Quantum Mechanics II

Scattering

Basics;
Scattering Phase-Shift;
Scattering Phase-Shift Examples

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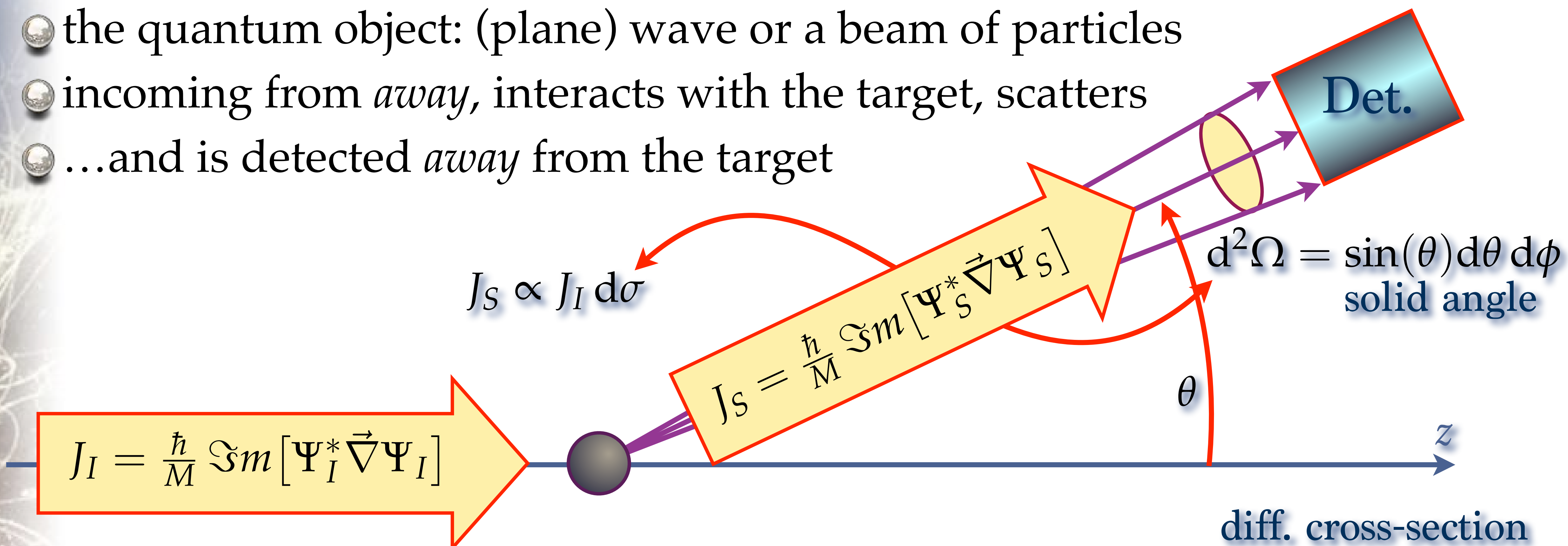
Scattering

Basics

- So far: quantum object (particle or wave)
  - subject to (classical) agents represented by a *surrounding* potential
- Turn this around: the (classical) scattering target is localized
  - the quantum object: (plane) wave or a beam of particles
  - incoming from *away*, interacts with the target, scatters
  - …and is detected *away* from the target

