the translation operator to find order:

$$T(\delta\mathbf{r}) = \mathbb{1} - \frac{i}{\hbar}\delta\mathbf{r}\cdot\mathbf{p}$$

where $\mathbf{p}$, an operator-valued vector (or vector operator), is the generator of translations in 3D Euclidean space and the linear momentum operator in quantum mechanics. Now consider a quantum particle in an arbitrary state $|\psi\rangle$. For an infinitesimal translation,

$$\langle\mathbf{r}|T(\delta\mathbf{r})|\psi\rangle = \psi(\mathbf{r}-\delta\mathbf{r}) \approx \psi(\mathbf{r}) - \delta\mathbf{r}\cdot\nabla\psi(\mathbf{r})$$

where we've used the Taylor expansion of ψ in the last equality. It follows that

$$\mathbf{p} = -i\hbar\nabla$$

in the position representation. In Cartesian components,

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}, \quad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

Using an arbitrary wave function $\psi(\mathbf{r})$, it's easy to verify the following commutation relations:

$$[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

3 Orbital Angular Momentum

In lecture #4, we worked out the general theory of rotations and the angular momentum operators $\mathbf{J}$ in quantum mechanics. We will now apply that general framework to the study of a single (spin-less) particle moving in three-dimensional space. For the majority of these notes, we'll make no assumptions about the Hamiltonian, but the theory of rotations is especially useful when the particle is under the influence of a central potential $V(r)$, i.e. one that depends only on the distance to some fixed location taken to be the origin.

3.1 Particle on a Ring

Before we dive in to the most general problem of a particle moving in three-dimensional space, let's first consider a particle confined to a circular ring of radius a. The circle is centered on the origin and lies in the xy plane. With a reference line along the x axis, let s be the arc length and ϕ be the angle subtended by a line between the particle and the origin. The generator of translation along the circumference of the circle is

$$\hat{p}_s = i\hbar \left.\frac{\partial T(s)}{\partial s}\right|_{s=0}$$

and since $s = a\phi$, we can associate with the translation operator T a rotation around the z axis. The corresponding generator of rotation is

$$L_z = i\hbar\frac{\partial T}{\partial \phi} = i\hbar\frac{\partial T}{\partial s}\frac{ds}{d\phi} = a\hat{p}_s$$

This expression is analogous to a classical particle executing circular motion with angular momentum $L_z = rp = mvr$. Consider an arbitrary wave function $\psi(\phi)$ which depends on the angular position of the particle. It follows that

$$L_z\psi(\phi) = a\hat{p}\psi(\phi) = -ai\hbar\frac{\partial\psi(\phi)}{\partial\phi}\frac{d\phi}{ds} = -i\hbar\frac{\partial\psi(\phi)}{\partial\phi}$$

We now search for eigenstates of the angular momentum operator such that

$$L_z\psi_m(\phi) = m\hbar\ \psi_m(\phi) = -i\hbar\frac{\partial\psi_m(\phi)}{\partial\phi}$$

where m is simply a unitless constant. This differential equation has the general solution

$$\psi_m(\phi) = Ae^{im\phi}$$

where A is a constant we can determine by enforcing normalization of the wave function:

$$1 = \int_0^{2\pi} d\phi\ |\psi_m(\phi)|^2 = 2\pi|A|^2 \quad \rightarrow \quad A = \frac{1}{\sqrt{2\pi}}$$

Despite there being no physical "boundary" on a ring, there is an important physical constraint that must be satisfied–the wave function must be *single-valued*. Each angular position ϕ is physically equivalent to the point $\phi + 2\pi$ in 3D Euclidean space, so the wave function

must satisfy the periodicity condition $\psi(\phi+2\pi) = \psi(\phi)$. Periodicity is indeed satisfied when

$$e^{i2\pi m} = 1$$

which holds if and only if

$$m = 0, \pm 1, \pm 2, \pm 3, \ldots$$

In other words, m can take only *integer values*. Evidently, the half-integer states are excluded in the case of orbital angular momentum. The eigenstates of L_z are

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad m = 0, \pm 1, \pm 2, \pm 3, \ldots$$

