

The Scattering and Shrinking of a Gaussian Wave Packet by Delta Function Potentials

by

Fei Sun

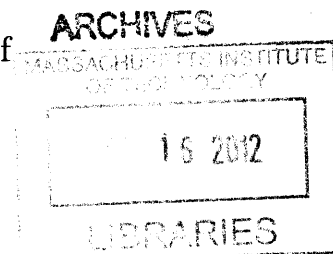
Submitted to the Department of Physics
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Abstract

In this thesis, we wish to test the hypothesis that scattering by a random potential causes localization of wave functions, and that this localization is governed by the Born postulate of quantum mechanics. We begin with a simple model system: a one-dimensional Gaussian wave packet incident from the left onto a delta function potential with a single scattering center. Then we proceed to study the more complicated models with double and triple scattering centers. Chapter 1 briefly describes the motivations behind this thesis and the phenomenon related to this research. Chapter 2 to Chapter 4 give the detailed calculations involved in the single, double and triple scattering cases; for each case, we work out the exact expressions of wave functions, write computer programs to numerically calculate the behavior of the wave packets, and use graphs to illustrate the results of the calculations. In Chapter 5, we study the parameters that determine how much the wave function shrinks, including the initial width, the initial position and the momentum of the Gaussian wave packet, and the strength of and the spacing between the delta functions; then we examine different combinations of the parameters in order to find a pattern to achieve maximum shrinking. Chapter 6 concludes the thesis with the essential results of this research as well as its implications and potentials.

Thesis Supervisor: Professor Edmund Bertschinger
Title: Thesis Supervisor, Department of Physics

0.1 Acknowledgments

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I also want to thank MIT's UROP office and Professor Bertschinger for giving me funding to do the research. Professor David Vogan from the Department of Mathematics and Robyn Sanderson from the Department of Physics also helped me in my research work. Professor Vogan gave me assistance on contour integrals, and Robyn Sanderson helped me with numerical simulations. I would like to thank them for all their interest and support.

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Chapter 1

Introduction

This thesis is motivated by the famous phenomenon that all wave functions collapse upon quantum measurements, and we want to explore the possible causes of this sudden collapse. One possible explanation of this collapse is that the measurement equipments or measurement procedures interfere with the wave packet in a certain way and make the wave function shrink. For example, the measurement equipments may emit particles such as photons or electrons in order to detect the position or momentum of the wave packet, and the emission process may interfere with the incoming wave packet in some way and to significantly change its shape. Another example can be that the measurement procedures create a certain potential around the wave packet, and this potential exerts some kind of influence upon the wave function. It is possible that such interferences may localize to a certain degree or even completely collapse the wave function during quantum measurements, and the localization or collapse is still guided by the Schrodinger equation. However, the physics of various measurement procedures can be extremely complicated and dramatically different from each other in reality. Thus to explore these ideas we begin with a simple model of a Gaussian wave packet scattered by a single delta function potential, and we add more delta functions to the potential later. Our hope is to deduce the localization of the wave function strictly from the Schrodinger equation. Although the localization achieved in these simple models are far from complete collapse, which is expected to happen during real quantum measurements, and these simple models are not even close to

real measurement equipments or procedures, at least these models provide us with a bridge between the sudden collapse of wave functions in quantum measurements and the gradual evolution of wave functions according to the Schrodinger equation.

Chapter 2

Single Scattering

In this chapter, we begin with a simple model system: a one-dimensional Gaussian wave packet incident from the left onto a delta function potential, $V(x) = V_0\delta(x)$, where the strength V_0 can be positive or negative. We wish to use this model to explore the possibility that scattering by a random potential causes localization of the wave function and that this localization is governed by the Schrodinger equation.

2.1 Fourier Transform

Suppose that we start with a Gaussian wave packet with its peak at $x = -x_i < 0$ traveling toward the delta function potential $V(x) = V_0\delta(x)$,

$$\psi(x, 0) = \left(\frac{1}{2\pi\sigma_0^2}\right)^{1/4} \exp\left\{-\frac{(x+x_i)^2}{4\sigma_0^2} + ik_0(x+x_i)\right\} \quad (2.1)$$

When $V_0 > 0$, plane waves are a complete set for the Hilbert space of the quantum system, but when $V_0 < 0$, however, a stationary bound state appears and can be added to the solution if boundary conditions and initial conditions require it. We want no trapped particles in our initial conditions, so we do not add the stationary bound state to $\psi(x, 0)$, and we break $\psi(x, 0)$, and consequently $\psi(x, t)$, into plane waves only by Fourier transform. The plane waves must obey the boundary conditions at

$x = 0$ that [1]

$$\psi_+ = \psi_- \quad (2.2)$$

$$\left(\frac{\partial\psi}{\partial x}\right)_+ - \left(\frac{\partial\psi}{\partial x}\right)_- = \frac{2mV_0}{\hbar^2}\psi \quad (2.3)$$

Therefore, for a plane wave e^{ikx} that encounters the single delta potential, it is scattered and becomes

$$e^{ikx} + \frac{-imV_0}{imV_0 + \hbar^2 k} e^{-ikx} \quad (x < 0) \quad (2.4)$$

$$e^{ikx} + \frac{-imV_0}{imV_0 + \hbar^2 k} e^{ikx} \quad (x > 0) \quad (2.5)$$

According to Fourier transform,

$$\tilde{\psi}(k) = \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} \psi(x, 0) \exp\{-ikx\} dx \quad (2.6)$$

$$\tilde{\psi}(k) = \left(\frac{2\sigma_0^2}{\pi}\right)^{1/4} \exp\{-(k - k_0)^2 \sigma_0^2 + ikx_i\} \quad (2.7)$$

and

$$\psi(x, 0) = \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} \tilde{\psi}(k) \exp\{ikx\} dk \quad (2.8)$$

$$\psi(x, 0) = \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} \left[\left(\frac{2\sigma_0^2}{\pi}\right)^{1/4} \exp\{-(k - k_0)^2 \sigma_0^2 + ikx_i\}\right] \exp\{ikx\} dk \quad (2.9)$$

From equation (2.4), equation (2.5), and equation (2.9), the wavefunction is

$$\psi(x, t) = \psi_0(x, t) + \psi_1(x, t) \quad (2.10)$$

where

$$\begin{aligned} \psi_0(x, t) &= \left(\frac{\sigma_0^2}{2\pi^3}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp\{-(k - k_0)^2 \sigma_0^2 + i[k(x + x_i) - \omega t]\} dk, \\ &= \left(\frac{\sigma_0^2}{2\pi\alpha^2}\right)^{\frac{1}{4}} \exp\left\{-\frac{(x + x_i)^2}{4\alpha} + \frac{i\sigma_0^2}{\alpha}[k_0(x + x_i) - \omega_0 t]\right\} \end{aligned} \quad (2.11)$$

$$\begin{aligned}
\psi_1(x, t) &= \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(|x| + x_i) - \omega t] \right\} \left(\frac{-imV_0}{imV_0 + \hbar^2 k} \right) dk, \\
&= \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(|x| + x_i) - \omega t] \right\} \left(\frac{-i\beta_0}{i\beta_0 + k} \right) dk \quad (2.12)
\end{aligned}$$

where

$$\omega \equiv \frac{\hbar k^2}{2m}, \quad \omega_0 \equiv \frac{\hbar k_0^2}{2m}, \quad \alpha \equiv \sigma_0^2 + \frac{i\hbar t}{2m}, \quad \beta_0 \equiv \frac{mV_0}{\hbar^2} \quad (2.13)$$

The first term in equation (2.10) represents a normalized Gaussian wave packet in free space:

$$|\psi_0(x, t)|^2 = (2\pi\sigma^2)^{-1/2} \exp \left[-\frac{(x + x_i - \hbar k_0 t/m)^2}{2\sigma^2} \right], \quad \sigma^2 = \sigma_0^2 + \left(\frac{\hbar t}{2m\sigma_0} \right)^2. \quad (2.14)$$

Here $-x_i < 0$, $\sigma_0 > 0$ and $\hbar k_0/m > 0$ are the initial position, width and mean velocity of the wavepacket, respectively. As time evolves, the wavepacket spreads.

2.2 The ψ_1 Integral

The scattered wave is given by the remaining term of equation (2.10), which requires evaluating the ψ_1 integral of equation (2.12). The ψ_1 integral is not elementary but may be done by contour integration. First complete the square to write

$$\psi_1(x, t) = A(x, t) \int_{-\infty}^{\infty} \frac{\exp[-\alpha(k - \kappa)^2]}{k + i\beta_0} dk \quad (2.15)$$

where

$$\kappa(x, t) \equiv \frac{k_0 \sigma_0^2}{\alpha} + i \frac{f(x)}{2\alpha}, \quad f(x) = |x| + x_i, \quad (2.16)$$

$$A(x, t) \equiv -i\beta_0 \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}} e^{\alpha\kappa^2 - k_0^2 \sigma_0^2} = -i\beta_0 \left(\frac{\alpha}{\pi} \right)^{\frac{1}{2}} \psi_0(|x|, t) \quad (2.17)$$

Since we do not add the stationary bound state to the solution, the integral is along the real k -axis. When $\beta_0 > 0$, the contour of the integral in the complex k plane is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour is always below the pole $k = -i\beta_0$.

Then we change variable from k to u ,

$$k = \kappa + u\alpha^{-1/2} \quad (2.18)$$

or

$$u = \alpha^{1/2}(k - \kappa) \quad (2.19)$$

so the integrand in equation (2.15) becomes

$$\frac{e^{-\alpha(k-\kappa)^2}}{k + i\beta_0} dk = \frac{e^{-u^2}}{u + z(x, t)} du \quad (2.20)$$

and the pole is now at

$$u_p(x, t) = \alpha^{1/2}(-\kappa - i\beta_0) = -\left[\frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{if(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2}\right] = -z(x, t) \quad (2.21)$$

where

$$z(x, t) \equiv \alpha^{1/2}(\kappa + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{if(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2} \quad (2.22)$$

At $t = 0$, $\alpha^{1/2} = \sigma_0$, and $\kappa = k_0 + i\frac{f(x)}{2\sigma_0^2}$, so

$$u(x, 0) = \sigma_0(k - k_0) - i\frac{f(x)}{2\sigma_0} \quad (2.23)$$

and the pole $k = -i\beta_0$ in the u -plane is initially at

$$u_p(x, 0) = -k_0\sigma_0 - i\left(\frac{f(x)}{2\sigma_0} + \beta_0\sigma_0\right) = -z(x, 0) \quad (2.24)$$

where

$$z(x, 0) = k_0\sigma_0 + i\left(\frac{f(x)}{2\sigma_0} + \beta_0\sigma_0\right) \quad (2.25)$$

According to equation (2.23), when $\text{Im}(k)=0$,

$$\text{Im}(u) = -\frac{f(x)}{2\sigma_0} \quad (2.26)$$

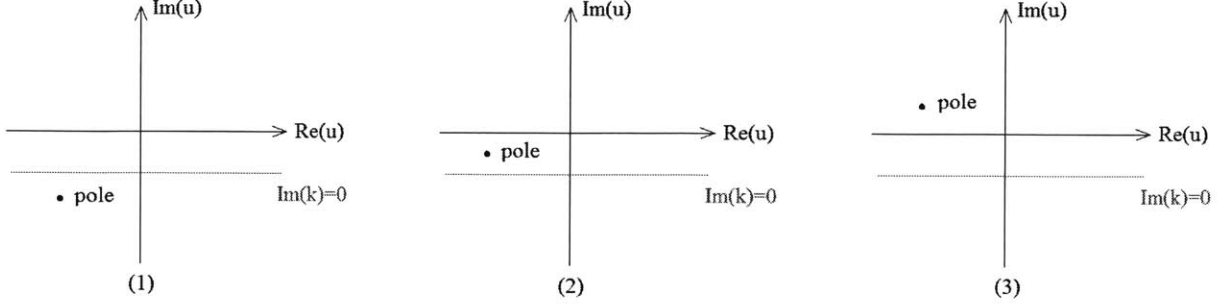


Figure 2-1: This is a schematic graph of the position of the pole $k = -i\beta_0$ in the u -plane for (1) $\beta_0 > 0$ (2) $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$ (3) $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, at $t = 0$. The integral is along the real k -axis. When $\beta_0 > 0$, the contour of integral is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour of integral is always below the pole $k = -i\beta_0$. The position of the pole is given by equation (2.24), and the line $\text{Im}(k)=0$ accords with equation (2.26).

Since $f(x)$ is always positive, then as shown in Figure2-1,

1. When $\beta_0 > 0$, $\text{Im}[z(x, 0)] > 0$ for all x , the pole lies below the real u -axis, and the real k -axis lies between the real u -axis and the pole.
2. When $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$, or equivalently, $\text{Im}[z(x, 0)] > 0$, the pole lies below the real u -axis but above the real k -axis.
3. When $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, or equivalently, $\text{Im}[z(x, 0)] < 0$, the pole lies above the real u -axis and the real k -axis lies below the real u axis.

In order to complete the contour integral, we first close the contour at positive and negative infinities. As shown in Figure 2-2, $|\text{Re}(u)| \rightarrow \infty$ and $0 > \text{Im}(u) > -\frac{f(x)}{2\sigma_0}$ along the vertical segments; since $\text{Im}(u)$ remains finite, the integrand in equation (2.20) vanishes along the vertical segments. The integral of equation (2.12) is along the real k -axis, but we want to replace it by the real u -axis to make the integral easier. With the integrand in equation (2.20) vanishing along the vertical segments,

1. if $\beta_0 > 0$, we simply shift the contour of integral from the real k -axis to the real u -axis without adding any residue, because $\int_{\text{Im}(u)=0} - \int_{\text{Im}(k)=0} = 0$;

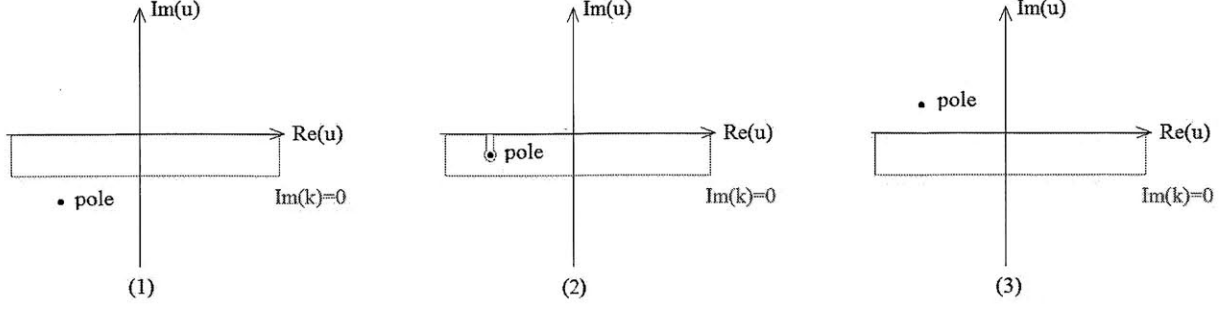


Figure 2-2: This is a schematic graph of shifting the contour of integral from the real k -axis to the real u -axis for (1) $\beta_0 > 0$ (2) $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$ (3) $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, at $t = 0$. The integral is originally along the real k -axis. When $\beta_0 > 0$, the contour of integral is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour of integral is always below the pole $k = -i\beta_0$. But we want to replace the original contour of integral, the real k -axis, by the real u -axis to make the integral easier, so we close the contour at positive and negative infinities.

2. if $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$, we need to add a residue when shifting the contour of integral from the real k -axis to the real u -axis, because $\int_{Im(u)=0} - \int_{Im(k)=0} = -2\pi i Res(u_p)$, which leads to $\int_{Im(k)=0} = \int_{Im(u)=0} + 2\pi i Res(u_p)$;
3. if $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, we simply shift the contour of integral from the real k -axis to the real u -axis without adding any residue, because $\int_{Im(u)=0} - \int_{Im(k)=0} = 0$.

Therefore, we add a residue to the solution of $\psi_1(x, 0)$ only when $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$. Since $\beta_0 > -\frac{f(x)}{2\sigma_0^2}$ is a necessary and sufficient condition for $Im[z(x, 0)] > 0$,

$$\psi_1(x, 0) = A(x, 0) \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z(x, 0)} + \theta(Im[z(x, 0)])\theta(-\beta_0)A(x, 0)2\pi i e^{-[u_p(x, 0)]^2} \quad (2.27)$$

where $\theta(x) = 1$ when $x > 0$ and $\theta(x) = 0$ when $x < 0$. The residue $2\pi i e^{-[u_p(x, 0)]^2}$ gives a contribution

$$\psi_{1, res}(x, 0) = A(x, 0)2\pi i e^{-u_p^2} = 2\pi\beta_0 \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}} \exp \left[\sigma_0^2\beta_0^2 + \beta_0(|x| + x_i - 2ik_0\sigma_0^2) - k_0^2\sigma_0^2 \right]. \quad (2.28)$$

For $\beta_0 > 0$, the residue contribution is unphysical at large distance because it diverges as $\exp(|\beta_0 x|)$, which agrees with equation (2.27). For $\beta_0 < 0$, when

$|x| > -2\sigma_0^2\beta_0 - x_i$, the residue contribution is added to the solution, but this residue contribution decays exponentially as $\exp(-|\beta_0 x|)$, so it does not violate the boundary conditions at positive and negative infinities.

For $t > 0$, when $\text{Im}(z)$ changes sign, we must add a residue to compensate for the discontinuity caused by the pole crossing the real u -axis. To illustrate the discontinuity, let $z = x + iy$,

$$f(x, y) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z} = \int_{-\infty}^{\infty} \frac{[(u + x) - iy]e^{-u^2} du}{(u + x)^2 + y^2} \quad (2.29)$$

$$f(x, y) - f(x, -y) = -2iy \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + x)^2 + y^2} \quad (2.30)$$

Let $u = -x + yt$, then $du = ydt$ and $(u + x)^2 + y^2 = y^2(1 + t^2)$, so

$$f(x, y) - f(x, -y) = \frac{-2iy}{y} \int_{-\infty}^{\infty} \frac{e^{-(x^2 - 2xyt + y^2 t^2)} dt}{1 + t^2} \quad (2.31)$$

Therefore,

$$\lim_{y \rightarrow 0^+} [f(x, y) - f(x, -y)] = -2ie^{-x^2} \lim_{y \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{e^{2xyt - y^2 t^2} dt}{1 + t^2} = -2\pi i e^{-x^2} = \lim_{y \rightarrow 0^+} (-2\pi i e^{-z^2}) \quad (2.32)$$

So the final result is,

$$\psi_1(x, t) = A(x, t) \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z(x, t)} + [\theta(\text{Im } z)\theta(-\beta_0) - \theta(-\text{Im } z)\theta(\beta_0)] A(x, t) 2\pi i e^{-[z(x, t)]^2} \quad (2.33)$$

The $-\theta(-\text{Im } z)\theta(\beta_0)$ in equation (2.33) arises in case (1) of Figure 2-2, when the pole $k = -i\beta_0$ moves up and crosses the real u -axis, as shown in case (1) of Figure 2-3. In case (1), the pole can only cross the real u -axis at $t > 0$, because at $t = 0$, $u_p(x, 0) = -z(x, 0)$, and $\text{Im}[z(x, 0)] > 0$ for all x at $t = 0$; and whether the pole crosses the real u -axis or not, the pole is always below the real k -axis, because for all $t > 0$, when $\beta_0 > 0$, $k = -i\beta_0$ must be below the line $\text{Im}(k) = 0$.

