

221B Lecture Notes

Scattering Theory I

1 Why Scattering?

Scattering of particles off target has been one of the most important applications of quantum mechanics. It is probably the most effective way to study the structure of matter at small distances. Due to the uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \quad (1)$$

in order to probe structure at the distance scale $\Delta x \simeq d$, we need momentum transfer $\Delta p \gtrsim \hbar/2d$ and hence need a high-momentum scattering experiment.

On the other hand, to study the excitation spectrum of a system, one can study the resonances and/or scattering at relatively low energies.

Rutherford scattering experiment, scattering of α -particles off gold foil, is the earliest important quantum mechanical scattering experiment of the first type, and revealed the fact that the positive charge in an atom is concentrated at the center rather than diffusely distributed throughout the atom.

For non-relativistic problems, time-independent formalism is convenient, where you study the stationary problem as in the bound state problems. It is somewhat confusing that you can study the scattering process as a stationary problem, but this becomes clear later once we discuss wave packets. For relativistic problems, however, time-dependent formalism is more convenient because one can keep manifest Lorentz covariance in the formulation.

2 Lippmann–Schwinger Equation

We first study time-independent formalism for scattering. Imagine a particle coming in and getting scattered by a short-ranged potential $V(\vec{x})$ located around the origin $\vec{x} \sim 0$. The time-independent Schrödinger equation is simply

$$\left(-\frac{\hbar^2 \vec{\nabla}^2}{2m} + V(\vec{x}) \right) \psi(\vec{x}) = E\psi(\vec{x}). \quad (2)$$

Because we assumed that the potential is short-ranged, $V(\vec{x}) \approx 0$ beyond a certain distance $|\vec{x}| \sim a$ where a is the “size” of the scatterer. Therefore, the Schrödinger equation Eq. (2) reduces to the free equation at $|\vec{x}| \gg a$

$$-\frac{\hbar^2 \vec{\nabla}^2}{2m} \psi(\vec{x}) = E \psi(\vec{x}), \quad (3)$$

and hence the energy eigenvalues and eigenfunctions are given by

$$-\frac{\hbar^2 \vec{\nabla}^2}{2m} e^{i\vec{k}\cdot\vec{x}} = \frac{\hbar^2 k^2}{2m} e^{i\vec{k}\cdot\vec{x}} = E e^{i\vec{k}\cdot\vec{x}}. \quad (4)$$

The question is how this eigenfunction is modified in the presence of the potential term in Eq. (2).

In order to answer this question, we first go to the “ket” notation $\langle \vec{x} | \psi \rangle = \psi(\vec{x})$ and rewrite Eq. (2) as

$$(H_0 + V)|\psi\rangle = E|\psi\rangle. \quad (5)$$

Here, $H_0 = \vec{p}^2/2m$ is the free-particle Hamiltonian operator. Because we are interested in the effect of the potential, we reorder it as

$$(E - H_0)|\psi\rangle = V|\psi\rangle. \quad (6)$$

Naively, we can write the solution to Eq. (6) as

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle. \quad (7)$$

But this is not correct because $E - H_0$ can be zero and this formal expression is ill-defined. First of all, we need to specify how we go around the pole of $1/(E - H_0)$; this corresponds to specifying a boundary condition to the solution. For our purpose, we choose $1/(E - H_0 + i\epsilon)$ where we take the limit $\epsilon \rightarrow +0$ at the end of the calculations. The meaning of this choice becomes clear when we discuss wave-packets in the next section. Second, because $E - H_0$ can be zero, there are solutions $(E - H_0)|\phi\rangle = 0$, which are nothing but the free plane wave solutions. Therefore, we can write the solution to this equation as

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0 + i\epsilon} V|\psi\rangle. \quad (8)$$

One can easily check that Eq. (8) satisfies the equation Eq. (6). This equation is called Lippmann–Schwinger equation. Because $|\phi\rangle$ is a solution to the free equation, we normally take it a plane wave $|\hbar\vec{k}\rangle$ with $E = \hbar^2\vec{k}^2/2m$ and momentum $\hbar\vec{k}$.

