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### **GULISTAN STATE UNIVERSITY**

# Classical and Quantum Scattering Theory. Born Approximation

**Electronic complex for undergraduate students** 

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Dean of the Faculty of Information Technology and Physics-Mathematics O. Murodov The electronic manual provides information about the classical and quantum scattering theory. Both theories deal with the interactions of particles, but they differ significantly in the way they describe these interactions due to the nature of classical versus quantum mechanics.

The electronic guide was created in accordance with the curriculum of the "Quantum mechanics" taught in the undergraduate education program 60530900-Physics. It can be used by undergraduate students, graduate students, and researchers conducting research on the physics of this period.

#### 1. INTRODUCTION

#### 1.1 Classical Scattering Theory

Imagine a particle incident on some scattering center (say, a proton fired at a heavy nucleus). It comes in with an energy E and an **impact parameter** b, and it emerges at some **scattering angle**  $\theta$ -see Figure 1.1. (I'll assume for simplicity that the target is azimuthally symmetrical, so the trajectory remains in one plane, and that the target is very heavy, so the recoil is negligible.) The essential problem of classical scattering



Figure 1 The classical scattering problem, showing the impact parameter b and the scattering angle  $\theta$ .

theory is this: Given the impact parameter, calculate the scattering angle. Ordinarily, of course, the smaller the impact parameter, the greater the scattering angle. **Example: Hard-sphere scattering**. Suppose the target is a billiard ball, of radius R, and the incident particle is a BB, which bounces off elastically (Figure 2). In terms of the angle  $\alpha$ , the impact parameter is  $b = R \sin \alpha$ , and the scattering angle is  $\theta = \pi - 2 \alpha$ , so

$$b = R\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = R\cos\left(\frac{\theta}{2}\right) \tag{1}$$

Evidently

$$\theta = \begin{cases} 2\cos^{-1}\left(\frac{b}{R}\right), & \text{if } b \le R \\ 0, & \text{if } b \ge R \end{cases}$$
(2)

More generally, particles incident within an infinitesimal patch of cross-sectional area d $\sigma$  will scatter into a corresponding infinitesimal solid angle d $\Omega$  (Figure 3). The larger d $\sigma$  is, the bigger d $\Omega$  will be; the proportionality factor,  $D(\Theta) = d\sigma / d\Omega$ , is called the **differential** (scattering) cross-section<sup>1</sup>

$$d\sigma = D(\Theta) \ d\Omega. \tag{3}$$

 $d\sigma = D(\Theta) d\Theta$ 





Figure 3: Particles incident in the area  $d\sigma$  scatter into the solid angle  $d\Omega$ .

In terms of the impact parameter and the azimuthal angle  $\varphi$ ,  $d\sigma = bdbd\varphi$  and  $d\Omega =$  $\sin\theta d\theta d\phi$ , so

$$D(\theta) = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right| \qquad (4)$$

(Since  $\theta$  is typically a decreasing function of b, the derivative is actually negative hence the absolute value sign.)

Example: Hard-sphere scattering (continued). In the case of hard-sphere scattering (Equation 1),

$$\frac{db}{dR} = -\frac{1}{2}R\sin\left(\frac{\theta}{2}\right), \quad (5)$$

So

$$D(\theta) = \frac{R\cos\left(\frac{\theta}{2}\right)}{\sin\theta} \left(\frac{R\sin\left(\frac{\theta}{2}\right)}{2}\right) = \frac{R^2}{4}$$
(6)

This example is unusual in that the differential cross-section is actually independent of  $\theta$ .

The **total cross-section** is the *integral* of  $D(\theta)$  overall solid angles:

$$\sigma = \int D(\theta) \, d\Omega \qquad (7)$$

roughly speaking, it is the total area of incident beam that is scattered by the target. For example, in the case of the hard sphere,

$$\sigma = (R^2/4) \int d\Omega = \pi R^2 \quad (8)$$

which is just what we would expect: It's the cross-sectional area of the sphere; BBs incident within this area will hit the target, and those farther out will miss it completely. But the virtue of the formalism developed here is that it applies just as well to "soft" targets (such as the Coulomb field of a nucleus) that are *not* simply "hit or miss."

