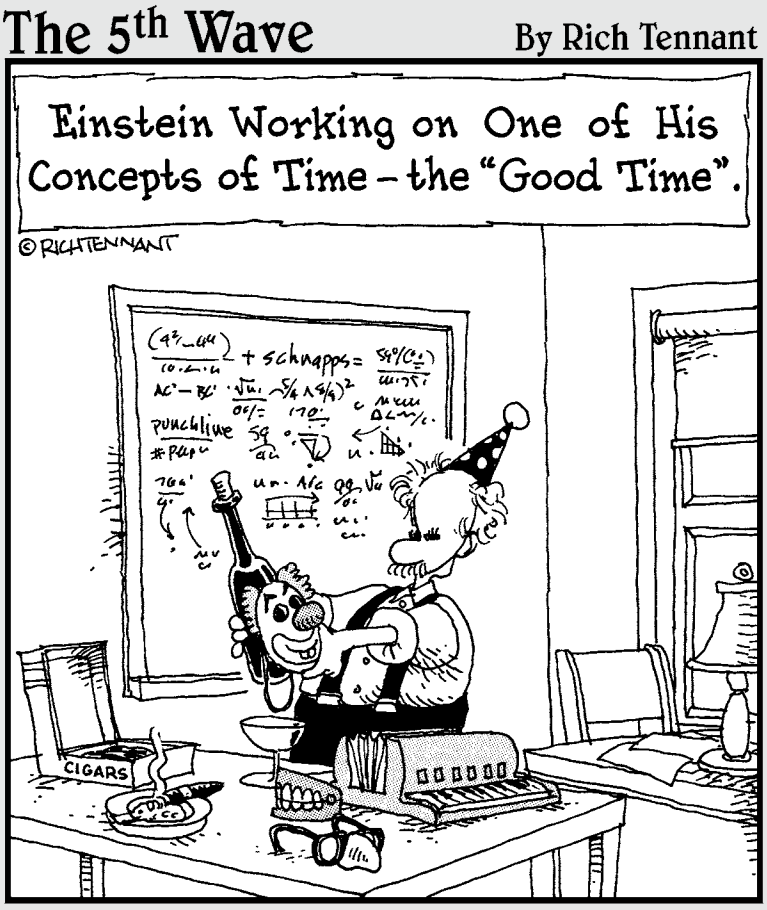
Part V

Group Dynamics: Introducing Multiple Particles



In this part . . .

This part introduces you to working with multiple particles at the same time. Now, all the particles in the system can interact not only with an overall potential but also with each other. You see how to deal with atoms (electron and nucleus systems) here, as well as systems of many atoms. After all, the whole world is made up of many-particle systems. Good thing quantum physics is up to the task.

Chapter 11

Giving Systems a Push: Perturbation Theory

In This Chapter

- Nondegenerate and degenerate perturbation theory
- Perturbing harmonic oscillators
- The Stark effect and perturbing hydrogen atoms

Problems in quantum physics can become pretty tough pretty fast — another way of saying that, unfortunately, you just can't find exact solutions to many quantum physics problems. This is particularly the case when you merge two kinds of systems. For example, you may know all about how square wells work and all about how electrons in magnetic fields work, but what if you combine the two? The wave functions of each system, which you know exactly, are no longer applicable — you need some sort of mix instead.

Perturbation theory to the rescue! This theory lets you handle mixes of situations, as long as the interference isn't too strong. In this chapter, you explore time-independent perturbation theory and degenerate and nondegenerate Hamiltonians. You also look at some examples that place harmonic oscillators and hydrogen atoms in electric fields.

Introducing Time-Independent Perturbation Theory

The idea behind time-independent perturbation theory is that you start with a known system — one whose wave functions you know and whose energy levels you know. Everything is all set up to this point. Then some new stimulus — a *perturbation* — comes along, disturbing the status quo. For example, you may apply an electrostatic or magnetic field to your known system, which changes that system somewhat.

Perturbation theory lets you handle situations like this — as long as the perturbation isn't too strong. In other words, if you apply a weak magnetic field to your known system, the energy levels will be mostly unchanged but with a correction. (***Note:*** That's why it's called *perturbation theory* and not *drastic-interference theory.)* The change you make to the setup is slight enough so that you can calculate the resulting energy levels and wave functions as *corrections* to the fundamental energy levels and wave functions of the unperturbed system.

So what does it mean to talk of perturbations in physics terms? Say that you have this Hamiltonian:

$$H = H_0 + \lambda W \quad (\lambda << 1)$$

Here, H_0 is a known Hamiltonian, with known eigenfunctions and eigenvalues, and λW is the so-called perturbation Hamiltonian, where $\lambda << 1$ indicates that the perturbation Hamiltonian is small.

Finding the eigenstates of the Hamiltonian in this equation is what solving problems like this is all about — in other words, here's the problem you want to solve:

$$H|\psi_n\rangle = (H_0 + \lambda W)|\psi_n\rangle = E_n|\psi_n\rangle \qquad (\lambda << 1)$$

The way you solve this equation depends on whether the exact, known solutions of H_0 are *degenerate* (that is, several states have the same energy) or nondegenerate. The next section solves the nondegenerate case.

Working with Perturbations to Nondegenerate Hamiltonians

Start with the case in which the unperturbed Hamiltonian, H_0, has *nondegenerate* solutions. That is, for every state $|\phi_n\rangle$, there's exactly one energy, E_n, that isn't the same as the energy for any other state: $H_0|\phi_n\rangle = E_n|\phi_n\rangle$ (just as a one-to-one function has only one *x* value for any *y*). You refer to these nondegenerate energy levels of the unperturbed Hamiltonian as $E^{(0)}{}_n$ to distinguish them from the corrections that the perturbation introduces, so the equation becomes

$$H_0|\phi_n\rangle = E^{(0)}{}_n|\phi_n\rangle$$

From here on, I refer to the energy levels of the perturbed system as E_n.

The idea behind perturbation theory is that you can perform expansions based on the parameter λ (which is much, much less than 1) to find the wave

functions and energy levels of the perturbed system. In this section, you go up to terms in λ^2 in the expansions.

A little expansion: Perturbing the equations

To find the energy of the perturbed system, E_n, start with the energy of the unperturbed system:

$$E_n = E^{(0)}{}_n + \ldots$$

Add the first-order correction to the energy, $\lambda E^{(1)}{}_n$:

$$E_n = E^{(0)}{}_n + \lambda E^{(1)}{}_n + \ldots \quad (\lambda << 1)$$

And add the second-order correction to the energy, $\lambda^2 E^{(2)}{}_n$, as well:

$$E_n = E^{(0)}{}_n + \lambda E^{(1)}{}_n + \lambda^2 E^{(2)}{}_n + \ldots \quad (\lambda << 1)$$

Now what about the wave function of the perturbed system, $|\psi_n\rangle$? Start with the wave function of the unperturbed system, $|\phi_n\rangle$:

$$|\psi_n\rangle = |\phi_n\rangle + \ldots$$

Add to it the first-order correction, $\lambda|\psi^{(1)}{}_n\rangle$:

$$|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi^{(1)}{}_n\rangle + \ldots \quad (\lambda << 1)$$

And then add to that the second-order correction to the wave function, $\lambda^2|\psi^{(2)}{}_n\rangle$:

$$|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi^{(1)}{}_n\rangle + \lambda^2|\psi^{(2)}{}_n\rangle + \ldots \quad (\lambda << 1)$$

Note that when $\lambda \to 0$, $E_n = E^{(0)}{}_n + \lambda E^{(1)}{}_n + \lambda^2 E^{(2)}{}_n + \ldots \quad (\lambda << 1)$ becomes the unperturbed energy:

$$E_n = E^{(0)}{}_n$$

And $|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi^{(1)}{}_n\rangle + \lambda^2|\psi^{(2)}{}_n\rangle + \ldots \quad (\lambda << 1)$ becomes the unperturbed wave function:

$$|\psi_n\rangle = |\phi_n\rangle$$

So your task is to calculate $E^{(1)}_n$ and $E^{(2)}_n$, as well as $\psi^{(1)}_n$ and $\psi^{(2)}_n$. So how do you do that in general? Time to start slinging some math. You start with three perturbed equations:

- **Hamiltonian:** $H|\psi_n\rangle = (H_0 + \lambda W)|\psi_n\rangle = E_n|\psi_n\rangle \quad (\lambda << 1)$
- **Energy levels:** $E_n = E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + \ldots \quad (\lambda << 1)$
- **Wave functions:** $|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi^{(1)}_n\rangle + \lambda^2|\psi^{(2)}_n\rangle + \ldots \quad (\lambda << 1)$

Combine these three equations to get this jumbo equation:

$$(H_0 + \lambda W)\left(|\phi_n\rangle + \lambda|\psi^{(1)}_n\rangle + \lambda^2|\psi^{(2)}_n\rangle + \ldots\right)$$
$$= \left(E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + \ldots\right)\left(|\phi_n\rangle + \lambda|\psi^{(1)}_n\rangle + \lambda^2|\psi^{(2)}_n\rangle + \ldots\right) \quad (\lambda << 1)$$

Matching the coefficients of λ and simplifying

You can handle the jumbo equation in the preceding section by setting the coefficients of λ on either side of the equal sign equal to each other.

Equating the zeroth order terms in λ on either side of this equation, here's what you get:

$$H_0|\phi_n\rangle = E^{(0)}_n|\phi_n\rangle$$

Now for the first-order terms in λ; equating them on either side of the jumbo equation gives you

$$H_0|\psi^{(1)}_n\rangle + W|\phi_n\rangle = E^{(0)}_n|\psi^{(1)}_n\rangle + E^{(1)}_n|\phi_n\rangle$$

Now equate the coefficients of λ^2 in the jumbo equation, giving you

$$H_0|\psi^{(2)}_n\rangle + W|\psi^{(1)}_n\rangle = E^{(0)}_n|\psi^{(2)}_n\rangle + E^{(1)}_n|\psi^{(1)}_n\rangle + E^{(2)}_n|\phi_n\rangle$$

Okay, that's the equation you derive from the second order in λ. Now you have to solve for $E^{(1)}_n$, $E^{(2)}_n$, and so on using the zeroth-order, first-order, and second-order equations.

