Lectures #17 - 18

Scattering

Method of partial waves.

Calculation of phase shifts

Scattering of two identical particles

Chapter 10, pages 393-398, Jasprit Singh, Quantum Mechanics

Chapter 13, pages 595-608, Bransden & Joachain, Quantum Mechanics

How to calculate differential cross section?

Step 1. Write the expression for the wave function $\psi(\mathbf{r})$.

Step 2. Determine the asymptotic behavior of this wave function for $r \to \infty$.

Step 3. Compare it with $\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \dfrac{f(\theta,\phi)}{r} e^{ikr}$.

Step 4. Determine $f(\theta,\phi)$ from this comparison.

Step 5. Calculate differential cross section using $\dfrac{d\sigma}{d\Omega} = \left| f(\theta,\phi) \right|^2$.

Note: this general procedure is used to derive formula for the differential cross section both using Born approximation and method of partial waves.

Step 1. Write the expression for the wave function $\psi(\mathbf{r})$.

Schrödinger equation … again

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(r)\psi(\mathbf{r})=E\psi(\mathbf{r})$$

For the spherically symmetric potentials, the wave function can be written in terms of spherical harmonics $Y_{lm}(\theta,\phi)$.

$$Y_{lm}(\theta,\phi)=(-1)^m\left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2}P_l^m(\cos\theta)\,e^{im\phi}$$

If we chose the z axes in the direction of the incident beam of particle there will be no dependence on the angle ϕ. Therefore, m=0.

$$Y_{l0}(\theta)=\left[\frac{(2l+1)}{4\pi}\right]^{1/2}P_l\,(\cos\theta)$$

Step 1. Write the expression for the wave function $\psi(\mathbf{r})$.

Schrödinger equation … again

Therefore, we can write our wave function as an expansion

$$\psi_k(\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1)\, i^l R_l(r) P_l(\cos\theta)$$

where l th term is called l th partial wave. The radial function R satisfies the radial Schrödinger equation (see the derivation in the Hydrogen atom lecture).

$$\left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{\hbar^2}{mr}\frac{d}{dr} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right\} R_l(r) = E\, R_l(r)$$

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right\} R_l(r) = 0$$

$$U(r) = \frac{2m}{\hbar^2} V(r)$$

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

Step 2. Determine the asymptotic behavior of this wave function for $r \to \infty$.

Solutions beyond the range of the potential

We suppose that the potential is negligible at r>a. Then, we can neglect the V(r) term in our equation

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 \right\} R_l(r) = 0 \qquad r > a$$

The solutions of this equation are given by:

$$R_l(r) = B_{kl}\, j_l(kr) + C_{kl} n_l(kr)$$

Spherical Bessel functions

Spherical Neumann functions

Step 2. Determine the asymptotic behavior of this wave function for $r \to \infty$.

Asymptotic behavior at $r \to \infty$

Asymptotic form of the Bessel functions:

$r \to \infty$ $\quad j_l(kr) \sim \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)$; $\quad n_l(kr) \sim -\frac{1}{kr} \cos\left(kr - \frac{l\pi}{2}\right)$

$$R_l(r) = B_{kl}\, j_l(kr) + C_{kl}\, n_l(kr)$$

$$R_l(r) \to \frac{1}{kr}\left\{ B_{kl} \sin\left(kr - \frac{l\pi}{2}\right) - C_{kl} \cos\left(kr - \frac{l\pi}{2}\right) \right\}$$

$$R_l(r) \to \frac{1}{kr}\sqrt{B_{kl}^2 + C_{kl}^2}\left\{ \frac{B_{kl}}{\sqrt{B_{kl}^2 + C_{kl}^2}} \sin\left(kr - \frac{l\pi}{2}\right) + \frac{-C_{kl}}{\sqrt{B_{kl}^2 + C_{kl}^2}} \cos\left(kr - \frac{l\pi}{2}\right) \right\}$$

Step 2. Determine the asymptotic behavior of this wave function for $r \to \infty$.