Finally, suppose we have a *beam* of incident particles, with uniform intensity (or **luminosity**, as particle physicists call it):

 $\mathcal{L}$  = number of incident particles per unit area, per unit time. (9)

The number of particles entering area  $d\sigma$  (and hence scattering into solid angle  $d\Omega$ ), per unit time, is  $dN = \mathcal{L} d\sigma = \mathcal{L} D(\theta) d\Omega$ , so

$$\mathbf{D}(\mathbf{\theta}) = \frac{1}{\mathcal{L}} \frac{dN}{d\Omega} \quad (10)$$

This is often taken as the *definition* of the differential cross-section, because it makes reference only to quantities easily measured in the laboratory: If the detector accepts particles scattering into a solid angle  $d\Omega$ , we simply count the *number* recorded, per unit time, divide by  $d\Omega$ , and normalize to the luminosity of the incident beam.

#### 1.2 Quantum Scattering Theory

In the quantum theory of scattering, we imagine an incident plane wave,  $\psi(z) = Ae^{ikz}$ , traveling in the z-direction, which encounters a scattering potential, producing an outgoing *spherical* wave (Figure 4). That is, we will look for solutions to the Schrodinger equation of the general form

$$\Psi(\mathbf{r}, \theta) \approx \mathbf{A} \left\{ e^{ikz} + f(\theta) \frac{e^{ikr}}{r} \right\}, \text{ for larger r. (12)}$$

(The spherical wave must carry a factor of 1/r, because this portion of  $|\Psi|^2$  must go like  $1/r^2$  to conserve probability.) The wave number *k* is related to the energy of the incident particles in the usual way:

$$\mathbf{K} \equiv \frac{\sqrt{2mk}}{\hbar} \quad (13)$$

(As before, I shall assume the target is azimuthally symmetrical; in the more general case the amplitude f of the outgoing spherical wave could depend on  $\varphi$  as well as  $\theta$ ) The whole problem is to determine the scattering amplitude  $f(\theta)$ ; it tells you the probability of scattering in a given direction  $\theta$ , and hence is related to the differential cross-section. Indeed, the probability that the incident particle, traveling at speed  $\vartheta$ , passes through the infinitesimal area d $\sigma$ , in time dt, is (see Figure 5)

 $dP = |\Psi_{incident}|^2 dV = |A|^2 (\vartheta dt) d\sigma$ 



Figure 4: Scattering of waves; incoming plane wave generates outgoing spherical wave.



**Figure 5:** The volume dV of incident beam that passes through area d $\sigma$  in time dt

But this is equal to the probability that the particle later emerges into the corresponding solid angle  $d\Omega$ 

$$d\mathbf{P} = |\Psi_{incident}|^2 dV = \frac{|A|^2 |f|^2}{r^2} (\vartheta dt) r^2 d\Omega,$$

from which it follows that  $d\sigma = |f|^2 d\Omega$ , so

$$\mathbf{D}(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (14)$$

Evidently the differential cross-section (which is the quantity of interest to the experimentalist) is equal to the absolute square of the scattering amplitude (which is obtained by solving the Schrodinger equation). In the next sections we will study two techniques for calculating the scattering amplitude: **partial wave analysis** and the **Born approximation**.

#### 2 PARTIAL WAVE ANALYSIS 2.1 Formalism

The Schrodinger equation for a spherically symmetrical potential V (r) admits the separable solutions

$$\Psi(\mathbf{r}, \theta, \varphi) = \mathbf{R}(\mathbf{r}) Y_l^m(\theta, \varphi), \qquad (15)$$

where  $Y_l^m$  is a spherical harmonic (Equation 4.32) and u(r) = r R(r) satisfies the "radial equation":

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = \text{Eu}$$
(16)

At very large r the potential goes to zero, and the centrifugal term is negligible, so

$$\frac{d^2u}{dr^2}\approx -k^2u$$

The general solution is

$$\mathbf{u}(\mathbf{r}) = \mathbf{C}e^{ikr} + De^{-ikr};$$

the first term represents an outgoing spherical wave, and the second an incoming one-for the scattered wave, we evidently want D = 0. At very large r, then,

$$\mathbf{R}(\mathbf{r})\approx\frac{e^{ikr}}{r},$$

as we already deduced (on qualitative grounds) in the previous section.

That's for very large r (more precisely, for  $kr \gg l$ ; in optics it would be called the **radiation zone**). As in one-dimensional scattering theory, we assume that the potential is "localized," in the sense that exterior to some finite scattering region it is essentially zero (Figure 6). In the intermediate region (where V can be ignored but the centrifugal term cannot), the radial equation becomes

$$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2u \tag{17}$$

and the general solution is a linear combination of spherical Bessel functions:

$$u(r) = \operatorname{Ar} j_l(kr) + Brn_l(kr) \quad (18)$$

However, neither  $j_l$  (which is something like a sine function) nor  $n_l$  (which is a sort of generalized cosine function) represents an outgoing (or an incoming) wave. What we need are the linear combinations analogous to  $e^{ikr}$  and  $e^{-ikr}$ ; these are known as **spherical Hankel functions**:

$$h_l^{(1)}(\mathbf{x}) \equiv j_l(\mathbf{x}) + in_l(\mathbf{x}); \ h_l^{(2)}(\mathbf{x}) \equiv j_l(\mathbf{x}) - in_l(\mathbf{x}).$$
 (19)