The $\theta(\text{Im } z)\theta(-\beta_0)$ in equation (2.33) arises in case (2) and case (3) of Figure 2-2 and Figure 2-3. When $\beta_0 < 0$, whether the pole crosses the real u -axis or not, the

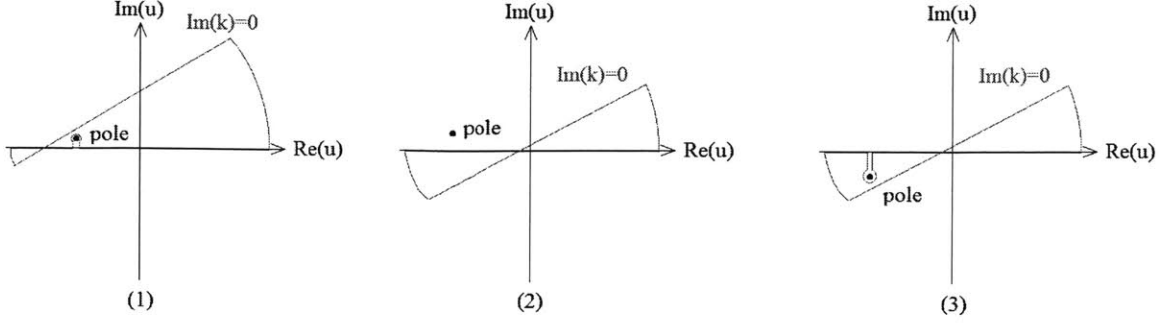


Figure 2-3: This is a schematic graph of the pole $k = -i\beta_0$ (1) moving up and crossing the real u -axis for $\beta_0 > 0$ (2) moving up and crossing the real u -axis for $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$ (3) moving down and crossing the real u -axis for $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, all for $t > 0$. The position of the pole is given by $u_p(x, t) = -z(x, t)$ as in equation (2.21). In case (1), the pole crossing the real u -axis results in a negative residue added to the solution, because the contour going around the pole is clockwise. In case (2), the pole crossing the real u -axis results in the residue removed from the solution, because the pole is no longer enclosed by the contour. In case (3), the pole crossing the real u -axis results in a positive residue added to the solution, because the contour going around the pole is counterclockwise.

pole $k = -i\beta_0$ is always above the real k -axis $\text{Im}(k) = 0$. At $t = 0$, if $0 > \beta_0 > -\frac{f(x)}{2\sigma_0^2}$, $\text{Im}[u_p(x, 0)] = -\text{Im}[z(x, 0)] < 0$, and the pole lies below the real u -axis as shown in case (2) of Figure 2-2, but at $t > 0$, it is possible though not necessary that the pole would move up and cross the real u -axis, so $\text{Im}[u_p(x, t)] = -\text{Im}[z(x, t)]$ becomes positive, and the residue contribution added to the solution at $t = 0$ should be removed then, as shown in case (2) of Figure 2-3. Similarly, at $t = 0$, if $\beta_0 < -\frac{f(x)}{2\sigma_0^2} < 0$, $\text{Im}[u_p(x, 0)] = -\text{Im}[z(x, 0)] > 0$, and the pole lies above the real u -axis as shown in case (3) of Figure 2-2, but at $t > 0$, it is possible though not necessary that the pole would move down and cross the real u -axis, so $\text{Im}[u_p(x, t)] = -\text{Im}[z(x, t)]$ becomes negative, and a residue contribution must be added to the solution then, as shown in case (3) of Figure 2-3. However, whether it is case (2) or case (3), it is always true for $\beta_0 < 0$ that we should add a residue contribution only when $\text{Im}[z(x, t)] > 0$.

The integral appearing in equation (2.33) can be written in terms of the Goodwin-

Staton integral (B. A. Mamedov, J. Quant. Spec. Rad. Trans. 105, 8, 2007),

$$G(z) \equiv \int_0^\infty \frac{e^{-t^2} dt}{t+z}. \quad (2.34)$$

Unfortunately, there is no simple way to write $G(z)$ in terms of more common special functions when z is complex. Therefore we resort to numerical integration, which can be done using the computer program, `wpscatt.c`.

2.3 Table of Notifications

Table 2.1: Table of Notifications

Notification	Definition	Equation
ω	$\frac{\hbar k^2}{2m}$	Eq. 2.13
ω_0	$\frac{\hbar k_0^2}{2m}$	Eq. 2.13
$\alpha(t)$	$\sigma_0^2 + \frac{i\hbar t}{2m}$	Eq. 2.13
$\sigma^2(t)$	$\sigma_0^2 + \left(\frac{\hbar t}{2m\sigma_0}\right)^2$	Eq. 2.14
β_0	$\frac{mV_0}{\hbar^2}$	Eq. 2.13
$f(x)$	$ x + x_i$	Eq. 2.16
$\kappa(x, t)$	$\frac{k_0\sigma_0^2}{\alpha} + i\frac{f(x)}{2\alpha}$	Eq. 2.16
$A(x, t)$	$-i\beta_0 \left(\frac{\sigma_0^2}{2\pi^3}\right)^{1/4} \exp(\alpha\kappa^2 - k_0^2\sigma_0^2) = -i\beta_0\left(\frac{\alpha}{\pi}\right)^{1/2}\psi_0(x , t)$	Eq. 2.17
k	$\kappa + u\alpha^{-1/2}$	Eq. 2.18
$z(x, t)$	$\alpha^{1/2}(\kappa + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{i(x +x_i)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2}$	Eq. 2.22
$z(x, 0)$	$k_0\sigma_0 + i\left(\frac{ x +x_i}{2\sigma_0} + \beta_0\sigma_0\right)$	Eq. 2.25
$\psi_{1,res}(x, t)$	$2\pi\beta_0\left(\frac{\sigma_0^2}{2\pi^3}\right)^{1/4} \exp[\alpha\beta_0^2 + \beta_0(x + x_i - 2ik_0\sigma_0^2) - k_0^2\sigma_0^2]$	Eq. 2.28

Chapter 3

Double Scattering

In this chapter, we add another scattering center, a delta function, to the potential of the single scattering case. The added delta function is at $x = -x_0$ and is of strength V , where V can be positive or negative. While we can only vary the initial width, the initial position and the momentum of the wave packet and the strength of the delta function in the single scattering case, now we can also alter the spacing between the two scattering center in the double scattering case to achieve maximum localization. The model is still simple, but it offers more insight than the single scattering model.

3.1 $\psi_A(x, t)$ and $\psi_B(x, t)$

As shown in Figure 3-1, suppose we start with a Gaussian wave packet with its peak at $x = -x_i < -x_0 < 0$ traveling toward a delta function potential $V(x) = V_0\delta(x) + V\delta(x + x_0)$. At $t > 0$,

$$\psi(x, t) = \psi_A(x, t) + \psi_B(x, t), \quad (x < -x_0) \quad (3.1)$$

$$\psi(x, t) = \psi_C(x, t) + \psi_D(x, t), \quad (-x_0 < x < 0) \quad (3.2)$$

$$\psi(x, t) = \psi_F(x, t), \quad (x > 0) \quad (3.3)$$

As in the single scattering case, we want no trapped particles in our initial condi-

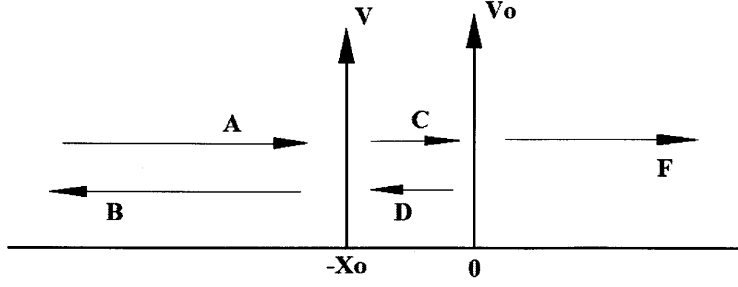


Figure 3-1: This is a schematic drawing for the scattering centers and the wavefunction in three different regions for the double scattering case.

tions, so we break $\psi(x, 0)$, and consequently $\psi(x, t)$, into plane waves only by Fourier transform. The wavefunction for $x > -x_0$ is the same as it is for the single scattering case with $V(x) = V_0\delta(x)$ except for normalization, so

$$\psi_C = C\left(\frac{\sigma_0^2}{2\pi^3}\right)^{-1/4}\psi_0, \psi_D = C\left(\frac{\sigma_0^2}{2\pi^3}\right)^{-1/4}\psi_1, \psi_F = C\left(\frac{\sigma_0^2}{2\pi^3}\right)^{-1/4}(\psi_0 + \psi_1) \quad (3.4)$$

where C is to be determined according to normalization.

For the region $x < -x_0$, due to the boundary conditions at $x = -x_0$,

$$\psi_A = C \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i) - \omega t]\right\} g_A(k) dk \quad (3.5)$$

where

$$g_A(k) = e^{2ikx_0} \left(\frac{i\beta_0}{k + i\beta_0}\right) \left(\frac{-i\beta}{k}\right) + 1 + \frac{i\beta}{k}, \beta \equiv \frac{mV}{\hbar^2}, \beta_0 \equiv \frac{mV_0}{\hbar^2} \quad (3.6)$$

and

$$\psi_B = C \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(-x + x_i) - \omega t]\right\} g_B(k) dk \quad (3.7)$$

where

$$g_B(k) = \frac{-i\beta}{k} e^{-2ikx_0} + \left(\frac{-i\beta_0}{k + i\beta_0}\right) \left(1 - \frac{i\beta}{k}\right) \quad (3.8)$$

Since $g_A(k) \approx 1$, the normalization factor C should be determined so that $\psi_A(x, 0) \approx$

$\psi_0(x, 0)$, so

$$\begin{aligned}\psi_A(x, 0) &\approx C \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i) - \omega t] \right\} dk \\ &= \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i) - \omega t] \right\} dk = \psi_0(x, 0)\end{aligned}\quad (3.9)$$

Therefore,

$$C = \left(\frac{\sigma_0^2}{2\pi^3} \right)^{\frac{1}{4}}, \quad (3.10)$$

and $\psi_C = \psi_0$, $\psi_D = \psi_1$, $\psi_F = \psi_0 + \psi_1$.

It appears that both ψ_A and ψ_B have two poles, one at $k = 0$, and the other at $k = -i\beta_0$; however, since

$$g_A(k) = e^{2ikx_0} \left(\frac{i\beta_0}{k + i\beta_0} \right) \left(\frac{-i\beta}{k} \right) + 1 + \frac{i\beta}{k} = \frac{-i\beta}{k} (e^{2ikx_0} - 1) + \frac{i\beta}{k + i\beta_0} e^{2ikx_0} + 1 \quad (3.11)$$

and by Taylor expansion,

$$\frac{-i\beta}{k} (e^{2ikx_0} - 1) = \frac{-i\beta}{k} [1 + 2ikx_0 + O(k^2) + \dots - 1] = -i\beta [2ix_0 + O(k) + \dots] \quad (3.12)$$

So ψ_A has no pole at $k = 0$. Similarly,

$$g_B(k) = \frac{-i\beta}{k} e^{-2ikx_0} + \left(\frac{-i\beta_0}{k + i\beta_0} \right) \left(1 - \frac{i\beta}{k} \right) = \frac{-i\beta}{k} (e^{-2ikx_0} - 1) - \frac{i(\beta_0 + \beta)}{k + \beta_0} \quad (3.13)$$

and by Taylor expansion,

$$\frac{-i\beta}{k} (e^{-2ikx_0} - 1) = \frac{-i\beta}{k} [1 - 2ikx_0 + O(k^2) + \dots - 1] = -i\beta [-2ix_0 + O(k) + \dots] \quad (3.14)$$

So ψ_B has no pole at $k = 0$ either.

From equation (3.5), equation (3.6), equation (3.7) and equation (3.8) we have,

$$\begin{aligned}\frac{\psi_A}{C} &= \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i + 2x_0) - \omega t] \right\} \left(\frac{i\beta}{k + i\beta_0} \right) dk \\ &\quad - \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i + 2x_0) - \omega t] \right\} \left(\frac{i\beta}{k} \right) dk\end{aligned}$$

$$\begin{aligned}
& + \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i) - \omega t] \right\} \left(\frac{i\beta}{k} \right) dk \\
& + \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_i) - \omega t] \right\} dk \quad (3.15)
\end{aligned}$$

$$\begin{aligned}
\frac{\psi_B}{C} &= \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(-x + x_i - 2x_0) - \omega t] \right\} \left(\frac{-i\beta}{k} \right) dk \\
& + \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(-x + x_i) - \omega t] \right\} \left(\frac{i\beta}{k} \right) dk \\
& - \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(-x + x_i) - \omega t] \right\} \left(\frac{i\beta_0 + i\beta}{k + i\beta_0} \right) dk \quad (3.16)
\end{aligned}$$

Now let

$$f_1(x) = x + x_i + 2x_0, \quad f_2(x) = x + x_i, \quad f_3(x) = -x + x_i - 2x_0, \quad f_4(x) = -x + x_i \quad (3.17)$$

$$\kappa_i(x, t) \equiv \frac{k_0 \sigma_0^2}{\alpha} + i \frac{f_i(x)}{2\alpha}, \quad d_i(x, t) \equiv e^{\alpha \kappa_i^2 - k_0^2 \sigma_0^2}, \quad \alpha \equiv \sigma_0^2 + \frac{i\hbar t}{2m} \quad (3.18)$$

Then

$$\begin{aligned}
\frac{\psi_A}{C} &= i\beta d_1(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_1)^2}}{k + i\beta_0} dk - i\beta d_1(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_1)^2}}{k} dk \\
& + i\beta d_2(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_2)^2}}{k} dk + d_2(x, t) \int_{-\infty}^{\infty} e^{-\alpha(k-\kappa_2)^2} dk \quad (3.19)
\end{aligned}$$

$$\begin{aligned}
\frac{\psi_B}{C} &= -i\beta d_3(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_3)^2}}{k} dk + i\beta d_4(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_4)^2}}{k} dk \\
& - i(\beta + \beta_0) d_4(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_4)^2}}{k + i\beta_0} dk \quad (3.20)
\end{aligned}$$

Since there is no pole at $k = 0$, let's first focus on the two integrals that have a pole at $k = -i\beta_0$ in equation (3.19) and equation (3.20),

$$I_A = \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_1)^2}}{k + i\beta_0} dk \quad (3.21)$$

$$I_B = \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_4)^2}}{k + i\beta_0} dk \quad (3.22)$$

Because we break $\psi(x, t)$ into plane waves only, the integrals are along the real k -axis. When $\beta_0 > 0$, the contour of integral is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour of integral is always below the pole $k = -i\beta_0$.

Then we change variable from k to u ,

$$k = \kappa_i + u\alpha^{-1/2} \quad (3.23)$$

or

$$u = \alpha^{1/2}(k - \kappa_i) \quad (3.24)$$

so the integrands in I_A and I_B become

$$\frac{e^{-\alpha(k-\kappa_1)^2}}{k+i\beta_0} dk = \frac{e^{-u^2}}{u+z_A(x,t)} du \quad (3.25)$$

$$\frac{e^{-\alpha(k-\kappa_4)^2}}{k+i\beta_0} dk = \frac{e^{-u^2}}{u+z_B(x,t)} du \quad (3.26)$$

The only difference between $I_{A,B}$ and the integral $I = \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa)^2}}{k+i\beta_0} dk$ in the single scattering case is that, the κ in I is replaced by $\kappa_{1,4}$ in $I_{A,B}$, and the only difference between κ and $\kappa_{1,4}$ is that, the $f(x)$ in κ is replaced by $f_{1,4}(x)$. Since $f_A(x)$ is always positive when $x < 0$, the analysis of I_B is exactly the same as the analysis of I . But $f_1(x)$ can be positive or negative, so the analysis of I_A is more complicated. When $f_1(x) > 0$, the analysis of I_A is reduced to the analysis of I ; when $f_1(x) < 0$, however, the analysis becomes different.

3.2 Analysis of I_A when $f_1(x) < 0$

For I_A , when $f_1(x) < 0$, the pole is at

$$u_{p,A}(x, t) = -z_A(x, t) \quad (3.27)$$

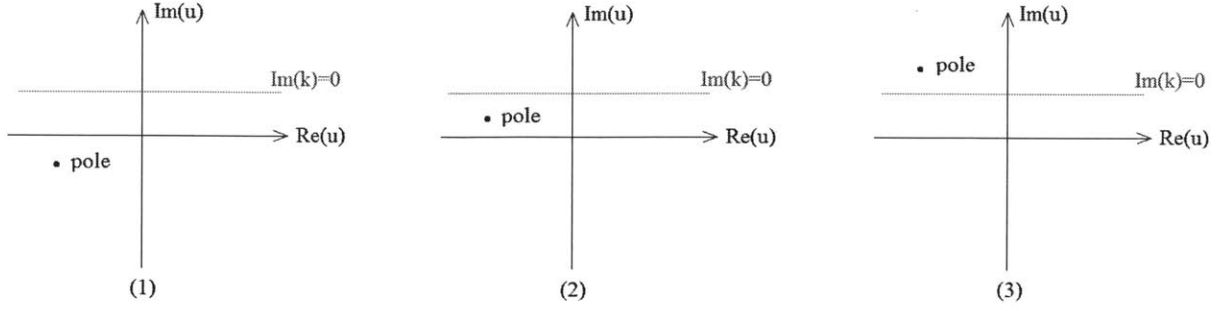


Figure 3-2: This is a schematic graph of the position of the pole $k = -i\beta_0$ at $t = 0$ in the u -plane for integral I_A when $f_1(x) < 0$. The three cases are (1) $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$, (2) $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$, and (3) $\beta_0 < 0$. The integral is along the real k -axis. When $\beta_0 > 0$, the contour of integral is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour of integral is always below the pole $k = -i\beta_0$. The position of the pole is given by equation (3.30), and the line $\text{Im}(k)=0$ always lies above the real u -axis when $f_1(x) < 0$, according to equation (3.32).

where

$$z_A(x, t) \equiv \alpha^{1/2}(\kappa_1 + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{if_1(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2} \quad (3.28)$$

At $t = 0$,

$$u(x, 0) = \sigma_0(k - k_0) - i\frac{f_1(x)}{2\sigma_0} \quad (3.29)$$

and the pole $k = -i\beta_0$ in the u -plane is initially at

$$u_{p,A}(x, 0) = -z_A(x, 0) \quad (3.30)$$

where

$$z_A(x, 0) = k_0\sigma_0 + i\left(\frac{f_1(x)}{2\sigma_0} + \beta_0\sigma_0\right) \quad (3.31)$$

According to equation (3.29), when $\text{Im}(k)=0$,

$$\text{Im}(u) = -\frac{f_1(x)}{2\sigma_0} > 0 \quad (3.32)$$

Therefore, as show in Figure 3-2,

1. When $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$, or equivalently, $\text{Im}[z_A(x, 0)] > 0$, the pole lies below the

real u -axis, and the real k -axis lies above the real u -axis.

2. When $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$, or equivalently, $\text{Im}[z_A(x, 0)] < 0$, the pole lies above the real u -axis but below the real k -axis.
3. When $\beta_0 < 0$, $\text{Im}[z_A(x, 0)] < 0$ for all x , the pole lies above the real k -axis and the real k -axis lies above the real u -axis.

