# 1 Scattering theory, lecture notes

A short exposition of basic topics in quantum scattering.

See: Griffiths D.J., *Introduction to quantum mechanics*, chapter 11.

Messia A. *Quantum mechanics*, vol. 2, chapter 19.

## 1.1 Elementary considerations

### 1.1.1 Scattering of plane waves

We consider the scattering of a stationary incident plane wave $\exp(i\mathbf{kx})$ on a potential $V(\mathbf{x})$ which is appreciably nonzero only in a neighborhood of $\mathbf{x}=0$, more exactly at $|\mathbf{x}|<a$.

The incoming wave mostly goes past $V(\mathbf{x})$ without change, but a small part of the wave is scattered into the outgoing wave. The outgoing wave is not a plane wave $\exp(i\mathbf{qx})$ but is similar to a spherical wave $r^{-1}\exp(ikr)$ although it has different amplitudes in different directions, so it is of the form $f(\hat{\mathbf{r}})r^{-1}\exp(ikr)$ at large $r\equiv|\mathbf{x}|$. (Here $\hat{\mathbf{r}}$ is the unit vector in the direction of the vector $\mathbf{x}$.) Therefore the total (stationary) wave function has the following asymptotic form,

$$\psi(\mathbf{x})\approx A\left[e^{i\mathbf{kx}}+f(\hat{\mathbf{r}})r^{-1}e^{ikr}\right],\quad r\gg a. \tag{1}$$

This is the boundary condition which is appropriate for scattering.

Remarks:

1. The spherical part $r^{-1}\exp(ikr)$ has the same wave number $k$ as the incident wave. This is because (by assumption) the scattering potential goes to zero at large $r\gg a$, so the energy of the outgoing particles is the same as that of the incoming particles.
2. The function $f(\hat{\mathbf{r}})$ defined by Eq. (1) has the dimension of *length*.

### 1.1.2 How to obtain the scattered wave

The function $\psi(\mathbf{x})$ must be a solution of the stationary Schrödinger equation,

$$-\frac{\hbar^2}{2\mu}\Delta\psi+V(\mathbf{x})\psi=E\psi. \tag{2}$$

(Here $\mu$ denotes the mass of the particle; later we shall have to use the letter $m$ as an index.) If we somehow find the solution of this equation which satisfies the boundary condition (1) at large $r$, we shall solve the scattering problem in principle.

Our considerations below are devoted to different ways of solving Eq. (2) with the boundary condition (1).

### 1.1.3 Scattering of wave packets

The consideration of plane waves is an idealization. A stationary plane wave $\exp(i\mathbf{kx})$ represents a particle with the energy

$$E=\frac{\hbar k^2}{2m} \tag{3}$$

moving with a definite momentum $\hbar\mathbf{k}$. The position of the particle is completely undefined. A more realistic consideration would be to use time-dependent wave packets with a finite width (much larger than the width $a$ of the potential). That calculation would be more complicated and the end result is almost the same as that of the plane wave calculation.

### 1.1.4 Scattering amplitude and cross-section

The function $f(\hat{\mathbf{r}})$ in Eq. (1) is the scattering amplitude into the direction $\hat{\mathbf{r}}$.

A simple consideration of the incoming and outgoing particle fluxes (omitted here) shows that the differential cross-section of scattering into the infinitesimal solid angle $d\Omega$ around the direction $\hat{\mathbf{r}}$ is

$$\frac{d\sigma}{d\Omega}=|f(\hat{\mathbf{r}})|^2.$$

The total cross-section is by definition

$$\sigma_{tot}=\int d^2\Omega\frac{d\sigma}{d\Omega}.$$

Note that the analogy with the hard-sphere scattering is incomplete: the total cross-section $\sigma_{tot}$ is not equal to the cross-section area that would catch all scattered particles because in general all particles are scattered, if only by a small angle.

## 1.2 Partial wave expansion

The method of partial wave expansion is a special trick to simplify the calculation of the scattering amplitude $f(\hat{\mathbf{r}})$, especially for *spherically symmetric* potentials $V(\mathbf{x})=V(r)$.

### 1.2.1 Definition

Partial wave expansion is an expansion of the wave function in spherical harmonics,

$$\psi(\mathbf{x})=\sum_{l,m}\frac{u_{lm}(r)}{r}Y_{lm}(\hat{\mathbf{r}}), \tag{4}$$

where $u_{lm}(r)$ are (complex) functions of the radius $r$. The hope is that the equation for $u_{lm}(r)$ is easier to solve than the original Schrödinger equation.

The spherical harmonics $Y_{lm}(\hat{\mathbf{r}})$ are orthogonal functions on the 2-sphere,

$$\int Y_{lm}(\hat{\mathbf{r}})Y_{l'm'}(\hat{\mathbf{r}})d^2\hat{\mathbf{r}}=\delta_{ll'}\delta_{mm'}.$$

### 1.2.2 Application to Schrödinger equation

If the wave function is expanded as in Eq. (4), the Schrödinger equation (2) is reduced to the following equation for $u_{lm}(r)$,

$$\frac{d^2}{dr^2}u_{lm}+\left[k^2-\frac{2\mu V(r)}{\hbar^2}-\frac{l(l+1)}{r^2}\right]u_{lm}=0. \tag{5}$$

Here $k$ is related to the energy $E$ by Eq. (3).