At large r,  $h_l^{(1)}(kr)$  (the "Hankel function of the first kind") goes like  $e^{ikr} / r$ , whereas )  $h_l^{(2)}(kr)$  (the "Hankel function of the second kind") goes like  $e^{-ikr}$ ; for outgoing waves we evidently need spherical Hankel functions of the *first* kind:

$$R(r) = Ch_l^{(1)}(kr).$$
 (20)



**Figure 1.6:** Scattering from a localized potential: the scattering region (shaded), the intermediate region (where V = 0), and the radiation zone (where kr >> 1).

Thus the exact wave function, in the exterior region [where V (r)= 0], is

$$\Psi(\mathbf{r},\boldsymbol{\theta},\boldsymbol{\varphi}) = \mathbf{A} \left\{ e^{ikz} + \sum_{l,m} C_{l,m} h_l^{(1)}(kr) Y_l^m(\boldsymbol{\theta},\boldsymbol{\varphi}), \right\} \quad (1.21)$$

Now, for very larger, the Hankel function goes like  $(-i)^{l+1}e^{ikr}/kr$  (Table 1.1), so

$$\Psi(\mathbf{r},\theta,\varphi) \approx A \left\{ e^{ikz} + f(\theta,\varphi) \frac{e^{ikr}}{r} \right\}, \quad (1.22)$$

Where

$$f(\theta, \varphi) = \frac{1}{k} \sum_{l,m} (-i)^{l+1} C_{l,m} Y_l^m(\theta, \varphi).$$
(1.23)

This confirms more rigorously the general structure postulated in Equation 11.12, and tells us how to compute the scattering amplitude,  $f(0, \langle I \rangle)$ , in terms of the

**partial wave amplitudes**  $C_{l,m}$ . Evidently the differential cross-section i  $D((\theta, \varphi) = |f(\theta, \varphi)|^2 = \frac{1}{k^2} \sum_{l,m} \sum_{l`m`} (i)^{l-l`} C^*_{l,m} C_{l`m`} (Y^m_l)^* Y^{m`}_{l`}, \quad (1.24)$  **Table 1.1:**Spherical Hankel functions,  $h_l^{(1)}(x)$  and  $h_l^{(2)}(x)$ .

$$h_{0}^{(1)} = -i\frac{e^{iz}}{z} \qquad h_{0}^{(2)} = i\frac{e^{-iz}}{z}$$

$$h_{1}^{(1)} = \left(-\frac{i}{z^{2}} - \frac{1}{z}\right)e^{iz} \qquad h_{1}^{(2)} = \left(\frac{i}{z^{2}} - \frac{1}{z}\right)e^{-iz}$$

$$h_{2}^{(1)} = \left(-\frac{3i}{z^{3}} - \frac{3}{z^{2}} + \frac{i}{z}\right)e^{iz} \qquad h_{2}^{(2)} = \left(\frac{3i}{z^{3}} - \frac{3}{z^{2}} - \frac{i}{z}\right)e^{-iz}$$

$$h_{2}^{(1)} = \left(-\frac{1}{z^{3}} - \frac{3}{z^{2}} + \frac{i}{z}\right)e^{iz} \qquad h_{2}^{(2)} = \left(\frac{3i}{z^{3}} - \frac{3}{z^{2}} - \frac{i}{z}\right)e^{-iz}$$

$$h_l^{(1)} \rightarrow \frac{1}{x} exp\left\{+i\left[x - \frac{\pi}{2}(l+1)\right]\right\}$$
$$h_l^{(2)} \rightarrow \frac{1}{x} exp\left\{-i\left[x - \frac{\pi}{2}(l+1)\right]\right\}$$

and the total cross-section is

$$\sigma = \frac{1}{k^2} \sum_{l,m} \sum_{l'm'} (i)^{l-l'} C_{l,m}^* C_{l'm'} \int (Y_l^m)^* Y_{l'}^{m'} \, \mathrm{d}\Omega = \frac{1}{k^2} \sum_{l,m} \left| C_{l,m} \right|^2.$$
(25)