To gain more insight into the Lippmann-Schwinger equation, let us take the position representation of this equation, by taking the inner product of Eq. (8) with the “bra” $\langle\vec{x}|$. We find

$$\begin{aligned}\psi(\vec{x}) &= \langle\vec{x}|\psi\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{k}\cdot\vec{x}} + \langle\vec{x}|\frac{1}{E - H_0 + i\epsilon}V|\psi\rangle \\ &= \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{k}\cdot\vec{x}} + \int d\vec{x}'\langle\vec{x}|\frac{1}{E - H_0 + i\epsilon}|\vec{x}'\rangle\langle\vec{x}'|V|\psi\rangle \\ &= \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{k}\cdot\vec{x}} + \int d\vec{x}'\langle\vec{x}|\frac{1}{E - H_0 + i\epsilon}|\vec{x}'\rangle V(\vec{x}')\psi(\vec{x}').\end{aligned}\quad (9)$$

At the very last step, we used the fact that the potential operator is diagonal in the position representation $\langle\vec{x}'|V|\vec{x}\rangle = V(\vec{x})\delta(\vec{x} - \vec{x}')$. Then the question is the exact form of the Green’s function

$$G(\vec{x}, \vec{x}') = \langle\vec{x}|\frac{1}{E - H_0 + i\epsilon}|\vec{x}'\rangle.\quad (10)$$

By inserting the complete set of states in the momentum representation, and using the fact that H_0 is diagonal in the momentum space, we find

$$\begin{aligned}G(\vec{x}, \vec{x}') &= \int d\vec{p}\langle\vec{x}|\vec{p}\rangle\frac{1}{E - \vec{p}^2/2m + i\epsilon}\langle\vec{p}|\vec{x}'\rangle \\ &= \int d\vec{p}\frac{e^{i\vec{x}\cdot\vec{p}/\hbar}}{(2\pi\hbar)^{3/2}}\frac{1}{E - \vec{p}^2/2m + i\epsilon}\frac{e^{-i\vec{x}'\cdot\vec{p}/\hbar}}{(2\pi\hbar)^{3/2}} \\ &= \int d\vec{p}\frac{e^{i(\vec{x}-\vec{x}')\cdot\vec{p}/\hbar}}{(2\pi\hbar)^3}\frac{1}{E - \vec{p}^2/2m + i\epsilon}.\end{aligned}\quad (11)$$

There are many ways to do this integration. One way is to use polar coordinates for \vec{p} defining the polar angle relative to the direction of $\vec{r} = \vec{x} - \vec{x}'$ such that

$$\begin{aligned}G(\vec{r}) &= \int_0^\infty p^2 dp \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^3} \frac{1}{E - p^2/2m + i\epsilon} \\ &= \frac{2\pi}{(2\pi\hbar)^3} \int_0^\infty p^2 dp \frac{e^{ipr/\hbar} - e^{-ipr/\hbar}}{ipr/\hbar} \frac{1}{E - p^2/2m + i\epsilon}\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} p dp \frac{e^{ipr/\hbar}}{ir} \frac{-2m}{p^2 - 2mE - i\epsilon} \\
&= \frac{1}{(2\pi\hbar)^2} \frac{2mi}{r} \int_{-\infty}^{\infty} dp \frac{pe^{ipr/\hbar}}{(p - \sqrt{2mE} - i\epsilon)(p + \sqrt{2mE} + i\epsilon)}. \quad (12)
\end{aligned}$$

Because of the numerator $e^{ipr/\hbar}$, we can extend the integration contour to go along the real axis and come back at the infinity on the upper half plane. Then the contour integral picks up only the pole at $p = \sqrt{2mE} + i\epsilon = \hbar k + i\epsilon$, and we find

$$\begin{aligned}
G(\vec{r}) &= \frac{1}{(2\pi\hbar)^2} \frac{2mi}{r} 2\pi i \frac{\hbar k e^{ikr}}{2\hbar k} \\
&= \frac{2m}{\hbar^2} \frac{e^{ikr}}{4\pi r}. \quad (13)
\end{aligned}$$