### 1.2.3 Asymptotic solutions at large $r$

We *assume* (only in this section; our further results do not use this assumption) that at large $r\gg a$ the potential $V(r)$ falls off faster than $r^{-2}$. Then we can disregard the $V(r)$ term and obtain the following asymptotic form of Eq. (5) at large $r$:

$$u''_{lm}-\frac{l(l+1)}{r^2}u+k^2u\approx 0.$$

The general solution of this equation is a combination of the spherical Hankel functions $h_l^{(1,2)}$,

$$\frac{u_{lm}(r)}{r} = A_{lm} h_l^{(1)}(kr) + B_{lm} h_l^{(2)}(kr).$$

Note that there are two asymptotic regions at large $r$: the first region where $V(r)$ can be disregarded but $l(l+1)r^{-2}$ is retained, and the second region where $l(l+1)r^{-2}$ is disregarded and the solution is simply the spherical wave $\exp(ikr)$.

If the potential does not fall off faster than $r^{-2}$, the asymptotic regime with Bessel functions never appears. Regardless of this, at sufficiently large $r$ such that the equation (5) becomes approximately

$$u''_{lm} + k^2 u_{lm} = 0,$$

the solutions are linear combinations of $\exp(\pm ikr)$. Ultimately we shall only need the asymptotics of this form, so our considerations apply also for potentials that fall off slower than $r^{-2}$. (However, the partial wave technique does not apply to the Coulomb potential $V \sim r^{-1}$.)

### 1.2.4 Spherical Bessel functions

The first few functions $h_l(z)$ are

$$h_0^{(1)}(z) = \frac{1}{iz}e^{iz},$$
$$h_1^{(1)}(z) = \left(-\frac{1}{z} - \frac{i}{z^2}\right)e^{iz},$$
$$h_2^{(1)}(z) = \left(\frac{i}{z} - \frac{3}{z^2} - \frac{3i}{z^3}\right)e^{iz},$$

while $h_l^{(2)}(z) = \left[h_l^{(1)}(z)\right]^*$. The factor at $e^{iz}$ is always a polynomial in $1/z$ of degree $l+1$, and the asymptotic behavior is

$$h_l^{(1)}(z) \sim \frac{e^{iz}}{i^{l+1}z}\left(1 + O\left(z^{-1}\right)\right), \quad z \to \infty. \tag{6}$$

The spherical Hankel functions $h_l^{(1,2)}$ belong to the family of Bessel functions. One defines the real functions $j_l(z)$ and $n_l(z)$ by $h_l^{(1,2)}(z) = j_l(z) \pm i n_l(z)$. The $j_l$s are called the spherical Bessel functions and the $n_l$s are the spherical Neumann functions. This relationship is quite similar to the relation between the functions $\exp(\pm ix)$ and $\cos x$, $\sin x$:

$$e^{\pm ix} = \cos x \pm i \sin x.$$

Unlike $\sin z$, the function $n_l(z)$ is infinite at the origin; also, none of the spherical Bessel functions are periodic.

### 1.2.5 Partial wave expansion of plane waves

Since a plane wave $\exp(i\mathbf{kx})$ is a solution of the Schrödinger equation with $V = 0$, we should also be able to expand it into partial waves. To simplify the expansion, we choose the $z$ axis along $\mathbf{k}$, so that the plane wave is independent of the asimuthal angle $\phi$. The resulting formula (the Rayleigh expansion) is

$$\exp(i\mathbf{kx}) = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta). \tag{7}$$

Here $\cos\theta \equiv \hat{\mathbf{k}}\hat{\mathbf{r}} = \hat{\mathbf{k}}\hat{\mathbf{z}}$. Note that $Y_{lm}(\theta,\phi) \propto \exp(im\phi)$ and therefore only the harmonics $Y_{lm}$ with $m = 0$ occur,

$$Y_{l0}(\hat{\mathbf{r}}) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta),$$

where $P_l(x)$ are the Legendre polynomials (see 1.2.13).

The function $j_l(kr)$ at large $kr$ contains both $\exp(ikr)$ and $\exp(-ikr)$,

$$j_l(z) \approx \frac{1 + O\left(z^{-1}\right)}{z} \sin\left(z - \frac{l\pi}{2}\right), \quad z \to \infty, \tag{8}$$

therefore (as expected) the plane wave $\exp(i\mathbf{kx})$ is neither purely outgoing nor purely incoming, but a mixture of the two.

### 1.2.6 Partial wave expansion of the scattered wave function

Suppose we know the wave function $\psi(\mathbf{x})$ for a particular scattering problem with a spherically symmetric potential $V(r)$. Then we can derive a partial wave expansion for the wave function and for the scattering quantities.