In the previous paragraph kept the possible  $\varphi$  dependence because it cost me nothing. But if (as is ordinarily the case) V is independent of  $\varphi$ , then only terms with m = 0 survive (remember,  $Y_l^m \sim e^{iz \varphi}$ ). Now

$$Y_l^0(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta), \qquad (26)$$

where  $P_l$  is the *l* th Legendre polynomial. So for the case of azimuthal symmetry, the exact wave function (in the exterior region) is

$$\Psi(\mathbf{r},\theta) = \mathbf{A} \{ e^{ikz} + \sum_{l=0} \sqrt{\frac{4l+1}{4\pi}} C_l h_l^{(1)}(kr) \,\theta P_l(\cos) \}; \qquad (27)$$

the scattering amplitude is

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (-i)^{l+1} \sqrt{\frac{l+1}{4\pi}} C_l P_l(\cos);$$
(28)

and the total cross-section is

$$\sigma = \frac{1}{k^2} \sum_{l=0}^{\infty} |C_l|^2 \quad (29)$$

#### 2.2 Strategy

All that remains is to determine the partial wave amplitudes  $C_l$ , for the potential in question. This is accomplished by solving the Schrodinger equation in the *interior* 

region [where V(r) is distinctly *nonzero*] and matching this to the exterior solution, using the appropriate boundary conditions. But first I need to do a little cosmetic work, because as it stands my notation is hybrid: I used *spherical* coordinates for the scattered wave, but *Canesian* coordinates for the incident wave. Before proceeding, it is useful to rewrite the wave function in a more consistent notation.

Of course,  $e^{ikz}$  satisfies the Schrodinger equation with V = 0. On the other hand, I just argued that the general solution to the Schrodinger equation with V = 0 can be written in the form

$$\sum_{l,m} \left[ A_{l,m} j_l(kr) + B_{l,m} n_l(kr) \right] Y_l^m(\theta,\varphi)$$

In particular, then, it must be possible to express  $e^{ikz}$  in this way. But  $e^{ikz}$  is finite at the origin, so no Neumann functions are allowed in the sum  $[n_l(kr)$  blows up at r = 0], and since  $z = r \cos \theta$  has no  $\varphi$  dependence, only m = 0 terms occur. The expansion of a plane wave in terms of spherical waves is sometimes called **Rayleigh's formula:** 

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos \theta).$$
 (30)

Thus the wave function, in the exterior region, can be written in the more consistent form

$$\Psi(\mathbf{r},\theta) = A \sum_{l=0}^{\infty} \left[ i^{l} (2l+1) j_{l}(kr) + \sqrt{\frac{2l+1}{4\pi}} C_{l} h_{l}^{(1)}(kr) \right] P_{l}(\cos\theta).$$
(31)

Example: Hard-sphere scattering. Suppose

$$V(r) = \begin{cases} \infty, & for \ r \le a \\ 0, & for \ r > a \end{cases}$$
(32)

The boundary condition, then, is

$$\Psi(a,\theta)=0,\qquad(33)$$

So

$$\sum_{l=0}^{\infty} \left[ i^{l} (2l+1) j_{l}(ka) + \sqrt{\frac{2l+1}{4\pi}} C_{l} h_{l}^{(1)}(ka) \right] P_{l}(\cos \theta) = 0$$
(34)

for all  $\theta$ , from which it follows that

$$C_l = -i^l \sqrt{4\pi (2l+1)} \frac{j_l(ka)}{h_l^{(1)}(ka)}.$$
 (35)

In particular, the total cross-section is

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left| \frac{j_l(ka)}{h_l^{(1)}(ka)} \right|^2.$$
(36)

That's the *exact* answer, but it's not terribly illuminating, so let's consider the limiting case of *low-energy scattering:*  $ka \ll 1$ . (Since  $k = 2\pi/\lambda$ ., this amounts to saying that the wavelength is much greater than the radius of the sphere.) Referring to Table 4.3, we note that  $n_l(z)$  is much larger than  $j_l(z)$ , for small z, so

$$\frac{j_l(z)}{h_l^{(1)}(z)} = \frac{j_l(z)}{j_l(z) + in_l(z)} \approx -i\frac{j_l(z)}{n_l(z)}$$

$$\approx -i \frac{\frac{2^{l} l! z^{l}}{(2l+1)!}}{-\frac{(2l)! z^{-l-1}}{2^{l} l!}} = \frac{i}{2l+1} \left[\frac{2^{l} l!}{(2l)!}\right]^{2} z^{2l+1},$$
(37)

and hence

$$\sigma \approx \frac{4\pi}{k} \sum_{l=0}^{\infty} \frac{1}{2l+1} \left[ \frac{2^{l} l!}{(2l)!} \right]^{4} (ka)^{4l+2}.$$