Going back to Eq. (9), we now obtain

$$\psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{x}} - \frac{2m}{\hbar^2} \int d\vec{x}' \frac{e^{ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|} V(\vec{x}') \psi(\vec{x}'). \quad (14)$$

This result allows a simple interpretation. The first term (plane wave) is the incident particle with a fixed three-momentum, while the second term is a spherical wave originated from the scattering. If we had chosen the opposite boundary condition $1/(E - H_0 - i\epsilon)$, we had obtained the second term coming from infinity and converging at the origin, which is practically impossible to arrange. This interpretation is further justified using wave-packets in the next section.

The experiment is done typically by placing the detector far away from the scatterer $|\vec{x}| \gg a$ where a is the “size” of the scatterer. The integration over \vec{x}' , on the other hand, is limited within the “size” of the scatterer because of the $V(\vec{x}')$ factor. Therefore, we are in the situation $|\vec{x}| \gg |\vec{x}'|$, and hence can use the approximation

$$|\vec{x} - \vec{x}'| \simeq \sqrt{\vec{x}^2 - 2\vec{x} \cdot \vec{x}'} \simeq |\vec{x}| - \frac{\vec{x} \cdot \vec{x}'}{|\vec{x}|}. \quad (15)$$

Under this limit, the Lippmann–Schwinger equation Eq. (14) becomes

$$\psi(\vec{x}) \simeq \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{x}} - \frac{2m}{\hbar^2} \frac{e^{ikr}}{4\pi r} \int d\vec{x}' e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}') \psi(\vec{x}'), \quad (16)$$

where $r = |\vec{x}|$ and $\vec{k}' = \vec{k} \frac{\vec{x}}{r}$ is the wave-vector of the scattered wave. Note that $|\vec{k}'| = \vec{k}$. It is customary to write this equation in the form

$$\psi(\vec{x}) \simeq \frac{1}{(2\pi\hbar)^{3/2}} \left(e^{i\vec{k}\cdot\vec{x}} + f(\vec{k}', \vec{k}) \frac{e^{ikr}}{r} \right), \quad (17)$$

with

$$f(\vec{k}', \vec{k}) = -\frac{(2\pi\hbar)^3}{4\pi} \frac{2m}{\hbar^2} \langle \hbar\vec{k}' | V | \psi \rangle, \quad (18)$$

which has a dimension of length. The advantage of using $f(\vec{k}', \vec{k})$ is that it is directly related to the scattering cross section

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}', \vec{k})|^2 \quad (19)$$

as we will see later.

3 Wave-Packets

The time-independent solution we discussed in the previous section is not easy to understand intuitively because both the incident and scattered waves appear and both waves are spread out over the entire space. What we normally picture as a scattering process is that there is a particle coming in with a fixed momentum, and it gets scattered to a different direction, or it does not get scattered and comes out with the same momentum. In fact, the time-dependent solution we discussed in the previous section actually gives precisely this picture once we form wave-packets out of it. We put in particles and detect particles far away from the scatterer, and we can use the asymptotic form Eq. (17).

3.1 Free Wave Packets

As an exercise, let us first study wave packets of plane waves. The plane wave $e^{i\vec{k}\cdot\vec{x}}$ has a definite momentum $\vec{p} = \hbar\vec{k}$ ($\Delta p = 0$), but is spread out in the whole space ($\Delta x = \infty$) consistent with the uncertainty principle. We can form a normalized wave-packet which has a momentum approximately

$\hbar\vec{k}$, but has a finite spatial extent d , by taking a linear combination of many plane waves. We take the so-called Gaussian wave packet

$$\psi_f(\vec{x}) = \left(\frac{d^2}{2\pi^3}\right)^{3/4} \int d\vec{q} e^{i\vec{q}\cdot\vec{x}} e^{-(\vec{q}-\vec{k})^2 d^2} = \left(\frac{1}{2\pi d^2}\right)^{3/4} e^{i\vec{k}\cdot\vec{x}} e^{-\vec{x}^2/4d^2}. \quad (20)$$

From the last expression, it is clear that the wave packet is concentrated around $\vec{x} \sim 0$ with the spread $\Delta x = d$, while from the middle expression, the momentum is distributed around $\hbar\vec{k}$ with $\Delta k = |\vec{q} - \vec{k}| = 1/2d$, consistent with the uncertainty principle.

