

4.2: Orbital Eigenfunctions- 2-D Case

Previously, we established that the operators \vec{J}^2, J_z have a common set of eigenkets ($|j, m\rangle$) with:

$$\vec{J}^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle \quad (4.2.1)$$

and

$$J_z |j, m\rangle = m\hbar |j, m\rangle \quad (4.2.2)$$

where j, m are integers or half odd integers, and we found the matrix elements of J_+, J_- (and hence those of J_x, J_y) between these eigenkets. This purely formal structure, therefore, nails down the allowed values of total angular momentum and of any measured component. But there are other things we need to know: for example, how is an electron in a particular angular momentum state in an atom affected by an external field? To compute that, we need to know the wave function ψ .

If a system has spherical symmetry, such as an electron in the Coulomb field of a hydrogen nucleus, then the Hamiltonian H and the operators \vec{J}^2, J_z have a common set of eigenkets $|E, j, m\rangle$. The spherically symmetric Hamiltonian is unchanged by rotation, so must commute with any rotation operator, $[H, \vec{J}^2] = 0$ and $[H, J_z] = 0$. Recall that commuting Hermitian operators can be diagonalized simultaneously -- and therefore have a common set of eigenkets.

Fortunately, many systems of interest do have spherical symmetry, at least to a good approximation, the basic example of course being the hydrogen atom, so the natural set of basis states is the common eigenkets of energy and angular momentum. It turns out that even when the spherical symmetry is broken, the angular momentum eigenkets may still be a useful starting point, with the symmetry breaking treated using perturbation theory.

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Two-Dimensional Models

As a warm-up exercise for the complications of the three-dimensional spherically symmetric model, it is worth analyzing a two-dimensional *circularly* symmetric model, that is,

$$H\psi(x, y) = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) + V(\sqrt{x^2 + y^2}) \psi(x, y) = E\psi(x, y). \quad (4.2.3)$$

(In this section, we'll denote the particle mass by M , to avoid confusion with the angular momentum quantum number m -- but be warned you are often going to find m used for both in the same discussion!)

The two-dimensional angular momentum operator is

$$L = \vec{r} \times \vec{p} = xp_y - yp_x = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right). \quad (4.2.4)$$

It is a straightforward exercise to check that for the circularly-symmetric Hamiltonian above,

$$[H, L] = 0. \quad (4.2.5)$$

Confirm that Equation 4.2.5 is accurate.

To take advantage of the circular symmetry, we switch to polar variables (r, ϕ) , where

$$r = \sqrt{x^2 + y^2}, \quad \phi = \tan^{-1}(y/x), \quad \text{so } x = r \cos \phi, \quad y = r \sin \phi. \quad (4.2.6)$$

Transforming the Hamiltonian and angular momentum into (r, ϕ) coordinates,

$$H\psi(r, \phi) = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) \psi(r, \phi) + V(r)\psi(r, \phi) = E\psi(r, \phi) \quad (4.2.7)$$

and

$$L = -i\hbar \frac{\partial}{\partial \phi}. \quad (4.2.8)$$

Confirm Equation 4.2.8 is correct.

The angular momentum eigenfunctions $\psi_m(r, \phi)$ satisfy

$$L\psi_m(r, \phi) = -i\hbar \frac{\partial}{\partial \phi} \psi_m(r, \phi) = m\hbar \psi_m(r, \phi) \quad (4.2.9)$$

equivalent to $L|m\rangle = m\hbar|m\rangle$. So $\psi_m(r, \phi) = R(r)e^{im\phi}$, and for this to be a single-valued wave function, m must be an integer. (This also ensures the hermiticity of the operator -- the integration-by-parts check has canceling contributions from $\phi = 0$ and $\phi = 2\pi$.)

Notice this means that *any* function of r multiplied by $e^{im\phi}$ is an eigenfunction of angular momentum with eigenvalue $m\hbar$, and in fact any eigenfunction of L with eigenvalue $m\hbar$ must be of this form. So we can factor out the r -dependence, and write a complete set of orthonormal eigenfunctions of L , normalized by integrating around the circle:

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad (4.2.10)$$

where ϕ is an integer.

It is interesting to note that this would be a complete set of wave functions for a particle confined to a ring -- rather like the original Bohr orbits. In fact, nanotech rings in which electrons have wave functions like this can be manufactured. Note also that in such rings one can also have *real* wave functions $\sqrt{1/\pi} \sin m\phi$, $\sqrt{1/\pi} \cos m\phi$, which are still energy eigenstates, but *not* angular momentum eigenstates, since they are standing waves, linear superpositions of waves going around the ring in opposite directions.