Asymptotic behavior at $r \to \infty$

$$R_l(r) \to \frac{1}{kr} \underbrace{\boxed{\sqrt{B_{kl}^2 + C_{kl}^2}}}_{A_{kl}} \left\{ \underbrace{\boxed{\frac{B_{kl}}{\sqrt{B_{kl}^2 + C_{kl}^2}}}}_{\cos\delta_l} \sin\left(kr - \frac{l\pi}{2}\right) + \underbrace{\boxed{\frac{-C_{kl}}{\sqrt{B_{kl}^2 + C_{kl}^2}}}}_{\sin\delta_l} \cos\left(kr - \frac{l\pi}{2}\right) \right\}$$

$$R_l(r) \to \frac{A_{lk}}{kr} \left\{ \cos\delta_l \sin\left(kr - \frac{l\pi}{2}\right) + \sin\delta_l \cos\left(kr - \frac{l\pi}{2}\right) \right\}$$

$$\boxed{R_l(r) \to \frac{A_{lk}}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)}$$

where $A_{lk} = \sqrt{B_{kl}^2 + C_{kl}^2}$ and $\delta_l = \tan^{-1} \frac{-C_{kl}}{B_{kl}}$

δ_l is called a phase shift for the l th partial wave

Step 3. Compare it with $\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta)}{r}e^{ikr}$.

How to calculate a scattering amplitude?

$$\psi_k(\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)\, i^l R_l(r) P_l(\cos\theta)$$

We substitute the asymptotic expression for the radial function R to this expansion:

$$r \to \infty \qquad \psi_k(\mathbf{r}) \to \sum_{l=0}^{\infty}(2l+1)\, i^l \frac{A_{lk}}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)P_l(\cos\theta)$$

and compare it with $\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta)}{r}e^{ikr}$.

Clearly, we need to transform this expression first. We use the expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty}(2l+1)\, i^l j_l(kr) P_l(\cos\theta).$$

For large r it becomes $e^{i\mathbf{k}\cdot\mathbf{r}} \to \sum_{l=0}^{\infty}(2l+1)\, i^l \frac{1}{kr}\sin\left(kr - \frac{\pi l}{2}\right)P_l(\cos\theta)$

where we used the asymptotic behavior of the spherical Bessel functions.

Step 3. Compare it with $\psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta)}{r} e^{ikr}$.

Next, we match both of the expressions:

$$\psi_k(\mathbf{r}) \to \sum_{l=0}^{\infty} (2l+1)\, i^l \frac{A_{lk}}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l \right) P_l(\cos\theta)$$

$$\parallel$$

$$\psi_k(\mathbf{r}) \to \sum_{l=0}^{\infty} (2l+1)\, i^l \frac{1}{kr} \sin\left(kr - \frac{\pi l}{2} \right) P_l(\cos\theta) + \frac{f(\theta)}{r} e^{ikr}$$

To obtain

$$\sum_{l=0}^{\infty} (2l+1)\, i^l \frac{A_{lk}}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l \right) P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} (2l+1)\, i^l \frac{1}{kr} \sin\left(kr - \frac{\pi l}{2} \right) P_l(\cos\theta) + \frac{f(\theta)}{r} e^{ikr}$$

Step 3. More transformations ...

First, we write out sine functions as exponentials:

$$\sum_{l=0}^{\infty}(2l+1)\,i^l\,\frac{A_{lk}}{2ikr}\left(e^{i\left(kr-\frac{l\pi}{2}+\delta_l\right)}-e^{-i\left(kr-\frac{l\pi}{2}+\delta_l\right)}\right)P_l(\cos\theta)$$

$$=\sum_{l=0}^{\infty}(2l+1)\,i^l\,\frac{1}{2ikr}\left(e^{i\left(kr-\frac{l\pi}{2}\right)}-e^{-i\left(kr-\frac{l\pi}{2}\right)}\right)P_l(\cos\theta)+\frac{f(\theta)}{r}e^{ikr}$$

$$e^{ikr}\sum_{l=0}^{\infty}(2l+1)\,i^l\,\frac{A_{lk}}{2ikr}e^{i\left(-\frac{l\pi}{2}+\delta_l\right)}P_l(\cos\theta)\;-e^{-ikr}\sum_{l=0}^{\infty}(2l+1)\,i^l\,\frac{A_{lk}}{2ikr}e^{i\left(\frac{l\pi}{2}-\delta_l\right)}P_l(\cos\theta)$$

$$=e^{ikr}\sum_{l=0}^{\infty}(2l+1)\,i^l\,\frac{1}{2ikr}e^{-\frac{il\pi}{2}}P_l(\cos\theta)\;-e^{-ikr}\sum_{l=0}^{\infty}(2l+1)\,i^l e^{\frac{il\pi}{2}}\frac{1}{2ikr}P_l(\cos\theta)+e^{ikr}\frac{f(\theta)}{r}$$

Next, we match the coefficients of e^{ikr} and e^{-ikr}.