Time evolution of course moves the wave packet. At time $t \neq 0$, the above wave function acquires a phase $e^{-iEt/\hbar}$ where $E = \hbar^2\vec{q}^2/2m$ for the plane wave with momentum $\hbar\vec{q}$. Therefore,

$$\begin{aligned} \psi_f(\vec{x}, t) &= \left(\frac{d^2}{2\pi^3}\right)^{3/4} \int d\vec{q} e^{i\vec{q}\cdot\vec{x}} e^{-i(\hbar^2\vec{q}^2/2m)t/\hbar} e^{-(\vec{q}-\vec{k})^2 d^2} \\ &= \left(\frac{d^2}{2\pi^3}\right)^{3/4} \left(\frac{\pi}{d^2 + i\hbar t/2m}\right)^{3/2} \exp\left(-\frac{\vec{x}^2 - 4i\vec{k}\cdot\vec{x}d^2 - 4\vec{k}^2 d^4}{4(d^2 + i\hbar t/2m)} - \vec{k}^2 d^2\right). \end{aligned} \quad (21)$$

This expression looks complicated, but it is easy to interpret the probability distribution $|\psi(\vec{x}, t)|^2$:

$$|\psi_f(\vec{x}, t)|^2 = \left(\frac{1}{2\pi d(t)^2}\right)^{3/2} e^{-(\vec{x}-\hbar\vec{k}t/m)^2/2d(t)^2}, \quad (22)$$

with

$$d(t) = \frac{(d^4 + (\hbar t/2m)^2)^{1/2}}{d}. \quad (23)$$

The wave packet is somewhat larger at $t \neq 0$ and is located at the position $\vec{x} \simeq \hbar\vec{k}t/m$ as expected.

As long as the experiment is done within the time $|t| \ll 2md^2/\hbar$, or in other words if the momentum is sufficiently well determined, we can ignore the change in the size of the wave packet. This corresponds to doing the integral over the phase factor $e^{-iEt/\hbar}$ with $E = \hbar^2\vec{q}^2/2m$ approximated as

$$E = \frac{\hbar^2\vec{k}^2}{2m} + \frac{\hbar^2\vec{k}\cdot(\vec{q}-\vec{k})}{m} + O(\vec{q}-\vec{k})^2 \quad (24)$$

and dropping the last correction. Then the wave packet is simply

$$\psi_f(\vec{x}, t) \simeq \left(\frac{1}{2\pi d^2}\right)^{3/4} e^{i\vec{k}\cdot\vec{x}} e^{-i(\hbar^2\vec{k}^2/2m)t/\hbar} e^{-(\vec{x}-\hbar\vec{k}t/m)^2/4d^2}. \quad (25)$$

3.2 Wave Packet with Scattering

We now take the wave packet out of Eq. (17) with the same Gaussian weight, and show that it gives the incoming wave at $t \ll 0$, while gives both the unscattered outgoing wave with the same momentum and the scattered outgoing wave emerging from the center at $t \gg 0$. This would match our intuition of a scattering experiment.

The wave packet we consider is therefore

$$\psi(\vec{x}, t) = \left(\frac{d^2}{2\pi^3}\right)^{3/4} \int d\vec{q} \left(e^{i\vec{q}\cdot\vec{x}} + f(\vec{q}', \vec{q}) \frac{e^{iqr}}{r} \right) e^{-i(\hbar^2\vec{q}^2/2m)t/\hbar} e^{-(\vec{q}-\vec{k})^2 d^2}. \quad (26)$$

Of course we assume that the transverse size of the wave packet is large enough $d \gg a$ so that entire scattering region is probed by the wave packet. The injection and detection time is not too long that the size of the wave packet does not increase significantly $|t| \ll 2md^2/\hbar$, but large enough that the entire packet exits the scattering region $|t| \gg md/\hbar k$, which is possible as long as the wave packet has a well-defined momentum $\Delta k = 1/2d \ll k$.

