1992

Φ 507 Problems Assigned: 4/27. Due: 5/4/92. file $\mathcal{H}14$ (14)

(44) Using the first Born approximation, find the differential and total scattering cross-sections for the central potentials: (A) $V(r) = V_0\, e^{-\alpha r}$, (B) $V(r) = V_0\, e^{-\alpha^2 r^2}$. With α held cnst, adjust V_0 so that each potential has the same "volume", i.e. so that $\int_0^\infty V(r)\cdot 4\pi r^2 dr = \Lambda$, cnst. Intercompare your results for $\frac{d\sigma}{d\Omega}$ & σ in parts (A) & (B).

[illegible] [20 pts]. The Green's fcn K for the time-dependent Schrödinger Eq. in prob #(43), viz. $K(\mathbf{r},t;\mathbf{r}_0,t_0) = \theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\, u_n(\mathbf{r})\, e^{-i\omega_n(t-t_0)}$ is hard to evaluate explicitly. Here we reformulate the "scattering problem" [i.e. how $\psi(\mathbf{r},t)$ evolves from some initial state $\psi(\mathbf{r}_0,0)$ by repeated interactions with a potential V] in terms of K_0, the Green's fcn for a free particle, which can be handled. As a compact notation, let $\xi = (x,t)$ stand for a space-time point ($x = x$ in 1D, $x = \mathbf{r}$ in 3D, etc.). Let $\hbar = 1$, and write $\mathcal{H}_0 = -(1/2m)\,\partial^2/\partial x^2$ for the free-particle Hamiltonian. The free-particle Green's fcn is then defined (1): $(i\frac{\partial}{\partial t} - \mathcal{H}_0) K_0(\xi,\xi') = i\,\delta(\xi-\xi')$, for $t > t'$, and zero otherwise. The Schrödinger Eq. (2): $(i\frac{\partial}{\partial t} - \mathcal{H}_0)\psi(\xi) = U(\xi)\psi(\xi)$, where now $U(\xi)$ now contains all interactions [$U(\xi) = V(\mathbf{r})\{\text{binding}\} + W(\xi)\{\text{coupling}\}$, W on @ $t=0$].

(A) Show that Eqs. (1) & (2) together give the usual integral equation for ψ, i.e. $\psi(\xi) = \phi(\xi) - i\int d\xi'\, K_0(\xi,\xi')\,U(\xi')\,\psi(\xi')$. Here $\phi(\xi) = \int d^3x_0\, K_0(\mathbf{r},t;\mathbf{r}_0,0)\,\psi(\mathbf{r}_0,0)$ is the initial state, and $\int d\xi' = \int_0^{t+} dt' \int_\infty dx'$. We could reference ϕ to $t' = (-)\infty$ [when free].

(B) Now construct K_0. Use above bound-state K, with $u_n(x) \to (1/\sqrt{2\pi})\, e^{ikx}$ for a free particle with energy $\omega_n \to k^2/2m$ in 1D [delta-fcn norm for the plane waves]. Show, when $\sum_n \to \int_{-\infty}^{+\infty} dk$, that: $K_0(\xi,\xi') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\, \exp[ik(x-x') - i\frac{k^2}{2m}(t-t')]$. By judicious choice of a convergence factor, evaluate this integral, and show that in 1D: $K_0(\xi,\xi') = \left(\frac{m/2\pi i}{t-t'}\right)^{1/2} \exp\left[\frac{im}{2}(x-x')^2/(t-t')\right]$. What would K_0 be in 3D? Sketch a graph of how K_0(1D) evolves in space & time.

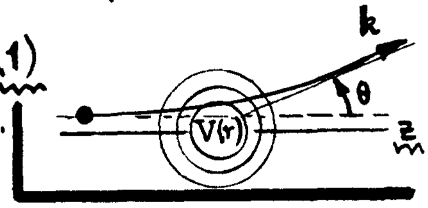
(C) Briefly discuss the successive (Born-type) iterations to the $\psi(\xi)$ integral equation in part (A). The resultant perturbation series is the Feynman-Hellman approach to QM.

(44) $\frac{d\sigma}{d\Omega}$ and σ in Born Approximation for: $V(r) = V_0 e^{-\alpha r}$, $V_0 e^{-\alpha^2 r^2}$.

1. From class notes, p. ScT 13, Eq. (31), the differential scattering cross section is:

$$\rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{2m}{\hbar^2 q}\right)^2 \left| \int_0^\infty r V(r) \sin qr \, dr \right|^2 ; \quad \text{w/ } q = 2k \sin\frac{\theta}{2}, \quad (1)$$

(momentum transfer).



for spherically symmetric potentials. So...