But we're assuming  $ka \ll 1$ , so the higher powers are negligible-in the low-energy approximation the scattering is dominated by the l = 0 term. (This means that the differential cross-section is independent of  $\theta$ , just as it was in the classical case.) Evidently

$$\sigma \approx 4\pi a^2,\tag{38}$$

for low-energy hard-sphere scattering. Surprisingly, the scattering cross-section is *four times* the geometrical cross-section-in fact, *a* is the *total suiface area of the sphere*. This "larger effective size" is characteristic of long-wavelength scattering (it would be true in optics, as well); in a sense, these waves "feel" their way around the whole sphere, whereas classical *particles* only see the head-on cross-section.

# THE BORN APPROXIMATION11.3.1Integral Form of the Schrodinger Equation

The time-independent Schrödinger equation,

$$-\frac{\hbar}{2m}\nabla^2\psi + V\psi = E\psi,\tag{39}$$

can be written more succiccntl as

$$(\nabla^2 + k^2)\psi = Q, \tag{40}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$
 and  $Q = \frac{2m}{\hbar^2}V\psi.$  (41)

This has the superficial form of the **Helmholtz equation**; note, however, that the "inhomogeneous" term (*Q*) *itself* depends on  $\psi$ . Suppose we could find a function G(**r**) that solves the Helmholtz equation with a *delta-function* "source":

$$(\nabla^2 + k^2)G(r) = \delta^3(r).$$
 (42)

Then we could express  $\psi$  as an integral:

$$\psi(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r_0}) Q(\mathbf{r_0}) d^3 \mathbf{r_0}.$$
 [((43)]

For it is easy to show that this satisfies Schrödinger's equation, in the fonn of Equation (40):

$$(\nabla^2 + k^2)\psi = \int [(\nabla^2 + k^2)G(r - r_0)]Q(r_0)d^3r_0 = \int \delta^2 (r - r_0)Q(r_0)d^3r_0 = Q(r_0).$$

 $G(\mathbf{r})$  is called the **Green's function** for the Helmholtz equation. (In general, the Green's function for a given differential equation represents the "response" to a delta-function source.)

Our first task<sup>5</sup> is to solve Equation (42) for  $G(\mathbf{r})$ . This is most easily accomplished by taking the Fourier transform, which turns the *differential* equation into an *algebraic* equation. Let

$$G(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{s}\cdot\mathbf{r}} g(\mathbf{s}) d^3 \mathbf{s}.$$
(44)

Then

$$(\nabla^2 + k^2)G(r) = \frac{1}{(2\pi)^{3/2}} \int [(\nabla^2 + k^2)e^{is \cdot r}] g(s) d^3s$$

But

$$\nabla^2 e^{is \cdot r} = -s^2 e^{is \cdot r},\tag{45}$$

and

$$\delta^3(\mathbf{r}) = \frac{1}{(2\pi)^3} \int e^{i s \cdot \mathbf{r}} d^3 \mathbf{s}, \qquad (46)$$

so Equation (42) says

$$\frac{1}{(2\pi)^{3/2}} \int (-s^2 + k^2) e^{is \cdot r} g(s) d^3 s = \frac{1}{(2\pi)^3} \int e^{is \cdot r} d^3 s$$

If follows that

$$g(\mathbf{s}) = \frac{1}{(2\pi)^{\frac{3}{2}}(k^2 - s^2)}$$
(47)

Putting this back into Equation (24), we find

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3} \int e^{is \cdot \mathbf{r}} \frac{1}{(k^2 - s^2)} d^3 \mathbf{s}.$$
 (48)

Now **r** is fixed, as far as the s integration is concerned, so we may as well choose spherical coordinates  $(s, \theta, \phi)$  with the polar axis along **r** (Figure 7). Then  $s \cdot \mathbf{r} = sr \cos \theta$ , the  $\phi$  integral is trivial  $(2\pi)$ , and the  $\theta$  integral is

$$\int e^{is \cdot r \cos\theta} \sin\theta \, d\theta = -\frac{e^{is \cdot r \cos\theta}}{isr} \Big|_{0}^{\pi} = \frac{2\sin(sr)}{sr}.$$
 (49)

Thus

$$G(\mathbf{r}) = \frac{1}{(2\pi)^2} \frac{2}{r} \int_0^\infty \frac{s\sin(sr)}{k^2 - s^2} ds = \frac{1}{4\pi^2} \int_{-\infty}^\infty \frac{s\sin(sr)}{k^2 - s^2} ds.$$
 (50)