Step 3. Even more transformations ...
Step 4. Determine $f(\theta)$ from this comparison.

$$e^{ikr}: \sum_{l=0}^{\infty}(2l+1)\, i^l \frac{A_{lk}}{2ikr} e^{i\left(-\frac{l\pi}{2}+\delta_l\right)} P_l(\cos\theta) = \sum_{l=0}^{\infty}(2l+1)\, i^l \frac{1}{2ikr} e^{-\frac{il\pi}{2}} P_l(\cos\theta) + \frac{f(\theta)}{r}$$

$$e^{-ikr}: \sum_{l=0}^{\infty}(2l+1)\, i^l \frac{A_{lk}}{2ikr} e^{i\left(\frac{l\pi}{2}-\delta_l\right)} P_l(\cos\theta) = \sum_{l=0}^{\infty}(2l+1)\, i^l e^{\frac{il\pi}{2}} \frac{1}{2ikr} P_l(\cos\theta)$$

The second equation gives the coefficients A_{kl}: $A_{lk} = e^{i\delta_l}$

We substitute this expression into the first equation and obtain:

Note: $i^l e^{-\frac{il\pi}{2}} = 1$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l}-1\right) P_l(\cos\theta)$$

Therefore, the problem of calculating the differential cross section is reduced to the calculation of the phase shifts.

Step 5. Calculate differential cross section using $\dfrac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2$.

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1)\, e^{i\delta_l} \sin\delta_l \; P_l(\cos\theta) \right|^2$$

$$= \frac{1}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)\; (2l'+1)\; e^{i(\delta_l - \delta_{l'})} \sin\delta_l \; \sin\delta_{l'} \; P_l(\cos\theta) P_{l'}(\cos\theta)$$

The total cross section is given by

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)\; (2l'+1)\; e^{i(\delta_l - \delta_{l'})} \; \sin\delta_l \; \sin\delta_{l'} \int_{-1}^{1} \mathrm{d}(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta)$$

Using the orthogonality condition for Legendre polynomials $\displaystyle\int_{-1}^{1} \mathrm{d}(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1} \delta_{ll'}$

we obtain for the total cross section $\displaystyle\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\; \sin^2\delta_l$

Optical theorem

The scattering amplitude for θ=0 is equal to

$$f(\theta=0)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\,\sin\delta_l\,\underbrace{P_l(1)}_{=1}$$

$$\mathrm{Im}[f(\theta=0)]=\mathrm{Im}\left\{\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\,\sin\delta_l\right\}=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

If we compare this expression with the total cross section

$$\sigma_{tot}=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\;\sin^2\delta_l$$

we obtain

$$\boxed{\sigma_{tot}=\frac{4\pi}{k}\mathrm{Im}\left[f(\theta=0)\right]}$$

Optical theorem

How to calculate phase shifts?

To calculate the phase shifts the radial function is calculated for regions $r<a$ (where potential is significant).

Then, the boundary condition is applied at $r=a$:

$$\left.\frac{1}{R_l}\frac{dR_l}{dr}\right|_{r=a^+} = \left.\frac{1}{R_l}\frac{dR_l}{dr}\right|_{r=a^-} \equiv \gamma_l$$

Using the formula for the wave function at $r > a$ we obtain

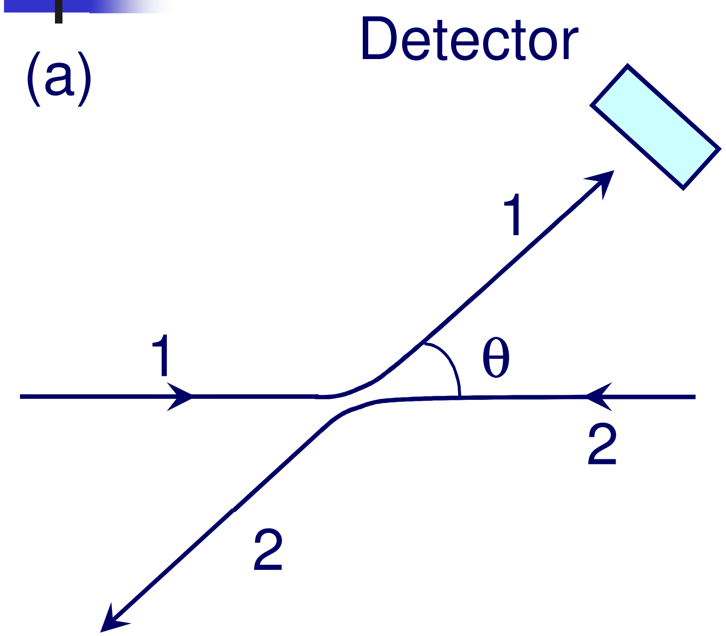
$$\frac{k\left[j_l\,'(ka)\cos\delta_l - n_l\,'(ka)\sin\delta_l\right]}{j_l(ka)\cos\delta_l - n_l(ka)\sin\delta_l} = \gamma_l$$