In order to complete the contour integral, we first close the contour at positive and negative infinities. As shown in Figure3-3, $|\text{Re}(u)| \rightarrow \infty$ and $0 < \text{Im}(u) < -\frac{f_1(x)}{2\sigma_0}$ along the vertical segments; since $\text{Im}(u)$ remains finite, the integrand in equation (3.25) vanishes along the vertical segments. The integral of I_A is along the real k -axis, but we want to replace it by the real u -axis to make the integral easier. With the integrand in equation (3.25) vanishing along the vertical segments,

1. if $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$, we simply shift the contour of integral from the real k -axis to the real u -axis without adding any residue, because $\int_{\text{Im}(u)=0} - \int_{\text{Im}(k)=0} = 0$;
2. if $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$, we need to add a residue when shifting the contour of integral from the real k -axis to the real u -axis, because $\int_{\text{Im}(u)=0} - \int_{\text{Im}(k)=0} = 2\pi i \text{Res}(u_p)$, which leads to $\int_{\text{Im}(k)=0} = \int_{\text{Im}(u)=0} - 2\pi i \text{Res}(u_p)$;
3. if $\beta_0 < 0$, we simply shift the contour of integral from the real k -axis to the real u -axis without adding any residue, because $\int_{\text{Im}(u)=0} - \int_{\text{Im}(k)=0} = 0$.

Therefore, when $f_1(x) < 0$, we add a residue to the solution of $I_A(x, 0)$ only if $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$. Since $\beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$ is a necessary and sufficient condition for $\text{Im}[z_A(x, 0)] < 0$,

$$I_A(x, 0) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_A(x, 0)} + \theta(-\text{Im}[z_A(x, 0)])\theta(\beta_0)2\pi i e^{-[u_{p,A}(x,0)]^2}, \quad f_1(x) < 0 \quad (3.33)$$

For $t > 0$, when $\text{Im}(z)$ changes sign, we must add a residue to compensate for the

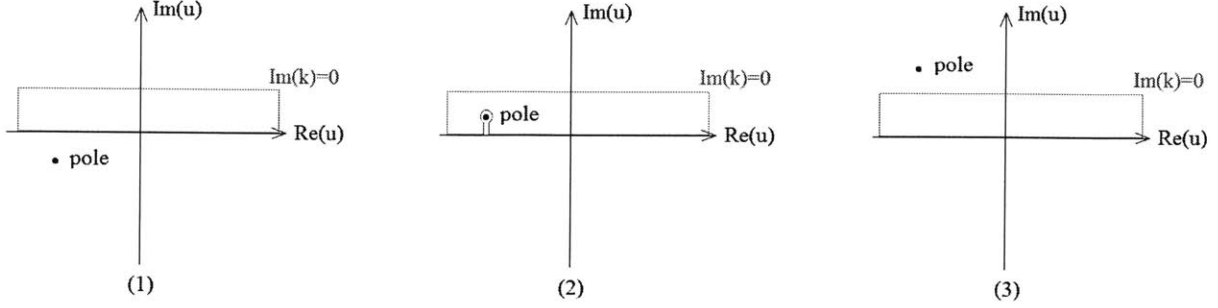


Figure 3-3: This is a schematic graph of shifting the contour of integral from the real k -axis to the real u -axis for (1) $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$, (2) $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$ (3) $\beta_0 < 0$, at $t = 0$. The integral is originally along the real k -axis. When $\beta_0 > 0$, the contour of integral is always above the pole $k = -i\beta_0$; when $\beta_0 < 0$, the contour of integral is always below the pole $k = -i\beta_0$. But we want to replace the original contour of integral, the real k -axis, by the real u -axis to make the integral easier, so we close the contour at positive and negative infinities.

discontinuity caused by the pole crossing the real u -axis, so

$$I_A(x, t) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_A(x, t)} + [\theta(\text{Im } z_A)\theta(-\beta_0) - \theta(-\text{Im } z_A)\theta(\beta_0)] 2\pi i e^{-[z_A(x, t)]^2}, \quad f_1(x) < 0 \quad (3.34)$$

The $\theta(\text{Im } z_A)\theta(-\beta_0)$ in equation (3.34) arises in case (3) of Figure 3-3, when the pole $k = -i\beta_0$ moves down and crosses the real u -axis, as shown in case (3) of Figure 3-4. In case (3), the pole can only cross the real u -axis at $t > 0$, because at $t = 0$, $u_{p,A}(x, 0) = -z_A(x, 0)$, and $\text{Im}[z_A(x, 0)] < 0$ for all x at $t = 0$; and whether the pole crosses the real u -axis or not, the pole is always above the real k -axis, because for all $t > 0$, when $\beta_0 < 0$, $k = -i\beta_0$ must be above the line $\text{Im}(k) = 0$.

The $-\theta(-\text{Im } z_A)\theta(\beta_0)$ in equation (3.34) arises in case (1) and case (2) of Figure 3-3 and Figure 3-4. When $\beta_0 > 0$, whether the pole crosses the real u -axis or not, the pole $k = -i\beta_0$ is always below the real k -axis $\text{Im}(k) = 0$. At $t = 0$, if $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$, $\text{Im}[u_{p,A}(x, 0)] = -\text{Im}[z_A(x, 0)] < 0$, and the pole lies below the real u -axis as shown in case (1) of Figure 3-3, but at $t > 0$, it is possible though not necessary that the pole would move up and cross the real u -axis, so $\text{Im}[u_{p,A}(x, t)] = -\text{Im}[z_A(x, t)]$ becomes positive, and a residue contribution must be added to the solution then, as shown in case (1) of Figure 3-4. Similarly, at $t = 0$, if $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$, $\text{Im}[u_{p,A}(x, 0)] =$

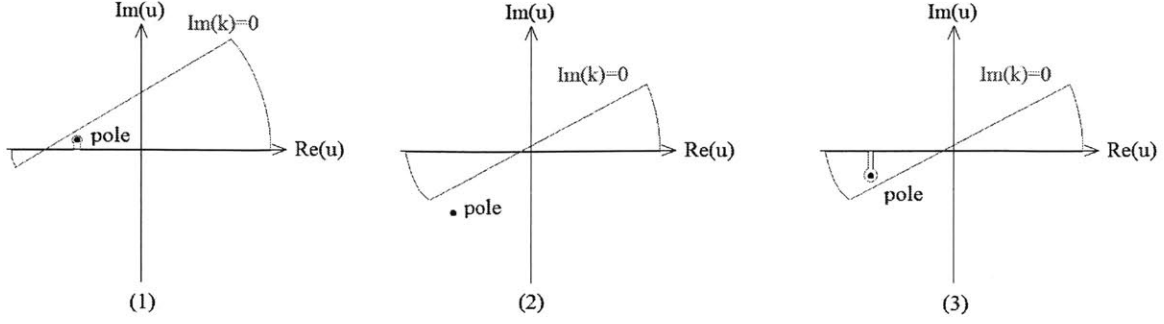


Figure 3-4: This is a schematic graph of the pole $k = -i\beta_0$ (1) moving up and crossing the real u -axis for $\beta_0 > -\frac{f_1(x)}{2\sigma_0^2} > 0$ (2) moving down and crossing the real u -axis for $0 < \beta_0 < -\frac{f_1(x)}{2\sigma_0^2}$ (3) moving down and crossing the real u -axis for $\beta_0 < 0$, all for $t > 0$. The position of the pole is given by $u_{p,A}(x, t) = -z_A(x, t)$ as in equation (3.27). In case (1), the pole crossing the real u -axis results in a negative residue added to the solution, because the contour going around the pole is clockwise. In case (2), the pole crossing the real u -axis results in the residue removed from the solution, because the pole is no longer enclosed by the contour. In case (3), the pole crossing the real u -axis results in a positive residue added to the solution, because the contour going around the pole is counterclockwise.

$-\text{Im}[z_A(x, 0)] > 0$, and the pole lies above the real u -axis as shown in case (2) of Figure 3-3, but at $t > 0$, it is possible though not necessary that the pole would move down and cross the real u -axis, so $\text{Im}[u_{p,A}(x, t)] = -\text{Im}[z_A(x, t)]$ becomes negative, and the residue contribution added to the solution at $t = 0$ must be removed then, as shown in case (2) of Figure 3-4. However, whether it is case (1) or case (2), it is always true for $\beta_0 > 0$ that we should add a residue contribution only when $\text{Im}[z_A(x, t)] < 0$.

Therefore, we conclude that, the final expression of I_A when $f_1(x) < 0$ is exactly the same as the final expression of I_A when $f_1(x) > 0$, except that $f(x)$ gets replaced by $f_1(x)$. That is to say, the final expressions of I_A , I_B and I are all of the same form, regardless of the sign of $f(x)$, $f_1(x)$, and $f_4(x)$, as shown in equation (3.35) and equation (3.36):

$$I_A(x, t) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_A(x, t)} + [\theta(\text{Im } z_A)\theta(-\beta_0) - \theta(-\text{Im } z_A)\theta(\beta_0)]2\pi i e^{-[z_A(x, t)]^2} \quad (3.35)$$

$$I_B(x, t) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_B(x, t)} + [\theta(\text{Im } z_B)\theta(-\beta_0) - \theta(-\text{Im } z_B)\theta(\beta_0)]2\pi i e^{-[z_B(x, t)]^2} \quad (3.36)$$

where

$$z_B(x, t) \equiv \alpha^{1/2}(\kappa_1 + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{if_4(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2} \quad (3.37)$$

Finally, according to equation (3.19) and equation (3.20),

$$\begin{aligned} \psi_A(x, t) = i\beta d_1 C \left\{ \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_A} + [\theta(\text{Im } z_A)\theta(-\beta_0) - \theta(-\text{Im } z_A)\theta(\beta_0)]2\pi i e^{-z_A^2} \right\} \\ + C[-\beta d_1 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_1} + i\beta d_2 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_2} + d_2\alpha^{-1/2}\pi^{1/2}] \end{aligned} \quad (3.38)$$

$$\begin{aligned} \psi_B(x, t) = C[-i\beta d_3 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_3} + i\beta d_4 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_4} - i(\beta + \beta_0)d_4 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_B}] \\ - i(\beta + \beta_0)d_4 C[\theta(\text{Im } z_B)\theta(-\beta_0) - \theta(-\text{Im } z_B)\theta(\beta_0)]2\pi i e^{-[z_B]^2} \end{aligned} \quad (3.39)$$

where

$$z_i(x, t) \equiv \alpha^{1/2}\kappa_i(x, t) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{if_i(x)}{2\alpha^{1/2}} \quad (3.40)$$

For the integral appearing in equation (3.38) and equation (3.39), we resort to numerical integration, which can be done using the computer program, `doublewpscott.c`.

3.3 Table of Notifications

Table 3.1: Table of Notifications

Notification	Definition	Equation
ω	$\frac{\hbar k^2}{2m}$	Eq. 2.13
ω_0	$\frac{\hbar k_0^2}{2m}$	Eq. 2.13
β	$\frac{mV}{\hbar^2}$	Eq. 3.6
β_0	$\frac{mV_0}{\hbar^2}$	Eq. 3.6
$g_A(k)$	$[e^{2ikx_0} (\frac{\beta_0}{\beta_0 - ik}) (\frac{\beta}{ik}) + 1 - \frac{\beta}{ik}]$	Eq. 3.6
$g_B(k)$	$[\frac{\beta}{ik} e^{-2ikx_0} + (\frac{-\beta_0}{\beta_0 - ik}) (1 + \frac{\beta}{ik})]$	Eq. 3.8
C	$(\frac{\sigma_0^2}{2\pi^3})^{1/4}$	Eq. 3.10
$\alpha(t)$	$\sigma_0^2 + \frac{i\hbar t}{2m}$	Eq. 3.18
$f_1(x)$	$x + x_i + 2x_0$	Eq. 3.17
$f_2(x)$	$x + x_i$	Eq. 3.17
$f_3(x)$	$-x + x_i - 2x_0$	Eq. 3.17
$f_4(x)$	$-x + x_i$	Eq. 3.17
$\kappa_i(x, t)$	$\frac{k_0 \sigma_0^2}{\alpha} + i \frac{f_i(x)}{2\alpha}$	Eq. 3.18
$d_i(x, t)$	$e^{\alpha \kappa_i^2 - k_0^2 \sigma_0^2}$	Eq. 3.18
k	$\kappa_i + u\alpha^{-1/2}$	Eq. 3.18
$z_A(x, t)$	$\alpha^{1/2}(\kappa_1 + i\beta_0) = \frac{k_0 \sigma_0^2}{\alpha^{1/2}} + \frac{if_1(x)}{2\alpha^{1/2}} + i\beta_0 \alpha^{1/2}$	Eq. 3.28
$z_B(x, t)$	$\alpha^{1/2}(\kappa_4 + i\beta_0) = \frac{k_0 \sigma_0^2}{\alpha^{1/2}} + \frac{if_4(x)}{2\alpha^{1/2}} + i\beta_0 \alpha^{1/2}$	Eq. 3.37
$z_i(x, t)$	$\alpha^{1/2} \kappa_i = \frac{k_0 \sigma_0^2}{\alpha^{1/2}} + \frac{if_i(x)}{2\alpha^{1/2}}$	Eq. 3.40

Chapter 4

Triple Scattering

In this chapter, we add one more scattering center, a delta function, to the potential of the double scattering case. The newly added delta function is at $x = -x_1$ and is of strength V_1 , where V_1 can be positive or negative. Again, the model is still simple, and is far from real quantum measurement equipments or procedures, but we hope that adding one more scattering center to our model can offer a better understanding of the importance of the spacing between the scattering centers.

4.1 Triple Scattering Solution

As shown in Figure 4-1, suppose we start with a Gaussian wave packet with its peak at $x = -x_i < -x_1 < -x_0 < 0$ traveling toward a delta function potential $V(x) = V_0\delta(x) + V\delta(x + x_0) + V_1\delta(x + x_1)$.

As in the single scattering case and the double scattering case, we want no trapped particles in our initial conditions, so we break $\psi(x, 0)$, and consequently $\psi(x, t)$, into plane waves only by Fourier transform. The wavefunction for $x > -x_1$ is the same as it is for the double scattering case with $V(x) = V_0\delta(x) + V\delta(x + x_0)$ except for normalizaton, so

$$\psi(x, t) = \frac{C_1}{C}\psi_A(x, t) + \frac{C_1}{C}\psi_B(x, t), \quad (-x_1 < x < -x_0) \quad (4.1)$$

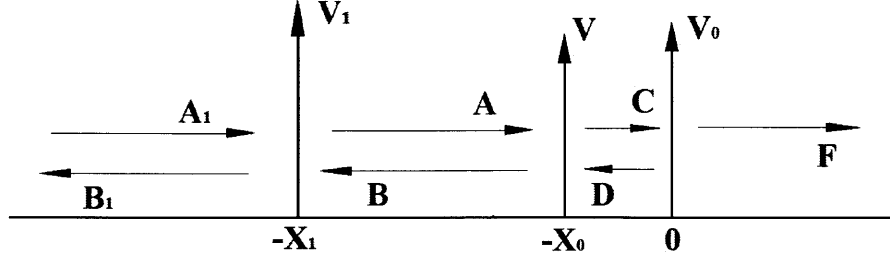


Figure 4-1: This is a schematic drawing for triple scattering case.

$$\psi(x, t) = \frac{C_1}{C} \psi_C(x, t) + \frac{C_1}{C} \psi_D(x, t), \quad (-x_0 < x < 0) \quad (4.2)$$

$$\psi(x, t) = \frac{C_1}{C} \psi_F(x, t), \quad (x > 0) \quad (4.3)$$

where C_1 is to be determined according to normalization.

For the region $x < -x_1$, due to the boundary conditions at $x = -x_1$,

$$\psi(x, t) = \psi_{A_1}(x, t) + \psi_{B_1}(x, t), \quad (x < -x_1) \quad (4.4)$$

$$\psi_{A_1} = C_1 \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(x + x_1) - \omega t] \right\} A_1(k) dk \quad (4.5)$$

where

$$A_1(k) = 1 + e^{2ikx_0} \beta \left(\frac{1 - \beta_1/\beta_0}{k + i\beta_0} \right) i + e^{2kix_1} \beta_1 \left(\frac{1 + \beta/\beta_0}{k + i\beta_0} \right) i + \left(\frac{i}{k} \right) h_A(k) + \left(\frac{\beta_1 \beta}{k^2} \right) f_A(k) \quad (4.6)$$

$$h_A(k) = \beta + \beta_1 + e^{2ikx_0} \left(\frac{\beta_1 \beta}{\beta_0} - \beta \right) - e^{2ikx_1} \left(\beta_1 + \frac{\beta_1 \beta}{\beta_0} \right) \quad (4.7)$$

$$f_A(k) = -1 + e^{2ik(x_1 - x_0)} + e^{2ikx_0} - e^{2ikx_1} \quad (4.8)$$

$$\beta \equiv \frac{mV}{\hbar^2}, \quad \beta_0 \equiv \frac{mV_0}{\hbar^2}, \quad \beta_1 \equiv \frac{mV_1}{\hbar^2} \quad (4.9)$$

and

$$\psi_{B_1} = C_1 \int_{-\infty}^{\infty} \exp \left\{ -(k - k_0)^2 \sigma_0^2 + i[k(-x + x_1) - \omega t] \right\} B_1(k) dk \quad (4.10)$$

where

$$B_1(k) = e^{2ik(x_0-x_1)} \left(\frac{\beta_1\beta}{\beta_0}\right) \left(\frac{1}{k+i\beta_0}\right) i - \frac{\beta_0 + \beta + \beta_1 + \beta_1\beta/\beta_0}{k+i\beta_0} i - \left(\frac{i}{k}\right) h_B(k) + \left(\frac{\beta_1\beta}{k^2}\right) f_B(k) \quad (4.11)$$

$$h_B(k) = \beta_1 e^{-2ikx_1} + \frac{\beta_1\beta}{\beta_0} e^{2ik(x_0-x_1)} + \beta e^{-2ikx_0} - \beta - \beta_1 - \frac{\beta_1\beta}{\beta_0} \quad (4.12)$$

$$f_B(k) = 1 - e^{2ik(x_0-x_1)} - e^{-2ikx_0} + e^{-2ikx_1} \quad (4.13)$$

Since $A_1(k) \approx 1$, the normalization factor C_1 should be determined so that $\psi_{A_1}(x, 0) \approx \psi_0(x, 0)$, so

$$\begin{aligned} \psi_{A_1}(x, 0) &\approx C_1 \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(x+x_i) - \omega t]\right\} dk \\ &= \left(\frac{\sigma_0^2}{2\pi^3}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(x+x_i) - \omega t]\right\} dk = \psi_0(x, 0) \end{aligned} \quad (4.14)$$

Therefore,

$$C_1 = \left(\frac{\sigma_0^2}{2\pi^3}\right)^{\frac{1}{4}} = C. \quad (4.15)$$

It appears that both ψ_{A_1} and ψ_{B_1} have poles at $k = 0$; however, according to Taylor expansion,

$$h_A(k) = \beta + \beta_1 + \left(\frac{\beta_1\beta}{\beta_0} - \beta\right)(1 + 2ikx_0) - \left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right)(1 + 2ikx_1) + O(k^2) + \dots \quad (4.16)$$

so

$$\frac{h_A(k)}{k} = \left(\frac{\beta_1\beta}{\beta_0} - \beta\right)2ix_0 - \left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right)2ix_1 + O(k) + \dots \quad (4.17)$$

and

$$\begin{aligned} f_A(k) &= -1 + \left[1 + (2ikx_1 - 2ikx_0) + \frac{(2ikx_1 - 2ikx_0)^2}{2}\right] + \left[1 + (2ikx_0) + \frac{(2ikx_0)^2}{2}\right] \\ &\quad - \left[1 + (2ikx_1) + \frac{(2ikx_1)^2}{2}\right] + O(k^3) + \dots \end{aligned} \quad (4.18)$$

so

$$\frac{f_A(k)}{k^2} = -4x_0^2 + 4x_0x_1 + O(k) + \dots \quad (4.19)$$

Therefore, ψ_{A_1} has no pole at $k = 0$. Similarly,

$$h_B(k) = \beta_1(1 - 2ikx_1) + \frac{\beta_1\beta}{\beta_0}(1 + 2ikx_0 - 2ikx_1) + \beta(1 - 2ikx_0) - \beta - \beta_1 - \frac{\beta_1\beta}{\beta_0} + O(k^2) + \dots \quad (4.20)$$

so

$$\frac{h_B(k)}{k} = \left(\frac{\beta_1\beta}{\beta_0} - \beta\right)2ix_0 - \left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right)2ix_1 + O(k) + \dots \quad (4.21)$$

and

$$f_B(k) = 1 - \left[1 + (2ikx_0 - 2ikx_1) + \frac{(2ikx_0 - 2ikx_1)^2}{2}\right] - \left[1 + (-2ikx_0) + \frac{(-2ikx_0)^2}{2}\right] + \left[1 + (-2ikx_1) + \frac{(-2ikx_1)^2}{2}\right] + O(k^3) + (4.22)$$

so

$$\frac{f_B(k)}{k^2} = 4x_0^2 - 4x_0x_1 + O(k) + \dots \quad (4.23)$$

Therefore, ψ_{B_1} has no pole at $k = 0$ either.