The first term in the parenthesis gives precisely the same wave packet as the free case, which comes in and goes out at the position $\vec{x} \simeq \hbar\vec{k}t/m$. We hence only need to discuss the second term. Because of the Gaussian damping factor, \vec{q} is highly concentrated around $\vec{q} \simeq \vec{k}$ and we can replace \vec{q} by \vec{k} almost everywhere. However, a care must be taken in the phase factors because the integral vanishes if the integrand oscillates very rapidly. The exponent in the phase factor is expanded as

$$iqr - i\frac{\hbar^2\vec{q}^2}{2m} \frac{t}{\hbar} = ikr - i\frac{\hbar^2\vec{k}^2}{2m} \frac{t}{\hbar} + i \left(r - \frac{\hbar k}{m} t \right) \frac{\vec{k}}{k} \cdot (\vec{q} - \vec{k}) + O(q - k)^2. \quad (27)$$

The phase factor is stationary only when $r - \frac{\hbar k}{m} t = 0$ but this is clearly possible only when $t > 0$. Therefore, this integral vanishes due to rapidly oscillating phase factor for $t \ll -md/\hbar k$, and only the plane wave piece remains:

$$\psi(\vec{x}, t) \simeq \left(\frac{1}{2\pi d^2}\right)^{3/4} e^{i\vec{k}\cdot\vec{x}} e^{-i(\hbar^2\vec{k}^2/2m)t/\hbar} e^{-(\vec{x}-\hbar\vec{k}t/m)^2/4d^2}, \quad \left(t \ll -\frac{md}{\hbar k} \right) \quad (28)$$

which is the same as Eq. (25). This is nothing but the incoming wave packet *before* the scattering takes place.

On the other hand, for $t \gg md/\hbar k$, the phase can be stationary (27), and the scattered wave contributes. \vec{q} integration in the scattered wave packet is

$$\begin{aligned} \int d\vec{q} f(\vec{q}', \vec{q}) \frac{1}{r} e^{ikr - i(\hbar^2 \vec{k}^2/2m)t/\hbar} e^{i(r - (\hbar k/m)t) \vec{k} \cdot (\vec{q} - \vec{k})/k} e^{-(\vec{q} - \vec{k})^2 d^2} \\ = f(\vec{k}', \vec{k}) \frac{1}{r} e^{ikr - i(\hbar^2 \vec{k}^2/2m)t/\hbar} \left(\frac{\pi}{d^2} \right)^{3/2} e^{-(r - (\hbar k/m)t)^2/4d^2}, \end{aligned} \quad (29)$$

and hence

$$\begin{aligned} \psi(\vec{x}, t) = \left(\frac{1}{2\pi d^2} \right)^{3/4} e^{-i(\hbar^2 \vec{k}^2/2m)t/\hbar} \\ \left(e^{i\vec{k} \cdot \vec{x}} e^{-(\vec{x} - \hbar \vec{k} t/m)^2/4d^2} + f(\vec{k}', \vec{k}) \frac{e^{ikr}}{r} e^{-(r - (\hbar k/m)t)^2/4d^2} \right). \quad \left(t \gg \frac{md}{\hbar k} \right) \end{aligned} \quad (30)$$

This wave packet consists of two pieces: one that went through the scattering region unscattered (the first term) and the other that emerged from scattering and expands as $r \simeq (\hbar k/m)t$ spherically. However, note that these two waves interfere at $\vec{x} \simeq (\hbar \vec{k}/m)t$.

I have plotted the scattered wave with the normalization $4\pi r^2 |\psi|^2$ as a function of r following its time-evolution, for a particular choice $f(\vec{k}', \vec{k}) = i/k$ (this satisfies the optical theorem discussed in the next section). The movie uses the exact integration over \vec{q} , without making the large $|t| \gg md/\hbar k$ approximation using the error function with complex arguments. It is clearly seen that the wave practically vanishes for negative t while it emerges from the origin for positive t . I took the unit $m = 1$, $k = 1$, $\hbar = 1$, and chose $d = 10$. You can download the movie from <http://hitoshi.berkeley.edu/221B/scatter.mov>.