The particle on a ring is a one-dimensional system even though it exists in a two-dimensional space–this is because there is only one degree of freedom ϕ. Let's briefly consider the free-particle Hamiltonian, written in terms of the angular momentum operator:

$$H = \frac{\hat{p}_s^2}{2m} = \frac{L_z^2}{2ma^2} = \frac{L_z^2}{2I}$$

where $I = mr^2$ is the moment of inertia of the particle about the origin. Since $[H, L_z] = 0$, the Hamiltonian and the z component of angular momentum share eigenstates. We can determine the energies of the particle by simply applying the Hamiltonian to an angular momentum eigenstate. For an arbitrary eigenstate $\psi_m(\phi)$,

$$H\psi_m(\phi) = \frac{1}{2I} L_z^2 \psi_m(\phi) = \frac{m^2\hbar^2}{2I} \psi_m(\phi)$$

The allowed energies of a particle on a ring are quantized and given by

$$E_m = \frac{m^2\hbar^2}{2I}$$

The eigenstates corresponding to $+|m|$ and $-|m|$ states have the same energy, so there are two energy states at every allowed energy except for the one corresponding to $m = 0$. Thus the particle-on-a-ring system exhibits *degeneracy*, which we first encountered in the free-particle system. For the particle-on-a-ring system, all states are two-fold degenerate except for $m = 0$, which is nondegenerate. The $\pm m$ degeneracy of the energy eigenstates corresponds to the angular momentum states with $L_z = +m\hbar$ and $L_z = -m\hbar$. That is, the two degenerate energy states represent states with opposite components of the angular momentum along the z-axis. The energy is the same regardless of the direction of rotation, which is analogous to the free particle in one dimension where the energy is independent of

the direction of travel.

3.2 Rotations of a Single-Particle System

In classical mechanics, the angular momentum of a single particle is an ordinary vector defined as $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ where $\mathbf{r}$ is the position vector locating the particle relative to some origin and $\mathbf{p}$ is the linear momentum of the particle. In quantum mechanics, angular momentum is defined as the generator of rotations. We begin with a definition of rotation operators on our single particle system, and then derive their generators. Let R be a proper rotation–an element of SO(3)–and define the unitary operator $U(R)$ by

$$U(R)|\mathbf{r}\rangle = |R\mathbf{r}\rangle$$

This equation says "the unitary operator U maps the state vector $|\mathbf{r}\rangle$ corresponding to position vector $\mathbf{r}$ to the state vector $|R\mathbf{r}\rangle$ corresponding to the rotated position vector $R\mathbf{r}$." We can undo the rotation, so $U(R^{-1})U(R)|\mathbf{r}\rangle = |\mathbf{r}\rangle$, and since U is unitary,

$$U^\dagger(R) = U(R^{-1})$$

We can then write the position-space wave function corresponding to a rotation as

$$\langle \mathbf{r}|U(R)|\psi\rangle = \langle R^{-1}\mathbf{r}|\psi\rangle = \psi(R^{-1}\mathbf{r}) \tag{3.1}$$

This is analogous to $\langle \mathbf{r}|T(\mathbf{a})|\psi\rangle = \psi(\mathbf{r}-\mathbf{a})$ for the translation operator. Using the axis-angle parameterization, we consider an infinitesimal rotation by $\delta\theta$ about an axis $\hat{\mathbf{n}}$. We have

$$\langle \mathbf{r}|U(\hat{\mathbf{n}}, \delta\theta)|\psi\rangle = \psi\Big(R^{-1}(\hat{\mathbf{n}}, \delta\theta)\mathbf{r}\Big) \tag{3.2}$$

where U may be expanded to first order in terms of the generator of rotation as

$$U(\hat{\mathbf{n}}, \delta\theta) = \mathbb{1} - \frac{i}{\hbar}\delta\theta\hat{\mathbf{n}} \cdot \mathbf{L} \qquad \text{(operator expression)}$$

and the infinitesimal classical rotation follows from the usual geometric argument

$$R^{-1}(\hat{\mathbf{n}}, \delta\theta)\mathbf{r} = \mathbf{r} - \delta\theta\hat{\mathbf{n}} \times \mathbf{r} \qquad \text{(vector expression)}$$

Since we are only considering terms that are first order in $\delta\theta$, we can approximate the wave function by its first order Taylor expansion:

$$\psi\Big(R^{-1}(\hat{\mathbf{n}}, \delta\theta)\mathbf{r}\Big) = \psi(\mathbf{r}) - \delta\theta(\hat{\mathbf{n}} \times \mathbf{r}) \cdot \nabla\psi$$