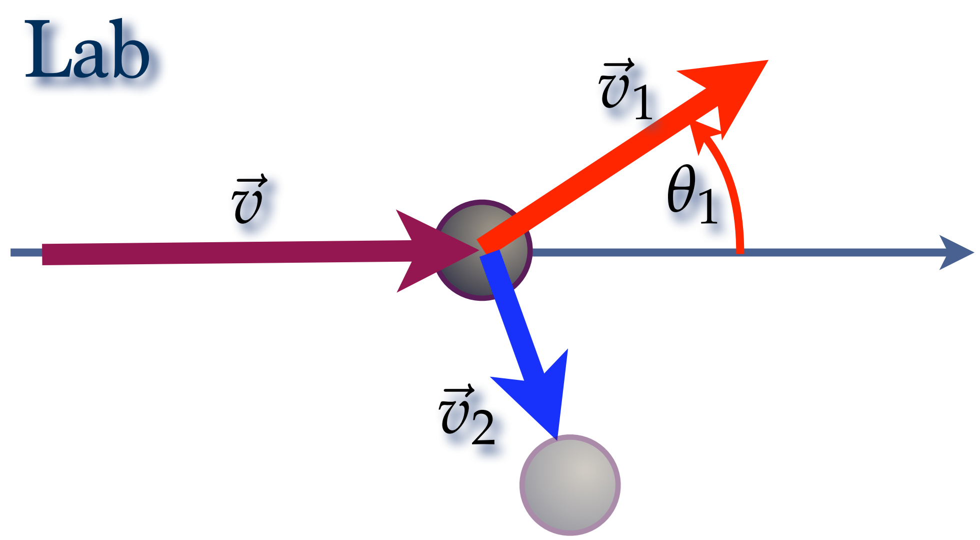


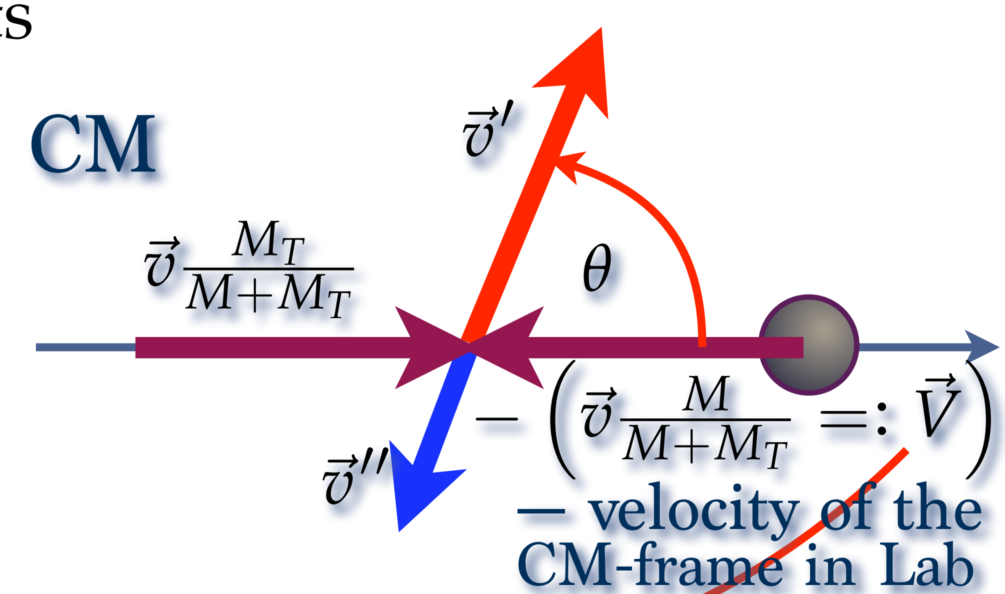
- Determine J_S/J_I as a function of θ: $\frac{J_S}{J_I} = \frac{\mathrm{d}\sigma}{r^2\mathrm{d}^2\Omega} =: \frac{1}{r^2}\underbrace{\left[\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} := \frac{\mathrm{d}\sigma}{\mathrm{d}^2\Omega}\right]}_{:=\,\sigma(\theta,\phi)}$ (diff. cross-section)

Scattering

Basics

- Linear momentum conservation: the target *does* move
  - Calculate in CM (center-of-mass)-frame
  - Compare with Lab-frame measurements





- Must be able to translate between the two

$$\left.\begin{aligned} v_1\cos(\theta_1) &= v'\cos(\theta) + V \\ v_1\sin(\theta_1) &= v'\sin(\theta) \end{aligned}\right\} \Rightarrow \tan(\theta_1) = \frac{\sin(\theta)}{\cos(\theta) + \frac{V}{v'}}$$