The remaining integral is not so simple. It pays to revert to exponential notation and factor the denominator:

$$G(\mathbf{r}) = \frac{i}{8\pi^2 r} \left\{ \int_{-\infty}^{\infty} \frac{se^{isr}}{(s-k)(s+k)} ds - \int_{-\infty}^{\infty} \frac{se^{-isr}}{(s-k)(s+k)} ds \right\}$$
  
=  $\frac{i}{8\pi^2 r} (I_1 - I_2).$  (51)

These two integrals can be evaluated using Cauchy's integral formula:

$$\oint \frac{f(z)}{(z - z_0)} dz = 2\pi i f(z_0),$$
(52)



**Figure 7:** Convenient coordinates for the integral in equation (48).

if  $z_0$  lies within the contour (otherwise the integral is zero). In the present case the integration is along the real axis, and it passes *right over* the pole singularities at  $\pm k$ . We have to decide how to skirt the poles-I'll go *over* the one at -k and *under* the one at +k (Figure 8). (You're welcome to choose some *other* convention if you like-even winding seven times around each pole; you'll get a

different Green's function, but, as I'll show you in a minute, they're all equally acceptable.)

For each integral in Equation (51) 1 must "close the contour" in such a way that the semicircle at infinity contributes nothing. In the case of  $I_1$ , the factor  $e^{isr}$ goes to zero when s has a large *positive* imaginary part; for this one I close *above* (Figure 9a). The contour encloses only the singularity at s = +k, so

$$I_1 = \oint \left[ \frac{se^{isr}}{s+k} \right] \frac{1}{s-k} ds = 2\pi i \left[ \frac{se^{isr}}{s+k} \right] \Big|_{s=k} = i\pi e^{ikr}.$$
 (53)

In the case of  $I_2$ , the factor  $e^{-isr}$  goes to zero when s has a large *negative* imaginary part, so we close *below* (Figure 9b); this time the contour encloses the singularity at s = -k (and it goes around in the *clockwise* direction, so we pick up a minus sign):

$$I_{2} = \oint \left[ \frac{se^{-isr}}{s-k} \right] \frac{1}{s+k} ds = -2\pi i \left[ \frac{se^{-isr}}{s-k} \right] \Big|_{s=-k} = -i\pi e^{ikr}.$$
(54)

Figure 11.8: Skirting the poles in the contour integral (Equation (51)).



Figure 11.9: Closing the contur in equations (53) and (54).

S = -k

Conclusion:

$$G(r) = \frac{i}{8\pi^2 r} \left[ \left( i\pi e^{ikr} \right) - \left( -i\pi e^{ikr} \right) \right] = -\frac{e^{ikr}}{4\pi r}.$$
 (55)

This, finally, is the Green's function for the Helmholtz equation-the solution to Equation (42). (Or rather, it is *a* Green's function for the Helmholtz equation, for we can add to  $G(\mathbf{r})$  any function  $G_0(\mathbf{r})$  that satisfies the *homogeneous* Helmholtz equation:

$$(\nabla^2 + k^2)G_0(r) = 0.$$
 (56)

clearly, the result (G +G<sub>0</sub>) still satisfies Equation (42). This ambiguity corresponds precisely to the ambiguity in how to skirt the poles-a different choice amounts to picking a different function  $G_0(r)$ .

Returning to Equation (43), the general solution to the Schrödinger equation takes the form

$$\psi(r) = \psi_0(r) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|r-r_0|}}{|r-r_0|} V(r_0)\psi(r_0)d^3r_0,$$
(57)

where  $\psi_0$  satisfies the *free* particle Schrödinger equation,

$$(\nabla^2 + k^2)\psi_0 = 0.$$
 (58)

Equation (57) is the **integral form of the Schrödinger equation** it is entirely equivalent to the more familiar differential form. At first glance it *looks* like an explicit *solution* to the Schrödinger equation (for any potential) - which is too good to be true. Don't be deceived: There's a  $\psi$  under the integral sign on the right-hand side, so we can't do the integral unless we already know the solution! Nevertheless, the integral form can be very powerful, and it is particularly well suited to scattering problems, as we'll see in the following section.