At this point, $\mathbf{r}$ may still be considered an ordinary vector in 3D Euclidean space. Substituting the appropriate expansions into Eq. (3.2), we find

$$\psi(\mathbf{r}) - \frac{i}{\hbar}\delta\theta\,(\hat{\mathbf{n}} \cdot \mathbf{L})\,\psi(\mathbf{r}) = \psi(\mathbf{r}) - \delta\theta(\hat{\mathbf{n}} \times \mathbf{r}) \cdot \nabla\psi$$

The zeroth order terms cancel, and $\delta\theta$ cancels from the first order terms, so we're left with

$$(\hat{\mathbf{n}} \cdot \mathbf{L})\,\psi(\mathbf{r}) = [(\hat{\mathbf{n}} \times \mathbf{r}) \cdot \mathbf{p}]\,\psi(\mathbf{r}) = \hat{\mathbf{n}} \cdot (\mathbf{r} \times \mathbf{p})\psi(\mathbf{r})$$

The position vector $\mathbf{r}$ becomes an operator-valued vector (or vector operator) in the second equality. Let's see how this works by looking at the z component of angular momentum, noting that $\hat{r}_i$ commutes with $\hat{p}_j$ when $i \neq j$:

$$L_z\psi = (x\hat{p}_y - y\hat{p}_x)\psi = (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\psi$$

Since ψ is arbitrary, $L_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$, and since $\hat{\mathbf{n}}$ is also arbitrary,

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

which is an *operator expression* that mirrors the classical definition of angular momentum! From now on, we refer to generators of rotation satisfying this operator expression as **orbital angular momentum**. Importantly, we derived this expression in a manner consistent with our general treatment of angular momentum in lecture #4, meaning we are free to make use of those results. As we learned in the previous section involving the particle on a ring, only the integer eigenstates are relevant when dealing with orbital angular momentum.

3.3 Eigenstates of Angular Momentum

In accordance with lecture #4, the standard basis of orbital angular momentum is formed by the simultaneous eigenstates of L^2 and L_z, which can be indexed by ℓ and m such that

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

$$L_z|\ell, m\rangle = m\hbar|\ell, m\rangle$$

The corresponding angular momentum eigenfunctions are $\psi_{\ell m}(\mathbf{r}) = \langle \mathbf{r}|\ell, m\rangle$, and

$$L^2\psi_{\ell m}(\mathbf{r}) = \ell(\ell+1)\hbar^2\psi_{\ell m}(\mathbf{r}) \tag{3.3}$$

$$L_z\psi_{\ell m}(\mathbf{r}) = m\hbar\psi_{\ell m}(\mathbf{r}) \tag{3.4}$$

The key to finding the wave functions is to first consider the "stretched states" with $m = \ell$. States with other values of m can be generated by applying the lowering operator L_-. Since the operator L^2 is pretty complicated, we will work with L_z and the raising operator L_+. For the stretched state $\psi_{\ell\ell}(\mathbf{r})$,

$$L_z\psi_{\ell\ell}(\mathbf{r}) = \ell\hbar\psi_{\ell\ell}(\mathbf{r}) \tag{3.5}$$

$$L_+\psi_{\ell\ell}(\mathbf{r}) = 0 \tag{3.6}$$

While nothing is really convenient about angular momentum, we can improve the situation slightly by using spherical coordinates (r, θ, ϕ) where

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}$$

The components of angular momentum can be found in spherical coordinates by applying the chain rule and working through a bit of algebra. I'll save you some time:

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

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

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\,\frac{\partial}{\partial\phi}$$

From L_x and L_y, we can compute the raising and lowering operators, given by

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

The component L_z is particularly simple in spherical coordinates—it is the generator of rotations about the z-axis, and ϕ is the azimuthal angle. Another striking feature of the angular momentum operators in spherical coordinates is that they do not depend on the radial coordinate r or the radial differential operator $\partial/\partial r$. The geometrical reason is that rotations in physical space change the direction of vectors, but not their magnitude; the motion of the tip of a given vector takes place on the surface of a sphere. This holds for infinitesimal rotations, which connect nearby points with the same r but different θ and ϕ.