From equation (4.5), equation (4.6), equation (4.7), and equation (4.8), we have

$$\begin{aligned} \frac{\psi_{A_1}}{C_1} &= \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i) - \omega t]\right\} dk \\ &- i\left(\frac{\beta_1\beta}{\beta_0} - \beta\right) \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_0) - \omega t]\right\} \left(\frac{1}{k + i\beta_0}\right) dk \\ &+ i\left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right) \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_1) - \omega t]\right\} \left(\frac{1}{k + i\beta_0}\right) dk \\ &\quad + i(\beta + \beta_1) \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i) - \omega t]\right\} \left(\frac{1}{k}\right) dk \\ &\quad + i\left(\frac{\beta_1\beta}{\beta_0} - \beta\right) \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_0) - \omega t]\right\} \left(\frac{1}{k}\right) dk \\ &\quad - i\left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right) \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_1) - \omega t]\right\} \left(\frac{1}{k}\right) dk \\ &\quad - \beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i) - \omega t]\right\} \left(\frac{1}{k^2}\right) dk \\ &\quad + \beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_0) - \omega t]\right\} \left(\frac{1}{k^2}\right) dk \\ &\quad - \beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_1) - \omega t]\right\} \left(\frac{1}{k^2}\right) dk \\ &\quad + \beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k - k_0)^2\sigma_0^2 + i[k(x + x_i + 2x_1 - 2x_0) - \omega t]\right\} \left(\frac{1}{k^2}\right) dk \quad (4.24) \end{aligned}$$

and from equation (4.10), equation (4.11), equation (4.12), and equation (4.13), we have

$$\begin{aligned}
\frac{\psi_{B_1}}{C_1} = & i\left(\frac{\beta_1\beta}{\beta_0}\right) \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i+2x_0-2x_1)-\omega t]\right\} \left(\frac{1}{k+i\beta_0}\right) dk \\
& -i(\beta_0+\beta+\beta_1+\frac{\beta_1\beta}{\beta_0}) \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i)-\omega t]\right\} \left(\frac{1}{k+i\beta_0}\right) dk \\
& +i(\beta+\beta_1+\frac{\beta_1\beta}{\beta_0}) \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i)-\omega t]\right\} \left(\frac{1}{k}\right) dk \\
& -i\beta \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i-2x_0)-\omega t]\right\} \left(\frac{1}{k}\right) dk \\
& -i\beta_1 \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i-2x_1)-\omega t]\right\} \left(\frac{1}{k}\right) dk \\
& -i\left(\frac{\beta_1\beta}{\beta_0}\right) \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i+2x_0-2x_1)-\omega t]\right\} \left(\frac{1}{k}\right) dk \\
& +\beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i)-\omega t]\right\} \left(\frac{1}{k^2}\right) dk \\
& -\beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i-2x_0)-\omega t]\right\} \left(\frac{1}{k^2}\right) dk \\
& +\beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i-2x_1)-\omega t]\right\} \left(\frac{1}{k^2}\right) dk \\
& -\beta_1\beta \int_{-\infty}^{\infty} \exp\left\{-(k-k_0)^2\sigma_0^2 + i[k(-x+x_i+2x_0-2x_1)-\omega t]\right\} \left(\frac{1}{k^2}\right) dk. \tag{4.25}
\end{aligned}$$

Now let

$$\begin{aligned}
g_1(x) &= x+x_i, \quad g_2(x) = x+x_i+2x_0 \\
g_3(x) &= x+x_i+2x_1, \quad g_4(x) = x+x_i+2x_1-2x_0 \\
g_5(x) &= -x+x_i, \quad g_6(x) = -x+x_i-2x_0 \\
g_7(x) &= -x+x_i-2x_1, \quad g_8(x) = -x+x_i+2x_0-2x_1
\end{aligned} \tag{4.26}$$

$$\kappa_i(x, t) \equiv \frac{k_0\sigma_0^2}{\alpha} + i\frac{g_i(x)}{2\alpha}, \quad d_i(x, t) \equiv e^{\alpha\kappa_i^2 - k_0^2\sigma_0^2}, \quad \alpha \equiv \sigma_0^2 + \frac{i\hbar t}{2m} \tag{4.27}$$

Then

$$\begin{aligned}
\frac{\psi_{A_1}}{C_1} = & d_1(x, t) \int_{-\infty}^{\infty} e^{-\alpha(k-\kappa_1)^2} dk - i\left(\frac{\beta_1\beta}{\beta_0} - \beta\right) d_2(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_2)^2}}{k+i\beta_0} dk \\
& +i\left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right) d_3(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_3)^2}}{k+i\beta_0} dk + i(\beta+\beta_1) d_4(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_1)^2}}{k} dk
\end{aligned}$$

$$\begin{aligned}
& +i\left(\frac{\beta_1\beta}{\beta_0} - \beta\right)d_2(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_2)^2}}{k} dk - i\left(\beta_1 + \frac{\beta_1\beta}{\beta_0}\right)d_3(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_3)^2}}{k} dk \\
& -\beta_1\beta d_1(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_1)^2}}{k^2} dk + \beta_1\beta d_2(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_2)^2}}{k^2} dk \\
& -\beta_1\beta d_3(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_3)^2}}{k^2} dk + \beta_1\beta d_4(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_4)^2}}{k^2} dk \quad (4.28)
\end{aligned}$$

$$\begin{aligned}
\frac{\psi_{B_1}}{C_1} = & i\left(\frac{\beta_1\beta}{\beta_0}\right)d_8(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_8)^2}}{k+i\beta_0} dk - i\left(\beta_0 + \beta + \beta_1 + \frac{\beta_1\beta}{\beta_0}\right)d_5(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_5)^2}}{k+i\beta_0} dk \\
& +i\left(\beta + \beta_1 + \frac{\beta_1\beta}{\beta_0}\right)d_5(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_5)^2}}{k} dk - i\beta d_6(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_6)^2}}{k} dk \\
& -i\beta_1 d_7(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_7)^2}}{k} dk - i\left(\frac{\beta_1\beta}{\beta_0}\right)d_8(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_8)^2}}{k} dk \\
& +\beta_1\beta d_5(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_5)^2}}{k^2} dk - \beta_1\beta d_6(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_6)^2}}{k^2} dk \\
& +\beta_1\beta d_7(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_7)^2}}{k^2} dk - \beta_1\beta d_8(x, t) \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_8)^2}}{k^2} dk \quad (4.29)
\end{aligned}$$

In equation (4.28) and equation (4.29), the integrals $I_i = \int_{-\infty}^{\infty} \frac{e^{-\alpha(k-\kappa_i)^2}}{k+i\beta_0} dk$ are of the same form as I_A and I_B in the double scattering case, so the analysis of I_A and I_B is applicable to I_i . Then by writing

$$k = \kappa_i + u\alpha^{-1/2} \quad (4.30)$$

and employing contour integration,

$$I_i(x, t) = \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z'_i(x, t)} + [\theta(\text{Im } z'_i)\theta(-\beta_0) - \theta(-\text{Im } z'_i)\theta(\beta_0)]2\pi i e^{-[z'_i(x, t)]^2} \quad (4.31)$$

where

$$z'_i(x, t) \equiv \alpha^{1/2}(\kappa_i + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{ig_i(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2} \quad (4.32)$$

Therefore,

$$\begin{aligned}
\frac{\psi_{A_1}}{C_1} = & \frac{d_1 \pi^{1/2}}{\alpha^{1/2}} - i \left(\frac{\beta_1 \beta}{\beta_0} - \beta \right) d_2 \left\{ \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z'_2} + [\theta(\text{Im } z'_2) \theta(-\beta_0) - \theta(-\text{Im } z'_2) \theta(\beta_0)] 2\pi i e^{-z_2'^2} \right\} \\
& + i \left(\frac{\beta_1 \beta}{\beta_0} + \beta_1 \right) d_3 \left\{ \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z'_3} + [\theta(\text{Im } z'_3) \theta(-\beta_0) - \theta(-\text{Im } z'_3) \theta(\beta_0)] 2\pi i e^{-z_3'^2} \right\} \\
& + i(\beta + \beta_1) d_1 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_1} + i \left(\frac{\beta_1 \beta}{\beta_0} - \beta \right) d_2 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_2} - i \left(\frac{\beta_1 \beta}{\beta_0} + \beta_1 \right) d_3 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_3} \\
& + \beta_1 \beta \alpha^{1/2} \left[-d_1 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_1)^2} + d_2 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_2)^2} - d_3 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_3)^2} + d_4 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_4)^2} \right] \quad (4.33)
\end{aligned}$$

$$\begin{aligned}
\frac{\psi_{B_1}}{C_1} = & -i(\beta_0 + \beta + \beta_1 + \frac{\beta_1 \beta}{\beta_0}) d_5 \left[\int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z'_5} + \left\{ \theta(\text{Im } z'_5) \theta(-\beta_0) - \theta(-\text{Im } z'_5) \theta(\beta_0) \right\} 2\pi i e^{-z_5'^2} \right] \\
& + i \left(\frac{\beta_1 \beta}{\beta_0} \right) d_8 \left\{ \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z'_8} + [\theta(\text{Im } z'_8) \theta(-\beta_0) - \theta(-\text{Im } z'_8) \theta(\beta_0)] 2\pi i e^{-z_8'^2} \right\} \\
& + i(\beta + \beta_1 + \frac{\beta_1 \beta}{\beta_0}) d_5 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_5} - i\beta d_6 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_6} - i\beta_1 d_7 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_7} - i \left(\frac{\beta_1 \beta}{\beta_0} \right) d_8 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{u + z_8} \\
& + \beta_1 \beta \alpha^{1/2} \left[d_5 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_5)^2} - d_6 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_6)^2} + d_7 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_7)^2} - d_8 \int_{-\infty}^{\infty} \frac{e^{-u^2} du}{(u + z_8)^2} \right] \quad (4.34)
\end{aligned}$$

where

$$z_i(x, t) \equiv \alpha^{1/2} \kappa_i(x, t) = \frac{k_0 \sigma_0^2}{\alpha^{1/2}} + \frac{i g_i(x)}{2\alpha^{1/2}} \quad (4.35)$$

For the integrals that appear in equation (4.33) and equation (4.34), we resort to numerical integration again, which can be done using the computer program, `triplewpscatt.c`.

4.2 Table of Notifications

Table 4.1: Table of Notifications

	Definition	Equation
ω	$\frac{\hbar k^2}{2m}$	Eq. 2.13
ω_0	$\frac{\hbar k_0^2}{2m}$	Eq. 2.13
β	$\frac{mV}{\hbar^2}$	Eq. 4.9
β_0	$\frac{mV_0}{\hbar^2}$	Eq. 4.9
β_1	$\frac{mV_1}{\hbar^2}$	Eq. 4.9
$A_1(k)$	$1 + e^{2ikx_0} \beta \left(\frac{1-\beta_1/\beta_0}{k+i\beta_0} \right) i + e^{2kix_1} \beta_1 \left(\frac{1+\beta/\beta_0}{k+i\beta_0} \right) i + \left(\frac{i}{k} \right) h_A + \left(\frac{\beta_1\beta}{k^2} \right) f_A$	Eq. 4.6
$h_A(k)$	$\beta + \beta_1 + e^{2ikx_0} \left(\frac{\beta_1\beta}{\beta_0} - \beta \right) - e^{2ikx_1} \left(\beta_1 + \frac{\beta_1\beta}{\beta_0} \right)$	Eq. 4.7
$f_A(k)$	$-1 + e^{2ik(x_1-x_0)} + e^{2ikx_0} - e^{2ikx_1}$	Eq. 4.8
$B_1(k)$	$e^{2ik(x_0-x_1)} \left(\frac{\beta_1\beta}{\beta_0} \right) \left(\frac{1}{k+i\beta_0} \right) i - \frac{\beta_0+\beta+\beta_1+\beta_1\beta/\beta_0}{k+i\beta_0} i - \left(\frac{i}{k} \right) h_B + \left(\frac{\beta_1\beta}{k^2} \right) f_B$	Eq. 4.11
$h_B(k)$	$\beta_1 e^{-2ikx_1} + \frac{\beta_1\beta}{\beta_0} e^{2ik(x_0-x_1)} + \beta e^{-2ikx_0} - \beta - \beta_1 - \frac{\beta_1\beta}{\beta_0}$	Eq. 4.12
$f_B(k)$	$1 - e^{2ik(x_0-x_1)} - e^{-2ikx_0} + e^{-2ikx_1}$	Eq. 4.13
C_1	$\left(\frac{\sigma_0^2}{2\pi^3} \right)^{1/4}$	Eq. 4.15
$\alpha(t)$	$\sigma_0^2 + \frac{\hbar t}{2m}$	Eq. 4.27
$g_1(x)$	$x + x_i$	Eq. 4.26
$g_2(x)$	$x + x_i + 2x_0$	Eq. 4.26
$g_3(x)$	$x + x_i + 2x_1$	Eq. 4.26
$g_4(x)$	$x + x_i + 2x_1 - 2x_0$	Eq. 4.26
$g_5(x)$	$-x + x_i$	Eq. 4.26
$g_6(x)$	$-x + x_i - 2x_0$	Eq. 4.26
$g_7(x)$	$-x + x_i - 2x_1$	Eq. 4.26
$g_8(x)$	$-x + x_i + 2x_0 - 2x_1$	Eq. 4.26
$\kappa_i(x, t)$	$\frac{k_0\sigma_0^2}{\alpha} + i \frac{f_i(x)}{2\alpha}$	Eq. 4.27
$d_i(x, t)$	$e^{\alpha\kappa_i^2 - k_0^2\sigma_0^2}$	Eq. 4.27
k	$\kappa_i + u\alpha^{-1/2}$	Eq. 4.30
$z'_i(x, t)$	$\alpha^{1/2}(\kappa_i + i\beta_0) = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{ig_i(x)}{2\alpha^{1/2}} + i\beta_0\alpha^{1/2}$	Eq. 4.32
$z_i(x, t)$	$\alpha^{1/2}\kappa_i = \frac{k_0\sigma_0^2}{\alpha^{1/2}} + \frac{ig_i(x)}{2\alpha^{1/2}}$	Eq. 4.35

Chapter 5

Results and Analysis

In this chapter, we present and analyze the results that our computer programs give for single, double and triple scattering. First, we use some special cases to check that our results are correct. For example, in the single scattering case, we set the strength of the delta function to be very large, and compare the results that our computer program gives to the results that Mathematica gives when the strength is infinitely large; in the double and triple scattering cases, we set the strength of one delta function to be zero, or set the distance between two scattering centers to be zero, in order to reduce triple scattering to double or to reduce double scattering to single scattering for verification. Second, we make spacetime color graphs for the probability density functions to show the evolution of the wave packet, and we also try different combinations of the parameters to explore the maximum probability.

5.1 Verification

First of all, we want to verify that our computer programs give correct results. For the single scattering case, if we set the strength of the delta function to be much larger than $\hbar^2 k_0/m$, the graphs of the probability density function should look very close to those of infinitely large strength. When $V_0 = \infty$, the exact expressions of

$\psi_0(x, t)$ and $\psi_1(x, t)$ are

$$\psi_0(x, t) = \left(\frac{\sigma_0^2}{2\pi\alpha^2} \right)^{\frac{1}{4}} \exp \left\{ -\frac{(x + x_i)^2}{4\alpha} + \frac{i\sigma_0^2}{\alpha} [k_0(x + x_i) - \omega_0 t] \right\} \quad (5.1)$$

$$\psi_1(x, t) = - \left(\frac{\sigma_0^2}{2\pi\alpha^2} \right)^{\frac{1}{4}} \exp \left\{ -\frac{(|x| + x_i)^2}{4\alpha} + \frac{i\sigma_0^2}{\alpha} [k_0(|x| + x_i) - \omega_0 t] \right\} \quad (5.2)$$

and we can use Mathematica to plot the graphs of $|\psi_0(x, t) + \psi_1(x, t)|^2$. Then we compare the graphs made by Mathematica to the graphs made by our computer program, with $V_0 = 1$ or 10 or 100 or 1000 (10^{-19} J*nm). Let $x_i = 8$ nm, $\sigma_0 = \sqrt{2}$ nm, and $k_0 = 3$ nm $^{-1}$. The graphs made by our computer program are shown on the left of Figure 5-1, and the difference between the graphs made by our computer program and the graph made by Mathematica with a delta function potential of infinite strength are shown on the right.

As we can see from Figure 5-1, the maximum difference times V_0 is approximately constant, which is around 0.2. This confirms that the difference between the graphs is due to the finite value of V_0 , instead of any mistake in `wpscatt.c`. In fact, according to the right column of Figure 5-1, the difference between the graphs is caused by a phase difference between a wave packet traveling towards a scattering center with infinite strength and a wave packet traveling towards a scattering center with finite strength.

We now proceed to the verification of double scattering cases. We set the strength of the scattering center on the left to be zero, or the strength of the scattering center on the right to be zero, or the distance between the two scattering centers to be zero. Then we compare the numerical results given by `doublewpscatt.c` to the corresponding results given by `wpscatt.c`. The numerical results have six significant figures, and we verify that the results from `doublewpscatt.c` are identical to the results from `wpscatt.c`.

The verification process for triple scattering case is similar. Since we have already verified that `doubelwpscatt.c` gives correct results, we can use `doublewpscatt.c` to verify the validity of `triplewpscatt.c`. We set the strength of one of the three scattering centers to be zero, or the distance between the left and the middle scattering centers to be

zero, or the distance between the middle and the right scattering centers to be zero. Then we compare the numerical results given by `triplewpscatt.c` to the corresponding results given by `doublewpscatt.c`. Again, the numerical results have six significant figures, and we verify that the results from `triplewpscatt.c` are identical to the results from `doublewpscatt.c`.