Therefore, the phase shift can be calculated using

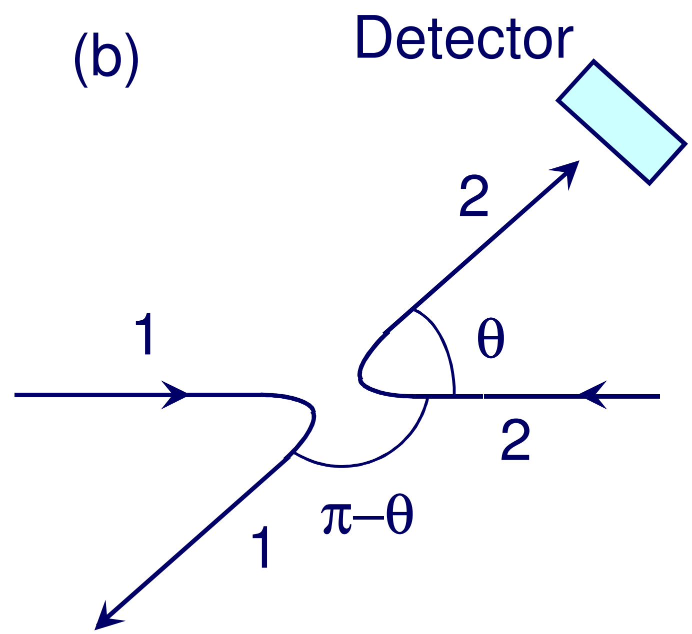
$$\tan\delta_l = \frac{k\ j_l\,'(ka) - \gamma_l\ j_l(ka)}{k\ n_l\,'(ka) - \gamma_l\ n_l(ka)}$$

if the solution R_l is known in the region where potential is significant.

Scattering of two identical particles in the center-of-mass frame



Particle 1 is scattered in the direction (θ,ϕ)



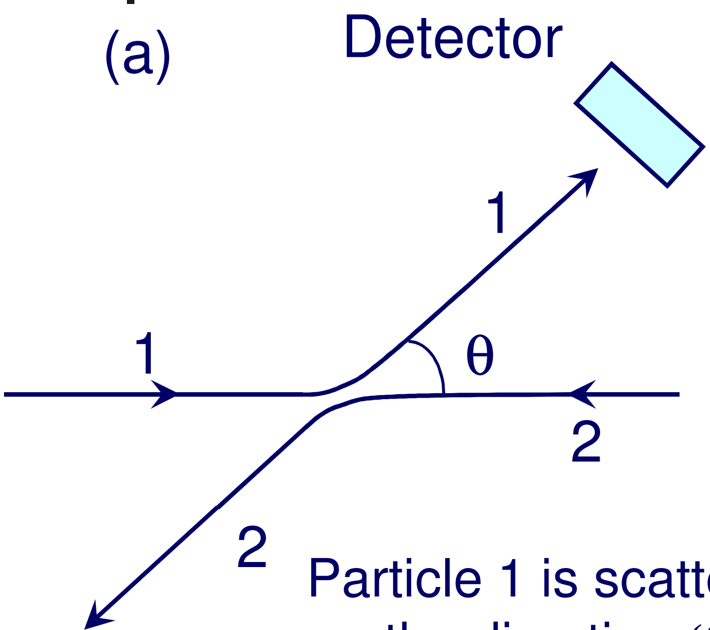
Particle 1 is scattered in the direction $(\pi-\theta,\pi+\phi)$

Since the particles are identical collisional processes (a) and (b) can not be distinguished. In center-of-mass system