The angular momentum operators are independent of the radial coordinate, so we consider wave functions $f(\theta, \phi)$ defined on the surface of the unit sphere. The wave functions are normalized by integrating over the unit sphere:

$$\langle f|f\rangle = \int d\Omega \; |f(\theta,\phi)|^2 = \int \sin\theta \, d\theta \, d\phi \; |f(\theta,\phi)|^2 = 1$$

where the inner product of two wave functions on the unit sphere is defined as

$$\langle f|g\rangle = \int d\Omega \; f^*(\theta,\phi) g(\theta,\phi)$$

Returning to Eqs. (3.5) and (3.6), we can solve for the stretched eigenfunctions on the unit sphere $f_{\ell\ell}(\theta, \phi)$. The L_z eigenvalue equation is

$$-i\hbar \frac{\partial}{\partial \phi} f_{\ell\ell}(\theta,\phi) = \ell\hbar f_{\ell\ell}(\theta,\phi)$$

which is almost exactly the same as the particle on a ring! The solution is

$$f_{\ell\ell}(\theta,\phi) = F_{\ell\ell}(\theta) e^{i\ell\phi}$$

where $F_{\ell\ell}(\theta)$ is a function of θ only, and ℓ must be an integer in order for the wave function to be single valued. From the L_+ equation, we find

$$0 = -i\hbar e^{i\phi}\left(i\frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi}\right) F_{\ell\ell} e^{i\ell\phi} = -i\hbar e^{i\phi}\left(i\frac{\partial}{\partial\theta} - (i\ell)\cot\theta \frac{\partial}{\partial\phi}\right) F_{\ell\ell} e^{i\ell\phi}$$

After simplifying the expression, we find

$$\frac{dF_{\ell\ell}}{d\theta} = \ell \cot\theta F_{\ell\ell}$$

which is a separable first-order differential equation. We can therefore apply separation of variables to solve for the function $F_{\ell\ell}(\theta)$. Start by moving all terms related to $F_{\ell\ell}$ to the

left-hand side, and all terms involving θ to the right-hand side:

$$\int \frac{dF_{\ell\ell}}{F_{\ell\ell}} = \ell \int \frac{\cos\theta}{\sin\theta} d\theta$$

The integral on the right can be solved by substitution with $u = \sin\theta$. The result is

$$\ln F_{\ell\ell} = \ell \ln \sin\theta + \ln A$$

where $\ln A$ is a constant of integration. It follows that

$$F_{\ell\ell}(\theta) = A \sin^\ell \theta$$

and thus,

$$f_{\ell\ell}(\theta, \phi) = A \sin^\ell \theta \; e^{i\ell\phi}$$

The constant A is chosen so that $f_{\ell\ell}$ satisfies the normalization condition for wave functions defined on the unit sphere. After a lengthy calculation, we end up with

$$A = \frac{(-1)^\ell}{2^\ell \ell!} \sqrt{\frac{(2\ell+1)!}{4\pi}}$$

which ensures

$$\langle f_{\ell\ell} | f_{\ell\ell} \rangle = \int d\Omega \; |f_{\ell\ell}|^2 = 1$$

The resulting wave function $f_{\ell\ell}$ is actually the stretched *spherical harmonic function*

$$Y_{\ell\ell}(\theta, \phi) = \frac{(-1)^\ell}{2^\ell \ell!} \sqrt{\frac{(2\ell+1)!}{4\pi}} \; \sin^\ell \theta \, e^{i\ell\phi}$$

To obtain states corresponding to other values of m, we apply the lowering operator L_-. For the sake of time (and personal sanity), we simply state the result for $m \geq 0$ as

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} \, e^{im\phi} P_\ell^m(\cos\theta) \qquad \text{(spherical harmonics)}$$

where $P_\ell^m(\cos\theta)$ are the **associated Legendre functions** defined by

$$P_\ell^m(x) \equiv (-1)^m (1-x^2)^{m/2} \left(\frac{d}{dx}\right)^m P_\ell(x)$$

and $P_\ell(x)$ are the **Legendre polynomials** defined by the *Rodriguez formula*

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

The eigenstates with negative values of m can be obtained from the relation

$$Y_\ell^{-m} = (-1)^m (Y_\ell^m)^* \qquad (m > 0)$$

where we are using associated Legendre polynomials with the property that for $m > 0$

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x)$$

In summary, the simultaneous eigenfunctions of L^2 and L_z are the spherical harmonics:

$$L^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi) \tag{3.7}$$

$$L_z Y_\ell^m(\theta,\phi) = m\hbar Y_\ell^m(\theta,\phi) \tag{3.8}$$

A more detailed treatment of spherical harmonics is beyond the scope of this course.