If you detect the wave at a direction different from the original plane wave, the first term simply does not contribute, and the only the second term is detected. The probability to detect a particle along the direction (θ, ϕ) in a solid angle $d\Omega = d \cos \theta d\phi$ is given by

$$\begin{aligned} P(\Omega) d\Omega &= \int_0^\infty r^2 dr d\Omega |\psi(\vec{x}, t)|^2 \\ &= \int_0^\infty r^2 dr \left(\frac{1}{2\pi d^2} \right)^{3/2} |f(\vec{k}', \vec{k})|^2 \frac{1}{r^2} e^{-(r - (\hbar k/m)t)^2/2d^2} d\Omega \end{aligned}$$

$$= \frac{1}{2\pi d^2} |f(\vec{k}', \vec{k})|^2 d\Omega. \quad (31)$$

At the last step, we assumed that t is sufficiently large so that the integration only for $r > 0$ can be approximated by a full Gaussian integral.

3.3 Scattering Cross Section

Now we are in the position to define the differential cross section. You wait for a particle to enter the detector in the solid angle $d\Omega$ for each particle you put in. The useful quantity is to detect the scattered particle for the given probability density of the particle you injected per unit area. The incoming wave packet was given in Eq. (25), and had the density of

$$\int dz |\psi_f(\vec{x}, t)|^2 = \int dz \left(\frac{1}{2\pi d^2} \right)^{3/2} e^{-(\vec{x} - \hbar\vec{k}t/m)^2/2d^2} = \frac{1}{2\pi d^2} e^{-(x^2+y^2)/2d^2} \quad (32)$$

where we assumed that \vec{k} is along the z -axis. At the location of the scatterer $x = y = 0$, the density is $1/2\pi d^2$. Therefore, the probability of the scattered particle to be detected at a given solid angle $d\Omega$ for a particle per area is

$$\frac{d\sigma}{d\Omega} = 2\pi d^2 P(\Omega) = |f(\vec{k}', \vec{k})|^2. \quad (33)$$

This is the definition of the differential cross section. It is usually phrased as the number of scattered particles in the solid angle $d\Omega$ per unit time per unit *luminosity*, which is the number of particles injected per unit area per unit time. Obviously two definitions are the same based on the probabilistic interpretation of quantum mechanics.

The total cross section is simply the differential cross section integrated over the entire solid angle

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}. \quad (34)$$

It is important to note, however, that the formula for the cross section does *not* take the unscattered wave into account. Therefore, the differential cross section at the forward direction is not the actual number of particles detected there, but rather the number of scattered particles slightly off from the forward direction extrapolated to the forward direction. The actual number of particles detected at the forward direction should take both the unscattered and scattered waves, and importantly their interference must be taken into

account. Because the total number of particles detected must equal the total number of particles injected, the scattered wave at the forward direction should satisfy a special requirement. This is the optical theorem discussed in the next section.

4 Optical Theorem

There are many ways to derive the optical theorem. Here we continue using the wave packets and require that the normalization of the wave function should always satisfy $\int d\vec{x} |\psi(\vec{x}, t)|^2 = 1$ for any t , as guaranteed by the unitarity of time evolution operator $e^{-iHt/\hbar}$. This requirement leads to a special requirement on the scattered wave, and hence $f(\vec{k}', \vec{k})$.

We start with the wave packet Eq. (26). When $t \ll -md/\hbar k$ (before the scattering), the scattered wave vanishes as discussed in the previous section, and hence the wave function is Eq. (28) which is properly normalized. On the other hand, when $t \gg md/\hbar k$ (after the scattering), the wave packet is Eq. (30), and its normalization is not obviously unity. We therefore require that

$$\int d\vec{x} \left(\frac{1}{2\pi d^2} \right)^{3/2} \left| e^{i\vec{k}\cdot\vec{x}} e^{-(\vec{x}-\hbar\vec{k}t/m)^2/4d^2} + f(\vec{k}', \vec{k}) \frac{e^{i\vec{k}r}}{r} e^{-(r-(\hbar k/m)t)^2/4d^2} \right|^2 = 1. \quad (35)$$

The absolute square of the first term is also properly normalized as it is the same as in the free case. Therefore, the cross term and the second term absolute squared must cancel.