in *elastic* collisions speeds are unchanged

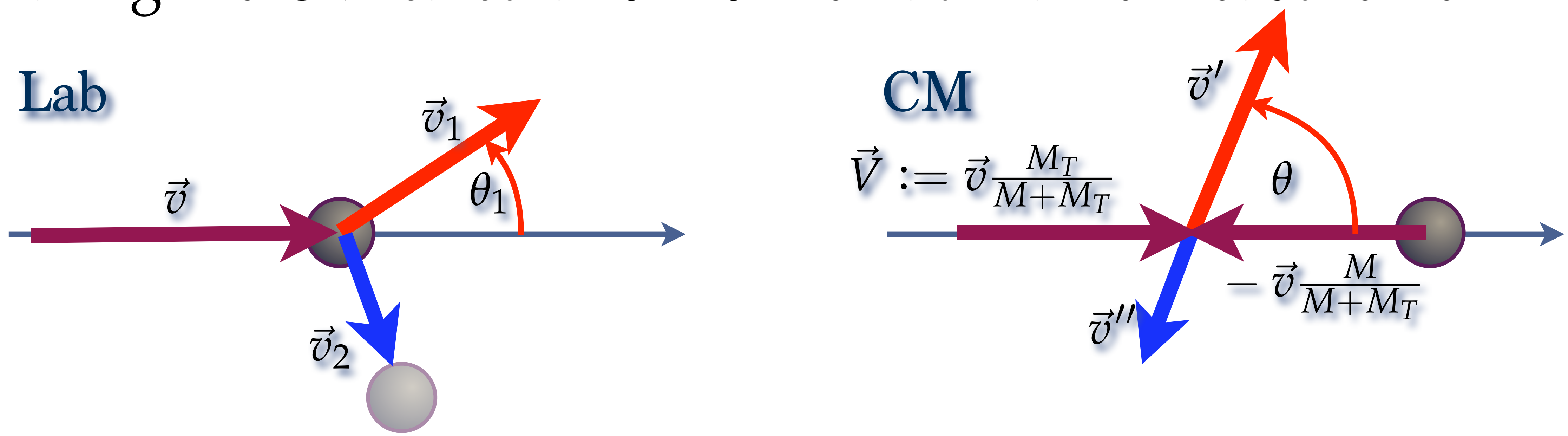
$$\left.\begin{aligned} \tfrac{1}{2}M\left(\tfrac{M_T\,v}{M+M_T}\right)^2 + \tfrac{1}{2}M_T\left(\tfrac{M\,v}{M+M_T}\right)^2 &\overset{!}{=} \tfrac{1}{2}M(v')^2 + \tfrac{1}{2}M(v'')^2 \\ M\left(\tfrac{M_T\,v}{M+M_T}\right) - M_T\left(\tfrac{M\,v}{M+M_T}\right) = 0 &\overset{!}{=} Mv' - M_T v'' \end{aligned}\right\} \Rightarrow \left\{\begin{aligned} v' &= \tfrac{M_T\,v}{M+M_T} \\ v'' &= \tfrac{M\,v}{M+M_T} \end{aligned}\right.$$

Scattering

Basics

$$\tan(\theta_1) = \frac{\sin(\theta)}{\cos(\theta) + \frac{V}{v'}}$$

- Relating the CM-calculation to the Lab-frame measurement:



- in particular, for the "differential cross-section"

$$\sigma_1(\theta,\phi)\,\sin(\theta_1)d\theta_1\,d\phi_1 = \sigma(\theta,\phi)\,\sin(\theta)d\theta\,d\phi$$

$$\underset{\text{Lab}}{\sigma_1(\theta,\phi)} = \sigma(\theta,\phi)\left(\frac{\partial(\theta,\phi)}{\partial(\theta_1,\phi_1)}\right) = \underset{\text{CM}}{\sigma(\theta,\phi)}\,\frac{\sqrt{(1+2\beta\cos(\theta)+\beta^2)^3}}{|1+\beta\cos(\theta)|}$$

$$\beta := \frac{V}{v'}$$

- There is no transformation in ϕ. In fact, for the most part, the target and so the scattered wave will be ϕ-independent. To first order at least.