3.4 Particle on a Sphere

Consider a free particle confined to the surface of a sphere with radius a and Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 \qquad \text{(position representation)}$$

where ∇^2 denotes the Laplacian. In spherical coordinates,

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

As it turns out, we can write $\mathbf{p}^2$ in terms of the L^2 operator as

$$\mathbf{p}^2 = -\hbar^2\nabla^2 = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L^2}{r^2}$$

For a particle confined to the sphere with radius a,

$$H = \frac{L^2}{2ma^2} = \frac{L^2}{2I}$$

where $I = ma^2$ is the moment of inertia of the particle about the origin. We can immediately write down the eigenfunctions of the Hamiltonian, since they are the same as the eigenfunctions of L^2, namely spherical harmonics $Y_\ell^m(\theta, \phi)$. Hence,

$$HY_\ell^m(\theta,\phi) = \frac{1}{2I}L^2 Y_\ell^m(\theta,\phi) = \frac{\ell(\ell+1)\hbar^2}{2I}Y_\ell^m(\theta,\phi)$$

and it follows that the energies of a particle on a sphere are

$$E_\ell = \frac{\ell(\ell+1)\hbar^2}{2I}$$

4 Central Potential

Consider a particle moving in 3D space under the influence of a conservative central force. The potential energy function $V(r)$ depends only on the particle's distance from the origin; thus we call it a **central potential**. This system exhibits a high degree of rotational symmetry. The Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(r)$$

commutes with all rotation operators $U(R)$ whose action on wave functions is given by Eq. (3.1). To see why this must be the case, consider the action of $U(R)$ on position and momentum. By definition, $U(R)$ implements a unitary transformation of the state vectors in a way that must correspond to a classical rotation. Hence,

$$U^\dagger(R)\mathbf{r}U(R) = R\mathbf{r} \quad \text{and} \quad U^\dagger(R)\mathbf{p}U(R) = R\mathbf{p}$$

This is the same operator expression we encountered in lecture #4 for the components of angular momentum. The potential energy depends only on the magnitude of $\mathbf{r}$, so

$$U^\dagger(R)V(r)U(R) = V\big(|R\mathbf{r}|\big) = V(r) \Rightarrow [V(r), U(R)] = 0$$

The kinetic energy depends on $\mathbf{p}^2 = \mathbf{p}\cdot\mathbf{p}$, so

$$U^\dagger(R)\mathbf{p}^2U(R) = (R\mathbf{p})\cdot(R\mathbf{p}) \Rightarrow [\mathbf{p}^2, U(R)] = 0$$

Since H commutes with $U(R)$ for any rotation R, and $U(R)$ is a function of $\mathbf{L}$, it follows that H commutes with $\mathbf{L}$ (or rather, the components of $\mathbf{L}$) and by extension, H commutes with L^2. In case you don't buy the argument above, I encourage you to compute the relevant

commutators. Nonetheless, a particle in a central potential has simultaneous eigenstates for H, L^2, and L_z given by

$$\psi(r, \theta, \phi) = \mathcal{R}(r) Y_\ell^m(\theta, \phi)$$

where $\mathcal{R}(r)$ where is a radial wave function normalized by the integral

$$\int_0^\infty r^2 \, dr \, |\mathcal{R}(r)|^2 = 1$$

Substitute ψ into the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r)\psi = E\psi$$

Expand the kinetic energy term in spherical coordinates:

$$\left[-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2mr^2} \right] \psi + V(r)\psi = E\psi$$

Note that L^2 acts non-trivially only on the spherical harmonic terms, bringing out a factor of $\ell(\ell+1)\hbar^2$. The overall factor of Y_ℓ^m cancels and we find an expression only in terms of the radial wave function. The so-called radial equation is

$$\left[-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \right] \mathcal{R} + V(r)\mathcal{R} = E\mathcal{R}$$

This expression can be simplified by defining an effective potential U_{eff} such that

$$-\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \mathcal{R}}{\partial r} \right) + V_{\text{eff}}(r)\mathcal{R} = E\mathcal{R}$$

where

$$V_{\text{eff}}(r) = \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)$$

The effective potential contains a *centrifugal term* in addition to the true potential. The radial equation becomes especially familiar by making the substitution

$$u(r) = r\mathcal{R}(r)$$

such that

$$-\frac{\hbar^2}{2m} \frac{du(r)}{dr} + V_{\text{eff}}(r)u(r) = Eu(r)$$

This version is easy to remember because it is almost the same as the one-dimensional

Schrödinger equation (usually written in terms of x with $-\infty < x < \infty$). The only differences are the presence of the centrifugal potential in the radial Schrödinger equation and the fact that r lies in the range $0 < r < \infty$. This is completely analogous to the classical particle in a central potential—due to rotational symmetry and conservation of angular momentum, the equation of motion for a single particle is effectively one dimensional despite having three degrees of freedom.