(To describe scattering, it is enough to know $\psi(\mathbf{x})$ asymptotically at large $r \equiv |\mathbf{x}|$.)

Assume that the wave function is asymptotically (for $r \gg a$) of the form (1). The plane wave is expanded as in Eq. (7), where the $z$ axis is chosen along the vector $\mathbf{k}$. The outgoing portion of the wave function contains only $\exp(ikr)$ and therefore it is expanded in partial waves using only $h_l^{(1)}$ but not $h_l^{(2)}$,

$$f(\hat{\mathbf{r}}) \frac{\exp(ikr)}{r} = \sum_{lm} C_{lm} h_l^{(1)}(kr) Y_{lm}(\hat{\mathbf{r}}),$$

where $C_{lm}$ are some complex coefficients (the partial wave amplitudes). Since the potential is spherically symmetric, the amplitude $f(\hat{\mathbf{r}})$ depends only on the angle $\theta$ but not on the angle $\phi$. Therefore only $Y_{lm}$ with $m = 0$ contribute to the expansion; we denote $C_l \equiv C_{l0}$.

So the partial wave expansion of $\psi$ at large $r$ is

$$\psi(\mathbf{x}) \approx A \sum_{l=0}^{\infty} \left[i^l (2l+1) j_l(kr) + \sqrt{\frac{2l+1}{4\pi}} C_l h_l^{(1)}(kr)\right] P_l(\cos\theta).$$

It follows that in the notation of 1.2.2 the function $u_l(r) \equiv u_{l0}(r)$ is

$$\frac{u_l(r)}{r} \approx i^l \sqrt{4\pi(2l+1)} j_l(kr) + C_l h_l^{(1)}(kr), \quad kr \gg 1. \tag{9}$$

### 1.2.7 Scattering quantities

At large $kr \gg 1$, the Hankel functions have the asymptotic (6). Therefore the scattering amplitude is expanded as

$$f(\hat{\mathbf{r}}) = f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} \frac{C_l}{i^{l+1}} \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta).$$

The differential cross-section is

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

and the total cross-section is found from the simple formula

$$\sigma_{tot} = \frac{1}{k^2} \sum_{l=0}^{\infty} |C_l|^2.$$

### 1.2.8 How to determine the partial wave amplitudes $C_l$

In 1.2.6 we have assumed that the wave function $\psi$ is known and we expanded it in partial waves. The various scattering quantities are easy to find if we know the coefficients $C_l$. However, the usual problem is the inverse: the function $\psi$ and the partial wave coefficients are unknown.

To obtain these coefficients, one must solve Eq. (5) *without* disregarding the $V(r)$ term. The boundary conditions for this second-order equation are the following: $u_l(r)/r$ remains finite at $r \to 0$, and the $r \to \infty$ behavior is given by Eq. (9). These two boundary conditions are sufficient to fix the solution $u_l(r)$ uniquely and to determine the coefficient $C_l$.

### 1.2.9 Which partial waves contribute

Usually, the coefficients $C_l$ are of the order $(ka)^l$ and decay quickly with $l$ when $ka \ll 1$ (the long-wave, or low-energy, limit). In the latter case, only a few partial waves, or even just the first one (the $l = 0$ or the s-wave), gives a good approximation to the scattering cross-section.

In the high-energy limit, the partial wave expansion is less effective since we have to add many terms $C_l$, $l = 0, 1, 2, ...$ to obtain a good approximation to $\sigma_{tot}$.

### 1.2.10 The method of phase shifts

Above we have described the scattering process using the the partial wave amplitudes $C_l$. The coefficients $C_l$ are complex numbers which we must obtain by solving the radial equation (5) with the boundary conditions (9). A procedure that does not require the spherical Bessel functions is the method of phase shifts.

When we solve Eq.(5) with the boundary conditions, the solution will presumably be found as an explicit function of $r$. At $r \to \infty$ (at $r$ sufficiently large that the $l(l+1)r^{-2}$ term can be disregarded) the equation becomes $u'' + k^2 u \approx 0$ and therefore the solution can be written in the form

$$u_l(r) \approx A_l \sin\left(kr - \frac{l\pi}{2} + \delta_l\right), \quad r \to \infty, \tag{10}$$

with some (complex) normalization constant $A_l$ and a (real) phase shift $\delta_l$. We chose sin and not cos for convenience: the phases $\delta_l = 0$ when there is no scattering, i.e. when $V(r) = 0$ (see 1.2.12 below).

The crucial point is that the phase shift $\delta_l$ is uniquely determined by the radial equation *without* using the boundary condition at large $r$. It is enough to use the regularity condition at $r = 0$.

On the other hand, the normalization constant $A_l$ can be determined only if we use the boundary condition (9). But it turns out (see below) that only the phase shifts $\delta_l$ are needed to describe the scattering.

