PHY456H1F: Quantum Mechanics II. Lecture L24 (Taught by Prof J.E. Sipe). 3D Scattering cross sections (cont.)

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Contents

1. Disclaimer.

Peeter's lecture notes from class. May not be entirely coherent.

2. Scattering cross sections.

READING: §20 [1]

Recall that we are studing the case of a potential that is zero outside of a fixed bound, $V(\mathbf{r}) = 0$ for $r > r_0$, as in figure (1)

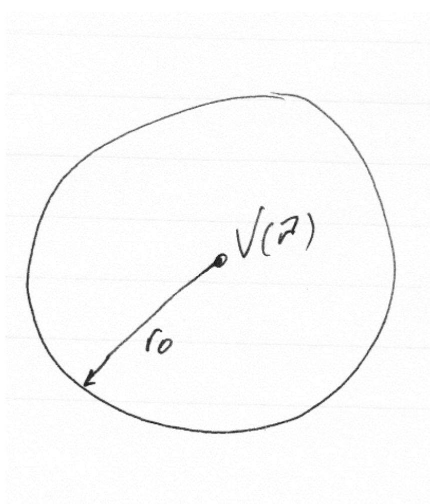

Figure 1: Bounded potential.

and were looking for solutions to Schrödinger's equation

$$-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2\psi_{\mathbf{k}}(\mathbf{r}) + V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) = \frac{\hbar^2\mathbf{k}^2}{2\mu}\psi_{\mathbf{k}}(\mathbf{r}), \tag{1}$$

in regions of space, where $r > r_0$ is very large. We found

$$\psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f_{\mathbf{k}}(\theta, \phi). \tag{2}$$

For $r \le r_0$ this will be something much more complicated.

To study scattering we'll use the concept of probability flux as in electromagnetism

$$\boldsymbol{\nabla} \cdot \mathbf{j} + \dot{\rho} = 0 \tag{3}$$

Using

$$\psi(\mathbf{r}, t) = \psi_{\mathbf{k}}(\mathbf{r})^* \psi_{\mathbf{k}}(\mathbf{r}) \tag{4}$$

we find

$$\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2\mu i}\Big(\psi_{\mathbf{k}}(\mathbf{r})^* \boldsymbol{\nabla}\psi_{\mathbf{k}}(\mathbf{r}) - (\boldsymbol{\nabla}\psi_{\mathbf{k}}^*(\mathbf{r}))\psi_{\mathbf{k}}(\mathbf{r})\Big) \tag{5}$$

when

$$-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2\psi_{\mathbf{k}}(\mathbf{r}) + V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) = i\hbar\frac{\partial\psi_{\mathbf{k}}(\mathbf{r})}{\partial t} \tag{6}$$

In a fashion similar to what we did in the 1D case, let's suppose that we can write our wave function

$$\psi(\mathbf{r}, t_{\text{initial}}) = \int d^3k\alpha(\mathbf{k}, t_{\text{initial}})\psi_{\mathbf{k}}(\mathbf{r}) \tag{7}$$

and treat the scattering as the scattering of a plane wave front (idealizing a set of wave packets) off of the object of interest as depicted in figure (2)

We assume that our incoming particles are sufficiently localized in k space as depicted in the idealized representation of figure (3)

we assume that $\alpha(\mathbf{k}, t_{\text{initial}})$ is localized.

$$\psi(\mathbf{r}, t_{\text{initial}}) = \int d^3k \left(\alpha(\mathbf{k}, t_{\text{initial}})e^{ik_z z} + \alpha(\mathbf{k}, t_{\text{initial}})\frac{e^{ikr}}{r} f_{\mathbf{k}}(\theta, \phi)\right) \tag{8}$$

We suppose that

$$\alpha(\mathbf{k}, t_{\text{initial}}) = \alpha(\mathbf{k})e^{-i\hbar k^2 t_{\text{initial}}/2\mu} \tag{9}$$

where this is chosen ($\alpha(\mathbf{k}, t_{\text{initial}})$ is built in this fashion) so that this is non-zero for z large in magnitude and negative.

This last integral can be approximated

$$\begin{aligned} \int d^3k\alpha(\mathbf{k}, t_{\text{initial}})\frac{e^{ikr}}{r} f_{\mathbf{k}}(\theta, \phi) &\approx \frac{f_{\mathbf{k}_0}(\theta, \phi)}{r}\int d^3k\alpha(\mathbf{k}, t_{\text{initial}})e^{ikr} \\ &\to 0 \end{aligned} \tag{10}$$