5.2 Spacetime Color Graphs

We can now confidently proceed to make spacetime color graphs of the probability density function in order to visualize the evolution of the wave packet scattered by a single delta function potential. One such color graph is shown in Figure 5-2, with $x_i = 8$ nm, $\sigma_0 = \sqrt{2}$ nm, $k_0 = 3$ nm⁻¹, and $V_0 = 0.15 * 10^{-19}$ J*nm. Since $\hbar k_0/m$ is the speed at which the peak of the wave packet approaches the scattering center, $x_i m/\hbar k_0$ is the time for the peak to travel from its initial position to the scattering center. We define $T_s \equiv t - x_i m/\hbar k_0$, so $T_s = 0$ is the moment when the center of the wave packet encounters the scattering center, which is indicated by the white line. A negative T_s indicates that the center has not arrived at the scattering center yet, and a positive T_s indicates that the center is already scattered by the scattering center. The vertical white line indicates the position of the scattering center.

Figure 5-2 has some important implications. First, we see that the transmitted wave spreads out over time. The initial Gaussian wave packet is a superposition of plane waves e^{ikx} with different k , and since these plane waves travel at different speeds, the wave packet gradually spreads out. We compare this spreading wave packet with an electromagnetic wave, and the results are shown in Table 5.1. The two waves have the same form at $t = 0$. but they have different time derivatives. As a result, the quantum wave packet gradually spreads out, while the shape of the electromagnetic wave stays unchanged.

Second, the localization happens on the left side of the scattering center, so the shrinking is mainly due to the interference between the incoming wave and the reflected wave. The transmission coefficient T and the reflection coefficient R can be

Table 5.1: A Quantum Wave Packet and an Electromagnetic Wave Packet

	Quantum Wave	Electromagnetic Wave
$\psi(x, 0)$	Eq. 2.1 = Eq. 2.9	same
Evolution	$i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = 0$	$\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} = 0$
$\frac{\partial^2}{\partial x^2}$	$-k^2$	same
$\frac{\partial}{\partial t}$	$-i \frac{\hbar k^2}{2m}$	$\pm ikc$
Define	$\sigma^2 = \sigma_0^2 + \left(\frac{\hbar t}{2m\sigma_0}\right)^2$	$\sigma_C^2 = \sigma_0^2$
$ \psi(x, t) ^2$	Eq. 2.14	$\frac{1}{\sqrt{2\pi\sigma_C^2}} \exp\left\{\frac{-(x+x_i \pm ct)^2}{2\sigma_C^2}\right\}$

easily calculated according to Eq. 2.4 and Eq. 2.5:

$$T = \frac{1}{1 + \left(\frac{mV_0}{\hbar^2 k}\right)^2}, \quad R = \frac{\left(\frac{mV_0}{\hbar^2 k}\right)^2}{1 + \left(\frac{mV_0}{\hbar^2 k}\right)^2} = \frac{1}{1 + \left(\frac{\hbar^2 k}{mV_0}\right)^2} \quad (5.3)$$

Therefore, the larger V_0 is, the smaller T is and the larger R is, as expected. Third, it is clear from the graph that the probability density function is significantly localized when the center of the wave packet encounters the scattering center. In other words, the delta function potential is essential to the shrinking of the wave function.

Then we proceed to add another scattering center with the same strength at $x = -1$ nm, and set all the other parameters the same as in the single scattering case. We define $T_d \equiv t - (x_i - x_0)m/\hbar k_0$, so $T_d = 0$ is the moment when the center of the wave packet encounters the first scattering center on the left, which is indicated by the lower white line. The spacetime color graph of the probability density function is shown in Figure 5-3. The upper white line indicates $T_s = 0$ or $T_d = 2.88$ fs, when the wave packet encounters the right scattering center. The vertical white lines indicate the positions of the scattering centers. We can tell from the graph that the maximum peak, which appears to the left of the first scattering center, becomes higher in the double scattering case than in the single scattering case, since the color that indicates the maximum peak in the single scattering case is yellow, but the color that indicates the maximum peak in the double scattering case is red. We are curious to see what will happen if we add more scattering centers.

So we proceed to add one more scattering center with the same strength at $x = -2nm$, and set all the other parameters the same as in the double scattering case. We define $T_t \equiv t - (x_i - x_1)m/\hbar k_0$, so $T_t = 0$ is the moment when the center of the wave packet encounters the first scattering center on the left, which is indicated by the lower white line. The middle white line indicates $T_d = 0$ or $T_t = 2.88$ fs, when the wave packet encounters the middle scattering center. The upper white line indicates $T_s = 0$ or $T_t = 5.76$ fs, when the wave packet encounters the right scattering center. The vertical white lines indicate the positions of the scattering centers. We use the same strength for all scattering centers here, because our simple models of multiple delta functions potential is the first step towards studying real materials, and real materials usually have periodic potentials.

The spacetime color graph of the probability density function is shown in Figure 5-4. We can tell from the graph that the maximum peak, which appears to the left of the first scattering center, becomes even higher in the triple scattering case than in the double scattering case, since the color that indicates the maximum peak in the triple scattering case is almost white now. In fact, the numerical value of the maximum peak is 0.436873 in the single scattering case, 0.689630 in the double scattering case, and 0.966902 in the triple scattering case. And here comes a significant implication: we can increase the maximum peak by adding one more scattering center, and repeat this process for N times until the maximum peak is so high that the wave function *collapses* when approaching the first scattering center on the left. This is theoretically possible: if N is the number of scattering centers in real materials, N should be a very large number that is on the order of Avogadro's number.

It is also possible that the increase of the maximum peak is related to the separation between the scattering centers, and the separation between the scattering centers reminds us of Bragg's law. Bragg's law states that the incident and reflected waves interfere with each other most constructively when [2]

$$n\lambda = 2d \sin \theta \tag{5.4}$$

where n is an integer, λ is the wavelength of the incident wave, and d is the separation between two scattering centers. In our case, $\sin \theta = 1$, and λ should be the wavelength of the incident wave when it reaches the first scattering center, since the wave spreads out over time. At $t = 0$, $\lambda \approx 2\pi/k_0$, according to Eq. 2.1. The spreading factor is, according to Eq. 2.14,

$$\sqrt{\sigma^2}/\sigma_0 = \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2}. \quad (5.5)$$

For $\sigma_0^2 = 2 \text{ nm}^2$, $t = \frac{m(x_i - x_1)}{\hbar k_0}$, $x_i = 8 \text{ nm}$, $x_1 = 2 \text{ nm}$, and $k_0 = 3 \text{ nm}^{-1}$, the spreading factor has a value of 1.12. The initial wavelength $2\pi/k_0$ has a value of 2.09, and the wavelength becomes 2.34 when the wave packet encounters the first scattering center. For $n = 1$, the left side of Eq. 5.4 is equal to 2.34, very roughly close to the value of right side, 2.

To take one step further, we try different combinations of the parameters σ_0 and k_0 in single scattering, while we set $x_i = 8 \text{ nm}$ and $\beta_0 = 1.64 \text{ nm}^{-1}$ (or $V_0 = 0.2 * 10^{-19} \text{ J*nm}$), and study how the maximum probability density changes. We vary σ_0 and k_0 instead of x_i and β_0 because σ_0 and k_0 are the two parameters associated with the wave packet only. In order to make the variables dimensionless, we define $W = \sigma_0\beta_0$ and $M = k_0x_0$. A color graph of the maximum probability density with different combinations of W and M is shown in Figure 5-5. When W is too small, the maximum probability density occurs at $x = -x_i$ and $t = 0$. In fact, when $W = 0$, the wave packet is initially localized at $x = -x_i$ and collapses very quickly over time. As W increases, however, the maximum probability density begins to occur around the scattering center, but Figure 5-5 does not show us any significantly indicative pattern of the maximum probability density. This implies that, the maximum probability density depends more on the parameters of the scattering centers than on the initial width or the average energy of the wave packet.

As the last step of our analysis, we try different combinations of the parameters V and V_0 in double scattering, while we set $\sigma_0 = \sqrt{2} \text{ nm}$, $k_0 = 3 \text{ nm}^{-1}$, $x_i = 8 \text{ nm}$, and $x_0 = 1 \text{ nm}$. Again we define dimensionless variables $W_L = \sigma_0\beta$ and let $W_R = W = \sigma_0\beta_0$, where β is proportional to V and β_0 is proportional to V_0 . A

color graph of the maximum probability density with different combinations of W_L and W_R is shown in Figure 5-6. We find that the maximum probability density increases as the strength of the left scattering center increases. We also find that the maximum probability density depends much more on W_L than on W_R . It seems that the strength of the left scattering center, which the wave packet encounters first, is more important than the strength of the right scattering center, which the wave packet encounters later. One way to interpret this is that, after the incident wave packet encounters the first scattering center, the transmitted wave is weaker than the incident wave, and this weakened wave then encounters the second scattering center. The reflected wave from the second scattering center is even weaker, and it needs to travel through two scattering centers to interfere with the incident wave left to the first scattering center, so its influence is relatively small.

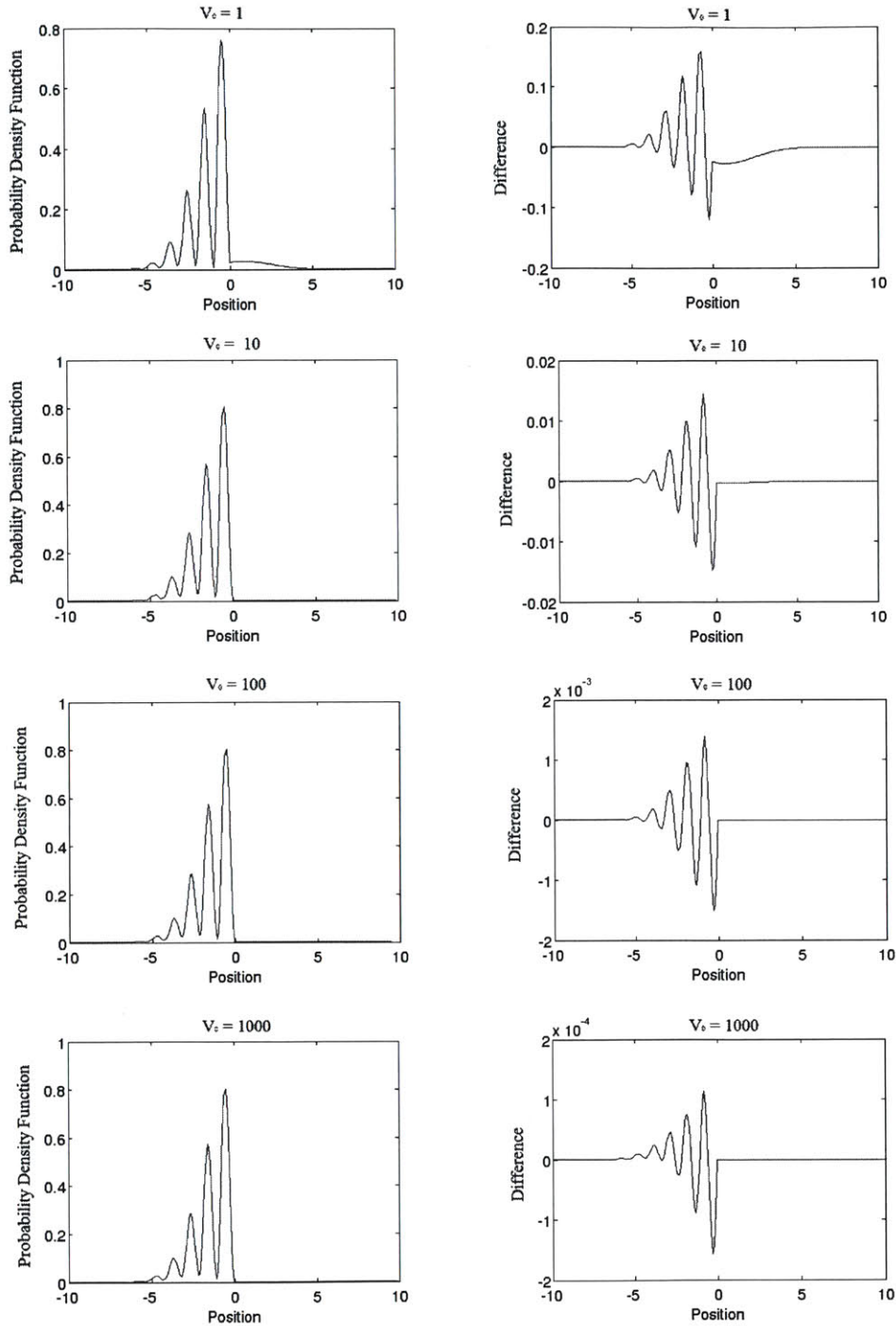


Figure 5-1: The graphs on the left are made by our computer program, *wpscatt.c*. The graphs on the right tell us the difference between the graphs made by our computer program and the graph made by Mathematica with a delta function potential of infinite strength. The parameters are set to be: $x_i = 8$ nm, $\sigma_0 = \sqrt{2}$ nm, $k_0 = 3$ nm⁻¹, and $t = 25$ fs.

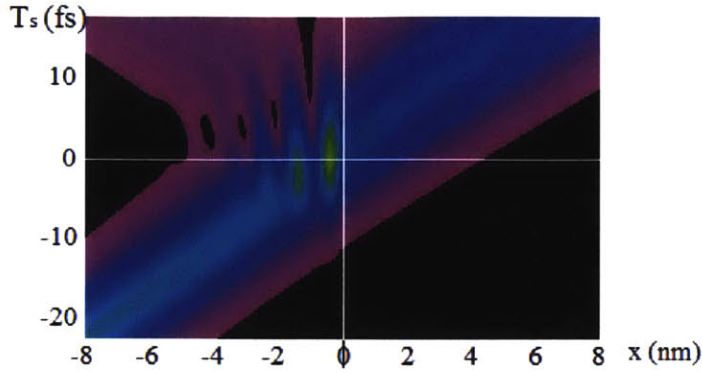


Figure 5-2: This is the spacetime color graph of $|\psi(x, t)|^2$ for single scattering; The parameters are set to be $x_i = 8$ nm, $\sigma_0 = \sqrt{2}$ nm, $k_0 = 3$ nm⁻¹, and $V_0 = 0.15 * 10^{-19}$ J*nm. White indicates 1.0, purple 0.001, and black any value below 0.001.

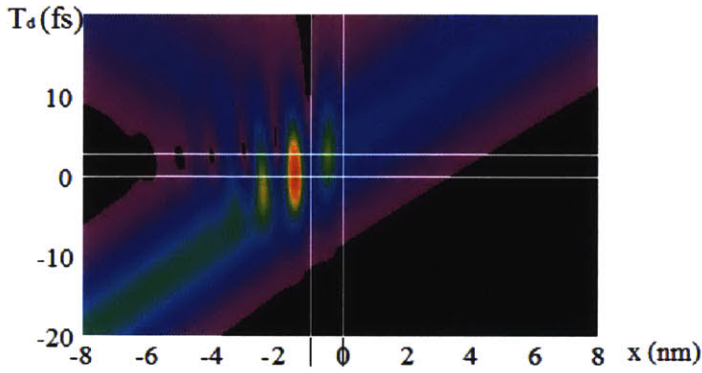


Figure 5-3: This is the spacetime color graph of $|\psi(x, t)|^2$ for double scattering; $x_0 = 1$ nm, $V_0 = 0.15 * 10^{-19}$ J*nm, and all the other parameters have the same values as in the single scattering graph . White indicates 1.0 and purple 0.001.

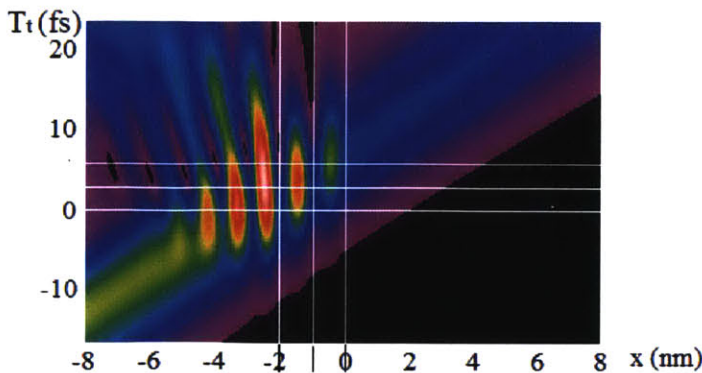


Figure 5-4: This is the spacetime color graph of $|\psi(x, t)|^2$ for triple scattering; $x_1 = 2$ nm, $V_1 = 0.15 * 10^{-19}$ J*nm, and all the other parameters have the same values as in the double scattering graph. White indicates 1.0 and purple 0.001.

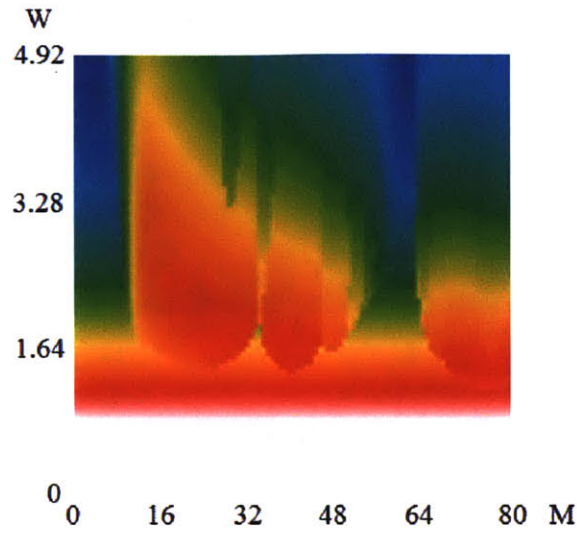


Figure 5-5: This is the color graph of the maximum probability density for different combinations of W and M in single scattering, where $W = \sigma_0\beta_0$ and $M = k_0x_0$. The other two parameters are set to be $x_i = 8$ nm, and $V_0 = 0.2 * 10^{-19}$ J*nm. White indicates 0.75 and purple 0.001. The vertical white lines indicate the position of the scattering centers.

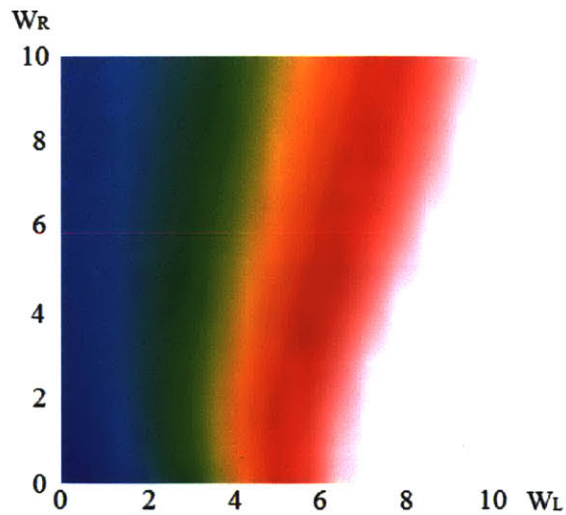


Figure 5-6: This is the color graph of the maximum probability density for different combinations of W_L and W_R in double scattering, where $W_L = \sigma_0\beta$ and $W_R = W = \sigma_0\beta_0$. The other parameters are set to be $\sigma_0 = \sqrt{2}$ nm, $k_0 = 3$ nm⁻¹, $x_i = 8$ nm, and $x_0 = 1$ nm. White indicates 3.0 and purple 0.001.