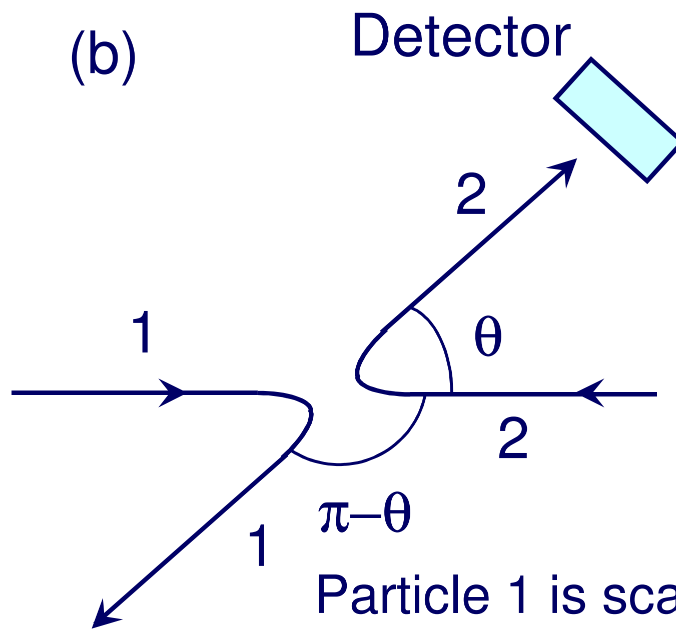
$$\left[-\frac{\hbar^2}{2\mu}\nabla^2+V(\mathbf{r})\right]\psi(\mathbf{r})=E\,\psi(\mathbf{r})$$

where $\mu=m/2$ is the reduced mass, $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$.

Scattering of two identical particles spinless bosons



Particle 1 is scattered in the direction (θ,φ)

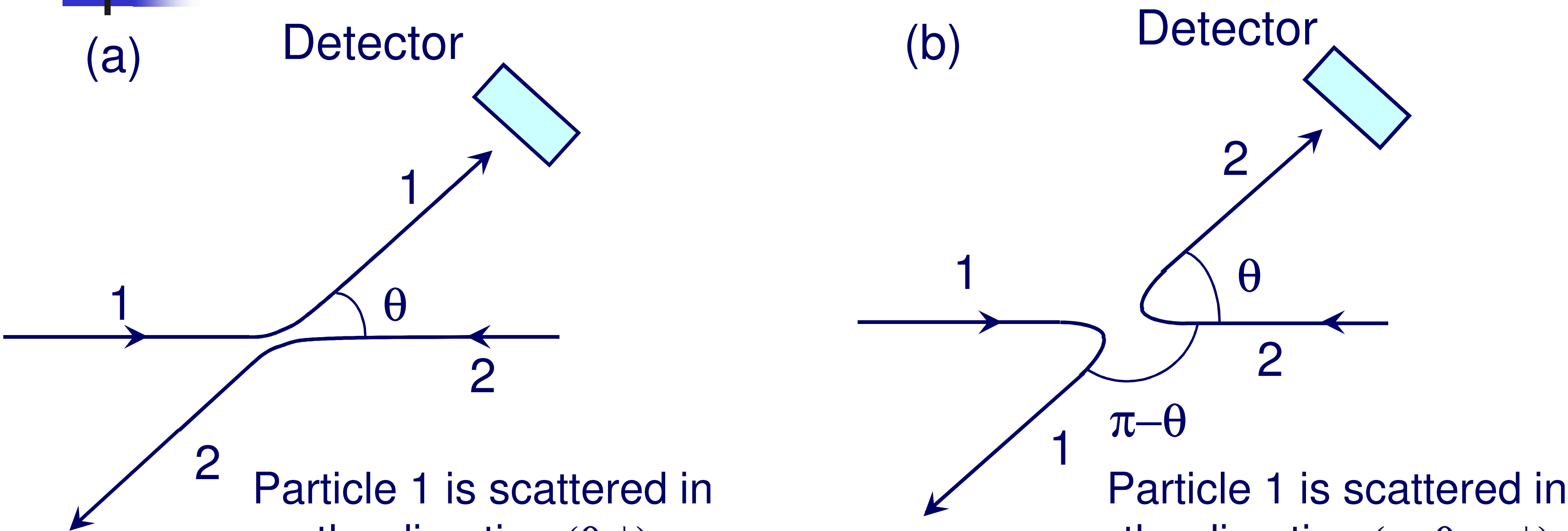


Particle 1 is scattered in the direction (π–θ,π+φ)

In classical mechanics the differential cross section for scattering in the direction (θ,φ) would be simply the sum of differential cross sections for observation of particles 1 and 2 in that direction. If the same were true in quantum mechanics we would obtain the “classical result”

$$\frac{d\sigma_{cl}}{d\Omega} = \left| f(\theta,\pi)\right|^2 + \left| f(\pi-\theta,\phi+\pi)\right|^2 ; \qquad \psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta,\phi)}{r} e^{ikr}$$