Start by noting that the unperturbed wave function, $|\phi_n\rangle$ isn't going to be very different from the perturbed wave function, $|\psi_n\rangle$, because the perturbation is small. That means that $\langle\phi_n|\psi_n\rangle \approx 1$. In fact, you can normalize $|\psi_n\rangle$ so that $\langle\phi_n|\psi_n\rangle$ is exactly equal to 1:

$$\langle\phi_n|\psi_n\rangle = 1$$

Given that $|\psi_n\rangle = |\phi_n\rangle + \lambda|\psi^{(1)}{}_n\rangle + \lambda^2|\psi^{(2)}{}_n\rangle + \ldots$, the equation becomes

$$\lambda\langle\phi_n|\psi^{(1)}{}_n\rangle + \lambda^2\langle\phi_n|\psi^{(2)}{}_n\rangle + \ldots = 0$$

And because the coefficients of λ must both vanish, you get the following:

$$\langle\phi_n|\psi^{(1)}{}_n\rangle = \langle\phi_n|\psi^{(2)}{}_n\rangle = 0$$

This equation is useful for simplifying the math.

Finding the first-order corrections

After matching the coefficients of λ and simplifying (see the preceding section), you want to find the first-order corrections to the energy levels and the wave functions. Find the first-order correction to the energy, $E^{(1)}{}_n$, by multiplying $H_0|\psi^{(1)}{}_n\rangle + W|\phi_n\rangle = E^{(0)}{}_n|\psi^{(1)}{}_n\rangle + E^{(1)}{}_n|\phi_n\rangle$ by $\langle\phi_n|$:

$$\langle\phi_n|H_0|\psi^{(1)}{}_n\rangle + \langle\phi_n|W|\phi_n\rangle = \langle\phi_n|E^{(0)}{}_n|\psi^{(1)}{}_n\rangle + \langle\phi_n|E^{(1)}{}_n|\phi_n\rangle$$

Then the first term can be neglected and we can use our simplification above to write the first order energy perturbation as:

$$E^{(1)}{}_n = \langle\phi_n|W|\phi_n\rangle$$

Swell, that's the expression you use for the first-order correction, $E^{(1)}{}_n$.

Now look into finding the first-order correction to the wave function, $|\psi^{(1)}{}_n\rangle$. You can multiply the wave-function equation by this next expression, which is equal to 1:

$$\sum_m |\phi_m\rangle\langle\phi_m|$$

So you have

$$\begin{aligned}\left|\psi^{(1)}{}_n\right\rangle &= \left(\sum_m \left|\phi_m\right\rangle\left\langle\phi_m\right|\right)\left|\psi^{(1)}{}_n\right\rangle \\ &= \sum_m \left\langle\phi_m\middle|\psi^{(1)}{}_n\right\rangle\left|\phi_m\right\rangle \qquad m \neq n\end{aligned}$$

Note that the $m = n$ term is zero because $\langle\phi_n|\psi^{(1)}{}_n\rangle = 0$.

So what is $\langle\phi_m|\psi^{(1)}{}_n\rangle$? You can find out by multiplying the first-order correction, $H_0\left|\psi^{(1)}{}_n\right\rangle + W\left|\phi_n\right\rangle = E^{(0)}{}_n\left|\psi^{(1)}{}_n\right\rangle + E^{(1)}{}_n\left|\phi_n\right\rangle$, by $\langle\phi_m|$ to give you

$$\left\langle\phi_m\middle|\psi^{(1)}{}_n\right\rangle = \frac{\left\langle\phi_m\middle|W\middle|\phi_n\right\rangle}{E^{(0)}{}_n - E^{(0)}{}_m}$$

And substituting that into $\left|\psi^{(1)}{}_n\right\rangle = \sum_m \left\langle\phi_m\middle|\psi^{(1)}{}_n\right\rangle\left|\phi_m\right\rangle$ gives you

$$\left|\psi^{(1)}{}_n\right\rangle = \sum_{m\neq n} \frac{\left\langle\phi_m\middle|W\middle|\phi_n\right\rangle}{E^{(0)}{}_n - E^{(0)}{}_m}\left|\phi_m\right\rangle$$

Okay, that's your term for the first-order correction to the wave function, $|\psi^{(1)}{}_n\rangle$. From $\left|\psi_n\right\rangle = \left|\phi_n\right\rangle + \lambda\left|\psi^{(1)}{}_n\right\rangle + \lambda^2\left|\psi^{(2)}{}_n\right\rangle + \ldots \quad (\lambda << 1)$, the wave function looks like this, made up of of zeroth-, first-, and second-order corrections:

$$\left|\psi_n\right\rangle = \left|\phi_n\right\rangle + \lambda\left|\psi^{(1)}{}_n\right\rangle + \lambda^2\left|\psi^{(2)}{}_n\right\rangle + \ldots \quad (\lambda << 1)$$

Ignoring the second-order correction for the moment and substituting $\left|\psi^{(1)}{}_n\right\rangle = \sum_{m\neq n} \frac{\left\langle\phi_m\middle|W\middle|\phi_n\right\rangle}{E^{(0)}{}_n - E^{(0)}{}_m}\left|\phi_m\right\rangle$ in for the first-order correction gives you this for the wave function of the perturbed system, to the first order:

$$\left|\psi_n\right\rangle = \left|\phi_n\right\rangle + \sum_{m\neq n} \frac{\left\langle\phi_m\middle|\lambda W\middle|\phi_n\right\rangle}{E^{(0)}{}_n - E^{(0)}{}_m}\left|\phi_m\right\rangle \ldots \quad (\lambda << 1)$$

That's the wave function of the perturbed system in terms of the perturbation. But that's still only the first-order correction. How about the second? Read on.

Finding the second-order corrections

Now find the second-order corrections to the energy levels and the wave functions (the preceding section covers first-order corrections). To find $E^{(2)}_n$, multiply both sides of $H_0\left|\psi^{(2)}_n\right\rangle + W\left|\psi^{(1)}_n\right\rangle = E^{(0)}_n\left|\psi^{(2)}_n\right\rangle + E^{(1)}_n\left|\psi^{(1)}_n\right\rangle + E^{(2)}_n\left|\phi_n\right\rangle$ by $\langle\phi_n|$:

$$\left\langle\phi_n\right|H_0\left|\psi^{(2)}_n\right\rangle + \left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle = \left\langle\phi_n\right|E^{(0)}_n\left|\psi^{(2)}_n\right\rangle + \left\langle\phi_n\right|E^{(1)}_n\left|\psi^{(1)}_n\right\rangle + \left\langle\phi_n\right|E^{(2)}_n\left|\phi_n\right\rangle$$

This looks like a tough equation until you realize that $\langle\phi_n|\psi^{(1)}_n\rangle$ is equal to zero, so you get

$$\left\langle\phi_n\right|H_0\left|\psi^{(2)}_n\right\rangle + \left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle = \left\langle\phi_n\right|E^{(0)}_n\left|\psi^{(2)}_n\right\rangle + \left\langle\phi_n\right|E^{(2)}_n\left|\phi_n\right\rangle$$

Because $\langle\phi_n|\psi^{(2)}_n\rangle$ is also equal to zero, and again neglecting the first term, you get

$$\left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle = \left\langle\phi_n\right|E^{(2)}_n\left|\phi_n\right\rangle$$

$E^{(2)}_n$ is just a number, so you have

$$\left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle = E^{(2)}_n\left\langle\phi_n|\phi_n\right\rangle$$

And of course, because $\langle\phi_n|\phi_n\rangle = 1$, you have

$$E^{(2)}_n = \left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle$$

Note that if $|\psi^{(1)}_n\rangle$ is an eigenstate of W, the second-order correction equals zero.

Okay, so $E^{(2)}_n = \langle\phi_n|W|\psi^{(1)}_n\rangle$. How can you make that simpler? Well, from using $\left|\psi^{(1)}_n\right\rangle = \sum_{m\neq n}\frac{\left\langle\phi_m\right|W\left|\phi_n\right\rangle}{E^{(0)}_n - E^{(0)}_m}\left|\phi_m\right\rangle$. Substituting that equation into $E^{(2)}_n = \left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle$ gives you

$$E^{(2)}_n = \left\langle\phi_n\right|W\left|\psi^{(1)}_n\right\rangle = \left\langle\phi_n\right|W\sum_{m\neq n}\frac{\left\langle\phi_m\right|W\left|\phi_n\right\rangle}{E^{(0)}_n - E^{(0)}_m}\left|\phi_m\right\rangle$$

$$= \sum_{m\neq n}\frac{\left|\left\langle\phi_m\right|W\left|\phi_n\right\rangle\right|^2}{E^{(0)}_n - E^{(0)}_m}$$

Now you have $E^{(1)}{}_n = \langle \phi_n | W | \phi_n \rangle$ and $E^{(2)}{}_n = \sum_{m \neq n} \frac{|\langle \phi_m | W | \phi_n \rangle|^2}{E^{(0)}{}_n - E^{(0)}{}_m}$. Here's the total energy with the first- and second-order corrections:

$$E_n = E^{(0)}{}_n + \lambda E^{(1)}{}_n + \lambda^2 E^{(2)}{}_n + \ldots \quad (\lambda << 1)$$

So from this equation, you can say

$$E_n = E_0 + \lambda \langle \phi_n | W | \phi_n \rangle + \lambda^2 \sum_{m \neq n} \frac{|\langle \phi_m | W | \phi_n \rangle|^2}{E^{(0)}{}_n - E^{(0)}{}_m} + \ldots \quad (\lambda << 1)$$

That gives you the first- and second-order corrections to the energy, according to perturbation theory.