Chapter 6

Conclusion

We start this paper with an attempt to explain the phenomenon that all wave functions collapse upon quantum measurements, and we build a simple model of a Gaussian wave packet scattered by delta function potentials. After we see that a single scattering center does cause the wave function to shrink, we add more scattering centers to explore further. The results show that, as we add one more scattering center to the single scattering case, the wave function shrinks more with the same parameters, and if we add two more scattering centers to the single scattering case, the wave function shrinks even more. This observation leads us to speculate that if we add N scattering centers to the single scattering case, where N is a number on the order of Avogadro's number, the wave function may shrink so much that it eventually collapses.

Another factor that may contribute to the shrinking of the wave function in double or triple scattering cases is the separation between the scattering centers. If the Bragg's law is also valid here, we show that the parameters we pick very roughly satisfy the Bragg's law. We also make another comparison between the results from quantum mechanics and those from classical physics. We compare the evolution of a Gaussian wave packet in quantum mechanics with an electromagnetic wave packet. The two waves have the same form at $t = 0$. but they have different time derivatives, which leads to that the quantum wave packet gradually spreads out, while the shape of the electromagnetic wave stays unchanged.

Overall, we do see some shrinking of the wave function after a wave packet is scattered by single or multiple scattering centers, but it is still far from complete collapse or localization. Although we have not validated the hypothesis that scattering by a random potential causes localization of wave functions in quantum measurements, at least we show the possibility of future validation.

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- [2] Bekefi and Barrett, *Electromagnetic Vibrations, Waves, and Radiation* (The MIT Press, Cambridge, MA, 1977), page 558.


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/* Integrate psi1(x,t) for all x for single scattering solution */
#define PI 3.1415926535898
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <assert.h>
int wgif(char *image, int np1, int np0, char *filegif);
/* Parameters of the integral: real and imaginary parts of z. */
double zr,zi;
double rombint(double f(),double a,double b,double tol);

int main(void)
{
double psi1integral, dps11(), psi2integral, dps22(), tol=1.0e-8, ulim=8.;
double a0, k0, h, m, V0, x0, w0, b0, ar, ai, kr, ki, c1, theta1, Ar, Ai, r, theta2, sqrar, sqrai, a2;
double Rr, Ri, psi1r, psi1i, c2, c3r, c3i, c4, theta3, psi0r, psi0i, psir, psii, time;
double t, x, dt, dx, tmax, tmin, xmax, xmin, tmax0, tmin0, xmax0, xmin0;
double a0max, k0max, p, pmax, pmax0, tm, xm, dt0, dx0, datamax, datamin;
int i, it, ix, nt, nx, ia0, ik0, na0, nk0, iwhile;
char **image, *imageptr, **image1, *image1ptr, filename[11];
FILE *fp;

/* These 8 parameters control the size and scale of the images. */
na0 = 1;
nk0 = 1;
nt = 201;
nx = 321;
a0max = 1.414;
k0max = 3.0;
tmin0 = 0.0;
tmax0 = 40.0;
xmin0 = -8.0;
xmax0 = 8.0;
/* These parameters control the color stretch of the image. */
datamax = 1.0;
datamin = 0.001;

V0 = 0.15;
h = 1.055;
m = 9.109;
x0 = 8.0;
b0 = m*V0/(h*h);

/* Allocate image storage for maximum probability density. */
image1 = (char **)malloc(na0*sizeof(char *));
assert(image1);
image1[0] = (char *)malloc(na0*nk0*sizeof(char));
assert(image1[0]);
for(ia0=0; ia0<na0; ia0++) image1[ia0] = image1[0] +ia0*nk0;

```

```

image1ptr = image1[0];
/* Open output data file for maximum probability density. */
if ((fp = fopen("maxprob.txt","w")) == NULL) {
    printf("Error opening file maxprob.txt\n");
    exit(1);
}

/* Loop over a0, k0. */
for (ia0=0; ia0<na0; ia0++) {
    a0 = (na0-ia0)*a0max/na0;
    for (ik0=0; ik0<nk0; ik0++) {
        k0 = (ik0+1)*k0max/nk0;
        image = (char **)malloc(nt*sizeof(char *));
        assert(image);
        image[0] = (char *)malloc(nt*nx*sizeof(char));
        assert(image[0]);
        for(it=0; it<nt; it++) image[it] = image[0] +it*nx;
        imageptr = image[0];
        w0 = h*k0*k0/(2.0*m);
        dt0=(tmax0-tmin0)/(nt-1);
        dx0=(xmax0-xmin0)/(nx-1);
        pmax=1.0e-20;
        pmax0=0.0;
        tm = 0.0;
        xm = 0.0;
/* Initialize search range for the maximum probability density. */
        tmin=tmin0;
        tmax=tmax0;
        dt=dt0;
        xmin=xmin0;
        xmax=xmax0;
        dx=dx0;
/* Refine calculation of the maximum probability density.
For each (a0,k0), vary (t,x) to find the maximum probability density.
pmax0 is the maximum probability density from the previous iteration,
pmax is the maximum probability density in the current iteration.
Stop when the change is less than 0.01%. */
        iwhile = 0;
        while (pmax > 1.0001*pmax0) {
            pmax0 = pmax;
            iwhile++;
/* Outer loop over t */
            for (it=0; it<nt; it++) {
                t = tmin+(nt-it-1)*dt;
/* Calculate a = ar+i*ai */
                ar = a0*a0;
                ai = h*t/(2.0*m);
/* Inner loop over x */
                for (ix=0; ix<nx; ix++) {

```

```

    x = xmin+ix*dx;
/* Calculate k = kr+i*ki, Ar, Ai, zr, zi, psi1integral, psi2integral */
kr = (k0*a0*a0*ar+(fabs(x)+x0)*0.5*ai)/(ar*ar+ai*ai);
ki = (-k0*a0*a0*ai+(fabs(x)+x0)*0.5*ar)/(ar*ar+ai*ai);
c1 = b0*sqrt(sqrt(a0*a0/(2.0*PI*PI*PI)))*exp(-k0*k0*a0*a0+ar*(kr*kr-ki*ki)-2.0*ai*kr*ki);
theta1 = 2.0*kr*ki*ar+ai*(kr*kr-ki*ki);
Ar = c1*sin(theta1);
Ai = -c1*cos(theta1);
r = sqrt(ar*ar+ai*ai);
theta2 = atan2(ai,ar);
sqrar = sqrt(r)*cos(theta2/2.0);
sqrai = sqrt(r)*sin(theta2/2.0);
zr = sqrar*kr-sqrai*(ki+b0);
zi = sqrai*kr+sqrar*(ki+b0);
psi1integral = rombint(dpsi1,-ulim,ulim,tol);
psi2integral = rombint(dpsi2,-ulim,ulim,tol);
/* Calculate Rr, Ri */
if (zi*b0<0.0) {
    Rr = fabs(zi)/zi*2.0*PI*exp(zi*zi-zr*zr)*sin(2.0*zr*zi);
    Ri = fabs(zi)/zi*2.0*PI*exp(zi*zi-zr*zr)*cos(2.0*zr*zi);
}
else {
    Rr = 0.0;
    Ri = 0.0;
}
/* Calculate wavefunction psi=A*psi1+psi0=psir+ipsii */
psi1r = psi2integral+zr*psi1integral+Rr;
psi1i = -zi*psi1integral+Ri;
c2 = sqrt(sqrt(a0*a0/(2.0*PI)));
c3r = sqrar/(sqrar*sqrar+sqrai*sqrai);
c3i = -sqrai/(sqrar*sqrar+sqrai*sqrai);
c4 = exp((-0.25*(x+x0)*(x+x0)*ar+a0*a0*ai*(k0*(x+x0)-w0*t))/(r*r));
theta3 = (0.25*(x+x0)*(x+x0)*ai+a0*a0*ar*(k0*(x+x0)-w0*t))/(r*r);
psi0r = c2*c4*(c3r*cos(theta3)-c3i*sin(theta3));
psi0i = c2*c4*(c3r*sin(theta3)+c3i*cos(theta3));
psir = Ar*psi1r-Ai*psi1i+psi0r;
psii = Ar*psi1i+Ai*psi1r+psi0i;
a2 = a0*a0+ai*ai/a0/a0;
time = (h*k0*t/m-x0)/sqrt(a2);
/* Find maximum probability density */
p = (psir*psir+psii*psii);
if (p > pmax) {
/* Record the new maximum. */
    pmax = p;
    tm = t;
    xm = x;
}
if (iwhile == 1) {
/* Produce spacetime image. */

```

```

        if ((i=255*p/datamax) < 255)
            image[it][ix] = i;
        else
            image[it][ix] = 255;
    }
/* End loop on x */
}
/* End loop on t */
}
/* Narrow the search for the maximum. */
    tmin = (tmin=tm-2*dt) > tmin0 ? tmin:tmin0;
    tmax = (tmax=tm+2*dt) < tmax0 ? tmax:tmax0;
    dt = (tmax-tmin)/(nt-1);
    xmin = (xmin=xm-2*dx) > xmin0 ? xmin:xmin0;
    xmax = (xmax=xm+2*dx) < xmax0 ? xmax:xmax0;
    dx = (xmax-xmin)/(nx-1);
/* End while loop (used to find maximum probability density). */
}
printf("%g %g %d %g %g %g\n",a0,k0,iwhile,tm,xm,pmax);
fprintf(fp,"%g %g %g %g %g\n",a0,k0,tm,xm,pmax);
/* Produce spacetime image. */
    sprintf(filename,"%dp%d_%d%d.gif",(int)(a0),(int)(10*(a0-(int)a0)),(int)(k0/10),(int)(k0-
10*(int)(k0/10)));
    wgif(imageptr,nx,nt,filename);
/* Produce maximum probability density image. */
    if ((i=255*pmax/datamax)<255)
        image1[ia0][ik0] = i;
    else
        image1[ia0][ik0] = 255;
/* End loop on k0 */
}
/* End loop on a0 */
}
fclose(fp);
/* Produce maximum probability density image. */
wgif(image1ptr,nk0,na0,"maxprob.gif");
free(image);
free(image1);
return 0;
}

double dps1(double u)
{
    return(exp(-u*u)/((u+zr)*(u+zr)+zi*zi));
}
double dps2(double u)
{
    return(u*exp(-u*u)/((u+zr)*(u+zr)+zi*zi));
}

```

```

/* Integrate psi(x,t) left to the first scattering center for double scattering solution. */
#define PI 3.1415926535898
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <assert.h>
int wgif(char *image, int np1, int np0, char *filegif);
/* Parameters of the integral: real and imaginary parts of z1, zA, z2, z3, z4, zB. */
double zr1, zi1, zrA, ziA, zr2, zi2, zr3, zi3, zr4, zi4, zrB, ziB;
double rombint(double f(),double a,double b,double tol);

int main(void)
{
    double
dpsi1(),dpsi2(),dpsi3(),dpsi4(),dpsi5(),dpsi6(),dpsi7(),dpsi8(),dpsi9(),dpsi10(),dpsi11(),dpsi12()
,IUE1,IUEA,IUE2,IUE3,IUE4,IUEB,IE1,IEA,IE2,IE3,IE4,IEB,RrA,RiA,RrB,RiB,Ir1,IrA,Ir2,Ir3,Ir4,
IrB,Ii1,IiA,Ii2,Ii3,Ii4,IiB, tol=1.0e-8, ulim=8.;
    double a0, k0, hbar, m, V, V0, x0, w0, xi, b, b0, ar, ai, r, theta, sqrar, sqrai;
    double psiAr, psiAi, psiBr, psiBi, psir, psii;
    double t, x, dt, dx, tmax, tmin, xmax, xmin, tmax0, tmin0, xmax0, xmin0;
    double a0max, k0max, p, pmax, pmax0, tm, xm, dt0, dx0, datamax, datamin;
    double kr1, ki1, kr2, ki2, kr3, ki3, kr4, ki4, theta1, theta2, theta3, theta4, dr1, di1, dr2, di2,
dr3, di3, dr4, di4;
    int i, it, ix, nt, nx, ia0, ik0, na0, nk0, iwhile;
    char **image, *imageptr, **image1, *image1ptr, filename[11];
    FILE *fp;

/* These 8 parameters control the size and scale of the images. */
    na0 = 1;
    nk0 = 1;
    nt = 201;
    nx = 141;
    a0max = 1.414;
    k0max = 3.0;
    tmin0 = 0.0;
    tmax0 = 40.0;
    xmin0 = -8.0;
    xmax0 = -1.0;
/* These parameters control the color stretch of the image. */
    datamax = 1.0;
    datamin = 0.001;

    hbar = 1.055;
    m = 9.109;
    V = 0.15;
    V0 = 0.15;
    x0 = 1.0;
    xi = 8.0;
    b = m*V/(hbar*hbar);

```

```
b0 = m*V0/(hbar*hbar);
```

```
/* Allocate image storage for maximum probability density. */
```

```
image1 = (char **)malloc(na0*sizeof(char *));
```

```
assert(image1);
```

```
image1[0] = (char *)malloc(na0*nk0*sizeof(char));
```

```
assert(image1[0]);
```

```
for(ia0=0; ia0<na0; ia0++) image1[ia0] = image1[0] +ia0*nk0;
```

```
image1ptr = image1[0];
```

```
/* Open output data file for maximum probability density. */
```

```
if ((fp = fopen("maxprob.txt","w")) == NULL) {
```

```
    printf("Error opening file maxprob.txt\n");
```

```
    exit(1);
```

```
}
```

```
/* Loop over a0, k0. */
```

```
for (ia0=0; ia0<na0; ia0++) {
```

```
    a0 = (na0-ia0)*a0max/na0;
```

```
    for (ik0=0; ik0<nk0; ik0++) {
```

```
        k0 = (ik0+1)*k0max/nk0;
```

```
        image = (char **)malloc(nt*sizeof(char *));
```

```
        assert(image);
```

```
        image[0] = (char *)malloc(nt*nx*sizeof(char));
```

```
        assert(image[0]);
```

```
        for(it=0; it<nt; it++) image[it] = image[0] +it*nx;
```

```
        imageptr = image[0];
```

```
        w0 = hbar*k0*k0/(2.0*m);
```

```
        dt0=(tmax0-tmin0)/(nt-1);
```

```
        dx0=(xmax0-xmin0)/(nx-1);
```

```
        pmax=1.0e-20;
```

```
        pmax0=0.0;
```

```
        tm = 0.0;
```

```
        xm = 0.0;
```

```
/* Initialize search range for the maximum probability density. */
```

```
    tmin=tmin0;
```

```
    tmax=tmax0;
```

```
    dt=dt0;
```

```
    xmin=xmin0;
```

```
    xmax=xmax0;
```

```
    dx=dx0;
```

```
/* Refine calculation of the maximum probability density.
```

```
For each (a0,k0), vary (t,x) to find the maximum probability density.
```

```
pmax0 is the maximum probability density from the previous iteration,
```

```
pmax is the maximum probability density in the current iteration.
```

```
Stop when the change is less than 0.01%. */
```

```
    iwhile = 0;
```

```
    while (pmax > 1.0001*pmax0) {
```

```
        pmax0 = pmax;
```

```
        iwhile++;
```

```

/* Outer loop over t */
  for (it=0; it<nt; it++) {
    t = tmin+(nt-it-1)*dt;
/* Calculate a = ar+i*ai */
    ar = a0*a0;
    ai = hbar*t/(2.0*m);
/* Inner loop over x */
    for (ix=0; ix<nx; ix++) {
/* Calculate k, d, z, psiintegral */
      r = sqrt(ar*ar+ai*ai);
      theta = atan2(ai,ar);
      sqrar = sqrt(r)*cos(theta/2.0);
      sqrai = sqrt(r)*sin(theta/2.0);
      kr1 = (k0*a0*a0*ar+0.5*(x+xi+2.0*x0)*ai)/(r*r);
      ki1 = (-k0*a0*a0*ai+0.5*(x+xi+2.0*x0)*ar)/(r*r);
      kr2 = (k0*a0*a0*ar+0.5*(x+xi)*ai)/(r*r);
      ki2 = (-k0*a0*a0*ai+0.5*(x+xi)*ar)/(r*r);
      kr3 = (k0*a0*a0*ar+0.5*(-x+xi-2.0*x0)*ai)/(r*r);
      ki3 = (-k0*a0*a0*ai+0.5*(-x+xi-2.0*x0)*ar)/(r*r);
      kr4 = (k0*a0*a0*ar+0.5*(-x+xi)*ai)/(r*r);
      ki4 = (-k0*a0*a0*ai+0.5*(-x+xi)*ar)/(r*r);
      theta1 = ai*(kr1*kr1-ki1*ki1)+2.0*ar*kr1*ki1;
      theta2 = ai*(kr2*kr2-ki2*ki2)+2.0*ar*kr2*ki2;
      theta3 = ai*(kr3*kr3-ki3*ki3)+2.0*ar*kr3*ki3;
      theta4 = ai*(kr4*kr4-ki4*ki4)+2.0*ar*kr4*ki4;
      dr1 = exp(ar*(kr1*kr1-ki1*ki1)-2.0*ai*kr1*ki1-k0*k0*a0*a0)*cos(theta1);
      di1 = exp(ar*(kr1*kr1-ki1*ki1)-2.0*ai*kr1*ki1-k0*k0*a0*a0)*sin(theta1);
      dr2 = exp(ar*(kr2*kr2-ki2*ki2)-2.0*ai*kr2*ki2-k0*k0*a0*a0)*cos(theta2);
      di2 = exp(ar*(kr2*kr2-ki2*ki2)-2.0*ai*kr2*ki2-k0*k0*a0*a0)*sin(theta2);
      dr3 = exp(ar*(kr3*kr3-ki3*ki3)-2.0*ai*kr3*ki3-k0*k0*a0*a0)*cos(theta3);
      di3 = exp(ar*(kr3*kr3-ki3*ki3)-2.0*ai*kr3*ki3-k0*k0*a0*a0)*sin(theta3);
      dr4 = exp(ar*(kr4*kr4-ki4*ki4)-2.0*ai*kr4*ki4-k0*k0*a0*a0)*cos(theta4);
      di4 = exp(ar*(kr4*kr4-ki4*ki4)-2.0*ai*kr4*ki4-k0*k0*a0*a0)*sin(theta4);
      zr1 = sqrar*kr1-sqrai*ki1;
      zi1 = sqrar*ki1+sqrai*kr1;
      zrA = sqrar*kr1-sqrai*(ki1+b0);
      ziA = sqrar*(ki1+b0)+sqrai*kr1;
      zr2 = sqrar*kr2-sqrai*ki2;
      zi2 = sqrar*ki2+sqrai*kr2;
      zr3 = sqrar*kr3-sqrai*ki3;
      zi3 = sqrar*ki3+sqrai*kr3;
      zr4 = sqrar*kr4-sqrai*ki4;
      zi4 = sqrar*ki4+sqrai*kr4;
      zrB = sqrar*kr4-sqrai*(ki4+b0);
      ziB = sqrar*(ki4+b0)+sqrai*kr4;
      IUE1 = rombint(dpsi1,-ulim,ulim,tol);
      IUEA = rombint(dpsi2,-ulim,ulim,tol);
      IUE2 = rombint(dpsi3,-ulim,ulim,tol);

```