The common eigenstates of the Hamiltonian and the angular momentum evidently have the form

$$|E, m\rangle = \psi_{E,m}(r, \phi) = R_{E,m}(r) \Phi_m(\phi). \quad (4.2.11)$$

We should emphasize that although the angular part of the wave function does not depend on the radial potential, the radial component $R_{E,m}(r)$ *does* depend on the angular momentum m . This becomes obvious on putting this $\psi_{E,m}(r, \phi)$ into the (r, ϕ) version of Schrödinger's equation,

$$-\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) R_{E,m}(r) \Phi_m(\phi) + V(r) R_{E,m}(r) \Phi_m(\phi) = E R_{E,m}(r) \Phi_m(\phi), \quad (4.2.12)$$

noting that $\partial^2/\partial \phi^2 \equiv -m^2$, and canceling out the common factor $\Phi_m(\phi)$ to give

$$-\frac{\hbar^2}{2M} \left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{m^2}{r^2} \right) R_{E,m}(r) + V(r) R_{E,m}(r) = E R_{E,m}(r). \quad (4.2.13)$$

In this one-dimensional equation for the radial wave function $R_{E,m}(r)$, the angular momentum term $\hbar^2 m^2 / 2Mr^2 = L^2 / 2Mr^2$ evidently is equivalent to a repulsive potential. It's called the "centrifugal barrier" and is easy to understand from classical mechanics. To see this, consider a classical particle bound (in two dimensions) by an attractive central force $V(r)$. Split the momentum into a radial component p_r and a component in the direction perpendicular to the radius, p_\perp . The angular momentum $L = rp_\perp$ and is constant (since the force is central). The energy

$$E = \frac{p_r^2}{2M} + \frac{p_\perp^2}{2M} + V(r) = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + V(r) \quad (4.2.14)$$

substituting $p_\perp = L/r$. Since $L = m\hbar$, the angular part is exactly equivalent to the above Schrödinger equation.

But what about the radial part? Why isn't p_r just equal to $-i\hbar \partial/\partial r$, and p_r^2 equal to $\hbar^2 \partial^2/\partial r^2$? We know the more complicated differentiation with respect to r in the Schrödinger equation above must be correct, because it came from $\partial^2/\partial x^2 + \partial^2/\partial y^2$ and $r = \sqrt{x^2 + y^2}$, $\phi = \tan^{-1}(y/x)$.

To see why p_r equal to $-i\hbar \partial/\partial r$ is incorrect, even though it satisfies $[r, p_r] = i\hbar$, recall what happens in x -space. We argued there that $p_x = -i\hbar \partial/\partial x$ for a plane wave because from the photon analogy, acting on the plane wave state $Ce^{ip_x x/\hbar}$ this operator gives the rate of change of phase and therefore the momentum. But a *radial* wave is a little different: picture a photon wave coming

out of a single narrow slit, that is, a slit having width far smaller than the photon wavelength. The photon wave will radiate outwards with equal amplitude in all directions (180°) but the *wave amplitude will decrease* with distance from the slit to conserve probability. For a long (narrow) slit, this is essentially a two-dimensional problem, so the wave function will be $\psi(r) \cong C e^{ip_r r/\hbar} / \sqrt{r}$. We know that if we measure the momentum of photons at different distances from the slit we'll get the same result. The wavelength determines the photon's momentum, and it isn't changing. The color stays the same. However, $-i\hbar\partial/\partial r$ operating on $\psi(r)$ doesn't just give p_r : it picks up *an extra term* from differentiating the \sqrt{r} , so it is obviously *not* giving us the right momentum. Fortunately, this is easy to fix: we define the operator

$$\hat{p}_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{2r}\right) \quad (4.2.15)$$

which eliminates the extra term, *and still satisfies* $[r, p_r] = i\hbar$.

However, there is still a small problem. If we substitute this \hat{p}_r in the classical expression for the energy, following the procedure we used successfully to find Schrödinger's equation in Cartesian coordinates, we find

$$\begin{aligned} H &= \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + V(r) \\ &= \frac{-\hbar^2 \left(\frac{\partial}{\partial r} + \frac{1}{2r}\right)^2}{2M} + \frac{L^2}{2Mr^2} + V(r) \\ &= \frac{-\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial}{\partial r} - \frac{1}{4r^2}\right)}{2M} + \frac{L^2}{2Mr^2} + V(r) \end{aligned} \quad (4.2.16)$$

This is almost -- but not quite -- the same as the equation we found by transforming from Cartesian coordinates. The difference is the term $\hbar^2/8Mr^2$. So which is right? Actually our first one was right -- this second one, derived directly from the classical Hamiltonian, does give the same result in the classical limit, because the difference between them vanishes for $\hbar \rightarrow 0$. We conclude that beginning with the classical Hamiltonian, and replacing dynamical variables with the appropriate quantum operators, cannot guarantee that we get the correct quantum Hamiltonian: it might be off by some term of order \hbar . This would become evident in predicting properties of truly quantum systems, such as atomic energy levels. Problems of this kind are common in constructing quantum theories starting from a classical theory: essentially, in a classical theory, the order of variables in an expression is irrelevant, but in the quantum theory there can only be *one* correct order of noncommuting variables such as $\partial/\partial r$ and r in any expression.

What can we say about the radial wave function $R_{E,m}(r)$? If both the energy and the potential at the origin are finite, then for small r :

$$R_{E,m}(r) \approx Ar^m \text{ or } Ar^{-m} \quad (4.2.17)$$

However, the wave function cannot be discontinuous, so $R_{E,m}(r) \approx Ar^{|m|}$. To make further progress in finding the wave function, we need to know the potential. Specific examples will be analyzed in due course. It is interesting to note that the allowed wave functions, proportional to $rme^{im\phi}$, $rme^{-im\phi}$, $m > 0$, are the complex functions z^m , $(z^*)^m$ if the two-dimensional space is mapped into the complex plane. Representing many-electron wave functions in the plane in this way was a key to understanding the quantum Hall effect.

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