Scattering

Scattering Phase-Shift

- Scattering is a 2-body interaction

$$\widehat{H} = -\frac{\hbar^2}{2M_1}\vec{\nabla}_1 - \frac{\hbar^2}{2M_2}\vec{\nabla}_2 + W(\vec{r}_1 - \vec{r}_2)$$

$$\vec{R} := \frac{M_1\vec{r}_1 + M_2\vec{r}_2}{M_1+M_2} \qquad \vec{r} := \vec{r}_1 - \vec{r}_2 \qquad \mu := \frac{M_1 M_2}{M_1+M_2}$$

CM-position — relative position — reduced mass

$$\widehat{H} = -\frac{\hbar^2}{2(M_1+M_2)}\vec{\nabla}_{\vec{R}} \;\; -\frac{\hbar^2}{2\mu} + W(\vec{r}) \;\Rightarrow\; \left[-\frac{\hbar^2}{2\mu} + W(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

motion as a whole (free particle) — relative dynamics

$$\psi(\vec{r}) = \psi_I(\vec{r}) + \psi_S(\vec{r})$$

incident — scattered

- Thus

$$\vec{J}_I := \frac{\hbar}{\mu}\,\Im m\left[\psi_I^*(\vec{r})\vec{\nabla}\psi_I(\vec{r})\right] \qquad \vec{J}_S := \frac{\hbar}{\mu}\,\Im m\left[\psi_S^*(\vec{r})\vec{\nabla}\psi_S(\vec{r})\right]$$

- Choose:

$$\psi_I(\vec{r}) = A\,e^{-i\vec{k}\cdot\vec{r}} \qquad \vec{J}_I = |A|^2\frac{\hbar\vec{k}}{\mu} \sim |A|^2\vec{v} \quad \text{uniform plane-wave}$$

$$\psi_S(\vec{r}) = A\,f(\theta,\phi)\,\frac{1}{r}\,e^{-i|\vec{k}||\vec{r}|} \qquad \vec{J}_S = |A|^2|f(\theta,\phi)|^2\frac{\hbar|\vec{k}|}{\mu}\frac{1}{r^2}\hat{\mathrm{e}}_r$$

spherical wave $\oint_{S^2} \mathrm{d}^2\vec{\sigma}\cdot\vec{J}_S = const.$

Scattering

Scattering Phase-Shift

- Simple example: spherical potential

$$\vec{\nabla}^2\psi(\vec{r}) + \big[k^2 - U(r)\big]\psi(\vec{r}) = 0 \qquad k := \frac{\sqrt{2\mu E}}{\hbar} \qquad U(r) := \frac{2\mu}{\hbar^2}W(r)$$

$$\psi(\vec{r}) = \sum_{\ell\, m} a_{\ell\, m}\, Y_\ell^m(\theta,\phi)\,\frac{u_\ell(r)}{r} \qquad u_\ell''(r) + \Big[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\Big]u_\ell(r) = 0$$

- Now: for very large r, ignore $U(r)$ and the centrifugal barrier

$$u_\ell''(r) + k^2 u_\ell(r) \sim 0 \quad \text{for } r \to \infty \qquad \Rightarrow \qquad u_\ell(r) \sim e^{\pm ikr}$$

- BTW, the Coulomb potential cannot be ignored for large r!
- Restrict to "short-range" potentials
- Know: $$\psi_I = e^{i\vec{k}\cdot\vec{r}} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos(\theta))$$
- Try: $$\psi = \psi_I + \psi_S = \sum_\ell (2\ell+1)\, i^\ell\, A_\ell\, R_\ell(r)\, P_\ell(\cos(\theta))$$
  - satisfying

$$\frac{1}{r}\Big[\frac{d^2}{dr^2}(rR_\ell)\Big] + \Big[k^2 - U - \frac{\ell(\ell+1)}{r^2}\Big]R_\ell = 0$$

where U = 0, spherical Bessel eq.