```

IUE3 = rombint(dpsi4,-ulim,ulim,tol);
IUE4 = rombint(dpsi5,-ulim,ulim,tol);
IUEB = rombint(dpsi6,-ulim,ulim,tol);
IE1 = rombint(dpsi7,-ulim,ulim,tol);
IEA = rombint(dpsi8,-ulim,ulim,tol);
IE2 = rombint(dpsi9,-ulim,ulim,tol);
IE3 = rombint(dpsi10,-ulim,ulim,tol);
IE4 = rombint(dpsi11,-ulim,ulim,tol);
IEB = rombint(dpsi12,-ulim,ulim,tol);
Ir1 = IUE1+zr1*IE1;
IrA = IUEA+zrA*IEA;
Ir2 = IUE2+zr2*IE2;
Ir3 = IUE3+zr3*IE3;
Ir4 = IUE4+zr4*IE4;
IrB = IUEB+zrB*IEB;
li1 = -zi1*IE1;
liA = -ziA*IEA;
li2 = -zi2*IE2;
li3 = -zi3*IE3;
li4 = -zi4*IE4;
liB = -ziB*IEB;
/* Calculate RrA, RiA */
if (ziA*b0<0.0) {
    RrA = -fabs(b0)/b0*2.0*PI*exp(ziA*ziA-zrA*zrA)*sin(2.0*zrA*ziA);
    RiA = -fabs(b0)/b0*2.0*PI*exp(ziA*ziA-zrA*zrA)*cos(2.0*zrA*ziA);
}
else {
    RrA = 0.0;
    RiA = 0.0;
}
/* Calculate RrB, RiB */
if (ziB*b0<0.0) {
    RrB = -fabs(b0)/b0*2.0*PI*exp(ziB*ziB-zrB*zrB)*sin(2.0*zrB*ziB);
    RiB = -fabs(b0)/b0*2.0*PI*exp(ziB*ziB-zrB*zrB)*cos(2.0*zrB*ziB);
}
else {
    RrB = 0.0;
    RiB = 0.0;
}
/* Calculate wavefunction psi */
psiAr = -b*(di1*(IrA+RrA)+dr1*(liA+RiA))+sqrt(PI)*(dr2*sqrar/r+di2*sqrar/r)
+b*(di1*Ir1+dr1*li1)-b*(di2*Ir2+dr2*li2);
psiAi = b*(dr1*(IrA+RrA)-di1*(liA+RiA))+sqrt(PI)*(di2*sqrar/r-dr2*sqrar/r)-b*(dr1*Ir1-
di1*li1)+b*(dr2*Ir2-di2*li2);
psiBr = (b+b0)*(di4*(IrB+RrB)+dr4*(liB+RiB))+b*(di3*Ir3+dr3*li3)-b*(di4*Ir4+dr4*li4);
psiBi = -(b+b0)*(dr4*(IrB+RrB)-di4*(liB+RiB))-b*(dr3*Ir3-di3*li3)+b*(dr4*Ir4-di4*li4);
psir = sqrt(sqrt(a0*a0/2.0/PI/PI/PI))*(psiAr+psiBr);
psii = sqrt(sqrt(a0*a0/2.0/PI/PI/PI))*(psiAi+psiBi);
/* Find maximum probability density */

```

```

        p = (psir*psir+psii*psii);
        if (p > pmax) {
/* Record the new maximum. */
            pmax = p;
            tm = t;
            xm = x;
        }
        if (iwhile == 1) {
/* Produce spacetime image. */
            if ((i=255*p/datamax) < 255)
                image[it][ix] = i;
            else
                image[it][ix] = 255;
        }
/* End loop on x */
    }
/* End loop on t */
}
/* Narrow the search for the maximum. */
    tmin = (tmin=tm-2*dt) > tmin0 ? tmin:tmin0;
    tmax = (tmax=tm+2*dt) < tmax0 ? tmax:tmax0;
    dt = (tmax-tmin)/(nt-1);
    xmin = (xmin=xm-2*dx) > xmin0 ? xmin:xmin0;
    xmax = (xmax=xm+2*dx) < xmax0 ? xmax:xmax0;
    dx = (xmax-xmin)/(nx-1);
/* End while loop (used to find maximum probability density). */
}
printf("%g %g %d %g %g %g\n",a0,k0,iwhile,tm,xm,pmax);
fprintf(fp,"%g %g %g %g %g\n",a0,k0,tm,xm,pmax);
/* Produce spacetime image. */
    sprintf(filename,"%dp%d_%d%d.gif",(int)(a0),(int)(10*(a0-(int)a0)),(int)(k0/10),(int)(k0-
10*(int)(k0/10)));
    wgif(imageptr,nx,nt,filename);
/* Produce maximum probability density image. */
    if ((i=255*pmax/datamax)<255)
        image1[ia0][ik0] = i;
    else
        image1[ia0][ik0] = 255;
/* End loop on k0 */
}
/* End loop on a0 */
}
fclose(fp);
/* Produce maximum probability density image. */
wgif(image1ptr,nk0,na0,"maxprob.gif");
free(image);
free(image1);
return 0;
}

```

```

double dpsi1(double u)
{
    return(u*exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1));
}
double dpsi2(double u)
{
    return(u*exp(-u*u)/((u+zrA)*(u+zrA)+ziA*ziA));
}
double dpsi3(double u)
{
    return(u*exp(-u*u)/((u+zr2)*(u+zr2)+zi2*zi2));
}
double dpsi4(double u)
{
    return(u*exp(-u*u)/((u+zr3)*(u+zr3)+zi3*zi3));
}
double dpsi5(double u)
{
    return(u*exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dpsi6(double u)
{
    return(u*exp(-u*u)/((u+zrB)*(u+zrB)+ziB*ziB));
}
double dpsi7(double u)
{
    return(exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1));
}
double dpsi8(double u)
{
    return(exp(-u*u)/((u+zrA)*(u+zrA)+ziA*ziA));
}
double dpsi9(double u)
{
    return(exp(-u*u)/((u+zr2)*(u+zr2)+zi2*zi2));
}
double dpsi10(double u)
{
    return(exp(-u*u)/((u+zr3)*(u+zr3)+zi3*zi3));
}
double dpsi11(double u)
{
    return(exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dpsi12(double u)
{
    return(exp(-u*u)/((u+zrB)*(u+zrB)+ziB*ziB));
}

```

```

/* Integrate psi(x,t) left to the scattering center at x=-x1 for triple scattering solution. */
#define PI 3.1415926535898
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <assert.h>
int wgif(char *image, int np1, int np0, char *filegif);
/* Parameters of the integral: real and imaginary parts of z1, z21, z22, z31, z32, z4, z51, z52,
z6, z7, z81, z82. */
double zr1, zr21, zr22, zr31, zr32, zr4, zr51, zr52, zr6, zr7, zr81, zr82;
double zi1, zi21, zi22, zi31, zi32, zi4, zi51, zi52, zi6, zi7, zi81, zi82;
double rombint(double f(),double a,double b,double tol);

int main(void)
{
    double dps1(), dps2(), dps3(), dps4(), dps5(), dps6(), dps7(), dps8(), dps9(), dps10(),
    dps11(), dps12(), dps13(), dps14(), dps15(), dps16(), dps17(), dps18(), dps19(), dps20(),
    dps21(), dps22(), dps23(), dps24(), dps25(), dps26(), dps27(), dps28(), dps29(), dps30(),
    dps31(), dps32(), dps33(), dps34(), dps35(), dps36(), dps37(), dps38(), dps39(), dps40(),
    dps41(), dps42(), dps43(), dps44(), dps45(), dps46(), dps47(), dps48(), IUE1, IUE21,
    IUE22, IUE31, IUE32, IUE4, IUE51, IUE52, IUE6, IUE7, IUE81, IUE82, IE1, IE21, IE22, IE31,
    IE32, IE4, IE51, IE52, IE6, IE7, IE81, IE82, IIUUE1, IIUUE21, IIUUE31, IIUUE4, IIUUE51,
    IIUUE6, IIUUE7, IIUUE81, IIUE1, IIUE21, IIUE31, IIUE4, IIUE51, IIUE6, IIUE7, IIUE81, IIE1,
    IIE21, IIE31, IIE4, IIE51, IIE6, IIE7, IIE81, tol=1.0e-8, ulim=8.;
    double lr1,lr21,lr22,lr31,lr32,lr4,lr51,lr52,lr6,lr7,lr81,lr82;
    double li1,li21,li22,li31,li32,li4,li51,li52,li6,li7,li81,li82;
    double llr1,llr21,llr31,llr4,llr51,llr6,llr7,llr81;
    double lli1,lli21,lli31,lli4,lli51,lli6,lli7,lli81;
    double Rr22,Rr32,Rr52,Rr82,Ri22,Ri32,Ri52,Ri82;
    double a0, k0, hbar, m, V, V0, V1, x0, x1, xi, w0, b, b0, b1, ar, ai, r, theta, sqrar, sqrai;
    double psiA1r, psiA1i, psiA2r, psiA2i, psir, psii;
    double t, x, dt, dx, tmax, tmin, xmax, xmin, tmax0, tmin0, xmax0, xmin0;
    double kr1, ki1, kr2, ki2, kr3, ki3, kr4, ki4, kr5, ki5, kr6, ki6, kr7, ki7, kr8, ki8, theta1, theta2,
    theta3, theta4, theta5, theta6, theta7, theta8, dr1, di1, dr2, di2, dr3, di3, dr4, di4, dr5, di5, dr6,
    di6, dr7, di7, dr8, di8;
    double DI1r,DI1i,DI2r,DI2i;
    double a0max, k0max, p, pmax, pmax0, tm, xm, dt0, dx0, datamax, datamin;
    int i, it, ix, nt, nx, ia0, ik0, na0, nk0, iwhile;
    char **image, *imageptr, **image1, *image1ptr, filename[11];
    FILE *fp;
/* These 8 parameters control the size and scale of the images. */
    na0 = 1;
    nk0 = 1;
    nt = 201;
    nx = 121;
    a0max = 1.414;
    k0max = 3.0;
    tmin0 = 0.0;
    tmax0 = 40.0;

```

```

xmin0 = -8.0;
xmax0 = -2.0;
/* These parameters control the color stretch of the image. */
datamax = 1.0;
datamin = 0.001;

hbar = 1.055;
m = 9.109;
V = 0.15;
V0 = 0.15;
V1 = 0.15;
x0 = 1.0;
x1 = 2.0;
xi = 8.0;
b = m*V/(hbar*hbar);
b0 = m*V0/(hbar*hbar);
b1 = m*V1/(hbar*hbar);

/* Allocate image storage for maximum probability density. */
image1 = (char **)malloc(na0*sizeof(char *));
assert(image1);
image1[0] = (char *)malloc(na0*nk0*sizeof(char));
assert(image1[0]);
for(ia0=0; ia0<na0; ia0++) image1[ia0] = image1[0] +ia0*nk0;
image1ptr = image1[0];
/* Open output data file for maximum probability density. */
if ((fp = fopen("maxprob.txt","w")) == NULL) {
    printf("Error opening file maxprob.txt\n");
    exit(1);
}

/* Loop over a0, k0. */
for (ia0=0; ia0<na0; ia0++) {
    a0 = (na0-ia0)*a0max/na0;
    for (ik0=0; ik0<nk0; ik0++) {
        k0 = (ik0+1)*k0max/nk0;
        image = (char **)malloc(nt*sizeof(char *));
        assert(image);
        image[0] = (char *)malloc(nt*nx*sizeof(char));
        assert(image[0]);
        for(it=0; it<nt; it++) image[it] = image[0] +it*nx;
        imageptr = image[0];
        w0 = hbar*k0*k0/(2.0*m);
        dt0=(tmax0-tmin0)/(nt-1);
        dx0=(xmax0-xmin0)/(nx-1);
        pmax=1.0e-20;
        pmax0=0.0;
        tm = 0.0;
        xm = 0.0;
    }
}

```

```

/* Initialize search range for the maximum probability density. */
tmin=tmin0;
tmax=tmax0;
dt=dt0;
xmin=xmin0;
xmax=xmax0;
dx=dx0;
/* Refine calculation of the maximum probability density.
For each (a0,k0), vary (t,x) to find the maximum probability density.
pmax0 is the maximum probability density from the previous iteration,
pmax is the maximum probability density in the current iteration.
Stop when the change is less than 0.01%. */
iwhile = 0;
while (pmax > 1.0001*pmax0) {
    pmax0 = pmax;
    iwhile++;
/* Outer loop over t */
    for (it=0; it<nt; it++) {
        t = tmin+(nt-it-1)*dt;
/* Calculate a = ar+ai */
        ar = a0*a0;
        ai = hbar*t/(2.0*m);
/* Inner loop over x */
        for (ix=0; ix<nx; ix++) {
            x = xmin+ix*dx;

/* Calculate k, d, z, psiintegral */
            r = sqrt(ar*ar+ai*ai);
            theta = atan2(ai,ar);
            squar = sqrt(r)*cos(theta/2.0);
            sqrai = sqrt(r)*sin(theta/2.0);
            kr1 = (k0*a0*a0*ar+0.5*(x+xi)*ai)/(r*r);
            ki1 = (-k0*a0*a0*ai+0.5*(x+xi)*ar)/(r*r);
            kr2 = (k0*a0*a0*ar+0.5*(x+xi+2.0*x0)*ai)/(r*r);
            ki2 = (-k0*a0*a0*ai+0.5*(x+xi+2.0*x0)*ar)/(r*r);
            kr3 = (k0*a0*a0*ar+0.5*(x+xi+2.0*x1)*ai)/(r*r);
            ki3 = (-k0*a0*a0*ai+0.5*(x+xi+2.0*x1)*ar)/(r*r);
            kr4 = (k0*a0*a0*ar+0.5*(x+xi+2.0*x1-2.0*x0)*ai)/(r*r);
            ki4 = (-k0*a0*a0*ai+0.5*(x+xi+2.0*x1-2.0*x0)*ar)/(r*r);
            kr5 = (k0*a0*a0*ar+0.5*(-x+xi)*ai)/(r*r);
            ki5 = (-k0*a0*a0*ai+0.5*(-x+xi)*ar)/(r*r);
            kr6 = (k0*a0*a0*ar+0.5*(-x+xi-2.0*x0)*ai)/(r*r);
            ki6 = (-k0*a0*a0*ai+0.5*(-x+xi-2.0*x0)*ar)/(r*r);
            kr7 = (k0*a0*a0*ar+0.5*(-x+xi-2.0*x1)*ai)/(r*r);
            ki7 = (-k0*a0*a0*ai+0.5*(-x+xi-2.0*x1)*ar)/(r*r);
            kr8 = (k0*a0*a0*ar+0.5*(-x+xi+2.0*x0-2.0*x1)*ai)/(r*r);
            ki8 = (-k0*a0*a0*ai+0.5*(-x+xi+2.0*x0-2.0*x1)*ar)/(r*r);
            theta1 = ai*(kr1*kr1-ki1*ki1)+2.0*ar*kr1*ki1;
            theta2 = ai*(kr2*kr2-ki2*ki2)+2.0*ar*kr2*ki2;

```