Scattering of two identical particles spinless bosons



Particle 1 is scattered in the direction (θ,ϕ)

Particle 1 is scattered in the direction $(\pi-\theta,\pi+\phi)$

In classical mechanics the differential cross section for scattering in the direction (θ,ϕ) would be simply the sum of differential cross sections for observation of particles 1 and 2 in that direction. If the same were true in quantum mechanics we would obtain the "classical result"

$$\cancel{\frac{d\sigma_{cl}}{d\Omega} = \left|f(\theta,\pi)\right|^2 + \left|f(\pi-\theta,\phi+\pi)\right|^2} \; ; \qquad \psi(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta,\phi)}{r} e^{ikr}$$

Scattering of two identical particles: spinless bosons

$$\frac{d\sigma_{cl}}{d\Omega} = |f(\theta,\pi)|^2 + |f(\pi-\theta,\phi+\pi)|^2$$

incorrect result

Spinless bosons: wave function must be symmetric under $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2 : \mathbf{r} \to -\mathbf{r}$.
Clearly, the function $\psi(\mathbf{r})$ which satisfies boundary condition

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow[r\to\infty]{} e^{i\,\mathbf{k}\cdot\mathbf{r}} + \frac{f(\theta,\phi)}{r} e^{ikr}$$

is not symmetric under $\mathbf{r} \to -\mathbf{r}$ interchange. However, we can make a symmetric combination $\psi^+(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + \psi_{\mathbf{k}}(-\mathbf{r});\quad \psi^+(\mathbf{r}) = \psi^+(-\mathbf{r})$.
The corresponding asymptotic form is

$$\psi^+(\mathbf{r}) \xrightarrow[r\to\infty]{} \left(e^{i\,\mathbf{k}\cdot\mathbf{r}} + e^{-i\,\mathbf{k}\cdot\mathbf{r}}\right) + \left[f(\theta,\phi) + f(\pi-\theta,\phi+\pi)\right]\frac{e^{ikr}}{r}$$

since $\mathbf{r} \to -\mathbf{r} : (r,\theta,\phi) \to (r,\pi-\theta,\phi+\pi)$.

Scattering of two identical particles: spinless bosons

Therefore, the differential cross section is

$$\frac{d\sigma}{d\Omega} = \left| f(\theta,\pi) + f(\pi-\theta,\phi+\pi) \right|^2$$

$$= \left| f(\theta,\pi) \right|^2 + \left| f(\pi-\theta,\phi+\pi) \right|^2 + 2\,\mathrm{Re}\left[f(\theta,\pi) f^*(\pi-\theta,\phi+\pi) \right]$$

and the total cross section is

$$\sigma_{tot} = \int \left| f(\theta,\pi) + f(\pi-\theta,\phi+\pi) \right|^2 d\Omega$$

Scattering of two identical spin ½ fermions

Note: we assume that particles interact through central forces.
Total wave function must be antisymmetric with respect of interchanging two particles.

Case 1: Singlet state, S=0 ⇒ the spatial wave function must be symmetric. The corresponding scattering amplitude is

$$\frac{d\sigma_s}{d\Omega} = \left| f_s(\theta) + f_s(\pi - \theta) \right|^2$$

Case 2: Triplet state, S=1 ⇒ the spatial wave function must be antisymmetric. The corresponding scattering amplitude is

$$\frac{d\sigma_t}{d\Omega} = \left| f_t(\theta) - f_t(\pi - \theta) \right|^2$$

Scattering of two identical spin ½ fermions

If the spins of both particles are randomly oriented the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{1}{4}\frac{d\sigma_s}{d\Omega} + \frac{3}{4}\frac{d\sigma_t}{d\Omega}$$

$$= \frac{1}{4}\left|f_s(\theta) + f_s(\pi-\theta)\right|^2 + \frac{3}{4}\left|f_t(\theta) - f_t(\pi-\theta)\right|^2$$

If the interaction is spin-independent, i.e. $f(\theta) = f_t(\theta) = f_s(\theta)$

$$\frac{d\sigma}{d\Omega} = \left|f(\theta)\right|^2 + \left|f(\pi-\theta)\right|^2 - \mathrm{Re}\left[f(\theta)f^*(\pi-\theta)\right]$$

Again, the result is different from the “classical” result.