Scattering

Scattering Phase-Shift

$$\psi = \sum_\ell (2\ell+1)\, i^\ell A_\ell\, R_\ell(r)\, P_\ell(\cos(\theta))$$

$$\psi_I = e^{i\vec{k}\cdot\vec{r}} = \sum_\ell (2\ell+1)\, i^\ell j_\ell(kr)\, P_\ell(\cos(\theta))$$

- As the solution of the spherical Bessel equation,

$$R_\ell = a_\ell\, j_\ell(kr) + b_\ell\, n_\ell(kr) \qquad a_\ell^2 + b_\ell^2 = 1$$

$$= \cos(\delta_\ell)\, j_\ell(kr) + \sin(\delta_\ell)\, n_\ell(kr)$$

$$\sim \cos(\delta_\ell)\,\frac{\sin(kr-\frac{1}{2}\pi\ell)}{kr} + \sin(\delta_\ell)\,\frac{-\cos(kr-\frac{1}{2}\pi\ell)}{kr} \quad \text{for } kr \gg 1$$

at the detector!

$$\sim \frac{\sin(kr-\frac{1}{2}\pi\ell + \delta_\ell)}{kr}$$

phase-shift

  - The phase-shifts are not multiples of $\pi/2$ and $n_\ell(kr)$ is not ruled out
  - …because the origin (where the $n_\ell(kr)$ diverge) is excluded by the target
- Equating

$$\psi(\vec{r}) = \psi_I(\vec{r}) + \psi_S(\vec{r}) = \psi_I(\vec{r}) + f(\theta,\phi)\,\frac{e^{ikr}}{r}$$

$$\sum_\ell (2\ell+1) i^\ell P_\ell(\cos(\theta)) \left[A_\ell \frac{\sin(kr-\frac{1}{2}\pi\ell+\delta_\ell)}{kr} - \frac{\sin(kr-\frac{1}{2}\pi\ell)}{kr}\right] = f(\theta,\phi)\,\frac{e^{ikr}}{r}$$

Scattering

Scattering Phase-Shift $\sum_\ell (2\ell+1) i^\ell P_\ell(\cos(\theta)) \Big[A_\ell \frac{\sin(kr-\frac{1}{2}\pi\ell+\delta_\ell)}{kr} - \frac{\sin(kr-\frac{1}{2}\pi\ell)}{kr} \Big] = f(\theta,\phi)\,\frac{e^{ikr}}{r}$

- Equating coefficients of e^{-ikr} (projecting w/ e^{-ikr}):

$$\sum_\ell (2\ell+1) i^\ell P_\ell(\cos(\theta)) \Big[A_\ell \exp(kr-\tfrac{1}{2}\pi\ell+\delta_\ell) - \exp(kr-\tfrac{1}{2}\pi\ell) \Big] = 0$$

- Projecting with $P_\ell(\cos(\theta))$: $\quad A_\ell = e^{i\delta_\ell}$
- Equating coefficients of e^{+ikr} (projecting w/ e^{+ikr}):

$$f(\theta,\phi) = \frac{1}{2ik} \sum_\ell (2\ell+1) i^\ell e^{-\pi\ell/2} \big[e^{2i\delta_\ell} - 1 \big] P_\ell(\cos(\theta))$$

$$= \frac{1}{k} \sum_\ell (2\ell+1)\, e^{i\delta_\ell} \sin(\delta_\ell)\, P_\ell(\cos(\theta))$$

This is indeed independent of ϕ

- Thus: $\quad \sigma(\theta,\phi) = \big| f(\theta,\phi) \big|^2$

$$\sigma := \int d^2\Omega\, \sigma(\theta,\phi) = \frac{4\pi}{k^2} \sum_\ell (2\ell+1) \sin^2(\delta_\ell)$$

- So, calculating $\sigma(\theta,\phi)$ and σ reduces to calculating δ_ℓ.

Scattering

Phase-Shift Examples

$$u_\ell''(r) + \left[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = 0$$

- A spherically limited potential

$$W(r) = \begin{cases} U(r) & \text{for } r < a \\ 0 & \text{for } r \geqslant a \end{cases}$$

- The inside solution $R_\ell(r) = u_\ell(r)/r$ must be regular at $r=0$,
  - so $u_\ell(r) \sim r^b$, we must have $b \geq 1$

$$@r \sim 0 \qquad u_\ell''(r) + \left[-\frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) \sim 0$$

$$b(b-1)r^{b-2} - \ell(\ell+1)r^{b-2} \sim 0 \qquad b = \begin{cases} \ell+1 & \text{regular} \\ -\ell & \text{singular} \end{cases}$$