```

theta3 = ai*(kr3*kr3-ki3*ki3)+2.0*ar*kr3*ki3;
theta4 = ai*(kr4*kr4-ki4*ki4)+2.0*ar*kr4*ki4;
theta5 = ai*(kr5*kr5-ki5*ki5)+2.0*ar*kr5*ki5;
theta6 = ai*(kr6*kr6-ki6*ki6)+2.0*ar*kr6*ki6;
theta7 = ai*(kr7*kr7-ki7*ki7)+2.0*ar*kr7*ki7;
theta8 = ai*(kr8*kr8-ki8*ki8)+2.0*ar*kr8*ki8;
dr1 = exp(ar*(kr1*kr1-ki1*ki1)-2.0*ai*kr1*ki1-k0*k0*a0*a0)*cos(theta1);
di1 = exp(ar*(kr1*kr1-ki1*ki1)-2.0*ai*kr1*ki1-k0*k0*a0*a0)*sin(theta1);
dr2 = exp(ar*(kr2*kr2-ki2*ki2)-2.0*ai*kr2*ki2-k0*k0*a0*a0)*cos(theta2);
di2 = exp(ar*(kr2*kr2-ki2*ki2)-2.0*ai*kr2*ki2-k0*k0*a0*a0)*sin(theta2);
dr3 = exp(ar*(kr3*kr3-ki3*ki3)-2.0*ai*kr3*ki3-k0*k0*a0*a0)*cos(theta3);
di3 = exp(ar*(kr3*kr3-ki3*ki3)-2.0*ai*kr3*ki3-k0*k0*a0*a0)*sin(theta3);
dr4 = exp(ar*(kr4*kr4-ki4*ki4)-2.0*ai*kr4*ki4-k0*k0*a0*a0)*cos(theta4);
di4 = exp(ar*(kr4*kr4-ki4*ki4)-2.0*ai*kr4*ki4-k0*k0*a0*a0)*sin(theta4);
dr5 = exp(ar*(kr5*kr5-ki5*ki5)-2.0*ai*kr5*ki5-k0*k0*a0*a0)*cos(theta5);
di5 = exp(ar*(kr5*kr5-ki5*ki5)-2.0*ai*kr5*ki5-k0*k0*a0*a0)*sin(theta5);
dr6 = exp(ar*(kr6*kr6-ki6*ki6)-2.0*ai*kr6*ki6-k0*k0*a0*a0)*cos(theta6);
di6 = exp(ar*(kr6*kr6-ki6*ki6)-2.0*ai*kr6*ki6-k0*k0*a0*a0)*sin(theta6);
dr7 = exp(ar*(kr7*kr7-ki7*ki7)-2.0*ai*kr7*ki7-k0*k0*a0*a0)*cos(theta7);
di7 = exp(ar*(kr7*kr7-ki7*ki7)-2.0*ai*kr7*ki7-k0*k0*a0*a0)*sin(theta7);
dr8 = exp(ar*(kr8*kr8-ki8*ki8)-2.0*ai*kr8*ki8-k0*k0*a0*a0)*cos(theta8);
di8 = exp(ar*(kr8*kr8-ki8*ki8)-2.0*ai*kr8*ki8-k0*k0*a0*a0)*sin(theta8);
zr1 = sqrar*kr1-sqrai*ki1;
zi1 = sqrar*ki1+sqrai*kr1;
zr21 = sqrar*kr2-sqrai*ki2;
zi21 = sqrar*ki2+sqrai*kr2;
zr22 = sqrar*kr2-sqrai*(ki2+b0);
zi22 = sqrar*(ki2+b0)+sqrai*kr2;
zr31 = sqrar*kr3-sqrai*ki3;
zi31 = sqrar*ki3+sqrai*kr3;
zr32 = sqrar*kr3-sqrai*(ki3+b0);
zi32 = sqrar*(ki3+b0)+sqrai*kr3;
zr4 = sqrar*kr4-sqrai*ki4;
zi4 = sqrar*ki4+sqrai*kr4;
zr51 = sqrar*kr5-sqrai*ki5;
zi51 = sqrar*ki5+sqrai*kr5;
zr52 = sqrar*kr5-sqrai*(ki5+b0);
zi52 = sqrar*(ki5+b0)+sqrai*kr5;
zr6 = sqrar*kr6-sqrai*ki6;
zi6 = sqrar*ki6+sqrai*kr6;
zr7 = sqrar*kr7-sqrai*ki7;
zi7 = sqrar*ki7+sqrai*kr7;
zr81 = sqrar*kr8-sqrai*ki8;
zi81 = sqrar*ki8+sqrai*kr8;
zr82 = sqrar*kr8-sqrai*(ki8+b0);
zi82 = sqrar*(ki8+b0)+sqrai*kr8;
IUE1 = rombint(dpsi1,-ulim,ulim,tol);
IUE21 = rombint(dpsi2,-ulim,ulim,tol);
IUE22 = rombint(dpsi3,-ulim,ulim,tol);

```

IUE31 = rombint(dpsi4,-ulim,ulim,tol);
IUE32 = rombint(dpsi5,-ulim,ulim,tol);
IUE4 = rombint(dpsi6,-ulim,ulim,tol);
IUE51 = rombint(dpsi7,-ulim,ulim,tol);
IUE52 = rombint(dpsi8,-ulim,ulim,tol);
IUE6 = rombint(dpsi9,-ulim,ulim,tol);
IUE7 = rombint(dpsi10,-ulim,ulim,tol);
IUE81 = rombint(dpsi11,-ulim,ulim,tol);
IUE82 = rombint(dpsi12,-ulim,ulim,tol);
IE1 = rombint(dpsi13,-ulim,ulim,tol);
IE21 = rombint(dpsi14,-ulim,ulim,tol);
IE22 = rombint(dpsi15,-ulim,ulim,tol);
IE31 = rombint(dpsi16,-ulim,ulim,tol);
IE32 = rombint(dpsi17,-ulim,ulim,tol);
IE4 = rombint(dpsi18,-ulim,ulim,tol);
IE51 = rombint(dpsi19,-ulim,ulim,tol);
IE52 = rombint(dpsi20,-ulim,ulim,tol);
IE6 = rombint(dpsi21,-ulim,ulim,tol);
IE7 = rombint(dpsi22,-ulim,ulim,tol);
IE81 = rombint(dpsi23,-ulim,ulim,tol);
IE82 = rombint(dpsi24,-ulim,ulim,tol);
IIUE1 = rombint(dpsi25,-ulim,ulim,tol);
IIUE21 = rombint(dpsi26,-ulim,ulim,tol);
IIUE31 = rombint(dpsi27,-ulim,ulim,tol);
IIUE4 = rombint(dpsi28,-ulim,ulim,tol);
IIUE51 = rombint(dpsi29,-ulim,ulim,tol);
IIUE6 = rombint(dpsi30,-ulim,ulim,tol);
IIUE7 = rombint(dpsi31,-ulim,ulim,tol);
IIUE81 = rombint(dpsi32,-ulim,ulim,tol);
IIE1 = rombint(dpsi33,-ulim,ulim,tol);
IIE21 = rombint(dpsi34,-ulim,ulim,tol);
IIE31 = rombint(dpsi35,-ulim,ulim,tol);
IIE4 = rombint(dpsi36,-ulim,ulim,tol);
IIE51 = rombint(dpsi37,-ulim,ulim,tol);
IIE6 = rombint(dpsi38,-ulim,ulim,tol);
IIE7 = rombint(dpsi39,-ulim,ulim,tol);
IIE81 = rombint(dpsi40,-ulim,ulim,tol);
IIE1 = rombint(dpsi41,-ulim,ulim,tol);
IIE21 = rombint(dpsi42,-ulim,ulim,tol);
IIE31 = rombint(dpsi43,-ulim,ulim,tol);
IIE4 = rombint(dpsi44,-ulim,ulim,tol);
IIE51 = rombint(dpsi45,-ulim,ulim,tol);
IIE6 = rombint(dpsi46,-ulim,ulim,tol);
IIE7 = rombint(dpsi47,-ulim,ulim,tol);
IIE81 = rombint(dpsi48,-ulim,ulim,tol);
Ir1 = IUE1+zr1*IE1;
Ir21 = IUE21+zr21*IE21;
Ir22 = IUE22+zr22*IE22;
Ir31 = IUE31+zr31*IE31;

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lr32 = IUE32+zr32*IE32;
lr4 = IUE4+zr4*IE4;
lr51 = IUE51+zr51*IE51;
lr52 = IUE52+zr52*IE52;
lr6 = IUE6+zr6*IE6;
lr7 = IUE7+zr7*IE7;
lr81 = IUE81+zr81*IE81;
lr82 = IUE82+zr82*IE82;
li1 = -zi1*IE1;
li21 = -zi21*IE21;
li22 = -zi22*IE22;
li31 = -zi31*IE31;
li32 = -zi32*IE32;
li4 = -zi4*IE4;
li51 = -zi51*IE51;
li52 = -zi52*IE52;
li6 = -zi6*IE6;
li7 = -zi7*IE7;
li81 = -zi81*IE81;
li82 = -zi82*IE82;
/* Calculate Rr22, Ri22 */
if (b0*zi22<0.0) {
    Rr22 = fabs(zi22)/zi22*2.0*PI*exp(zi22*zi22-zr22*zr22)*sin(2.0*zr22*zi22);
    Ri22 = fabs(zi22)/zi22*2.0*PI*exp(zi22*zi22-zr22*zr22)*cos(2.0*zr22*zi22);
}
else {
    Rr22 = 0.0;
    Ri22 = 0.0;
}
/* Calculate Rr32, Ri32 */
if (b0*zi32<0.0) {
    Rr32 = fabs(zi32)/zi32*2.0*PI*exp(zi32*zi32-zr32*zr32)*sin(2.0*zr32*zi32);
    Ri32 = fabs(zi32)/zi32*2.0*PI*exp(zi32*zi32-zr32*zr32)*cos(2.0*zr32*zi32);
}
else {
    Rr32 = 0.0;
    Ri32 = 0.0;
}
/* Calculate Rr52, Ri52 */
if (b0*zi52<0.0) {
    Rr52 = fabs(zi52)/zi52*2.0*PI*exp(zi52*zi52-zr52*zr52)*sin(2.0*zr52*zi52);
    Ri52 = fabs(zi52)/zi52*2.0*PI*exp(zi52*zi52-zr52*zr52)*cos(2.0*zr52*zi52);
}
else {
    Rr52 = 0.0;
    Ri52 = 0.0;
}
/* Calculate Rr82, Ri82 */
if (b0*zi82<0.0) {

```

```

Rr82 = fabs(zi82)/zi82*2.0*PI*exp(zi82*zi82-zr82*zr82)*sin(2.0*zr82*zi82);
Ri82 = fabs(zi82)/zi82*2.0*PI*exp(zi82*zi82-zr82*zr82)*cos(2.0*zr82*zi82);
}
else {
  Rr82 = 0.0;
  Ri82 = 0.0;
}
/* Calculate wavefunction psi */
Ilr1 = IIUUE1+2.0*zr1*IIUE1+(zr1*zr1-zi1*zi1)*IIE1;
Ilr21 = IIUUE21+2.0*zr21*IIUE21+(zr21*zr21-zi21*zi21)*IIE21;
Ilr31 = IIUUE31+2.0*zr31*IIUE31+(zr31*zr31-zi31*zi31)*IIE31;
Ilr4 = IIUUE4+2.0*zr4*IIUE4+(zr4*zr4-zi4*zi4)*IIE4;
Ilr51 = IIUUE51+2.0*zr51*IIUE51+(zr51*zr51-zi51*zi51)*IIE51;
Ilr6 = IIUUE6+2.0*zr6*IIUE6+(zr6*zr6-zi6*zi6)*IIE6;
Ilr7 = IIUUE7+2.0*zr7*IIUE7+(zr7*zr7-zi7*zi7)*IIE7;
Ilr81 = IIUUE81+2.0*zr81*IIUE81+(zr81*zr81-zi81*zi81)*IIE81;
Ili1 = -2.0*zi1*IIUE1-2.0*zi1*zr1*IIE1;
Ili21 = -2.0*zi21*IIUE21-2.0*zi21*zr21*IIE21;
Ili31 = -2.0*zi31*IIUE31-2.0*zi31*zr31*IIE31;
Ili4 = -2.0*zi4*IIUE4-2.0*zi4*zr4*IIE4;
Ili51 = -2.0*zi51*IIUE51-2.0*zi51*zr51*IIE51;
Ili6 = -2.0*zi6*IIUE6-2.0*zi6*zr6*IIE6;
Ili7 = -2.0*zi7*IIUE7-2.0*zi7*zr7*IIE7;
Ili81 = -2.0*zi81*IIUE81-2.0*zi81*zr81*IIE81;
DI1r = -(dr1*lr1-di1*li1)+(dr2*lr21-di2*li21)-(dr3*lr31-di3*li31)+(dr4*lr4-di4*li4);
DI1i = -(di1*lr1+dr1*li1)+(di2*lr21+dr2*li21)-(di3*lr31+dr3*li31)+(di4*lr4+dr4*li4);
DI2r = (dr5*lr51-di5*li51)-(dr6*lr6-di6*li6)+(dr7*lr7-di7*li7)-(dr8*lr81-di8*li81);
DI2i = (di5*lr51+dr5*li51)-(di6*lr6+dr6*li6)+(di7*lr7+dr7*li7)-(di8*lr81+dr8*li81);
psiA1r = (b1*b/b0-b)*(di2*(lr22+Rr22)+dr2*(li22+Ri22))-
(b1*b/b0+b1)*(di3*(lr32+Rr32)+dr3*(li32+Ri32))+sqrt(PI)*(dr1*sqrar/r+di1*sqrar/r)-
(b+b1)*(di1*lr1+dr1*li1)-(b1*b/b0-b)*(di2*lr21+dr2*li21)+
(b1*b/b0+b1)*(di3*lr31+dr3*li31)+b1*b*(sqrar*DI1r-sqrar*DI1i);
psiA1i = -(b1*b/b0-b)*(dr2*(lr22+Rr22)-di2*(li22+Ri22))+b1*b/b0+b1*(dr3*(lr32+Rr32)-
di3*(li32+Ri32))+sqrt(PI)*(di1*sqrar/r-dr1*sqrar/r)+(b+b1)*(dr1*lr1-di1*li1)+(b1*b/b0-
b)*(dr2*lr21-di2*li21)-(b1*b/b0+b1)*(dr3*lr31-di3*li31)+b1*b*(sqrar*DI1i+sqrar*DI1r);
psiA2r = -(b1*b/b0)*(di8*(lr82+Rr82)+dr8*(li82+Ri82))+
(b0+b+b1+b1*b/b0)*(di5*(lr52+Rr52)+dr5*(li52+Ri52))+b1*(di7*lr7+dr7*li7)+
(b1*b/b0)*(di8*lr81+dr8*li81)+b*(di6*lr6+dr6*li6)-
(b+b1+b1*b/b0)*(di5*lr51+dr5*li51)+b1*b*(sqrar*DI2r-sqrar*DI2i);
psiA2i = (b1*b/b0)*(dr8*(lr82+Rr82)-di8*(li82+Ri82))-(b0+b+b1+b1*b/b0)*(dr5*(lr52+Rr52)-
di5*(li52+Ri52))-b1*(dr7*lr7-di7*li7)-(b1*b/b0)*(dr8*lr81-di8*li81)-b*(dr6*lr6-di6*li6)+
(b+b1+b1*b/b0)*(dr5*lr51-di5*li51)+b1*b*(sqrar*DI2i+sqrar*DI2r);
psir = sqrt(sqrt(a0*a0/2.0/(PI*PI*PI)))*(psiA1r+psiA2r);
psii = sqrt(sqrt(a0*a0/2.0/(PI*PI*PI)))*(psiA1i+psiA2i);
/* Find maximum probability density */
p = (psir*psir+psii*psii);
if (p > pmax) {
/* Record the new maximum. */
  pmax = p;

```

```

        tm = t;
        xm = x;
    }
    if (iwhile == 1) {
/* Produce spacetime image. */
        if ((i=255*p/datamax) < 255)
            image[it][ix] = i;
        else
            image[it][ix] = 255;
    }
/* End loop on x */
    }
/* End loop on t */
    }
/* Narrow the search for the maximum. */
    tmin = (tmin=tm-2*dt) > tmin0 ? tmin:tmin0;
    tmax = (tmax=tm+2*dt) < tmax0 ? tmax:tmax0;
    dt = (tmax-tmin)/(nt-1);
    xmin = (xmin=xm-2*dx) > xmin0 ? xmin:xmin0;
    xmax = (xmax=xm+2*dx) < xmax0 ? xmax:xmax0;
    dx = (xmax-xmin)/(nx-1);
/* End while loop (used to find maximum probability density). */
    }
printf("%g %g %d %g %g %g\n",a0,k0,iwhile,tm,xm,pmax);
fprintf(fp,"%g %g %g %g %g\n",a0,k0,tm,xm,pmax);
/* Produce spacetime image. */
    sprintf(filename,"%dp%d_%d%d.gif",(int)(a0),(int)(10*(a0-(int)a0)),(int)(k0/10),(int)(k0-
10*(int)(k0/10)));
    wgif(imageptr,nx,nt,filename);
/* Produce maximum probability density image. */
    if ((i=255*pmax/datamax)<255)
        image1[ja0][ik0] = i;
    else
        image1[ja0][ik0] = 255;
/* End loop on k0 */
    }
/* End loop on a0 */
    }
    fclose(fp);
/* Produce maximum probability density image. */
    wgif(image1ptr,nk0,na0,"maxprob.gif");
    free(image);
    free(image1);
    return 0;
}

double dps1(double u)
{
    return(u*exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1));
}

```

```

}
double dps2(double u)
{
return(u*exp(-u*u)/((u+zr21)*(u+zr21)+zi21*zi21));
}
double dps3(double u)
{
return(u*exp(-u*u)/((u+zr22)*(u+zr22)+zi22*zi22));
}
double dps4(double u)
{
return(u*exp(-u*u)/((u+zr31)*(u+zr31)+zi31*zi31));
}
double dps5(double u)
{
return(u*exp(-u*u)/((u+zr32)*(u+zr32)+zi32*zi32));
}
double dps6(double u)
{
return(u*exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dps7(double u)
{
return(u*exp(-u*u)/((u+zr51)*(u+zr51)+zi51*zi51));
}
double dps8(double u)
{
return(u*exp(-u*u)/((u+zr52)*(u+zr52)+zi52*zi52));
}
double dps9(double u)
{
return(u*exp(-u*u)/((u+zr6)*(u+zr6)+zi6*zi6));
}
double dps10(double u)
{
return(u*exp(-u*u)/((u+zr7)*(u+zr7)+zi7*zi7));
}
double dps11(double u)
{
return(u*exp(-u*u)/((u+zr81)*(u+zr81)+zi81*zi81));
}
double dps12(double u)
{
return(u*exp(-u*u)/((u+zr82)*(u+zr82)+zi82*zi82));
}
double dps13(double u)
{
return(exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1));
}

```

```

double dpsi14(double u)
{
    return(exp(-u*u)/((u+zr21)*(u+zr21)+zi21*zi21));
}
double dpsi15(double u)
{
    return(exp(-u*u)/((u+zr22)*(u+zr22)+zi22*zi22));
}
double dpsi16(double u)
{
    return(exp(-u*u)/((u+zr31)*(u+zr31)+zi31*zi31));
}
double dpsi17(double u)
{
    return(exp(-u*u)/((u+zr32)*(u+zr32)+zi32*zi32));
}
double dpsi18(double u)
{
    return(exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dpsi19(double u)
{
    return(exp(-u*u)/((u+zr51)*(u+zr51)+zi51*zi51));
}
double dpsi20(double u)
{
    return(exp(-u*u)/((u+zr52)*(u+zr52)+zi52*zi52));
}
double dpsi21(double u)
{
    return(exp(-u*u)/((u+zr6)*(u+zr6)+zi6*zi6));
}
double dpsi22(double u)
{
    return(exp(-u*u)/((u+zr7)*(u+zr7)+zi7*zi7));
}
double dpsi23(double u)
{
    return(exp(-u*u)/((u+zr81)*(u+zr81)+zi81*zi81));
}
double dpsi24(double u)
{
    return(exp(-u*u)/((u+zr82)*(u+zr82)+zi82*zi82));
}
double dpsi25(double u)
{
    return(u*u*exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1)/((u+zr1)*(u+zr1)+zi1*zi1));
}
double dpsi26(double u)

```

```

{
  return(u*u*exp(-u*u)/((u+zr21)*(u+zr21)+zi21*zi21)/((u+zr21)*(u+zr21)+zi21*zi21));
}
double dps27(double u)
{
  return(u*u*exp(-u*u)/((u+zr31)*(u+zr31)+zi31*zi31)/((u+zr31)*(u+zr31)+zi31*zi31));
}
double dps28(double u)
{
  return(u*u*exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dps29(double u)
{
  return(u*u*exp(-u*u)/((u+zr51)*(u+zr51)+zi51*zi51)/((u+zr51)*(u+zr51)+zi51*zi51));
}
double dps30(double u)
{
  return(u*u*exp(-u*u)/((u+zr6)*(u+zr6)+zi6*zi6)/((u+zr6)*(u+zr6)+zi6*zi6));
}
double dps31(double u)
{
  return(u*u*exp(-u*u)/((u+zr7)*(u+zr7)+zi7*zi7)/((u+zr7)*(u+zr7)+zi7*zi7));
}
double dps32(double u)
{
  return(u*u*exp(-u*u)/((u+zr81)*(u+zr81)+zi81*zi81)/((u+zr81)*(u+zr81)+zi81*zi81));
}
double dps33(double u)
{
  return(u*exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1)/((u+zr1)*(u+zr1)+zi1*zi1));
}
double dps34(double u)
{
  return(u*exp(-u*u)/((u+zr21)*(u+zr21)+zi21*zi21)/((u+zr21)*(u+zr21)+zi21*zi21));
}
double dps35(double u)
{
  return(u*exp(-u*u)/((u+zr31)*(u+zr31)+zi31*zi31)/((u+zr31)*(u+zr31)+zi31*zi31));
}
}
double dps36(double u)
{
  return(u*exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dps37(double u)
{
  return(u*exp(-u*u)/((u+zr51)*(u+zr51)+zi51*zi51)/((u+zr51)*(u+zr51)+zi51*zi51));
}
}
double dps38(double u)

```

```

{
return(u*exp(-u*u)/((u+zr6)*(u+zr6)+zi6*zi6)/((u+zr6)*(u+zr6)+zi6*zi6));
}
double dpsi39(double u)
{
return(u*exp(-u*u)/((u+zr7)*(u+zr7)+zi7*zi7)/((u+zr7)*(u+zr7)+zi7*zi7));
}
double dpsi40(double u)
{
return(u*exp(-u*u)/((u+zr81)*(u+zr81)+zi81*zi81)/((u+zr81)*(u+zr81)+zi81*zi81));
}
double dpsi41(double u)
{
return(exp(-u*u)/((u+zr1)*(u+zr1)+zi1*zi1)/((u+zr1)*(u+zr1)+zi1*zi1));
}
double dpsi42(double u)
{
return(exp(-u*u)/((u+zr21)*(u+zr21)+zi21*zi21)/((u+zr21)*(u+zr21)+zi21*zi21));
}
double dpsi43(double u)
{
return(exp(-u*u)/((u+zr31)*(u+zr31)+zi31*zi31)/((u+zr31)*(u+zr31)+zi31*zi31));
}
double dpsi44(double u)
{
return(exp(-u*u)/((u+zr4)*(u+zr4)+zi4*zi4)/((u+zr4)*(u+zr4)+zi4*zi4));
}
double dpsi45(double u)
{
return(exp(-u*u)/((u+zr51)*(u+zr51)+zi51*zi51)/((u+zr51)*(u+zr51)+zi51*zi51));
}
double dpsi46(double u)
{
return(exp(-u*u)/((u+zr6)*(u+zr6)+zi6*zi6)/((u+zr6)*(u+zr6)+zi6*zi6));
}
double dpsi47(double u)
{
return(exp(-u*u)/((u+zr7)*(u+zr7)+zi7*zi7)/((u+zr7)*(u+zr7)+zi7*zi7));
}
double dpsi48(double u)
{
return(exp(-u*u)/((u+zr81)*(u+zr81)+zi81*zi81)/((u+zr81)*(u+zr81)+zi81*zi81));
}
}

```