5 Two-Body Central Force Motion

The Hamiltonian for two bodies with a potential energy of interaction that depends on the magnitude of the distance separating the two bodies is given by

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

where $\mathbf{p}_1$ is the momentum for particle 1 and $\mathbf{p}_2$ is the momentum for particle 2. Technically, a system made of two particles is described by a state living in the tensor product of the individual single-particle vector spaces. A two-particle Hamiltonian is therefore an operator on this tensor product space. We will explore tensor products later in the course (or in Phys 438B) when we study multiparticle quantum systems and/or inclusion of spin states.

The two-body position basis states are described by the state vector $|\mathbf{r}_1, \mathbf{r}_2\rangle$, and the position-space wave function for the system in the state $|\Psi\rangle$ is

$$\langle \mathbf{r}_1, \mathbf{r}_2 | \Psi \rangle = \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

We call $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ the *configuration space wave function* because it depends on the entire configuration of the system. The wave function therefore depends on a $3 + 3 = 6$ dimensional configuration space, while the particles are each moving in a three-dimensional space.

We can define a total translation operator $T(\mathbf{a})$ that translates both particles equally:

$$\langle \mathbf{r}_1, \mathbf{r}_2 | T(\mathbf{a}) | \Psi \rangle = \Psi(\mathbf{r}_1 - \mathbf{a}, \mathbf{r}_2 - \mathbf{a})$$

The corresponding generator of total translation is the total momentum

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$

The Hamiltonian commutes with all translations because the distance between the particles is not changed when both particles are displaced by the same amount. It follows that H

commutes with the total momentum.

The Hamiltonian is invariant under rotations. The total rotation operator acts on the configuration space wave function according to

$$\langle \mathbf{r}_1, \mathbf{r}_2 | U(R) | \Psi \rangle = \Psi(R^{-1}\mathbf{r}_1, R^{-1}\mathbf{r}_2)$$

and the corresponding generator of rotations is the total angular momentum

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 \quad \text{where } \mathbf{L}_k = \mathbf{r}_k \times \mathbf{p}_k$$

The Hamiltonian commutes with all rotations and hence with the total angular momentum.

To solve the eigenvalue equation $H\Psi = E\Psi$, we first introduce a change of coordinates. The natural coordinates for the two-body central force problem are relative coordinates $\mathbf{r}$ and the center of mass coordinates $\mathbf{R}$. The corresponding position operators are

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M}$$

where $M = m_1 + m_2$ is the total mass of the two-particle system. We also define the corresponding generators of translation $\mathbf{p}$ and $\mathbf{P}$, corresponding to translation of $\mathbf{r}$ and $\mathbf{R}$ respectively, which can be written in the position representation as

$$\mathbf{p} = -i\hbar\nabla_{\mathbf{r}} \quad \text{and} \quad \mathbf{P} = -i\hbar\nabla_{\mathbf{R}}$$

By the multidimensional chain rule, we can relate these operators to $\mathbf{p}_1$ and $\mathbf{p}_2$ as

$$\mathbf{p}_1 = -i\hbar\nabla_1 = -i\hbar\left(\nabla_1\mathbf{R}\cdot\nabla_{\mathbf{R}} + \nabla_1\mathbf{r}\cdot\nabla_{\mathbf{r}}\right) = -i\hbar\left(\frac{m_1}{M}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}\right)$$

$$\mathbf{p}_2 = -i\hbar\nabla_2 = -i\hbar\left(\nabla_2\mathbf{R}\cdot\nabla_{\mathbf{R}} + \nabla_2\mathbf{r}\cdot\nabla_{\mathbf{r}}\right) = -i\hbar\left(\frac{m_2}{M}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}\right)$$

In case this application of the chain rule looks unfamiliar, let's write out the x component of $\mathbf{p}_1$ and use a test wave function $\Psi(\mathbf{R}, \mathbf{r})$:

$$\frac{\partial\Psi}{\partial x_1} = \sum_{i=1}^{3}\left(\frac{\partial R_i}{\partial x_1}\frac{\partial\Psi}{\partial R_i} + \frac{\partial r_i}{\partial x_1}\frac{\partial\Psi}{\partial r_i}\right)$$