  - As long as $r^2 U(r) < \infty$ for $r \sim 0$, one solution is regular, one singular
  - Turns out, if $r^4 U(r) \sim \infty$ for $r \sim 0$, both solutions are singular @ $r \sim 0$.
  - Assume that $r^2 U(r) < \infty$ for $r \sim 0$, solve the radial equation, compute

$$\gamma_\ell^{(\text{in})} := \left[\frac{\mathrm{d} \ln\left(r u_\ell^{(\text{in})}(r)\right)}{\mathrm{d}r}\right]_{r \to a}$$

and match this to the logarithmic derivative computed from the outside

  - Matching $u_\ell(r)$ itself will match the amplitudes & the normalization

Scattering

Phase-Shift Examples

$$u_\ell''(r) + \left[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = 0$$

- The outside solution is $R_\ell(r) = \cos(\delta_\ell)\, j_\ell(kr) - \sin(\delta_\ell)\, n_\ell(kr)$
  - so

$$\gamma_\ell^{\text{(out)}} := \left[\frac{\mathrm{d}\ln\big(R_\ell^{\text{(out)}}(r)\big)}{\mathrm{d}r}\right]_{r\to a}$$

$$= \left[\frac{k\big[\cos(\delta_\ell)\, j_\ell'(z) - \sin(\delta_\ell)\, n_\ell'(z)\big]}{\cos(\delta_\ell)\, j_\ell(z) - \sin(\delta_\ell)\, n_\ell(z)}\right]_{z\to ka} \overset{!}{=} \gamma_\ell^{\text{(in)}}$$

  - This is the equation that determines the phase-shifts, δ_ℓ

$$\tan\delta_\ell = \frac{k\, j_\ell'(ka) - \gamma_\ell^{\text{(in)}}\, j_\ell(ka)}{k\, n_\ell'(ka) - \gamma_\ell^{\text{(in)}}\, n_\ell(ka)}$$

  - Quick example: impenetrable sphere. The inside solution = 0, $\gamma_\ell^{\text{(in)}} \to \infty$

$$\tan\delta_\ell = \frac{j_\ell(ka)}{n_\ell(ka)}$$

$$j_\ell(z) = 2^\ell z^\ell \sum_{s=0}^{\infty} \frac{(-1)^s (s+\ell)!}{s!(2s+2\ell+1)!} z^{2s} \approx \frac{z^\ell}{(2\ell+1)!!}$$

$$n_\ell(z) = \frac{(-1)^{\ell+1}}{2^\ell z^{\ell+1}} \sum_{s=0}^{\infty} \frac{(-1)^s (s-\ell)!}{s!(2s-2\ell)!} z^{2s} \approx -\frac{(2\ell-1)!!}{z^{\ell+1}}$$

$z \ll 1$

$$\tan\delta_\ell \approx -\frac{(2\ell+1)}{[(2\ell+1)!!]^2}(ka)^{2\ell+1} \qquad ka \ll 1$$

Lowest-ℓ terms contribute most.

Scattering

Phase-Shift Examples

$$\tan\delta_\ell \approx -\frac{(2\ell+1)}{[(2\ell+1)!!]^2}(ka)^{2\ell+1} \quad ka \ll 1$$

- For very low energies, $ka \ll 1$,

$$\sigma = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2(\delta_\ell) = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\frac{\tan^2(\delta_\ell)}{1+\tan^2(\delta_\ell)}$$

$$\approx \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\tan^2(\delta_\ell) = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\left(-\frac{(2\ell+1)}{[(2\ell+1)!!]^2}(ka)^{2\ell+1}\right)^2$$

$$= 4\pi a^2\left[1 + \tfrac{1}{3}(ka)^4 + \tfrac{1}{405}(ka)^8 + \dots\right]$$

rapid convergence

4 × the geometric cross-section

- For very high energies,

$$\tan(\delta_\ell) = \frac{j_\ell(ka)}{n_\ell(ka)} \approx \frac{\frac{1}{ka}\sin(ka-\ell\pi/2)}{-\frac{1}{ka}\cos(ka-\ell\pi/2)} = -\tan\left(ka-\ell\tfrac{\pi}{2}\right)$$

must sum over all ℓ

- Summation (Sakuri, 1982) produces $\sigma = 2\pi a^2$
- …still 2 × the geometric cross-section