To obtain just one real number $\delta_l$ from a complicated equation (5) by matching the solution to a simple sine curve is an easier task than that of matching to a combination (9) of spherical Bessel functions and obtaining a complex number $C_l$. This is the advantage of the method of phase shifts.

### 1.2.11 Relation of phase shifts to partial wave amplitudes

Assume that in Eq. (10) the phase shift $\delta_l$ is known but the amplitude $A_l$ is not yet known. From Eqs. (6), (8), and (9), we find the large-$r$ asymptotic of $u_l$ as

$$\frac{u_l(r)}{r} \approx -\frac{i^l\sqrt{4\pi(2l+1)}}{2i}\frac{\exp\left(-ikr + i\frac{l\pi}{2}\right)}{kr} + \left[\frac{i^l\sqrt{4\pi(2l+1)}}{2i} + \frac{C_l}{i^{l+1}}\right]\frac{\exp\left(ikr - i\frac{l\pi}{2}\right)}{kr}.$$

On the other hand, the same asymptotic must be reproduced by the ansatz (10),

$$\frac{u_l(r)}{r} \approx \frac{A_l}{r}\frac{\exp\left(ikr - i\frac{l\pi}{2} + i\delta_l\right) - \exp\left(-ikr + i\frac{l\pi}{2} - i\delta_l\right)}{2i}.$$

The coefficients at $\exp(\pm ikr)$ must be equal in these expressions. Therefore the phase shifts $\delta_l$ are related to the partial wave amplitudes $C_l$ by the formula

$$\frac{C_l}{i^{l+1}\sqrt{4\pi(2l+1)}} = e^{i\delta_l}\sin\delta_l = \frac{e^{2i\delta_l} - 1}{2i}, \tag{11}$$

and the amplitude $A_l$ must be

$$A_l = \frac{e^{i\delta_l}}{k} i^l \sqrt{4\pi(2l+1)}. \tag{12}$$

### 1.2.12 Physical interpretation of phase shifts

Suppose that there is no scattering (set $V = 0$). Then $f(\hat{\mathbf{r}}) \equiv 0$, all $C_l = 0$, and the solutions of the radial equation (5) are the pure spherical Bessel functions $j_l$. The functions $j_l$ have the asymptotic (8). Therefore the asymptotic form of the radial solution at large $r$ would be

$$u_l(r) \approx A_l \sin\left(kr - \frac{l\pi}{2}\right).$$

Comparing this to the asymptotic formula (10), we find that the phase shifts $\delta_l$ are all zero when there is no scattering. Also, it follows the only effect of scattering is to introduce phase shifts into the partial waves, while the intensities $|A_l|$ of the partial waves remain unchanged, according to Eq. (12).

Note that the phase shifts $\delta_l$ are defined only up to a multiple of $\pi$. This is because $A_l \sin(... + \delta_l)$ merely changes sign if we add $\pi$ to the phase shift $\delta_l$, while the constant $A_l$ is still undetermined and can absorb this sign. Compare with Eq. (11) which contains only $\exp(2i\delta_l)$. Therefore we may always assume that $0 \le \delta_l < \pi$.

### 1.2.13 Some properties of Legendre polynomials

The Legendre polynomials $P_l(x)$ can be derived from the generating function,

$$\frac{1}{\sqrt{1 - 2xz + z^2}} = \sum_{l=0}^{\infty} P_l(x) z^l.$$

This relation can be used as a convenient *definition* of the polynomials $P_l(x)$.

It follows immediately that

$$\frac{1}{1-z} = \sum_{l=0}^{\infty} P_l(1) z^l \;\Rightarrow\; P_l(1) = 1 \text{ for all } l.$$

The Legendre polynomials are orthogonal on the $[-1, 1]$ range:

$$\int_{-1}^{1} P_l(x) P_m(x)\, dx = \frac{2}{2l+1}\delta_{lm}.$$

This relation can be derived directly from the generating function: since

$$\int_{-1}^{1}\frac{dx}{\sqrt{(1-2ax+a^2)(1-2bx+b^2)}}=\frac{1}{\sqrt{ab}}\ln\frac{1+\sqrt{ab}}{1-\sqrt{ab}}\equiv g(ab)$$

is a function only of $ab$ (this is an elementary but cumbersome calculation), it follows that

$$\int_{-1}^{1}P_l(x)P_m(x)\,dx=0\text{ if }l\neq m.$$

The normalization factor $2l+1$ appears in the Taylor expansion of $g(ab)$ because

$$\frac{d}{ds}\left[sg\left(s^2\right)\right]=\frac{2}{1-s^2}=2\left(1+s^2+s^4+\ldots\right),\quad s\equiv\sqrt{ab},$$

and so

$$sg\left(s^2\right)=2\sum_{l=0}^{\infty}\frac{s^{2l+1}}{2l+1}.$$

### 1.2.14 Scattering quantities in terms of phase shifts

It follows from Eq. (11) that the scattering amplitude $f(\hat{\mathbf{r}})$ is

$$f(\hat{\mathbf{r}})=f(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\left[e^{i\delta_l}\sin\delta_l\right]P_l(\cos\theta).$$

Using the orthogonality of $P_l(x)$, we find that the total scattering cross-section is expressed as

$$\sigma_{tot}=2\pi\int_0^{\pi}d\theta\sin\theta\,|f(\theta)|^2=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l. \qquad (13)$$

This is interpreted as the sum of contributions

$$\sigma_l\equiv\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$

of each partial wave with index $l$.