Note that for this equation to converge, the term in the summation must be small. And note in particular what happens to the expansion term if the energy levels are degenerate:

$$\frac{|\langle \phi_m | W | \phi_n \rangle|^2}{E^{(0)}{}_n - E^{(0)}{}_m}$$

In that case, you're going to end up with an $E^{(0)}{}_n$ that equals an $E^{(0)}{}_m$, which means that the energy-corrections equation blows up, and this approach to perturbation theory is no good — which is to say that you need a different approach to perturbation theory (coming up later in "Working with Pertubations to Degenerate Hamiltonians") to handle systems with degenerate energy states.

In the next section, I show you an example to make the idea of perturbing nondegenerate Hamiltonians more real.

Perturbation Theory to the Test: Harmonic Oscillators in Electric Fields

Consider the case in which you have a small particle oscillating in a harmonic potential, back and forth, as Figure 11-1 shows.

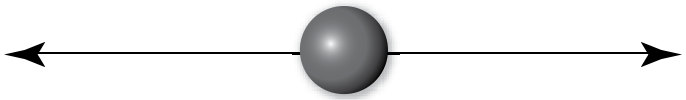


Figure 11-1: A harmonic oscillator.

Here's the Hamiltonian for that particle, where the particle's mass is *m,* its location is *x,* and the angular frequency of the motion is ω:

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Now assume that the particle is charged, with charge *q,* and that you apply a weak electric field, ε, as Figure 11-2 shows.

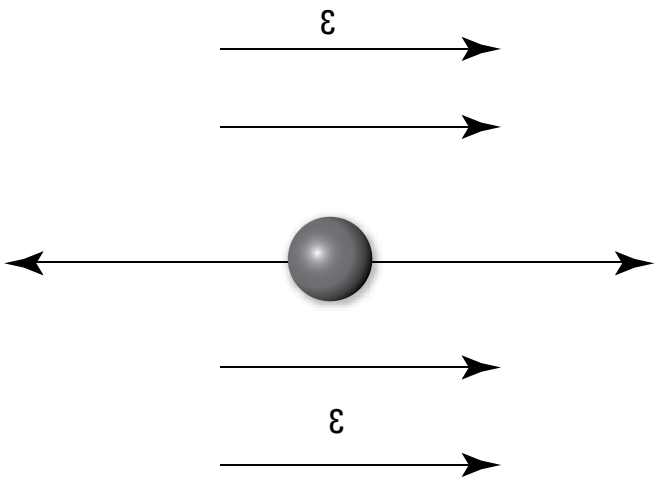


Figure 11-2: Applying an electric field to a harmonic oscillator.

The force due to the electric field in this case is the perturbation, and the Hamiltonian becomes

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + q\varepsilon x$$

In this section, you find the energy and wave functions of the perturbed system and compare them to the exact solutions.

Finding exact solutions

So what are the energy eigenvalues of the preceding Hamiltonian for the harmonic oscillator in an electric field? First solve for the eigenvalues exactly; then use perturbation theory. You can solve for the exact energy eigenvalues by making one of the following substitutions:

- $y = x + \frac{q\varepsilon}{m\omega^2}$
- $x = y - \frac{q\varepsilon}{m\omega^2}$

Substituting the equation solved for *x* into $\mathrm{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + q\varepsilon x$ gives you $\mathrm{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dy^2} + \frac{1}{2}m\omega^2 y^2 - \frac{q^2\varepsilon^2}{2m\omega^2}$

The last term is a constant, so the equation is of the form

$$\mathrm{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dy^2} + \frac{1}{2}m\omega^2 y^2 + C$$

where $C = \frac{-q^2\varepsilon^2}{m\omega^2}$. $\mathrm{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dy^2} + \frac{1}{2}m\omega^2 y^2 + C$ is just the Hamiltonian of a harmonic oscillator with an added constant, which means that the energy levels are simply

$$\mathrm{E}_n = \left(n + \frac{1}{2}\right)\hbar\omega + C$$

Substituting in for C gives you the exact energy levels:

$$\mathrm{E}_n = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{q^2\varepsilon^2}{2m\omega^2}$$

Great — that's the exact solution.

Applying perturbation theory

As soon as you have the exact eigenvalues for your charged oscillator (see the preceding section), you have something to compare the solution from perturbation theory to. Now you can find the energy and wave functions of the perturbed system.

Energy of the charged oscillator

So what is the energy of the charged oscillator, as given by perturbation theory? You know that the corrected energy is given by

$$E_n = E_0 + \lambda\left\langle \phi_n \middle| W \middle| \phi_n \right\rangle + \lambda^2 \sum_{m \neq n} \frac{\left|\left\langle \phi_m \middle| W \middle| \phi_n \right\rangle\right|^2}{E^{(0)}{}_n - E^{(0)}{}_m} + \ldots \quad (\lambda << 1)$$

where λW is the perturbation term in the Hamiltonian. That is, here, λW = $q\varepsilon x$. Now take a look at the corrected energy equation using $q\varepsilon x$ for λW. The first-order correction is $\lambda\left\langle \phi_n \middle| W \middle| \phi_n \right\rangle$, which, using λW = $q\varepsilon x$, becomes

$$\langle \phi_n | q\varepsilon x | \phi_n \rangle \text{ or } q\varepsilon \langle \phi_n | x | \phi_n \rangle$$

But $\langle \phi_n | x | \phi_n \rangle = 0$, because that's the expectation value of x, and harmonic oscillators spend as much time in negative x territory as in positive x territory — that is, the average value of x is zero. So the first-order correction to the energy, as given by perturbation theory, is zero.

Okay, what's the second-order correction to the energy, as given by perturbation theory? Here it is:

$$\lambda^2 \sum_{m \neq n} \frac{\left|\left\langle \phi_m \middle| W \middle| \phi_n \right\rangle\right|^2}{E^{(0)}{}_n - E^{(0)}{}_m} + \ldots \quad (\lambda << 1)$$

And because λW = $q\varepsilon x$, you have

$$q^2\varepsilon^2 \sum_{m \neq n} \frac{\left|\left\langle \phi_m \middle| x \middle| \phi_n \right\rangle\right|^2}{E^{(0)}{}_n - E^{(0)}{}_m} + \ldots$$

Cast this in terms of bras and kets (see Chapter 4), changing $\langle \phi_m |$ to $\langle m |$ and $| \phi_n \rangle$ to $| n \rangle$, making the second-order energy correction into this expression:

$$q^2\varepsilon^2 \sum_{m \neq n} \frac{\left|\left\langle m \middle| x \middle| n \right\rangle\right|^2}{E^{(0)}{}_n - E^{(0)}{}_m} + \ldots$$

You can decipher this step by step. First, the energy is

$$E^{(0)}{}_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

That makes figuring out the second-order energy a little easier.

Also, the following expressions turn out to hold for a harmonic oscillator:

- $\left\langle n+1\left| x \right| n\right\rangle = \left(n+1\right)^{1/2} \frac{\hbar^{1/2}}{\left(2m\omega\right)^{1/2}}$
- $\left\langle n-1\left| x \right| n\right\rangle = n^{1/2} \frac{\hbar^{1/2}}{\left(2m\omega\right)^{1/2}}$
- $\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n-1} = \hbar\omega$
- $\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n+1} = -\hbar\omega$

With these four equations, you're ready to tackle $q^2\varepsilon^2 \sum_{m\neq n} \frac{\left|\left\langle m\left| x \right| n\right\rangle\right|^2}{\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{m}} + \ldots$, the second-order correction to the energy. Omitting higher-power terms, the summation in this equation becomes

$$q^2\varepsilon^2 \frac{\left|\left\langle n+1\left| x \right| n\right\rangle\right|^2}{\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n+1}} + \ldots$$
$$q^2\varepsilon^2 \frac{\left|\left\langle n-1\left| x \right| n\right\rangle\right|^2}{\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n-1}} \ldots$$

And substituting in the for $\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n+1}$ and $\mathrm{E}^{(0)}{}_{n} - \mathrm{E}^{(0)}{}_{n-1}$ gives you

$$q^2\varepsilon^2 \frac{\left|\left\langle n+1\left| x \right| n\right\rangle\right|^2}{-\hbar\omega} + \ldots$$
$$q^2\varepsilon^2 \frac{\left|\left\langle n-1\left| x \right| n\right\rangle\right|^2}{\hbar\omega} \ldots$$

Now, substituting in for $\langle n+1 | x | n \rangle$ and $\langle n-1 | x | n \rangle$ gives you

$$q^2\varepsilon^2 \frac{\left(n+1\right)\hbar}{\left(-\hbar\omega\right)\left(2m\omega\right)} + \ldots$$
$$q^2\varepsilon^2 \frac{n\hbar}{\left(\hbar\omega\right)\left(2m\omega\right)} \ldots$$

or

$$-q^2\varepsilon^2 \frac{\left(n+1\right)}{2m\omega^2} + \ldots$$
$$q^2\varepsilon^2 \frac{n}{2m\omega^2} \ldots$$

So the second-order correction is

$$\frac{-q^2\varepsilon^2}{2m\omega^2}\ldots$$

Therefore, according to perturbation theory, the energy of the harmonic oscillator in the electric field should be

$$\mathrm{E}_n = \left(n+\frac{1}{2}\right)\hbar\omega - \frac{q^2\varepsilon^2}{2m\omega^2}$$

Compare this result to the earlier equation for the exact energy levels, $\mathrm{E}_n = \left(n+\frac{1}{2}\right)\hbar\omega - \frac{q^2\varepsilon^2}{2m\omega^2}$ — they're the same! In other words, perturbation theory has given you the same result as the exact answer. How's that for agreement?

Of course, you can't expect to hit the same answer every time using perturbation theory, but this result is impressive!

