AQT May 13th, 2011

Recap: scattering off a central potential

$$V(\vec{x}) = V(r) \qquad r = |\vec{x}|.$$

$$H = \frac{\vec{P}^2}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{2mr^2}\vec{L}^2 + V(r)$$

Obtain the partial wave amplitudes[1] by a product ansatz with fixed $\vec{L}^2$ (eigenvalue $\hbar^2 \ell(\ell+1)$)

$$\psi_\ell(r,\theta,\varphi) = R_\ell(r)\, Y_\ell^m(\theta,\varphi)$$

R_ℓ solves the radial equation

$$-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_\ell}{dr}\right) + \left[\frac{\ell(\ell+1)}{r^2} + U(r)\right]R_\ell = k^2 R_\ell$$

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

Discuss today how to get the $a_\ell(k)$ from the solution R_ℓ.

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[1] scattering amplitude $\quad f(k,\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,a_\ell(k)\,P_\ell(\cos\theta)$

uniform convergence on Rollnik class.

②

Strategy:

1. restrict to a finite-range potential
   ($V(r) = 0$ for $r \geq R$).
   Then for $|\vec{x}| \geq R$, the solution is the one with $V \equiv 0$. Then, we have to satisfy <u>two</u> boundary conditions:
   (a) the one at $|\vec{x}| = R$
   (b) the asymptotic condition (Sommerfeld radiation condition)
   $$\psi(\vec{x}) = e^{ikx_3} + f(k,\theta)\,\frac{e^{ikr}}{r}$$
   Thus, we first need to find the general solution for $V = 0$, then choose coeff's to satisfy (a) and (b). Note that e^{ikx_3} is also a solution for $V = 0$, so we'll also need to express it in terms of radial functions (since $[H, \vec{L}] = 0$, can do this).

[2. This extends by a continuity argument to potentials that decrease faster than $\frac{1}{r}$ as $r \to \infty$.]

3. For $r \leq R$, need to solve the radial Schrö. eq. in that potential, then piece together the solution.

Solution of the radial Schrödinger equation.

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

Introduce dimensionless variables:

$$\rho = kr$$

Write $R_\ell(r) = \tilde{R}_\ell(kr)$. Then $R_\ell' = k\tilde{R}_\ell'$, $R_\ell'' = k^2\tilde{R}_\ell''$

Call $\tilde{U}(kr) = \frac{1}{k^2}U(r)$. Then

$$-\tilde{R}_\ell'' - \frac{2}{\rho}\tilde{R}_\ell' + \left[\frac{\ell(\ell+1)}{\rho^2} + \tilde{U}(\rho)\right]\tilde{R}_\ell = \tilde{R}_\ell$$

Special case $U = 0$:

$$\tilde{R}_\ell'' + \frac{2}{\rho}\tilde{R}_\ell' + \left(1 - \frac{\ell(\ell+1)}{\rho^2}\right)\tilde{R}_\ell = 0.$$

Define W_ℓ by $\tilde{R}_\ell(\rho) = \rho^\ell W_\ell(\rho)$. Then

$$\tilde{R}_\ell' = \ell\rho^{\ell-1}W_\ell + \rho^\ell W_\ell'$$
$$\tilde{R}_\ell'' = \ell(\ell-1)\rho^{\ell-2}W_\ell + 2\ell\rho^{\ell-1}W_\ell' + \rho^\ell W_\ell''$$

so

$$\rho^\ell W_\ell'' + W_\ell'\left[2\ell\rho^{\ell-1} + \frac{2}{\rho}\rho^\ell\right] + W_\ell\left[\ell(\ell-1)\rho^{\ell-2} + \frac{2}{\rho}\ell\rho^{\ell-1} + \left(1 - \frac{\ell(\ell+1)}{\rho^2}\right)\rho^\ell\right] = 0$$

i.e.

$$\boxed{W_\ell'' + \frac{2\ell+2}{\rho}W_\ell' + W_\ell = 0} \qquad (*)_\ell$$

valid for all $\ell \geq 0$.

④ <u>Claim.</u> If w_0 solves $w_0'' + \frac{2}{\rho} w_0' + w_0 = 0$, then w_ℓ, defined recursively by

$$w_{\ell+1} = \frac{1}{\rho} \frac{d}{d\rho} w_\ell ,$$

solves $(*)_\ell$ for all $\ell \geq 1$.

Proof. Induction on ℓ. $\ell = 0$ is given.