### 1.2.15 Optical theorem derived from phase shifts

The optical theorem connects the total scattering cross-section $\sigma_{tot}$ and the imaginary part of the scattering amplitude Im $f\left(\hat{\mathbf{k}}\right)$ evaluated at $\hat{\mathbf{r}}=\hat{\mathbf{k}}$, i.e. for particles scattered in the forward direction.

Since $\hat{\mathbf{r}}=\hat{\mathbf{k}}$ corresponds to $\cos\theta=1$ and $\theta=0$, we find

$$\begin{aligned}\text{Im } f(\theta)_{\theta=0}&=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,\text{Im}\left[e^{i\delta_l}\sin\delta_l\right]\\&=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,2\sin^2\delta_l.\end{aligned}$$

Comparing this with Eq. (13), we find the relation

$$\sigma_{tot}=\frac{2\pi}{k}\text{Im } f(\theta)_{\theta=0}. \qquad (14)$$

This is the optical theorem derived for spherically symmetric potentials. (Of course, this theorem holds for arbitrary potentials.)

### 1.2.16 Finding the phase shifts $\delta_l$ by WKB approximation

The phase shifts $\delta_l$ must be obtained by solving the radial equation (5). This equation has the form of a Schrödinger equation of a particle with mass $\mu$ moving at the energy level $E=0$ between $r=0$ and $r=\infty$ in the potential

$$U(r)\equiv V(r)+\frac{\hbar^2}{2\mu}\left(\frac{l(l+1)}{r^2}-k^2\right).$$

Typically there will be a turning point at small $r$ where $U(r)=0$. We assume that the potential $V(r)$ does not go to the negative infinity faster than $r^{-2}$, more precisely, that $U(r)>0$ as $r\to 0$, and that there is *only one* turning point at $r=r_0$ where $U(r_0)=0$.

From the standard formula of the WKB approximation near a turning point we find the approximate wave function for $r\gg r_0$ as

$$u_l(r)\approx A\sin\left[\frac{\pi}{4}+\int_{r_0}^{r}\sqrt{k^2-\frac{l(l+1)}{r^2}-\frac{2\mu V(r)}{\hbar^2}}dr\right].$$

It is clear that at very large $r$ this function is of the form (10) where the phase $\delta_l$ is defined by

$$\delta_l^{WKB}=\lim_{r\to\infty}\left[\frac{\pi}{4}+\int_{r_0}^{r}\sqrt{k^2-\frac{l(l+1)}{r^2}-\frac{2\mu V(r)}{\hbar^2}}dr-\frac{l\pi}{2}-kr\right]. \qquad (15)$$

This is the *approximate* formula expressing the phase shifts $\delta_l$ through the potential $V(r)$. The actual phase shifts $\delta_l$ are not precisely equal to $\delta_l^{WKB}$ but we can expect that $\delta_l\approx\delta_l^{WKB}$ if the potential $V(r)$ changes sufficiently slowly with $r$.

### 1.2.17 Applicability of the phase shift method

The limit in Eq. (16) exists if the potential $V(r)$ falls off rapidly enough. This can be seen by rewriting

$$\begin{aligned}&\int_{r_0}^{r}\left[\sqrt{k^2-\frac{l(l+1)}{r^2}-\frac{2\mu V(r)}{\hbar^2}}-k\right]dr\\&=-\int_{r_0}^{r}\frac{\frac{l(l+1)}{r^2}+\frac{2\mu}{\hbar^2}V(r)}{\sqrt{k^2-\frac{l(l+1)}{r^2}-\frac{2\mu V(r)}{\hbar^2}}+k}dr.\end{aligned}$$

The latter integral converges at $r\to\infty$ if and only if the integral of $V(r)$ converges,

$$\int_{r_0}^{\infty}V(r)\,dr<\infty.$$

Therefore a sufficient condition for the convergence is a fast decay $V(r)\sim r^{-n}$, with $n>1$.

The Coulomb potential $V(r)\sim r^{-1}$ does not satisfy the convergence condition and the method of phase shifts does not work in its present form.