#### 3. The First Born Approximation

Suppose V ( $r_0$ ) is localized about  $r_0 = 0$  that is, the potential drops to zero outside some finite region (as is typical for a scattering problem), and we want to calculate  $\psi(r)$  at pointsfar *away* from the scattering center. Then  $|r| \gg |r_0|$  for all points that contribute to the integral in Equation (57), so

$$|r - r_0|^2 = r^2 + r_0^2 - 2r \cdot r_0 \cong r^2 \left(1 - 2\frac{r \cdot r_0}{r^2}\right),\tag{59}$$

and hence

$$|r - r_0| \cong r - \hat{r} \cdot r_0. \tag{60}$$

Let

$$k \equiv k\hat{r}; \tag{61}$$

then

$$e^{ik|r-r_0|} \cong e^{ikr}e^{-ik\cdot r_0},\tag{62}$$

and therefore

$$\frac{e^{ik|r-r_0|}}{|r-r_0|} \cong \frac{e^{ikr}}{r} e^{-ik \cdot r_0}.$$
 (63)

[In the *denominator* we can afford to make the more radical approximation  $|r - r_0| \cong r$ ; in the *exponent* we need to keep the next term. If this puzzles you, try writing out the next term in the expansion of the denominator. What we are doing is expanding in powers of the small quantity  $(r_0/r)$  and dropping all but the lowest order.]

In the case of scattering, we want

$$\psi_0(r) = A e^{ikz},\tag{64}$$

representing an incident plane wave. For large r, then,

$$\psi(r) \cong Ae^{ikz} - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-ik \cdot r_0} V(r_0) \psi(r_0) d^3 r_0.$$
(65)

This is in the standard form Equation (12), and we can read off the scattering amplitude:

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2 A} \int e^{-ik\cdot r_0} V(r_0)\psi(r_0)d^3r_0.$$
(66)

So far, this is *exact*. Now we invoke the **Born approximation:** Suppose the incoming plane wave is *not substantially altered by the potential;* then it makes sense to use

$$\psi(r_0) \approx \psi(r_0) = Ae^{ikz_0} = Ae^{ik' \cdot r_0}.$$
(67)

where

$$k' \equiv k\hat{z},\tag{68}$$

inside the integral. (This would be the *exact* wave function, if V were zero; it is essentially a *weak potential* approximation.) In the Born approximation, then,

$$f(\theta,\phi) \cong -\frac{m}{2\pi\hbar^2} \int e^{-i(k'-k)\cdot r_0} V(r_0)\psi(r_0)d^3r_0.$$
(69)

(In case you have lost track of the definitions of k and k', they both have magnitude k, but the former points in the direction of the incident beam, while the latter points toward the detector-see Figure (10).

In particular, for **low-energy** (long-wavelength) **scattering**, the exponential factor is essentially constant over the scattering region, and the Born approximation simplifies to

$$f(\theta,\phi) \cong -\frac{m}{2\pi\hbar^2} \int V(r) d^3r,$$
 (low energy). (70)

(I dropped the subscript on r, since there is no occasion for confusion at this point.)



Figure 10: Two wave vectors in the Born approximation: *k* points in the *incident* direction, *k'* in the *scattered* direction.

#### Example: Low-energy soft-sphere scattering. Suppose

$$V(r) = \begin{cases} V_0, & \text{if } r \le a, \\ 0, & \text{if } r > a. \end{cases}$$
(71)

In this case the low-energy scattering amplitude is

$$f(\theta,\phi) \cong -\frac{m}{2\pi\hbar^2} V_0\left(\frac{4}{3}\pi a^3\right) \tag{72}$$

(independent of  $\theta$  and  $\phi$ ), the differential cross-section is

$$\frac{d\sigma}{d\Omega} = |f|^2 \cong \left(\frac{2mV_0 a^3}{3\hbar^2}\right)^2,\tag{73}$$

and the total cross-section is

$$\sigma \cong 4\pi \left(\frac{2mV_0 a^3}{3\hbar^2}\right)^2. \tag{74}$$

For a spherically symmetrical potential, V(r) = V(r), (but *not* necessarily at low energy), the Born approximation again reduces to a simpler form. Define

$$\kappa = k' - k, \tag{75}$$

and let the polar axis for the  $r_0$  integral lie along  $\kappa$ , so that

$$(k'-k)\cdot r_0 = \kappa r_0 \cos\theta_0. \tag{76}$$

Then

$$f(\theta) \cong -\frac{m}{2\pi\hbar^2} \int e^{ikr_0\cos\theta_0} V(r_0) r_0^2 \sin\theta_0 dr_0 d\theta_0 d\phi_0.$$
(77)

The  $\phi_0$  integral is trivial (2 $\pi$ ), and the  $\theta_0$  integral is one we have encountered before (see Equation 11.49). Dropping the subscript on *r*, we are left with

$$f(\theta) \cong -\frac{2m}{\hbar^2 \kappa} \int_0^\infty r V(r) \sin(\kappa r) dr, \quad (spherial symmetr). \tag{78}$$