$\ell \mapsto \ell+1$. Let w_ℓ solve $(*)_\ell$, and $v = \frac{1}{\rho} w_\ell'$.

By differentiation of $(*)_\ell$, have

$$w_\ell''' + \frac{2\ell+2}{\rho} w_\ell'' + \left(1 - \frac{2\ell+2}{\rho^2}\right) w_\ell' = 0. \quad (**)$$

We have

$$v' = \left(\frac{1}{\rho} w_\ell'\right)' = -\frac{1}{\rho^2} w_\ell' + \frac{1}{\rho} w_\ell''$$

$$v'' = \frac{2}{\rho^3} w_\ell' - \frac{2}{\rho^2} w_\ell'' + \frac{1}{\rho} w_\ell'''$$

$$\overset{(**)}{=} w_\ell''\left(-\frac{2}{\rho^2} - \frac{2\ell+2}{\rho^2}\right) + w_\ell'\left(\frac{2\ell+2}{\rho^3} - \frac{1}{\rho} + \frac{2}{\rho^3}\right)$$

$$= -w_\ell'' \frac{2\ell+4}{\rho^2} + \frac{w_\ell'}{\rho^2} \frac{2\ell+4}{\rho} - \frac{w_\ell'}{\rho}.$$

hence

$$v'' + v = -\frac{2(\ell+2)}{\rho}\left[\frac{w_\ell''}{\rho} - \frac{w_\ell'}{\rho^2}\right] = -\frac{2(\ell+2)}{\rho} v'$$

so $v'' + \frac{2(\ell+1)+2}{\rho} v' + v = 0$

i.e. v solves $(*)_{\ell+1}$.

Thus everything is reduced to solving $(*)_0$,

$$w_0'' + \frac{2}{\rho} w_0' + w_0 = 0.$$

Let $v_0 = \rho w_0$. Then

$$w_0 = \frac{v_0}{\rho}, \quad w_0' = \frac{v_0'}{\rho} - \frac{1}{\rho^2} v_0, \quad w_0'' = \frac{v_0''}{\rho} - \frac{2}{\rho^2} v_0' + \frac{2}{\rho^3} v_0$$

so

$$w_0'' + \frac{2}{\rho} w_0' + w_0 = \frac{1}{\rho}(v_0'' + v_0) = 0$$

$$\Leftrightarrow \quad v_0'' + v_0 = 0.$$

Thus v_0 is a linear combination of $\sin\rho, \cos\rho$, (or of $e^{i\rho}, e^{-i\rho}$), and w_ℓ is a lin comb. of spherical Bessel functions:

$$j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho} \qquad \text{Bessel}$$

$$n_\ell(\rho) = \text{— " ——} \quad \frac{\cos\rho}{\rho} \qquad \text{Neumann}$$

$$h_\ell^{(+)}(\rho) = -i(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{e^{i\rho}}{\rho} \qquad \text{Hankel of 1}^{\text{st}} \text{ kind}$$

$$h_\ell^{(-)}(\rho) = i(-\rho)^\ell \text{ — " ——} \quad \frac{e^{-i\rho}}{\rho} \qquad \text{— " —— 2}^{\text{nd}} \text{ kind.}$$

Of course, $h_\ell^{(-)}(\rho) = \overline{h_\ell^{(+)}(\rho)}$, $h_\ell^{(+)}(\rho) = j_\ell(\rho) + i n_\ell(\rho)$.

⑥ Asymptotic behaviour

small ρ: n_ℓ, $h_\ell^{(\pm)}$ are singular, j_ℓ is regular.

$$j_\ell(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \rho^{2k}$$

lowest contr. term is $k=\ell$ $\rightarrow$ $2\ell(2\ell-2)\cdots 2 = 2^\ell \ell!$

minus sign cancels

$$\rightarrow j_\ell(\rho) = \rho^\ell \cdot \frac{2^\ell \ell!}{(2\ell+1)!} + O(\rho^{\ell+2}) \quad \text{for } |\rho| \text{ small}$$

$$n_\ell(\rho) = -\frac{(2\ell+1)!}{2^\ell \ell!} \frac{1}{\rho^{\ell+1}} + O(\rho^{-\ell}) \quad \text{—''—}$$