Wave functions of the charged oscillator

Now figure out what the charged oscillator's wave function looks like in the presence of the electric field. Here's the wave function of the perturbed system, to the first order:

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{m\neq n} \frac{\langle\phi_m|\lambda W|\phi_n\rangle}{E^{(0)}_n - E^{(0)}_m}|\phi_m\rangle\ldots \quad (\lambda << 1)$$

Using the $\langle n|$ and $|n\rangle$ bras and kets you're used to for harmonic oscillators, this becomes

$$|\psi_n\rangle = |n\rangle + \sum_{m\neq n} \frac{\langle m|\lambda W|n\rangle}{E^{(0)}_n - E^{(0)}_m}|\phi_m\rangle\ldots \quad (\lambda << 1)$$

Because $\lambda W = q\varepsilon x$, this becomes

$$|\psi_n\rangle = |n\rangle + q\varepsilon\sum_{m\neq n} \frac{\langle m|x|n\rangle}{E^{(0)}_n - E^{(0)}_m}|m\rangle\ldots \quad (\lambda << 1)$$

Evidently, as with the energy, only two terms contribute, because $\langle n|x|n\rangle = 0$. In particular, the two terms that contribute are

- $\left\langle n+1 \middle| x \middle| n \right\rangle = \left(n+1\right)^{1/2} \frac{\hbar^{(1/2)}}{\left(2m\omega\right)^{(1/2)}}$
- $\left\langle n-1 \middle| x \middle| n \right\rangle = n^{1/2} \frac{\hbar^{(1/2)}}{\left(2m\omega\right)^{(1/2)}}$

Note also that $E^{(0)}{}_{n} - E^{(0)}{}_{n-1} = \hbar\omega$ and $E^{(0)}{}_{n} - E^{(0)}{}_{n+1} = -\hbar\omega$.

These four equations mean that

$$\left|\psi_{n}\right\rangle = \left|n\right\rangle + \frac{q\varepsilon}{\hbar\omega} \frac{\hbar^{1/2}}{\left(2m\omega\right)^{1/2}} \left(n^{1/2} \left|n-1\right\rangle - (n+1)^{1/2} \left|n+1\right\rangle \right)$$

Note what this equation means: Adding an electric field to a quantum harmonic oscillator spreads the wave function of the harmonic oscillator.

Originally, the harmonic oscillator's wave function is just the standard harmonic oscillator wave function, $|\psi_n\rangle = |n\rangle$. Applying an electric field spreads the wave function, adding a component of $|n-1\rangle$, which is proportional to the electric field, ε, and the charge of the oscillator, *q,* like this:

$$\left|\psi_{n}\right\rangle = \left|n\right\rangle + \frac{q\varepsilon}{\hbar\omega} \frac{\hbar^{1/2}}{\left(2m\omega\right)^{1/2}} \left(n^{1/2} \left|n-1\right\rangle - \ldots \right)$$

And the wave function also spreads to the other adjacent state, $|n+1\rangle$, like this:

$$\left|\psi_{n}\right\rangle = \left|n\right\rangle + \frac{q\varepsilon}{\hbar\omega} \frac{\hbar^{1/2}}{\left(2m\omega\right)^{1/2}} \left(n^{1/2} \left|n-1\right\rangle - \left(n+1\right)^{1/2} \left|n+1\right\rangle \right)$$

You end up mixing states. That blending between states means that the perturbation you apply must be small with respect to the separation between unperturbed energy states, or you risk blurring the whole system to the point that you can't make any predictions about what's going to happen.

In any case, that's a nice result — blending the states in proportion to the strength of the electric field you apply — and it's typical of the result you get with perturbation theory.

Okay, that's how nondegenerate perturbation theory works. As you can see, it's strongly dependent on having the energy states separate so that your

solution can blend them. But what happens when you have a system where the energies are degenerate? You take a look at that in the next section.

Working with Perturbations to Degenerate Hamiltonians

This section tackles systems in which the energies are degenerate. Take a look at this unperturbed Hamiltonian:

$$H_0 \left|\phi_{n_\alpha}\right\rangle = E^{(0)}{}_n \left|\phi_{n_\alpha}\right\rangle \quad (\alpha = 1,2,3\ldots)$$

In other words, several states have the same energy. Say the energy states are *f*-fold degenerate, like this:

$$H_0 \left|\phi_{n_\alpha}\right\rangle = E^{(0)}{}_n \left|\phi_{n_\alpha}\right\rangle \quad (\alpha = 1,2,3,\ldots,f)$$

How does this affect the perturbation picture? The complete Hamiltonian, H, is made up of the original, unperturbed Hamiltonian, H_0, and the perturbation Hamiltonian, H_ρ:

$$H\left|\psi_n\right\rangle = \left(H_0 + H_\rho\right)\left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$$

In zeroth-order approximation, you can write the eigenfunction $|\psi_n\rangle$ as a combination of the degenerate states $|\phi_{n_\alpha}\rangle$:

$$\left|\psi_n\right\rangle = \sum_{\alpha=1}^{f} a_\alpha \left|\phi_{n_\alpha}\right\rangle \ldots$$

Note that in what follows, you assume that $\langle\phi_n|\phi_n\rangle = 1$ and $\langle\phi_m|\phi_n\rangle = 0$ if *m* is not equal to *n*. Also, you assume that the $|\psi_n\rangle$ are normalized — that is, $\langle\psi_n|\psi_n\rangle = 1$.

Plugging this zeroth-order equation into the complete Hamiltonian equation, you get

$$\sum_\alpha \left[E^{(0)}{}_n \left|\phi_{n_\alpha}\right\rangle + H_\rho \left|\phi_{n_\alpha}\right\rangle\right] a_\alpha = E_n \sum_\alpha a_\alpha \left|\phi_{n_\alpha}\right\rangle$$

Now multiplying that equation by $\langle\phi_{n_\beta}|$ gives you

$$\sum_\alpha \left[\left\langle \phi_{n_\beta} \middle| \mathrm{E}^{(0)}{}_n \middle| \phi_{n_\alpha} \right\rangle + \left\langle \phi_{n_\beta} \middle| \mathrm{H}_\rho \middle| \phi_{n_\alpha} \right\rangle \right] a_\alpha = \mathrm{E}_n \sum_\alpha a_\alpha \left\langle \phi_{n_\beta} \middle| \phi_{n_\alpha} \right\rangle$$

Using the fact that $\langle\phi_n|\phi_n\rangle = 1$ and $\langle\phi_m|\phi_n\rangle = 0$ if *m* is not equal to *n* gives you

$$a_\beta \mathrm{E}_n = a_\beta \mathrm{E}^{(0)}{}_n + \sum_{\alpha=1}^{f} a_\alpha \left\langle \phi_{n_\beta} \middle| \mathrm{H}_\rho \middle| \phi_{n_\alpha} \right\rangle$$

Physicists often write that equation as

$$\sum_{\alpha=1}^{f} a_\alpha \mathrm{H}_{\rho_{\alpha\beta}} - \left(a_\beta \mathrm{E}_n - a_\beta \mathrm{E}^{(0)}{}_n \right) = 0 \quad (\beta = 1,2,3,\ldots,f)$$

where $\mathrm{H}_{\rho_{\alpha\beta}} = \left\langle \phi_{n_\alpha} \middle| \mathrm{H}_\rho \middle| \phi_{n_\beta} \right\rangle$. And people also write that equation as

$$\sum_{\alpha=1}^{f} a_\alpha \mathrm{H}_{\rho_{\alpha_\beta}} - a_\beta \mathrm{E}^{(1)}{}_n = 0 \quad (\beta = 1,2,3,\ldots,f)$$

where $\mathrm{E}^{(1)}{}_n = \mathrm{E}_n - \mathrm{E}^{(0)}{}_n$. That's a system of linear equations, and the solution exists only when the determinant to this array is nonvanishing:

$$\begin{bmatrix} \mathrm{H}_{\rho 11} - \mathrm{E}_n^{(1)} & \mathrm{H}_{\rho 12} & \mathrm{H}_{\rho 13} & \ldots & \mathrm{H}_{\rho 1f} \\ \mathrm{H}_{\rho 21} & \mathrm{H}_{\rho 22} - \mathrm{E}_n^{(1)} & \mathrm{H}_{\rho 23} & \ldots & \mathrm{H}_{\rho 2f} \\ & \vdots & & & \\ \mathrm{H}_{\rho f1} & \mathrm{H}_{\rho f2} & \mathrm{H}_{\rho f3} & \ldots & \mathrm{H}_{\rho ff} - \mathrm{E}_n^{(1)} \end{bmatrix}$$

The determinant of this array is an *f*th degree equation in $\mathrm{E}^{(1)}{}_n$, and it has *f* different roots, $\mathrm{E}^{(1)}{}_{n_\alpha}$. Those *f* different roots are the first-order corrections to the Hamiltonian. Usually, those roots are different because of the applied perturbation. In other words, the perturbation typically gets rid of the degeneracy.

So here's the way you find the eigenvalues to the first order — you set up an *f*-by-*f* matrix of the perturbation Hamiltonian, H_ρ, where $\mathrm{H}_{\rho_{\alpha\beta}} = \langle\phi_{n_\alpha}|\mathrm{H}_\rho|\phi_{n_\beta}\rangle$:

$$\begin{bmatrix} H_{\rho 11} & H_{\rho 12} & H_{\rho 13} & \dots & H_{\rho 1f} \\ H_{\rho 21} & H_{\rho 22} & H_{\rho 23} & \dots & H_{\rho 2f} \\ & \vdots & & & \\ H_{\rho f1} & H_{\rho f2} & H_{\rho f3} & \dots & H_{\rho ff} \end{bmatrix}$$

Then diagonalize this matrix and determine the *f* eigenvalues $E^{(1)}{}_{n_\alpha}$ and the matching eigenvectors:

$$\begin{bmatrix} a_{\alpha 1} \\ a_{\alpha 2} \\ a_{\alpha 3} \\ . \\ . \\ . \\ a_{\alpha f} \end{bmatrix} = a_\beta \quad \beta = 1,2,3,\dots f$$

Then you get the energy eigenvalues to first order this way:

$$E_{n_\alpha} = E^{(0)}{}_n + E^{(1)}{}_{n_\alpha} \quad (\alpha = 1,2,3,\dots,f)$$

And the eigenvectors are

$$|\psi_{n_\alpha}\rangle = \sum_{\beta=1}^{f} a_{\alpha\beta} |\phi_{n_\beta}\rangle$$

In the next section, you look at an example to clarify this idea.