The angular dependence of f is carried by  $\kappa$ ; from Figure 10 we see that

$$\kappa = 2k \sin(\theta/2). \tag{79}$$

**Example: Yukawa scattering.** The **Yukawa potential** (which is a crude model for the binding force in an atomic nucleus) has the form

$$V(r) = \beta \frac{e^{-\mu r}}{r},\tag{80}$$

where  $\beta$  and  $\mu$  are contacts. The Born approximation gives

$$f(\theta) \cong -\frac{2m\beta}{\hbar^2\kappa} \int_0^\infty e^{-\mu r} \sin(\kappa r) dr = -\frac{2m\beta}{\hbar^2(\mu^2 + \kappa^2)}.$$
 (81)

**Example: Rutherford scattering.** If we put in  $\beta = q_1 q_2 / 4\pi\epsilon_0$ ,  $\mu = 0$ , the Yukawa potential reduces to the Coulomb potential, describing the electrical interaction of two point charges. Evidently the scattering amplitude is

$$f(\theta) \cong -\frac{2mq_1q_2}{4\pi\epsilon_0\hbar^2\kappa^2},\tag{82}$$

or (using Equations (79) and (41)),

$$f(\theta) \cong -\frac{q_1 q_2}{16\pi\epsilon_0 E \sin^2\left(\frac{\theta}{2}\right)}.$$
(83)

The differential cross-section is the square of this:

$$\frac{d\sigma}{d\Omega} = \left[\frac{q_1 q_2}{16\pi\epsilon_0 E \sin^2(\theta/2)}\right]^2,\tag{84}$$

which is precisely the Rutherford formula (Equation 11). It happens that for the Coulomb potential, classical mechanics, the Born approximation, and quantum field theory all yield the same result. In computer parlance, the Rutherford formula is amazingly "robust."

#### 4. The Born Series

The *Born* approximation is similar in spirit to the **impulse approximation** in classical scattering theory. In the impulse approximation we begin by pretending that the particle keeps going in a straight line (Figure 11), and compute the transverse impulse that would be delivered to it in that case:

$$I = \int F_{\perp} dt.$$
(85)

If the deflection is relatively small, this should be a good approximation to the transverse momentum imparted to the particle, and hence the scattering angle is  $\theta \cong \tan^{-1}(I/p).$ (86)

where p is the incident momentum. This is, if you like, the "first-order" impulse approximation (the *zeroth-order* is what we *started* with: no deflection at all). Likewise, in the *zeroth*-order Born approximation the incident plane wave passes by with no modification, and what we explored in the previous section is really the first-order conection to this. But the same idea can be iterated to generate a series of higher-order conections, which presumably converge to the exact answer.



Scattering center

**Figure 11:** The impulse approximation assumes that the particle continues undeflected, and calculates the transverse momentum delivered.



Figure 12: Diagrammatic interpretation of the Born series, Equation (91).

The integral form of the Schrödinger equation reads

$$\psi(r) = \psi_0 + \int g(r - r_0) V(r_0) \psi(r_0) d^3 r_0, \qquad (87)$$

where  $\psi_0$  is the incident wave,

$$g(\mathbf{r}) \equiv -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r}$$
(88)

is the Green's function (into which I have now incorporated the factor  $2m/\hbar^2$ , for convenience), and V is the scattering potential. Schematically,

$$\psi = \psi_0 + \int g V \psi. \tag{89}$$

Suppose we take this expression for  $\psi$ , and plug it in under the integral sign:

$$\psi = \psi_0 + \int g V \psi_0 + \int g V g V \psi. \tag{90}$$

Iterating this procedure, we obtain a formal series for  $\psi$ :

$$\psi = \psi_0 + \int gV\psi_0 + \int gVgV\psi_0 + \int gVgVgV\psi_0 + \dots + \int (gV)^n\psi_0 + \dots$$
(91)

In each term only the incident wave function  $(\psi_0)$  appears, together with more and more powers of gV. The *first Born* approximation truncates the series after the second term, but it is clear now how one generates the higher-order conections.

The *Born* series can be represented diagrammatically as shown in Figure 12. In zeroth order  $\psi$  is untouched by the potential; in first order it is "kicked" once, and then "propagates" out in some new direction; in second order it is kicked, propagates to a new location, is kicked again, and then propagates out; and so on. In this context the Green's function is sometimes called the **propagator**-it tells you how the disturbance propagates between one interaction and the next. The *Born* series was the inspiration for Feynman's formulation of relativistic quantum mechanics, which is expressed entirely in terms of **vertex factors** (*V*) and propagators (*g*), connected together in **Feynman diagrams**.

#### LITERATURE

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