$\rho \to \infty$

$$(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho} = (-\rho)^\ell \left[\frac{1}{\rho^{\ell+1}} \left(\frac{d}{d\rho}\right)^\ell \sin\rho + O\left(\frac{1}{\rho^{\ell+2}}\right)\right]$$

$$= \frac{1}{\rho}\left(-\frac{d}{d\rho}\right)^\ell \sin\rho + O\left(\frac{1}{\rho^2}\right)$$

$$= \frac{1}{\rho}\sin\left(\rho - \ell\frac{\pi}{2}\right) + O\left(\frac{1}{\rho^2}\right)$$

$$\left(-\frac{d}{dx}\sin x = -\cos x = \sin\left(x - \frac{\pi}{2}\right)\right)$$

Thus, for $\rho \to \infty$,

$$j_\ell(\rho) = \frac{1}{\rho}\sin\left(\rho - \ell\frac{\pi}{2}\right) + O\left(\frac{1}{\rho^2}\right)$$

$$n_\ell(\rho) = -\frac{1}{\rho}\cos\left(\rho - \ell\frac{\pi}{2}\right) + O\left(\frac{1}{\rho^2}\right)$$

$$h_\ell^{(1)}(\rho) = -\frac{i}{\rho}e^{i(\rho - \ell\frac{\pi}{2})} + \dots$$

Expansion for the plane wave.

only j_ℓ can contribute because $e^{ik\rho\cos\theta}$ is regular at $\rho = 0$.

$$e^{ikx_3} = e^{i\overbrace{kr}^{\rho}\cos\theta} = \sum_{\ell=0}^{\infty} c_\ell\, j_\ell(\rho)\, P_\ell(\cos\theta)$$

$$Y_\ell^0(\theta,\varphi) = \sqrt{\tfrac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) \qquad \qquad \frac{2^\ell \ell!}{(2\ell+1)!}\rho^\ell + \dots$$

conv. in L^2 sense at fixed ρ, but LHS is analytic in ρ and $w = \cos\theta$. Thus, compare coeff's of ρ^ℓ, and then use

$$P_\ell(w) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dw}\right)^\ell (w^2-1)^\ell = \frac{(2\ell)!}{2^\ell(\ell!)^2}w^\ell + O(w^{\ell-1})$$

$$\frac{i^\ell \rho^\ell w^\ell}{\ell!} = c_\ell \frac{2^\ell \ell!}{(2\ell+1)!}\rho^\ell \cdot \frac{(2\ell)!}{2^\ell(\ell!)^2}w^\ell + \dots$$

$$\Longrightarrow \boxed{c_\ell = i^\ell(2\ell+1)}$$

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\underbrace{j_\ell(kr)}_{\frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2}\right)} P_\ell(\cos\theta)$$

$r \to \infty$

$$= \frac{1}{k}\sum(2\ell+1)\, i^\ell\, \frac{e^{i(kr-\ell\frac{\pi}{2})} - e^{-i(kr-\ell\frac{\pi}{2})}}{2ir} P_\ell(\cos\theta)$$

$$f(k,\theta)\frac{e^{ikr}}{r} = \frac{1}{k}\sum(2\ell+1)\, a_\ell(k)\,\frac{e^{ikr}}{r} P_\ell(\cos\theta).$$

e^{-ikr} needs to get cancelled.

8

Finite-range potential U: continuous spectrum & eigenfunctions.

$U(r) = 0$ for $r \geq R$. Thus for $r \geq R$,

$$R_\ell(r) = B_\ell \left(h_\ell^{(-)}(kr) + S_\ell(E)\, h_\ell^{(+)}(kr) \right) \qquad (\ast\ast\ast)$$

$\left(E = \frac{\hbar^2 k^2}{2m}\right)$ B_ℓ, $S_\ell(E)$ constants (in r) of the general solution.

(We shall choose B_ℓ such that the first term cancels the $\frac{e^{-ikr}}{r}$ piece of the plane wave)

Claim: $|S_\ell(E)| = 1$.

Proof. ψ solves $H\psi = E\psi$, ψ is independent of t.
Thus $\Psi_t = e^{-\frac{i}{\hbar}Et}\psi$ solves $i\hbar\dot{\Psi} = H\Psi$, hence
$\frac{\partial}{\partial t}|\Psi_t|^2 + \nabla \cdot J_{\Psi_t} = 0$. But $|\Psi_t|^2 = |\psi|^2$ is
independent of t, so $\nabla J_{\Psi_t} = 0 \rightarrow \nabla J_\psi = 0$.
In particular, $\frac{\partial}{\partial r} J_r = 0$.