Testing Degenerate Perturbation Theory: Hydrogen in Electric Fields

In this section, you see whether degenerate perturbation theory can handle the hydrogen atom, which has energy states degenerate in different angular momentum quantum numbers, when you remove that degeneracy by applying an electric field. This setup is called the *Stark effect.*

Specifically, suppose you apply an electric field, ε, to a hydrogen atom in the $n = 2$ excited state. That state has four eigenfunctions that have the same energy, where the quantum numbers are $|nlm\rangle$ (note that you're renaming these eigenfunctions $|1\rangle$, $|2\rangle$, and so on to make the calculation easier):

- $|1\rangle = |200\rangle$
- $|2\rangle = |211\rangle$
- $|3\rangle = |210\rangle$
- $|4\rangle = |21-1\rangle$

All these unperturbed states have the same energy, $E = -R/4$, where R is the *Rydberg constant,* 13.6 eV. But at least some of these states will have their energies changed when you apply the electric field.

What does the electric field, ε, cause the perturbation Hamiltonian, H_p, to become? Here's the perturbation Hamiltonian:

$$H_p = e\varepsilon z$$

So you have to evaluate this equation for the various states. For example, what is the following expression equal to, where $\langle 1| = \langle 200|$ and $|3\rangle = |210\rangle$?

$$\langle 1|H_p|3\rangle$$

You solve for the unperturbed hydrogen wave functions in Chapter 9. In general, here's what the wave function $\psi_{nlm}(r, \theta, \phi)$ looks like for hydrogen:

$$\psi_{nlm}(r,\theta,\phi) = \frac{\left(\frac{2}{nr^0}\right)^{3/2}\left[(n-l-1)!\right]^{1/2}}{\left[2n(n+1)!\right]^{1/2}} e^{-r/nr_0}\left(\frac{2r}{nr_0}\right)^{l} L_{n-l-1}{}^{2l+1}\left(\frac{2r}{nr_0}\right) Y_{lm}(\theta,\phi)$$

where $L_{n-l-1}{}^{2l+1}(2r/nr_0)$ is a generalized Laguerre polynomial. Doing all the math gives you the following result, where a_0 is the Bohr radius of the atom:

$$\langle 1|H_p|3\rangle = e\varepsilon\langle 1|z|3\rangle = -3e\varepsilon a_0$$

The $\langle 1|H_p|3\rangle$ is just one term you have to compute, of course. Here's the full matrix for the perturbation Hamiltonian connecting all states, where $H_{p_{\alpha\beta}} = \langle\alpha|H_p|\beta\rangle$:

$$\begin{bmatrix} H_{\rho 11} & H_{\rho 12} & H_{\rho 13} & H_{\rho 14} \\ H_{\rho 21} & H_{\rho 22} & H_{\rho 23} & H_{\rho 24} \\ H_{\rho 31} & H_{\rho 32} & H_{\rho 33} & H_{\rho 34} \\ H_{\rho 41} & H_{\rho 42} & H_{\rho 43} & H_{\rho 44} \end{bmatrix}$$

Doing the math gives you this remarkably simple result:

$$\begin{bmatrix} H_{\rho 11} & H_{\rho 12} & H_{\rho 13} & H_{\rho 14} \\ H_{\rho 21} & H_{\rho 22} & H_{\rho 23} & H_{\rho 24} \\ H_{\rho 31} & H_{\rho 32} & H_{\rho 33} & H_{\rho 34} \\ H_{\rho 41} & H_{\rho 42} & H_{\rho 43} & H_{\rho 44} \end{bmatrix} = -3e\varepsilon a_0 \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Diagonalizing this matrix gives you these eigenvalues — the first-order corrections to the unperturbed energies:

- $E^{(1)}_1 = -3e\varepsilon a_0$
- $E^{(1)}_2 = 0$
- $E^{(1)}_3 = 3e\varepsilon a_0$
- $E^{(1)}_4 = 0$

where $E^{(1)}_1$ is the first-order correction to the energy of the |1> eigenfunction, $E^{(1)}_2$ is the first-order correction to the energy of the |2> eigenfunction, and so on. Adding these corrections to the unperturbed energy for the $n = 2$ state gives you the final energy levels:

- $E_1 = \frac{-R}{4} - 3e\varepsilon a_0$
- $E_2 = \frac{-R}{4}$
- $E_3 = \frac{-R}{4} + 3e\varepsilon a_0$
- $E_4 = \frac{-R}{4}$

where R is the Rydberg constant. Note this result: The Stark effect removes the energy degeneracy in |200> and |210> (the |1> and |3> eigenfunctions), but the degeneracy in |211> and |21 – 1> (the |2> and |4> eigenfunctions) remains.

Chapter 12

Wham-Blam! Scattering Theory

In This Chapter

- Switching between lab and center-of-mass frames
- Solving the Schrödinger equation
- Finding the wave function
- Putting the Born approximation to work

Your National Science Foundation grant finally came through, and you built your new synchrotron — a particle accelerator. Electrons and anti-electrons accelerate at near the speed of light along a giant circular track enclosed in a vacuum chamber and collide, letting you probe the structure of the high-energy particles you create. You're sitting at the console of your giant new experiment, watching the lights flashing and the signals on the screens approvingly. Millions of watts of power course through the thick cables, and the radiation monitors are beeping, indicating that things are working. Cool.

You're accelerating particles and smashing them against each other to observe how they scatter. But this is slightly more complex than observing how pool balls collide. Classically, you can predict the exact angle at which colliding objects will bounce off each other if the collision is *elastic* (that is, momentum and kinetic energy are both conserved). Quantum mechanically, however, you can only assign probabilities to the angles at which things scatter.

Physicists use large particle accelerators to discover more about the structure of matter, and that study is central to modern physics. This chapter serves as an introduction to that field of study. You get to take a look at particle scattering on the subatomic level.

Introducing Particle Scattering and Cross Sections

Think of a scattering experiment in terms of *particles in* and *particles out.* Look at Figure 12-1, for example. In the figure, particles are being sent in a

stream from the left and interacting with a target; most of them continue on unscattered, but some particles interact with the target and scatter.

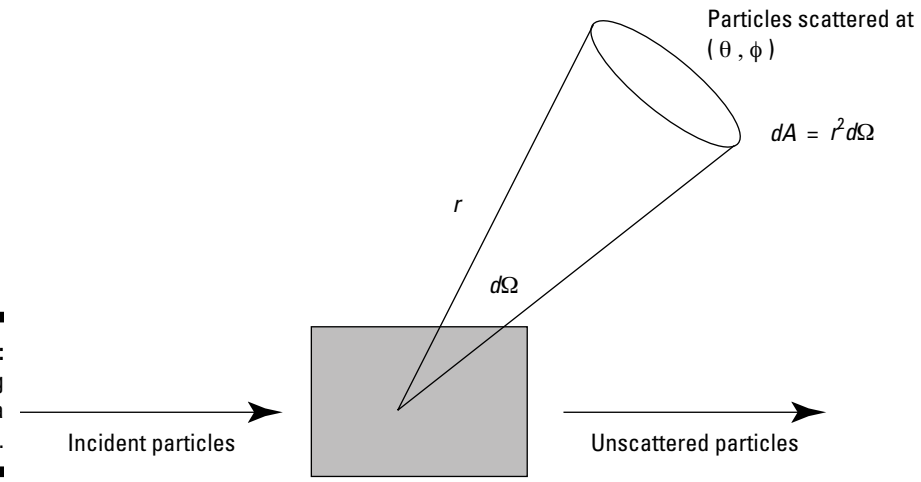


Figure 12-1: Scattering from a target.

Those particles that do scatter do so at a particular angle in three dimensions — that is, you give the scattering angle as a solid angle, $d\Omega$, which equals $\sin\theta\, d\theta\, d\phi$, where ϕ and θ are the spherical angles I introduce in Chapter 8.

The number of particles scattered into a specific $d\Omega$ per unit time is proportional to a very important quantity in scattering theory: the differential cross section.

The *differential cross section* is given by $\frac{d\sigma(\phi,\theta)}{d\Omega}$, and it's a measure of the number of particles per second scattered into $d\Omega$ per incoming flux. The *incident flux,* J (also called the *current density*), is the number of incident particles per unit area per unit time. So $\frac{d\sigma(\phi,\theta)}{d\Omega}$ is

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{1}{\mathrm{J}}\frac{d\mathrm{N}(\phi,\theta)}{d\Omega}$$

where $N(\phi, \theta)$ is the number of particles at angles ϕ and θ.

The differential cross section $\frac{d\sigma(\phi,\theta)}{d\Omega}$ has the dimensions of area, so calling

it a cross section is appropriate. The cross section is sort of like the size of the bull's eye when you're aiming to scatter incident particles through a specific solid angle.

The *differential cross section* is the cross section for scattering to a specific solid angle. The *total cross section,* σ, is the cross section for scattering of any kind, through any angle. So if the differential cross section for scattering to a particular solid angle is like the bull's eye, the total cross section corresponds to the whole target.