Since R_1 and r_1 are the only components that depend on x_1, we find

$$\frac{\partial \Psi}{\partial x_1} = \frac{m_1}{M}\frac{\partial \Psi}{\partial R_1} + \frac{\partial \Psi}{\partial r_1}$$

and hence,

$$\hat{p}_{1x} = -i\hbar\left(\frac{m_1}{M}\frac{\partial}{\partial R_1} + \frac{\partial}{\partial r_1}\right)$$

which is exactly the x component of the expression above. Thus, we've established that

$$\mathbf{p}_1 = \frac{m_1}{M}\mathbf{P} + \mathbf{p}$$

$$\mathbf{p}_2 = \frac{m_2}{M}\mathbf{P} - \mathbf{p}$$

Solving for $\mathbf{P}$ and $\mathbf{p}$, it follows that

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$

$$\mathbf{p} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{M}$$

Evidently, the operator $\mathbf{P}$ exactly coincides with the generator of translations defined earlier for the two-particle system. The transformation $(\mathbf{r}_1, \mathbf{r}_2) \mapsto (\mathbf{R}, \mathbf{r})$ is an example of a "canonical transformation" in quantum mechanics. A canonical transformation is one that preserves the canonical commutation relations:

$$[R_i, P_j] = [r_i, p_j] = i\hbar\delta_{ij} \qquad [R_i, r_j] = [R_i, p_j] = [P_i, r_j] = [P_i, p_j] = 0$$

where r_i, R_i, p_i, P_i refer to the components of $\mathbf{r}$, $\mathbf{R}$, $\mathbf{p}$, and $\mathbf{P}$, respectively.

We can now transform the Hamiltonian to the new set of coordinates. The potential energy operator becomes $V(|\mathbf{r}_1 - \mathbf{r}_2|) = V(|\mathbf{r}|) = V(r)$ where r is the distance between the two particles. The kinetic energy operators take a bit more work:

$$\mathbf{p}_1^2 = \frac{m_1^2}{M^2}\mathbf{P}^2 + \mathbf{p}^2 + \frac{m_1}{M}\mathbf{P}\cdot\mathbf{p} + \frac{m_1}{M}\mathbf{p}\cdot\mathbf{P}$$

where $\mathbf{p}$ commutes with $\mathbf{P}$, so

$$\mathbf{p}_1^2 = \frac{m_1^2}{M^2}\mathbf{P}^2 + \mathbf{p}^2 + \frac{2m_1}{M}\mathbf{P}\cdot\mathbf{p}$$

A similar expression holds for $\mathbf{p}_2^2$. The kinetic energy operator is

$$\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu}$$

where μ denotes the *reduced mass* defined as

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

The Hamiltonian can be written as the sum of a center of mass term and a relative term,

$$H = H_{\text{CM}} + H_{\text{rel}} = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + V(r)$$

where

$$H_{\text{CM}} = \frac{\mathbf{P}^2}{2M}$$

and

$$H_{\text{rel}} = \frac{\mathbf{p}^2}{2\mu} + V(r)$$

The Hamiltonian H_{CM} is a free particle Hamiltonian–the kinetic energy of the center of mass–while H_{rel} is the kinetic energy about the center of mass plus the potential energy. Since $[H_{\text{CM}}, H_{\text{rel}}] = 0$, the Hamiltonians share an eigenbasis. The eigenstates of H_{CM} are those of the total momentum operator. In position space,

$$\langle \mathbf{R}|\mathbf{P}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{P}\cdot\mathbf{R}/\hbar}$$

are the eigenstates of H_{CM}. In the exponential, $\mathbf{P}$ is a vector of eigenvalues (P_x, P_y, P_z), not the momentum operator, and the center of mass position vector $\mathbf{R}$ has Cartesian components (R_1, R_2, R_3). It is common to analyze the two body problem in the center of mass frame where $\mathbf{P} = 0$. From now on, we'll concentrate on the relative Hamiltonian

$$H = \frac{\mathbf{p}^2}{2\mu} + V(r)$$

which is nearly identical to the Hamiltonian for a single-particle in a central potential. When the mass of one particle is much greater than the other, say $m_2 \gg m_1$, the reduced mass simplifies to the mass of the lighter particle, the relative position vector simplifies to the position of the lighter particle, and the relative momentum simplifies to the momentum of the lighter particle.