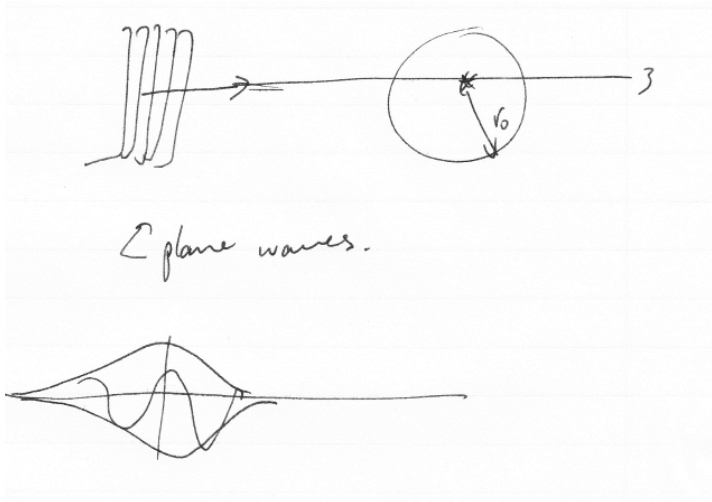

Figure 2: plane wave front incident on particle

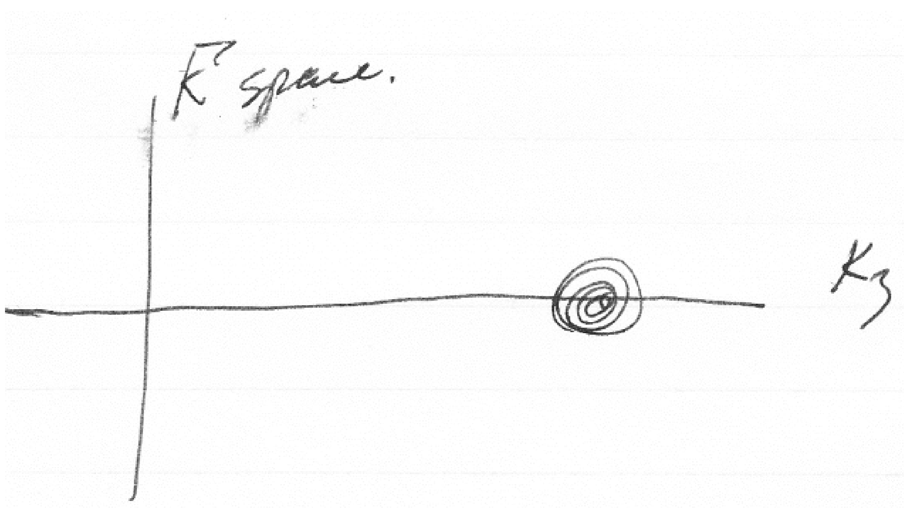

Figure 3: k space localized wave packet

This is very much like the 1D case where we found no reflected component for our initial time. We'll normally look in a locality well away from the wave front as indicted in figure (4)

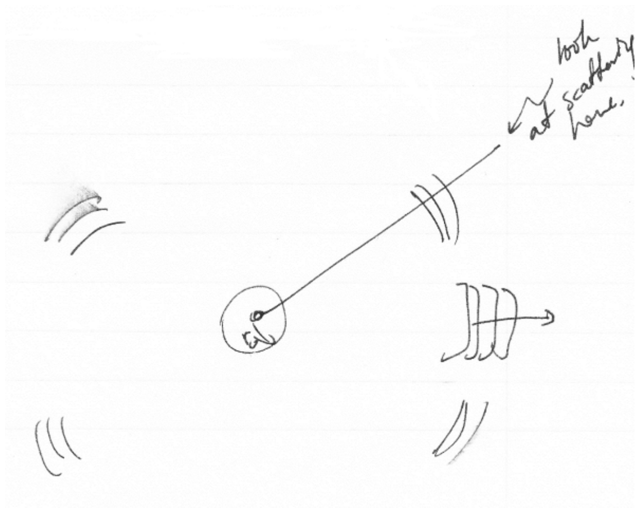

Figure 4: point of measurement of scattering cross section

There are situations where we do look in the locality of the wave front that has been scattered.

2.1.

Our income wave is of the form

$$\psi_i = A e^{ikz} e^{-i\hbar k^2 t/2\mu} \tag{11}$$

Here we've made the approximation that $k = |\mathbf{k}| \sim k_z$. We can calculate the probability current

$$\mathbf{j} = \hat{\mathbf{z}} \frac{\hbar k}{\mu} A \tag{12}$$

(notice the $v = p/m$ like term above, with $p = \hbar k$).
For the scattered wave (dropping A factor)

$$\begin{aligned}
\mathbf{j} &= \frac{\hbar}{2\mu i} \left(f_{\mathbf{k}}^*(\theta,\phi) \frac{e^{-ikr}}{r} \boldsymbol{\nabla} \left(f_{\mathbf{k}}(\theta,\phi) \frac{e^{ikr}}{r} \right) - \boldsymbol{\nabla} \left(f_{\mathbf{k}}^*(\theta,\phi) \frac{e^{-ikr}}{r} \right) f_{\mathbf{k}}(\theta,\phi) \frac{e^{ikr}}{r} \right) \\
&\approx \frac{\hbar}{2\mu i} \left(f_{\mathbf{k}}^*(\theta,\phi) \frac{e^{-ikr}}{r} ik\hat{\mathbf{r}} f_{\mathbf{k}}(\theta,\phi) \frac{e^{ikr}}{r} - f_{\mathbf{k}}^*(\theta,\phi) \frac{e^{-ikr}}{r} (-ik\hat{\mathbf{r}}) f_{\mathbf{k}}(\theta,\phi) \frac{e^{ikr}}{r} \right)
\end{aligned}$$