$$J_r = \mathrm{Re}\Big(\overline{\psi}(r,\theta,\varphi)\, \tfrac{\hbar}{mi} \underbrace{\nabla}_{\to \frac{\partial}{\partial r}} \psi(r,\theta,\varphi)\Big)_r = \tfrac{\hbar}{m}|Y_\ell^m(\theta,\varphi)|^2\, \mathrm{Re}\Big(\overline{R_\ell(r)} \cdot \tfrac{\partial}{\partial r} R_\ell(r)\Big)$$

For large r,

$$J_r \sim \frac{1}{r^2}\left(1 - |S_\ell(E)|^2\right)$$

[$\frac{d}{d\rho}(-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{e^{\pm i\rho}}{\rho}$: the leading term as $r \to \infty$ is again the one where the action $\frac{d}{d\rho}$ acts on $e^{\pm i\rho}$, so $\frac{\partial}{\partial r} R_\ell \sim (-h_\ell^{(-)} + S_\ell h_\ell^{(+)})$

$$\mathrm{Re}\,\overline{(h_\ell^{(-)} + S_\ell h_\ell^{(+)})}\,(-h_\ell^{(-)} + S_\ell h_\ell^{(+)}) = -|h_\ell^{(-)}|^2 + |S_\ell|^2 |h_\ell^{(+)}|^2 \sim \frac{1}{r^2}(1 - |S_\ell|^2)$$

Thus $S_\ell(E) = e^{2i\delta_\ell(E)}$ with $\delta_\ell(E) \in \mathbb{R}$,

and

$$R_\ell(r) = B_\ell e^{i\delta_\ell}\left(h_\ell^{(-)}(kr)e^{-i\delta_\ell} + h_\ell^{(+)}(kr)e^{i\delta_\ell}\right)$$

$$= 2B_\ell e^{i\delta_\ell}\left(j_\ell(kr)\cos\delta_\ell - n_\ell(kr)\sin\delta_\ell\right)$$

<u>Asymptotic condition.</u>

For $r \geq R$, $\psi(r,\theta,\varphi) \sim e^{ikr\cos\theta} + f(k,\theta)\frac{e^{ikr}}{r}$

so ψ is independent of φ, (1) Write

$$\psi(r,\theta) = \sum_{\ell \geq 0} R_\ell(r)\, P_\ell(\cos\theta) \cdot i^\ell (2\ell+1)$$

with R_ℓ as in ~~(xxx)~~.

$$\left(\psi(r,\theta) - e^{ikr\cos\theta}\right) \sim f(k,\theta)\frac{e^{ikr}}{r} \qquad (4*)$$

contains only e^{ikr}/r as $r \to \infty$. Thus we require the $h_\ell^{(-)}$ term to cancel the $h_\ell^{(-)}$ in $e^{ikr\cos\theta}$. Since $j_\ell(kr) = \frac{1}{2}(h_\ell^{(+)} + h_\ell^{(-)})$ it follows that $B_\ell = \frac{1}{2}$.

The coefficient of $h_\ell^{(+)}$ is then obtained by comparing coefficients in ~~the asymptotics of~~ (4*):

(1) better? a factor $e^{im\varphi}$ is irrelevant for $|f(k,\theta)|$?

10

Hankel asymptotics

$$\frac{1}{2}\left(S_\ell(E)-1\right) h_\ell^{(1)}(kr) \sim \frac{1}{2}\left(e^{2i\delta_\ell(E)}-1\right)\left(\frac{-i}{kr}\right) e^{i\left(kr-\ell\frac{\pi}{2}\right)} \quad i^{\ell} \quad i^{-\ell}$$

$$\sim \frac{e^{ikr}}{kr}\, a_\ell(k)$$

$$\rightarrow a_\ell(k) = \frac{1}{2i}\left(e^{2i\delta_\ell(E)}-1\right) = e^{i\delta_\ell}\sin\delta_\ell .$$

The optical theorem

$$\operatorname{Im} f(k,0) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\, \underbrace{\operatorname{Im}(a(k))}_{\sin^2\delta_\ell} \cdot \underbrace{P_\ell(1)}_{1}$$

$$= \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

On the other hand

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int |f(k,\theta)|^2 d\Omega = \frac{4\pi}{k^2}\sum(2\ell+1)\underbrace{|a_\ell(k)|^2}_{\sin^2\delta_\ell},$$

$$\Longrightarrow \boxed{\sigma = \frac{4\pi}{k}\operatorname{Im} f(k,0)}$$

total cross section

Im of forward scattering amplitude