### 1.2.18 Langer's trick: replacing $l(l+1)$ by $\left(l+\frac{1}{2}\right)^2$

The formula (16) is applicable when the limit exists and when WKB approximation for the potential $U(r)$ is valid, i.e. when the potential $V(r)$ changes slowly with $r$. However, there is always a certain error in this approximation. This can be seen by setting $V = 0$ in Eq. (16) and computing the integral exactly:

$$\int_{r_0}^{r} \sqrt{k^2 - \frac{l(l+1)}{r^2}} dr = \sqrt{k^2 r^2 - l(l+1)} + \sqrt{l(l+1)} \left[ \arcsin \frac{\sqrt{l(l+1)}}{k^2 r^2} - \frac{\pi}{2} \right].$$

Here we have set

$$r_0 = \frac{\sqrt{l(l+1)}}{k}.$$

We obtain

$$\delta_l^{WKB} = -\frac{\pi}{2} \left( \sqrt{l(l+1)} - l - \frac{1}{2} \right).$$

However, the exact result should be $\delta_l = 0$ since there is no scattering. The discrepancy is small when $l$ is large.

Langer's trick is to replace $l(l+1)$ by $l(l+1) + \frac{1}{4} = \left(l + \frac{1}{2}\right)^2$ in the WKB formula (16). This replacement compensates for some of the error that inevitably occurs when applying the WKB approximation to the equation (5). In particular, the no-scattering result $\delta_l = 0$ is reproduced.

The improved WKB formula for the phase shift $\delta_l$ is

$$\delta_l \approx \frac{\pi}{2} \left( l + \frac{1}{2} \right) - kr_0 - \int_{r_0}^{\infty} \left[ k - \sqrt{k^2 - \frac{\left(l + \frac{1}{2}\right)^2}{r^2} - \frac{2\mu V(r)}{\hbar^2}} \right] dr. \tag{16}$$

## 1.3 Integral representation of the scattering amplitude

A method that works well at high energies is based on the integral representation of the scattering amplitude. The integral representation gives rise to an expansion in powers of $V$ (the Born expansion). The Born approximation is the simplest application of this expansion.

Below we do *not* assume that the potential $V(x)$ is spherically symmetric.

### 1.3.1 Integral equation for the wave function

The wave function $\psi(\mathbf{x})$ in a scattering situation is the solution of the Schrödinger equation (2) which is asymptotically of the form (1) at large $r$. Rewrite the Schrödinger equation so that the potential is at the right-hand side,

$$-\frac{\hbar^2}{2\mu} \left( \Delta + k^2 \right) \psi = -V\psi. \tag{17}$$

If $V\psi$ were a known function, $F(\mathbf{x}) \equiv -V(\mathbf{x})\psi(x)$, the solution of Eq. (17) with the boundary condition (1) would be found using the outgoing-wave Green's function $G(\mathbf{x} - \mathbf{x}')$ of the Helmholtz operator $\Delta + k^2$, namely

$$\psi(\mathbf{x}) = e^{i\mathbf{kx}} + \int G\left(\mathbf{x} - \mathbf{x}'\right) F\left(\mathbf{x}'\right) d^3\mathbf{x}', \tag{18}$$

where

$$G\left(\mathbf{x} - \mathbf{x}'\right) = \frac{\mu}{2\pi\hbar^2} \frac{\exp\left(ik\left|\mathbf{x} - \mathbf{x}'\right|\right)}{\left|\mathbf{x} - \mathbf{x}'\right|}. \tag{19}$$

The Green's function (19) is chosen so that for *any* $F(\mathbf{x})$, the wave function $\psi(\mathbf{x})$ given by Eq. (18) satisfies the boundary condition (1) and solves Eq. (17) with $F(\mathbf{x})$ at the RHS.

In our case the function $F(\mathbf{x})$ is unknown and we cannot compute $\psi(\mathbf{x})$ directly from Eq. (18). Instead, we obtain the integral equation

$$\psi(\mathbf{x}) = e^{i\mathbf{kx}} - \int G\left(\mathbf{x} - \mathbf{x}'\right) V\left(\mathbf{x}'\right) \psi\left(\mathbf{x}'\right) d\mathbf{x}', \tag{20}$$

from which we need to find $\psi(\mathbf{x})$.

### 1.3.2 On derivation of the Green's function

The above Green's function $G(\mathbf{x} - \mathbf{x}')$ is the solution of the equation

$$-\frac{\hbar^2}{2\mu} \left( \Delta_{(\mathbf{x})} + k^2 \right) G\left(\mathbf{x} - \mathbf{x}'\right) = \delta\left(\mathbf{x} - \mathbf{x}'\right) \tag{21}$$

with the outgoing-wave boundary condition,

$$G\left(\mathbf{x} - \mathbf{x}'\right) \propto \frac{\exp\left(ik\left|\mathbf{x} - \mathbf{x}'\right|\right)}{\left|\mathbf{x} - \mathbf{x}'\right|}, \quad |\mathbf{x}| \to \infty.$$

This follows from the formula

$$\left( \Delta + k^2 \right) \frac{e^{ikr}}{r} = -4\pi\delta(r).$$

We omit the derivation of this mathematical statement which can be found in many textbooks, e.g. in Griffiths.