You can relate the total cross section to the differential cross section by integrating the following:

$$\sigma = \int \frac{d\sigma(\phi,\theta)d\Omega}{d\Omega} = \int_0^{2\pi}\int_0^{\pi} \frac{d\sigma(\phi,\theta)}{d\Omega}\sin\theta\, d\theta\, d\phi$$

Translating between the Center-of-Mass and Lab Frames

Now you can start getting into the details of scattering, beginning with a discussion of the center-of-mass frame versus the lab frame. Experiments take place in the *lab frame,* but you do scattering calculations in the *center-of-mass frame,* so you have to know how to translate between the two frames. This section explains how the frames differ and shows you how to relate the scattering angles and cross sections when you change frames.

Framing the scattering discussion

Look at Figure 12-2 — that's scattering in the lab frame. One particle, traveling at v_{1lab}, is incident on another particle that's at rest ($v_{2lab} = 0$) and hits it. After the collision, the first particle is scattered at angle θ_1, traveling at v'_{1lab}, and the other particle is scattered at angle θ_2 and velocity v'_{2lab}.

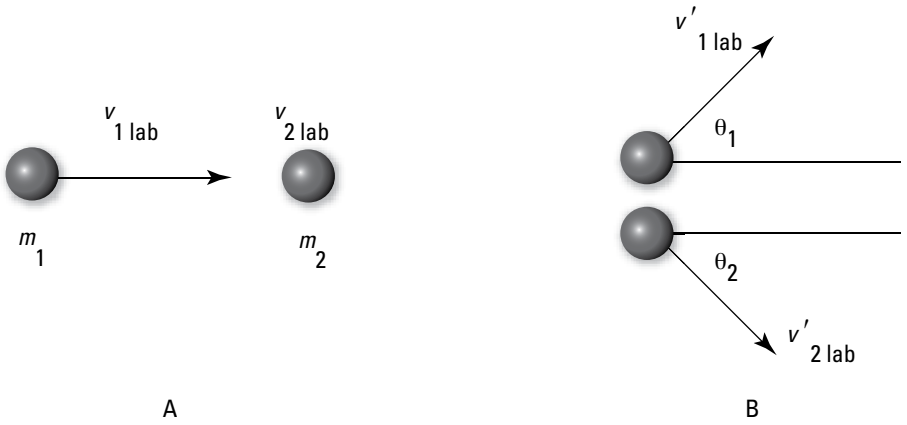


Figure 12-2: Scattering in the lab frame.

Now in the center-of-mass frame, the center of mass is stationary and the particles head toward each other with velocities v_{1c} and v_{2c}, respectively. After they collide, they head away from each other with velocities v'_{1c} and v'_{2c}, at angles θ and $\pi - \theta$.

You have to move back and forth between these two frames — the lab frame and the center-of-mass frame — so you need to relate the velocities and angles (in a nonrelativistic way).

Relating the scattering angles between frames

To relate the angles θ_1 and θ, you start by noting that you can connect v_{1lab} and v_{1c} using the velocity of the center of mass, v_{cm}, this way:

$$\boldsymbol{v}_{1lab} = \boldsymbol{v}_{1c} + \boldsymbol{v}_{cm}$$

In addition, here's what can say about the velocity of particle 1 after it collides with particle 2:

$$\boldsymbol{v}'_{1lab} = \boldsymbol{v}'_{1c} + \boldsymbol{v}_{cm}$$

Now you can find the components of these velocities:

- $\boldsymbol{v}'_{1lab} \cos\theta_1 = \boldsymbol{v}'_{1c} \cos\theta + \boldsymbol{v}_{cm}$
- $\boldsymbol{v}'_{1lab} \sin\theta_1 = \boldsymbol{v}'_{1c} \sin\theta$

Dividing the equation in the second bullet by the one in the first gives you

$$\tan\theta_1 = \frac{\sin\theta}{\cos\theta + \boldsymbol{v}_{cm} / \boldsymbol{v}'_{1c}}$$

But wouldn't it be easier if you could relate θ_1 and θ by something that didn't involve the velocities, only the masses, such as the following?

$$\tan\theta_1 = \frac{\sin\theta}{\cos\theta + m_1 / m_2}$$

Well, you can. To see that, start with

$$\boldsymbol{v}_{cm} = \frac{m_1}{m_1 + m_2}\boldsymbol{v}_{1lab}$$

And you can show that

$$\boldsymbol{v}_{1c} = \frac{m_2}{m_1 + m_2}\boldsymbol{v}_{1lab}$$

You can also use the conservation of momentum to say what happens after the collision. In fact, because the center of mass is stationary in the center-of-mass frame, the total momentum before and after the collision is zero in that frame, like this:

$$m_1\boldsymbol{v}_{1c} + m_2\boldsymbol{v}_{2c} = 0$$

Therefore

$$\boldsymbol{v}_{2c} = -\frac{m_1}{m_2}\boldsymbol{v}_{1c}$$

And after the collision, $m_1\boldsymbol{v}'_{1c} + m_2\boldsymbol{v}'_{2c} = 0$, which means that

$$\boldsymbol{v}'_{2c} = -\frac{m_1}{m_2}\boldsymbol{v}'_{1c}$$

Also, if the collision is elastic (and you assume all collisions are elastic in this chapter), kinetic energy is conserved in addition to momentum, so that means the following is true:

$$\frac{1}{2}m_1{v_{1c}}^2+\frac{1}{2}m_2{v_{2c}}^2=\frac{1}{2}m_1{v'_{1c}}^2+\frac{1}{2}m_2{v'_{2c}}^2$$

Substituting $\boldsymbol{v}_{2c}=-\frac{m_1}{m_2}\boldsymbol{v}_{1c}$ and $\boldsymbol{v}'_{2c}=-\frac{m_1}{m_2}\boldsymbol{v}'_{1c}$ into this equation gives you

$v'_{1c} = v_{1c}$
and $v'_{2c} = v_{2c}$

Given these two equations, you can redo $\boldsymbol{v}_{1c}=\frac{m_2}{m_1+m_2}\boldsymbol{v}_{1lab}$ as

$$\boldsymbol{v}'_{1c}=\boldsymbol{v}_{1c}=\frac{m_2}{m_1+m_2}\boldsymbol{v}_{1lab}$$

Dividing the magnitude of each side of $\boldsymbol{v}_{cm}=\frac{m_1}{m_1+m_2}\boldsymbol{v}_{1lab}$ by the magnitude of the above equation gives you

$$\frac{v_{cm}}{v'_{1c}}=\frac{m_1}{m_2}$$

And because you saw earlier that $\tan\theta_1=\frac{\sin\theta}{\cos\theta+v_{cm}/v'_{1c}}$, substituting $\frac{v_{cm}}{v'_{1c}}=\frac{m_1}{m_2}$ into this equation gives you at last

$$\tan\theta_1=\frac{\sin\theta}{\cos\theta+m_1/m_2}$$

Okay, that relates θ_1 and θ, which is what you were trying to do. Using the relation $\cos\theta_1=\frac{1}{\left(\tan^2\theta_1+1\right)^{1/2}}$, you can rewrite $\tan\theta_1=\frac{\sin\theta}{\cos\theta+m_1/m_2}$ as the following:

$$\cos\theta_1=\frac{\cos\theta+m_1/m_2}{\left[1+m_1^2/m_2^2+2\cos\theta\left(m_1/m_2\right)\right]^{1/2}}$$

You can also relate θ_2 and θ. You can show that $\tan\theta_2=\cot\left(\theta/2\right)$, which, using a little trig, means that

$$\theta_2=\frac{\pi-\theta}{2}$$

Okay, now you've related the angles between the lab and center-of-mass frames. How about relating the cross sections in the two frames? That's in the next section.

Translating cross sections between the frames

The preceding section relates θ_1 and θ and θ_2 — the angles of the scattered particles in the lab frame and the center-of-mass frame. Now how about relating the differential cross section — the bull's eye when you're aiming to scatter the particles at a particular angle — between the lab and center-of-mass frames?

The differential $d\sigma$ (total cross section) is infinitesimal in size, and it stays the same between the two frames. But the angles that make up $d\Omega$, the scattering angle, vary when you translate between frames. You get to take a look at how that works now, relating the lab differential cross section:

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{lab}$$

to the center-of-mass differential cross section:

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$

In the lab frame, $d\Omega_1 = \sin\theta_1\, d\theta_1\, d\phi_1$. And in the center-of-mass frame, $d\Omega = \sin\theta\, d\theta\, d\phi$. Because $d\sigma_{lab} = d\sigma_{cm}$, the following equation is true:

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} d\Omega_1 = \left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm} d\Omega$$

Putting that equation with the equations for the lab frame and the center-of-mass frame, you have

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = \left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm} \frac{\sin\theta}{\sin\theta_1}\frac{d\theta}{d\theta_1}\frac{d\phi}{d\phi_1}$$

Because you have cylindrical symmetry here, $\phi = \phi_1$, so

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = \left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm} \frac{\sin\theta}{\sin\theta_1}\frac{d\theta}{d\theta_1} = \left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm} \frac{d(\cos\theta)}{d(\cos\theta_1)}$$

You've already seen that $\cos\theta_1 = \dfrac{\cos\theta + m_1/m_2}{\left[1 + m_1^2/m_2^2 + 2\cos\theta\left(m_1/m_2\right)\right]^{1/2}}$, so

$\dfrac{d(\cos\theta_1)}{d(\cos\theta)} = \dfrac{1 + \cos\theta\left(m_1/m_2\right)}{\left[1 + m_1^2/m_2^2 + 2\cos\theta\left(m_1/m_2\right)\right]^{3/2}}$. Therefore

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = \frac{\left[1 + m_1^2/m_2^2 + 2\cos\theta\left(m_1/m_2\right)\right]^{3/2}}{1 + \cos\theta\left(m_1/m_2\right)} \left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$

You can also show that

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_2}\right|_{lab} = 4\sin\left(\frac{\theta}{2}\right)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$

Trying a lab-frame example with particles of equal mass

Say you have two particles of equal mass colliding in the lab frame (where one particle starts at rest). You want to show that the two particles end up traveling at right angles with respect to each other in the lab frame.