Scattering

Phase-Shift Examples

$$u_\ell''(r) + \left[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = 0$$

- Consider a finite-strength spherical potential barrier
  - $U(r) = V_0 > 0$ for $0 \le r \le a$ (inside), $U(r) = 0$ outside.

$$K_0 := \frac{\sqrt{2MV_0}}{\hbar} \quad k := \frac{\sqrt{2ME}}{\hbar} \quad \varkappa := \sqrt{K_0^2 - k^2}$$

  - Focus on $\ell = 0$

$$\underset{0 \le r \le a}{u_0^{(\text{in})}(r)} = \begin{cases} A \sinh(\varkappa r) \\ A' \sin(\varkappa r) \end{cases} \qquad \underset{r \ge a}{u_0^{(\text{out})}(r)} = \sin(kr + \delta_0)$$

  - Equating at $r = a$ the outside and the inside logarithmic derivative

$$ka \cot(ka + \delta_0) \overset{!}{=} \varkappa a \coth(\varkappa a) \quad E < V_0 \quad \delta_0 = \tan^{-1}\left(\tfrac{k}{\varkappa} \tanh(\varkappa a)\right) - ka$$

$$ka \cot(ka + \delta_0) \overset{!}{=} \varkappa' a \cot(\varkappa' a) \quad E > V_0 \quad \delta_0 = \tan^{-1}\left(\tfrac{k}{\varkappa'} \tan(\varkappa' a)\right) - ka$$

  - However, for low energies, $ka \ll 1 \quad k \ll K_0 \quad \varkappa \approx K_0$

$$\tan(\delta_\ell) \sim (ka)^{2\ell+1} \ll 1 \qquad ka + \delta_0 \ll 1 \qquad \cot(ka + \delta_0) \approx \frac{1}{ka + \delta_0}$$

$$\frac{ka}{ka + \delta_0} \approx \frac{K_0 a}{\tanh(K_0 a)} \quad \Rightarrow \quad \delta_0 \approx ka\left(\frac{\tanh(K_0 a)}{K_0 a} - 1\right)$$

$$\sigma_0 \approx 4\pi a^2 \left(\frac{\tanh(K_0 a)}{K_0 a} - 1\right)^2$$

Scattering

Phase-Shift Examples

$$u_\ell''(r) + \left[k^2 - U(r) - \tfrac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = 0$$

- Consider a spherical δ-function bubble
- Focus on $\ell = 0$

$$\int_{a-\epsilon}^{a+\epsilon} \mathrm{d}r\, u_0''(r) = u_0'(a+\epsilon) - u_0'(r-\epsilon) = \tfrac{\lambda}{a} u_0(a)$$

$$\lim_{\epsilon\to 0}\left[\frac{a u_0'(a+\epsilon)}{u_0(a)} - \frac{a u_0'(r-\epsilon)}{u_0(a)}\right] = \lambda$$

- The solution is

$$u_0(r) = \begin{cases} A\sin(kr) & \text{for } r < a \\ \sin(kr+\delta_0) & \text{for } r > a \end{cases}$$

- …for which the boundary condition is

$$k\left[\cot(ka+\delta_0) - \cot(ka)\right] = \lambda$$

- and produces:

$$\delta_0 = \tan^{-1}\left(\frac{\tan(ka)}{1+\lambda\frac{\tan(ka)}{ka}}\right) - ka$$

- while continuity yields:

$$A = \sqrt{\frac{\tan^2(ka)+1}{\tan^2(ka) + \left(1+\lambda\frac{\tan(ka)}{ka}\right)^2}}$$

just like a particle in a hard box

$$E_n \approx \frac{n^2\pi^2\hbar^2}{2\mu a^2}$$

Resonances!

$$\tan(k_n a) \approx 0$$

$$k_n \approx n\frac{\pi}{a}$$

Quantum Mechanics II

Now, go forth and calculate!!

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