Note that Eq. (21) does not determine $G(\mathbf{x} - \mathbf{x}')$ uniquely but allows to add an arbitrary solution of the homogeneous equation. For example, a function $G(\mathbf{x} - \mathbf{x}') + g(\mathbf{x}') \exp(i\mathbf{qx})$ is also a solution of Eq. (21) for any $\mathbf{q}$ and $g(\mathbf{x}')$. It is only with the help of the boundary condition (1) that one can fix $G(\mathbf{x} - \mathbf{x}')$ uniquely.

### 1.3.3 Iterative solution of the integral equation for $\psi(\mathbf{x})$

The equation (20) can be solved approximately if we assume that the second term at the RHS (the term containing $V$) is a small correction to the first one.

We expect that this assumption is justified for high energies, i.e. $\hbar^2 k^2 \gg 2\mu V$, when the kinetic energy of the particle is much larger than the potential $V$ and scattering cross-section is small.

In this case we form successive approximations by starting with the unperturbed plane wave $\exp(i\mathbf{kx})$ and substituting the previous approximation into Eq. (20):

$$\begin{aligned}
\psi^{(0)}(\mathbf{x}) &= e^{i\mathbf{kx}}, \\
\psi^{(1)}(\mathbf{x}) &= e^{i\mathbf{kx}} - \int G\left(\mathbf{x} - \mathbf{x}'\right) V\left(\mathbf{x}'\right) \psi^{(0)}\left(\mathbf{x}'\right) d^3\mathbf{x}', \\
\psi^{(2)}(\mathbf{x}) &= e^{i\mathbf{kx}} - \int G\left(\mathbf{x} - \mathbf{x}'\right) V\left(\mathbf{x}'\right) \psi^{(1)}\left(\mathbf{x}'\right) d^3\mathbf{x}', \\
&\ldots\ldots
\end{aligned}$$

This is the iterative solution of the integral equation (20).

Symbolically, we can denote the integration with the Green's function by the operator $\hat{G}$, i.e.

$$\left(\hat{G}f\right)(\mathbf{x}) \equiv \int G\left(\mathbf{x} - \mathbf{x}'\right) f\left(\mathbf{x}'\right) d^3\mathbf{x}',$$

and write the integral equation as

$$\psi = \psi^{(0)} - \hat{G}V\psi.$$

Then the iterations are

$$\psi^{(1)}(\mathbf{x}) = \psi^{(0)} - \hat{G}V\psi^{(0)},$$
$$\psi^{(2)}(\mathbf{x}) = \psi^{(0)} - \hat{G}V\psi^{(0)} + \hat{G}V\hat{G}V\psi^{(0)},$$
$$\ldots\ldots$$
$$\psi^{(n)}(\mathbf{x}) = \psi^{(0)} - \hat{G}V\psi^{(0)} + \ldots + \left(-\hat{G}V\right)^{n}\psi^{(0)}.$$

This symbolic expression helps to visualize the structure of the $n$-th approximation to the wave function.

This form of the wave function is called the Born expansion.

### 1.3.4 Asymptotic form of the Green's function

We need the asymptotic expression of the Green's function at large $r$ to derive the integral representation for the scattering amplitude (1.3.5).

At large $r \gg r'$, the above Green's function $G(\mathbf{x}-\mathbf{x}')$ has the asymptotic form

$$G\left(\mathbf{x}-\mathbf{x}'\right) \approx \frac{\mu}{2\pi\hbar^2}\frac{\exp\left(ikr - i\mathbf{k}'\mathbf{x}'\right)}{r}\left[1 + O\left(\frac{r'}{r}\right)\right], \qquad (22)$$

where we denoted

$$r \equiv |\mathbf{x}|, \quad r' \equiv \left|\mathbf{x}'\right|, \quad \mathbf{k}' \equiv k\hat{\mathbf{r}} = k\mathbf{r}/r.$$

The formula (22) follows from the Taylor series expansion in $r'/r$, e.g.

$$\left|\mathbf{x}-\mathbf{x}'\right| = r\sqrt{1 - 2\frac{\mathbf{x}\mathbf{x}'}{r^2} + \frac{r'^2}{r^2}} = r\left(1 - \frac{\mathbf{x}\mathbf{x}'}{r^2} + O\left(\frac{r'^2}{r^2}\right)\right).$$

Note that under the exponential we may only neglect terms that are small by their absolute value but not terms that are small in comparison with other terms.

### 1.3.5 Integral representation of the scattering amplitude

The integral representation of the wave function gives us the scattering amplitude directly.

The term $\hat{G}V\psi$ corresponds to the outgoing spherical wave in the asymptotic formula (1),

$$f(\hat{\mathbf{r}})\frac{e^{ikr}}{r} \approx -\int G\left(\mathbf{x}-\mathbf{x}'\right)V\left(\mathbf{x}'\right)\psi\left(\mathbf{x}'\right)d^3\mathbf{x}', \quad r \to \infty.$$

Therefore we shall find $f(\hat{\mathbf{r}})$ if we use the asymptotic form (22) of the Green's function:

$$f(\hat{\mathbf{r}}) = -\frac{\mu}{2\pi\hbar^2}\int V\left(\mathbf{x}'\right)e^{-i\mathbf{k}'\mathbf{x}'}\psi\left(\mathbf{x}'\right)d^3\mathbf{x}'. \qquad (23)$$

Here $\mathbf{k}' \equiv k\hat{\mathbf{r}}$.