Note that if $m_1 = m_2$, then $\cos\theta_1 = \dfrac{\cos\theta + m_1/m_2}{\left[1 + m_1^2/m_2^2 + 2\cos\theta\left(m_1/m_2\right)\right]^{1/2}}$ gives $\tan(\theta_1) = \tan(\theta/2)$, so $\theta_1 = \theta/2$. And $\left.\dfrac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = \dfrac{\left[1 + m_1^2/m_2^2 + 2\cos\theta\left(m_1/m_2\right)\right]^{3/2}}{1 + \cos\theta\left(m_1/m_2\right)} \left.\dfrac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$ becomes

$$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = 4\cos\left(\frac{\theta}{2}\right)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$

Note also that $\tan(\theta_2) = \cot(\theta/2)$, or $\tan(\theta_2) = \tan(\pi/2 - \theta/2)$.

You know that $\theta_1 = \theta/2$, and $\tan(\theta_2) = \tan(\pi/2 - \theta/2)$ tells you that the following is true:

$$\theta_2 = \pi/2 - \theta/2$$

So substituting $\theta_1 = \theta/2$ into the preceding equation gives you

$$\theta_2 = \pi/2 - \theta_1$$
$$\theta_2 + \theta_1 = \pi/2$$

Therefore, θ_2 and θ_1, the angles of the particles in the lab frame after the collision, add up to $\pi/2$ — which means θ_2 and θ_1 are at right angles with respect to each other. Cool.

In this case, you can use the relations you've already derived to get these relations in the special case where $m_1 = m_2$:

- $$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = 4\cos(\theta_1)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$
- $$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_1}\right|_{lab} = 4\cos\left(\frac{\theta}{2}\right)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$
- $$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_2}\right|_{lab} = 4\cos(\theta_2)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$
- $$\left.\frac{d\sigma(\phi,\theta)}{d\Omega_2}\right|_{lab} = 4\cos\left(\frac{\theta}{2}\right)\left.\frac{d\sigma(\phi,\theta)}{d\Omega}\right|_{cm}$$

Tracking the Scattering Amplitude of Spinless Particles

In the earlier section "Translating between the Center-of-Mass and Lab Frames," you see how to translate from the lab frame to the center-of-mass frame and back again, and those translations work classically as well as in quantum physics (as long as the speeds involved are nonrelativistic). Now

you look at the elastic scattering of two spinless nonrelativistic particles from the time-independent quantum physics point of view.

Assume that the interaction between the particles depends only on their relative distance, $|r_1 - r_2|$. You can reduce problems of this kind to two decoupled problems (see Chapter 9 for details). The first decoupled equation treats the center of mass of the two particles as a free particle, and the second equation is for an effective particle of mass $\frac{m_1 m_2}{m_1 + m_2}$.

The first decoupled equation, the free-particle equation of the center of mass, is of no interest to you in scattering discussions. The second equation is the one to concentrate on, where $\mu = \frac{m_1 m_2}{m_1 + m_2}$:

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

You can use the preceding equation to solve for the probability that a particle is scattered into a solid angle $d\Omega$ — and you give this probability by the differential cross section, $\frac{d\sigma}{d\Omega}$.

In quantum physics, wave packets represent particles. In terms of scattering, these wave packets must be wide enough so that the spreading that occurs during the scattering process is negligible (however, the wave packet can't be so spread that it encompasses the whole lab, including the particle detectors). Here's the crux: After the scattering, the wave function breaks up into two parts — an unscattered part and a scattered part. That's how scattering works in the quantum physics world.

The incident wave function

Assume that the scattering potential $V(r)$ has a very finite range, *a*. Outside that range, the wave functions involved act like free particles. So the incident particle's wave function, outside the limit of $V(r)$ — that is, outside the range *a* from the other particle — is given by this equation, because $V(r)$ is zero:

$$\nabla^2\phi_{inc}(r) + k_0^2\phi_{inc}(r) = 0$$

where $k_0^2 = \frac{2\mu E_0}{\hbar^2}$.

The form $\nabla^2\phi_{inc}(r) + k_0^2\phi_{inc}(r) = 0$ is the equation for a plane wave, so $\phi_{inc}(r)$ is $\phi_{inc}(r) = Ae^{i\boldsymbol{k}_0\cdot\boldsymbol{r}}$, where A is a constant and $\boldsymbol{k}_0 \cdot \boldsymbol{r}$ is the dot product between the incident wave's wave vector and $\boldsymbol{r}$. In other words, you're treating the incident particle as a particle of momentum $p = \hbar k$.

The scattered wave function

After the scattering of the spinless particles, the nonscattered wave function isn't of much interest to you, but the scattered wave function is. Although the incident wave function has the form $\phi_{inc}(r) = Ae^{i\mathbf{k}_0\cdot\mathbf{r}}$, the scattered wave function has a slightly different form:

$$k^2 = \frac{2\mu E_0}{\hbar^2}$$

The $f(\phi, \theta)$ part is called the *scattering amplitude*, and your job is to find it. Here, A is a normalization factor and

$$|k| = \frac{2\mu E}{\hbar^2}$$

where E is the energy of the scattered particle.

Relating the scattering amplitude and differential cross section

The scattering amplitude of spinless particles turns out to be crucial to understanding scattering from the quantum physics point of view. To see that, take a look at the current densities, J_{inc} (the flux density of the incident particle) and J_{sc} (the current density for the scattered particle):

- $J_{inc} = \frac{i\hbar}{2\mu}\left(\phi_{inc}\nabla\phi^*_{inc} - \phi^*_{inc}\nabla\phi_{inc}\right)$
- $J_{sc} = \frac{i\hbar}{2\mu}\left(\phi_{sc}\nabla\phi^*_{sc} - \phi^*_{sc}\nabla\phi_{sc}\right)$

Inserting your expressions for ϕ_{inc} and ϕ_{sc} into these equations gives you the following, where $f(\phi, \theta)$ is the scattering amplitude:

- $J_{inc} = |A|^2 \frac{\hbar k_0}{\mu}$
- $J_{sc} = |A|^2 \frac{\hbar k}{\mu r^2}\left|f(\phi,\theta)\right|^2$

Now in terms of the current density, the number of particles $dN(\phi, \theta)$ scattered into $d\Omega$ and passing through an area $dA = r^2 d\Omega$ is

$$dN(\phi, \theta) = J_{sc} r^2 d\Omega$$

Plugging in $J_{sc} = |A|^2 \frac{\hbar k}{\mu r^2} |f(\phi,\theta)|^2$ into the preceding equation gives you

$$\frac{dN(\phi,\theta)}{d\Omega} = |A|^2 \frac{\hbar k}{\mu} |f(\phi,\theta)|^2$$

Also, recall from the beginning of the chapter that $\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{1}{J}\frac{dN(\phi,\theta)}{d\Omega}$. You get

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{1}{J_{inc}}\frac{dN(\phi,\theta)}{d\Omega} = \frac{k}{k_0}|f(\phi,\theta)|^2$$

And here's the trick — for elastic scattering, $k = k_0$, which means that this is your final result:

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = |f(\phi,\theta)|^2$$

The problem of determining the differential cross section breaks down to determining the scattering amplitude.

Finding the scattering amplitude

To find the scattering amplitude — and therefore the differential cross section — of spinless particles, you work on solving the Schrödinger equation: $\frac{-\hbar^2}{2\mu}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$. You can also write this as

$$(\nabla^2 + k^2)\psi(r) = \frac{2\mu}{\hbar^2}V(r)\psi(r)$$

You can express the solution to that differential equation as the sum of a homogeneous solution and a particular solution:

$$\psi(r) = \psi_h(r) + \psi_p(r)$$

The homogeneous solution satisfies this equation:

$$(\nabla^2 + k^2)\psi(r) = 0$$

And the homogeneous solution is a plane wave — that is, it corresponds to the incident plane wave:

$$Ae^{ik_0 \cdot r}$$

To take a look at the scattering that happens, you have to find the particular solution. You can do that in terms of *Green's functions*, so the solution to $\left(\nabla^2 + k^2\right)\psi(r) = \frac{2\mu}{\hbar^2}\mathrm{V}(r)\psi(r)$ is

$$\psi(r) = Ae^{k_0 \cdot r} + \frac{2\mu}{\hbar^2}\int \mathrm{G}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{V}(r')\psi(r')d^3\boldsymbol{r}'$$

where $\mathrm{G}(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{(2\pi)^3}\int \frac{e^{iq|\boldsymbol{r}-\boldsymbol{r}'|}}{k^2-q^2}d^3\boldsymbol{q}$.

This integral breaks down to

$$\mathrm{G}(\boldsymbol{r}-\boldsymbol{r}') = \frac{-1}{4\pi^2 i|\boldsymbol{r}-\boldsymbol{r}'|}\int \frac{qe^{iq|\boldsymbol{r}-\boldsymbol{r}'|}}{q^2-k^2}dq$$

You can solve the preceding equation in terms of incoming and/or outgoing waves. Because the scattered particle is an outgoing wave, the Green's function takes this form:

$$\mathrm{G}(\boldsymbol{r}-\boldsymbol{r}') = \frac{-e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}$$

You already know that

$$\psi(r) = Ae^{ik_0 \cdot r} + \frac{2\mu}{\hbar^2}\int \mathrm{G}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{V}(r')\psi(r')d^3r'$$

So substituting $\mathrm{G}(\boldsymbol{r}-\boldsymbol{r}') = \frac{-e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}$ into the preceding equation gives you

$$\psi(r) = Ae^{ik_0 \cdot r} - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{V}(r')\psi(r')d^3r'$$

Wow, that's an integral equation for $\psi(r)$, the wave equation — how do you go about solving this whopper? Why, you use the Born approximation, of course.