The second term absolute squared is obtained easily as

$$\begin{aligned} & \int d\vec{x} \left(\frac{1}{2\pi d^2} \right)^{3/2} \left| f(\vec{k}', \vec{k}) \frac{e^{i\vec{k}r}}{r} e^{-(r-(\hbar k/m)t)^2/4d^2} \right|^2 \\ &= \left(\frac{1}{2\pi d^2} \right)^{3/2} \int d\Omega r^2 dr |f(\vec{k}', \vec{k})|^2 \frac{1}{r^2} e^{-(r-(\hbar k/m)t)^2/2d^2} \\ &= \frac{1}{2\pi d^2} \sigma, \end{aligned} \quad (36)$$

where σ is the total cross section Eq. (34). The cross term is slightly more complicated but is straightforward to calculate. Note that it is important only in the forward region where both the unscattered and scattered waves

coexist, and we can replace $f(\vec{k}', \vec{k})$ by $f(0) = f(\vec{k}, \vec{k})$. It is:

$$\begin{aligned}
& \int d\vec{x} \left(\frac{1}{2\pi d^2} \right)^{3/2} e^{-i\vec{k}\cdot\vec{x}} e^{-(\vec{x} - (\hbar\vec{k}/m)t)^2/4d^2} f(0) \frac{e^{ikr}}{r} e^{-(r - (\hbar k/m)t)^2/4d^2} + \text{c.c.} \\
&= \left(\frac{1}{2\pi d^2} \right)^{3/2} \int d\cos\theta d\phi r^2 dr \frac{1}{r} f(0) e^{ikr - ikr \cos\theta} \\
&\quad e^{-(r^2 - (2\hbar kr \cos\theta/m)t + (\hbar k/m)^2 t^2)/4d^2} e^{-(r^2 - (2\hbar kr/m)t + (\hbar k/m)^2 t^2)/4d^2} + \text{c.c.} \\
&= 2\pi \left(\frac{1}{2\pi d^2} \right)^{3/2} \int_0^\infty dr f(0) \frac{1}{\frac{2\hbar kt}{4md^2} - ik} \\
&\quad \left[e^{-(2r^2 - (4\hbar kr/m)t + 2(\hbar k/m)^2 t^2)/4d^2} - e^{-(2r^2 + 2(\hbar k/m)^2 t^2)/4d^2} e^{2ikr} \right] + \text{c.c.}
\end{aligned} \tag{37}$$

The term $2\hbar kt/4md^2$ in the denominator is negligible compared to k within our assumption that the size of the wave packet does not grow significantly ($\hbar t/md^2 \ll 1$) and can be dropped. The second term in the square bracket is exponentially suppressed at large time compared to the first term where the exponent vanishes at $r = \hbar kt/m$. Therefore,

$$\begin{aligned}
&= 2\pi \left(\frac{1}{2\pi d^2} \right)^{3/2} \int_0^\infty dr \frac{i}{k} f(0) e^{-(r - (\hbar k/m)t)^2/2d^2} + \text{c.c.} \\
&= -\frac{4\pi}{k} \frac{1}{2\pi d^2} \Im f(0).
\end{aligned} \tag{38}$$

Requiring that the second term absolute squared Eq. (36) and the cross term Eq. (38) cancel exactly, we find

$$\sigma = \frac{4\pi}{k} \Im f(0). \tag{39}$$

This is what is called the optical theorem.

The meaning of this theorem is clear. Because the scattered wave takes the probability away to different directions, the total probability for the particle to go to the forward direction (unscattered) should decrease. This decrease is caused by the interference between the unscattered and scattered waves and hence is proportional to $f(0)$. On the other hand, the amount of decrease in the forward direction should equal the total probability at other directions, which is proportional to the total cross section.