We find that the radial portion of the current density is

$$\begin{aligned}
\hat{\mathbf{r}} \cdot \mathbf{j} &= \frac{\hbar}{2\mu i} |f|^2 \frac{2ik}{r^2} \\
&= \frac{\hbar k}{\mu} \frac{1}{r^2} |f|^2,
\end{aligned}$$

and the flux through our element of solid angle is

$$
\begin{aligned}
\hat{\mathbf{r}} dA \cdot \mathbf{j} &= \frac{\text{probability}}{\text{unit area per time}} \times \text{area} \\
&= \frac{\text{probability}}{\text{unit time}} \\
&= \frac{\hbar k}{\mu} \frac{\left|f_{\mathbf{k}}(\theta, \phi)\right|^2}{r^2} r^2 d\Omega \\
&= \frac{\hbar k}{\mu} \left|f_{\mathbf{k}}(\theta, \phi)\right|^2 d\Omega \\
&= j_{\text{incoming}} \underbrace{\left|f_{\mathbf{k}}(\theta, \phi)\right|^2}_{d\sigma/d\Omega} d\Omega.
\end{aligned}
$$

We identify the scattering cross section above

$$
\frac{d\sigma}{d\Omega} = \left|f_{\mathbf{k}}(\theta, \phi)\right|^2 \tag{13}
$$

$$
\sigma = \int \left|f_{\mathbf{k}}(\theta, \phi)\right|^2 d\Omega \tag{14}
$$

We've been somewhat unrealistic here since we've used a plane wave approximation, and can as in figure (5)

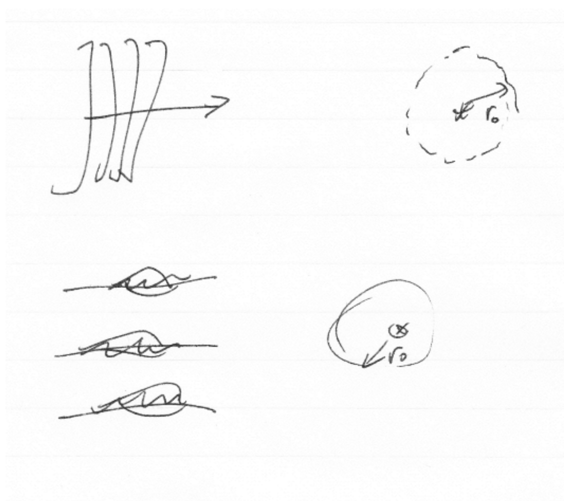

Figure 5: Plane wave vs packet wave front

will actually produce the same answer. For details we are referred to [2] and [3].

2.2. *Working towards a solution*

We've done a bunch of stuff here but are not much closer to a real solution because we don't actually know what $f_{\mathbf{k}}$ is.

Let's write Schrödinger

$$-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2\psi_{\mathbf{k}}(\mathbf{r}) + V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) = \frac{\hbar^2\mathbf{k}^2}{2\mu}\psi_{\mathbf{k}}(\mathbf{r}), \tag{15}$$

instead as

$$(\boldsymbol{\nabla}^2 + \mathbf{k}^2)\psi_{\mathbf{k}}(\mathbf{r}) = s(\mathbf{r}) \tag{16}$$

where

$$s(\mathbf{r}) = \frac{2\mu}{\hbar}V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) \tag{17}$$

where $s(\mathbf{r})$ is really the particular solution to this differential problem. We want

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}^{\text{homogeneous}}(\mathbf{r}) + \psi_{\mathbf{k}}^{\text{particular}}(\mathbf{r}) \tag{18}$$

and

$$\psi_{\mathbf{k}}^{\text{homogeneous}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \tag{19}$$

References

[1] BR Desai. *Quantum mechanics with basic field theory*. Cambridge University Press, 2009. 2

[2] A. Messiah, G.M. Temmer, and J. Potter. *Quantum mechanics: two volumes bound as one*. Dover Publications New York, 1999. 2.1

[3] JR Taylor. *Scattering Theory: the Quantum Theory of Nonrelativistic Scattering*, volume 1. 1972. 2.1