The Born Approximation: Rescuing the Wave Equation

Okay, your dilemma is to solve the following equation for $\psi(r)$, where $\phi_{inc} = Ae^{ik_0 r}$:

$$\psi(r) = \phi_{inc} - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i\boldsymbol{k}|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} V(r')\psi(r')d^3\boldsymbol{r}'$$

You can do that with a series of successive approximations, called the *Born approximation* (this is a famous result). To start, the zeroth order Born approximation is just $\psi_0(r) = \phi_{inc}(r)$. And substituting this zeroth-order term, $\psi_0(r)$, into the first equation in this section gives you the first-order term:

$$\psi_1(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i|\boldsymbol{r}-\boldsymbol{r}_1|}}{|\boldsymbol{r}-\boldsymbol{r}_1|} V(r_1)\phi_{inc}(r_1)d^3\boldsymbol{r}_1$$

which, using $\psi_0(r) = \phi_{\text{inc}}(r)$ gives you

$$\psi_1(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}_1|}}{|\boldsymbol{r}-\boldsymbol{r}_1|} V(r_1)\phi_{inc}(r_1)d^3\boldsymbol{r}_1$$

You get the second-order term by substituting this equation into $\psi(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i\boldsymbol{k}|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} V(r')\psi(r')d^3\boldsymbol{r}'$:

$$\psi_2(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}_2|}}{|\boldsymbol{r}-\boldsymbol{r}_2|} V(r_2)\psi_1(r_2)d^3\boldsymbol{r}_2$$

And substituting $\psi_1(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i|\boldsymbol{r}-\boldsymbol{r}_1|}}{|\boldsymbol{r}-\boldsymbol{r}_1|} V(r_1)\phi_{inc}(r_1)d^3\boldsymbol{r}_1$ into the preceding equation gives you

$$\psi_2(r) =$$

$$\phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}_2|}}{|\boldsymbol{r}-\boldsymbol{r}_2|} V(r_2)\phi_{inc}(r_2)d^3\boldsymbol{r}_2$$

$$+\frac{\mu^2}{4\pi^2\hbar^4}\int \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}_2|}}{|\boldsymbol{r}-\boldsymbol{r}_2|} V(r_2)\psi_1(r_2)d^3r_2\int \frac{e^{ik|\boldsymbol{r}_2-\boldsymbol{r}_1|}}{|\boldsymbol{r}_2-\boldsymbol{r}_1|} V(r_1)\phi_{inc}(r_1)d^3\boldsymbol{r}_1$$

The pattern continues for the higher terms, which you can find by plugging lower-order terms into higher ones.

Exploring the far limits of the wave function

Now that you've used the Born approximation (see the preceding section), take a look at the case where r is large — in scattering experiments, $r >> r'$, where r is the distance from the target to the detector and r' is the size of the detector. What happens to $\psi(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}'-\mathbf{r}'|}}{r} V(r')\psi(r')d^3\mathbf{r}'$, the exact integral equation for the wave function, when $r >> r'$? Here's the answer:

$$\psi(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i(kr-\mathbf{k}\cdot\mathbf{r}')}}{r} V(r')\psi(r')d^3\mathbf{r}'$$

Because $r >> r'$, you can say that $k|r - r'| \approx kr - \mathbf{k}\cdot\mathbf{r}'$, where $\mathbf{k}\cdot\mathbf{r}'$ is the dot product of $\mathbf{k}$ and $\mathbf{r}'$ ($\mathbf{k}$ is the wave vector of the scattered particle). And

$$\frac{1}{|r-r'|} \approx \frac{1}{r}$$

Using the last two equations in $\psi(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}'-\mathbf{r}'|}}{r} V(r')\psi(r')d^3\mathbf{r}'$ gives you

$$\psi(r) = Ae^{ik_0\cdot r} + \frac{Ae^{ikr}}{r} f(\phi,\theta) \qquad r \to \infty$$

And here

$$f(\theta,\phi) = \frac{-\mu}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}'} \mathrm{V}(r')\psi(r')d^3r' = \frac{-\mu}{2\pi\hbar^2}\langle\phi|\mathrm{V}|\psi\rangle$$

The differential cross section is given by $\frac{d\sigma(\phi,\theta)}{d\Omega} = |f(\phi,\theta)|^2$, which in this case becomes

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^2}\left|\int e^{-\mathbf{k}\cdot\mathbf{r}'} V(r')\psi(r')d^3r'\right|^2 = \frac{\mu^2}{4\pi^2\hbar^2}\left|\langle\phi|V|\psi\rangle\right|^2$$

Using the first Born approximation

If the potential is weak, the incident plane wave is only a little distorted and the scattered wave is also a plane wave. That's the assumption behind the first Born approximation, which you take a look at here. So if you make the assumption that the potential is weak, you can determine from the equation

$$\psi_1(r) = \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{i|\mathbf{r}-\mathbf{r}_1|}}{|\mathbf{r}-\mathbf{r}_1|} \mathrm{V}(r_1)\phi_{inc}(r_1)d^3\mathbf{r}_1$$ that

$$\psi(r) \approx \phi_{inc}(r) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \mathrm{V}(r')\phi_{inc}(r')d^3\mathbf{r}'$$

Okay, so what is $f(\theta, \phi)$? Well

$$f(\phi,\theta) = \frac{-\mu}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}'} \mathrm{V}(r')\psi(r')d^3\mathbf{r}'$$

And this equals the following, where $\boldsymbol{q} = \boldsymbol{k_0} - \boldsymbol{k}$:

$$f(\phi,\theta) = \frac{-\mu_2}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}'} \mathrm{V}(r')\psi(r')d^3\mathbf{r}' = \frac{-\mu}{2\pi\hbar^2}\int e^{-i\mathbf{q}\cdot\mathbf{r}'} \mathrm{V}(r')d^3\mathbf{r}'$$

And because $\frac{d\sigma(\phi,\theta)}{d\Omega} = |f(\phi,\theta)|^2$, you have

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4}\left|\int e^{-i\mathbf{q}\cdot\mathbf{r}'} \mathrm{V}(r')d^3\mathbf{r}'\right|^2$$

When the scattering is elastic, the magnitude of $\boldsymbol{k}$ is equal to the magnitude of $\boldsymbol{k_0}$, and you have

$$q = |\boldsymbol{k_0} - \boldsymbol{k}| = 2k\sin(\theta/2)$$

where θ is the angle between $\boldsymbol{k_0}$ and $\boldsymbol{k}$.

In addition, if you say that V(r) is spherically symmetric, and you can choose the z axis along $\boldsymbol{q}$, then $\boldsymbol{q} \cdot \boldsymbol{r}' = qr'\cos\theta'$, so

$$f(\phi,\theta) = \frac{-\mu}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}'} V(r')d^3r' = \frac{-\mu}{2\pi\hbar^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} e^{-iqr'\cos\theta'} V(r')r'^2\sin\theta'\,dr'\,d\theta'\,d\phi'$$

That equals

$$f(\phi,\theta) = \frac{-\mu}{2\pi\hbar^2}\int_0^{\infty} r'^2\mathrm{V}(r')dr'\int_0^{\pi} e^{-iqr'\cos\theta'}\sin\theta' d\theta'\int_0^{2\pi} d\varphi' = \frac{-2\mu}{q\hbar^2}\int_0^{\infty} r'\mathrm{V}(r')\sin(qr')dr'$$

You know that $\frac{d\sigma(\phi,\theta)}{d\Omega} = \left|f(\phi,\theta)\right|^2$, so

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{4\mu^2}{q^2\hbar^4}\left|\int_0^\infty r' \mathrm{V}(r')\sin(qr')dr'\right|^2$$

You've come far in this chapter — from the Schrödinger equation all the way through the Born approximation, and now to the preceding equation for weak, spherically symmetric potentials. How about you put this to work with some concrete numbers?

Putting the Born approximation to work

In this section, you find the differential cross section for two electrically charged particles of charge Z_1e and Z_2e. Here, the potential looks like this:

$$V(r) = \frac{Z_1 Z_2 e^2}{r}$$

So here's what the differential cross section looks like in the first Born approximation:

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{4Z_1^2 Z_2^2 e^4 \mu^2}{q^2\hbar^4}\left|\int_0^\infty \sin(qr')dr'\right|^2$$

And because $\int_0^\infty \sin(qr')dr' = \frac{1}{q}$, you know that

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{4Z_1^2 Z_2^2 e^4 \mu^2}{q^4\hbar^4}$$

And because $q = 2k\sin(\theta/2)$, the following is true:

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{4Z_1^2 Z_2^2 e^4 \mu^2}{q^4\hbar^4} = \frac{Z_1^2 Z_2^2 e^4}{16E^2}\sin^{-4}\left(\frac{\theta}{2}\right)$$

where E is the kinetic energy of the incoming particle: $E = \frac{\hbar^2 k^2}{2\mu}$.

Now get more specific; say that you're smashing an alpha particle, $Z_1 = 4$, against a gold nucleus, $Z_2 = 79$. If the scattering angle in the lab frame is 60°, what is it in the center-of-mass frame?

The ratio of the particles' mass in this case, m_1/m_2, is 0.02, so the scattering angle in the center-of-mass frame, θ, is the following, where $\theta_{lab} = 60°$:

$$\tan\theta_{lab} = \frac{\sin\theta}{\cos\theta + m_1/m_2}$$

Solving that equation for θ gives you θ = 61°. So what's the cross section for this scattering angle? Take a look:

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = \frac{4Z_1^2Z_2^2e^4\mu^2}{q^4\hbar^4} = \frac{Z_1^2Z_2^2e^4}{16E^2}\sin^{-4}\left(\frac{\theta}{2}\right)$$

Plugging in the numbers if the incident alpha particle's energy is 8 MeV gives you the following:

$$\frac{d\sigma(\phi,\theta)}{d\Omega} = 3.1\times10^{-29}\,\mathrm{m}^2$$

That's the size of the target — the cross section — you have to hit to create the scattering angle seen.