This is the integral representation of the scattering amplitude $f(\hat{\mathbf{r}})$. It contains the *exact* wave function $\psi(\mathbf{x})$ and therefore is *not* an integral equation for $f(\hat{\mathbf{r}})$, unlike Eq. (20) which is a closed integral equation for $\psi(\mathbf{x})$ that contains no other functions.

### 1.3.6 The Born approximation

The formula (23) is exact, but we cannot use it to obtain $f(\hat{\mathbf{r}})$ unless we know $\psi(\mathbf{x})$. One way is to use the above iterative solution for $\psi(\mathbf{x})$. The Born approximation is the result of using the lowest-order approximation $\psi^{(0)}(\mathbf{x}') = \exp(i\mathbf{k}\mathbf{x}')$ instead of $\psi(\mathbf{x}')$ in Eq. (23):

$$f(\hat{\mathbf{r}}) \approx -\frac{\mu}{2\pi\hbar^2}\int V\left(\mathbf{x}'\right)e^{i\left(\mathbf{k}-\mathbf{k}'\right)\mathbf{x}'}d^3\mathbf{x}'. \qquad (24)$$

In other words: the scattering amplitude $f(\hat{\mathbf{r}})$ is determined by the Fourier component of the potential in the direction $\mathbf{k}-\mathbf{k}'$.

The assumption underlying the Born approximation is that the further terms of the Born expansion are negligible.

### 1.3.7 The Born approximation for spherically symmetric potentials

The formula (24) is simpler for spherically symmetric potentials $V(\mathbf{x}) \equiv V(r)$. The Fourier transform of the potential is

$$\tilde{V}(q) \equiv \int e^{-i\mathbf{q}\mathbf{x}}V(\mathbf{x})\,d^3\mathbf{x} = \frac{4\pi}{q}\int rV(r)\sin(qr)\,dr.$$

Therefore Eq. (24) gives (with $\mathbf{q} \equiv \mathbf{k}-\mathbf{k}'$)

$$f(\hat{\mathbf{r}}) \approx -\frac{2\mu}{|\mathbf{k}-\mathbf{k}'|\hbar^2}\int rV(r)\sin\left(\left|\mathbf{k}-\mathbf{k}'\right|r\right)dr. \qquad (25)$$

### 1.3.8 Applicability of the Born approximation

The scattering amplitude (25) is real which contradicts the optical theorem (14). But this does not mean that the Born approximation cannot be used.

In fact, the Born approximation can be used only if the scattering amplitude $f$ is small because we neglect the terms $\hat{G}V\hat{G}V\psi^{(0)}$ which are of order $f^2$. The optical theorem says that the imaginary part of $f$ is of order $k\sigma \sim k|f|^2$ and this quantity is much smaller than $|f|$. The Born approximation already neglects the quadratic terms and so the imaginary part of $f$ cannot be retained within that approximation.

This consideration gives a method to verify the applicability of the Born approximation. First we find the scattering amplitude $f$ from Eq. (24), then the total cross-section $\sigma_{tot}$, and then we check using the optical theorem that the imaginary part of the forward scattering amplitude is negligible.

### 1.3.9 High-energy behavior of the scattering cross-section

The Born approximation is valid for high energies, so we can use it to study the high-energy asymptotic of the scattering cross-section.

If the function $V(r)$ is significantly nonzero for $r < a$, then $\tilde{V}(q)$ is significantly nonzero for $q < a^{-1}$. Since $\mathbf{q} \equiv \mathbf{k}-\mathbf{k}'$, we get for the scattering angle $\theta$ the equation

$$q = 2k\sin\frac{\theta}{2}, \quad \cos\theta \equiv \hat{\mathbf{k}}\hat{\mathbf{k}}' = \hat{\mathbf{k}}\hat{\mathbf{r}}.$$

It follows that the high-energy scattering occurs predominantly within the narrow forward cone $\theta < \theta_{\max} \sim (ka)^{-1}$.

The total cross-section is (after some algebra)

$$\sigma_{tot} = \frac{\mu^2}{2\pi\hbar^4 k^2}\int_0^{2k}\tilde{V}^2(q)\,q\,dq.$$

It follows that $\sigma_{tot} \sim k^{-2} \sim E^{-1}$ at high energies $E$.

A necessary condition for the applicability of the Born approximation is $\sigma_{tot} \ll 4\pi a^2$, and $ka \gg 1$ (see Messia, vol. 2, chapter 19, section 8). Here $a$ is the typical size of the domain where $V(\mathbf{x})$ significantly differs from 0 , so $4\pi a^2$ is the surface area of a sphere with radius $a$.