(A) $V(r) = V_0 e^{-\alpha r}$.

tabulated: Dwight # (860.81).

$$\int_0^\infty r V(r) \sin qr \, dr = V_0 \int_0^\infty r e^{-\alpha r} \sin qr \, dr = V_0 \cdot 2\alpha q / (\alpha^2 + q^2)^2. \quad (2)$$

So// $$d\sigma/d\Omega = \left(\frac{4mV_0\alpha}{\hbar^2}\right)^2 / (\alpha^2 + q^2)^4, \quad q = 2k\sin(\theta/2) \text{ as above.} \quad (3)$$

For total cross section $\sigma = \int_{4\pi} (d\sigma/d\Omega) d\Omega$, use $d\Omega = \frac{2\pi}{k^2} q\, dq$*, so here...

$$\rightarrow \sigma = \left(\frac{4mV_0\alpha}{\hbar^2}\right)^2 \frac{2\pi}{k^2} \int_0^{2k} \frac{q\,dq}{(\alpha^2+q^2)^4} = \left(\frac{4mV_0\alpha}{\hbar^2}\right)^2 \frac{\pi}{3k^2} \left[\frac{1}{\alpha^6} - \frac{1}{(\alpha^2 + 4k^2)^3}\right], \text{ Dwight \#(90.4).}$$

So// $$\sigma = \frac{4\pi}{3} \left(\frac{4mV_0}{\hbar^2 \alpha^2}\right)^2 \left[3\alpha^4 + 12\alpha^2 k^2 + 16k^4\right] / (\alpha^2 + 4k^2)^3 \quad (4)$$

(B) $V(r) = V_0 e^{-\alpha^2 r^2}$.

tabulated: Dwight # (861.21)

$$\int_0^\infty r V(r) \sin qr \, dr = V_0 \int_0^\infty r e^{-\alpha^2 r^2} \sin qr \, dr = V_0 \cdot (q\sqrt{\pi}/4\alpha^3) e^{-q^2/4\alpha^2}. \quad (5)$$

So// $$d\sigma/d\Omega = \pi \left(\frac{mV_0}{2\hbar^2 \alpha^3}\right)^2 e^{-q^2/4\alpha^2}, \quad q = 2k\sin(\theta/2) \text{ as above.} \quad (6)$$

$$\sigma = \pi \left(\frac{mV_0}{2\hbar^2\alpha^3}\right)^2 \frac{2\pi}{k^2} \int_0^{2k} e^{-(q^2/4\alpha^2)} q\,dq = \left(\frac{\pi m V_0}{\hbar^2 \alpha^2}\right)^2 \frac{1}{k^2}\left[1 - e^{-(k^2/\alpha^2)}\right]. \quad (7)$$

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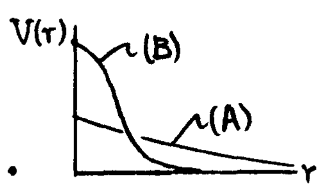
2. Adjust the coefficients V_0 in parts (A) & (B) to same "volume" Λ...

(A) $\Lambda = \int_0^\infty V_0^{(A)} e^{-\alpha r} \cdot 4\pi r^2 dr \Rightarrow V_0^{(A)} = \alpha^3 \Lambda / 8\pi$;

(B) $\Lambda = \int_0^\infty V_0^{(B)} e^{-\alpha^2 r^2} \cdot 4\pi r^2 dr \Rightarrow V_0^{(B)} = \alpha^3 \Lambda / \pi^{3/2}$. (8)



$V_0^{(B)}$ must be (and is) larger than $V_0^{(A)}$ because the Gaussian falls off much faster

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* $d\Omega = 2\pi \sin\theta\, d\theta = 2\pi \left(2\sin\frac{\theta}{2}\right) d\left(2\sin\frac{\theta}{2}\right) = (2\pi/k^2)\, q\, dq$. $0 \leq \theta \leq \pi \Rightarrow 0 \leq q \leq 2k$.

than the exponential. The differential cross-sections in Eqs. (3) & (6) are now:

$$\rightarrow \left(\frac{d\sigma}{d\Omega}\right)_A = \frac{S}{[1+(q^2/\alpha^2)]^4}, \quad \left(\frac{d\sigma}{d\Omega}\right)_B = S\,e^{-\frac{1}{4}q^2/\alpha^2}; \quad q = 2k\sin\frac{\theta}{2};$$

w/ $\underline{S} = (m\Lambda/2\pi\hbar^2)^2 = \text{cnst}$ [S has dim^{n}s of an area]. (9)

And the total cross sections of Eqs. (4) & (7) can be written as:

$$\rightarrow \sigma_A = 4\pi S\left\{\frac{1+4\epsilon+(16/3)\epsilon^2}{(1+4\epsilon)^3}\right\}, \quad \sigma_B = 4\pi S\left\{\frac{1}{\epsilon}(1-e^{-\epsilon})\right\};$$

w/ $\underline{\epsilon} = k^2/\alpha^2 = (2m/\hbar^2\alpha^2)E$, a dimensionless energy parameter. (10)

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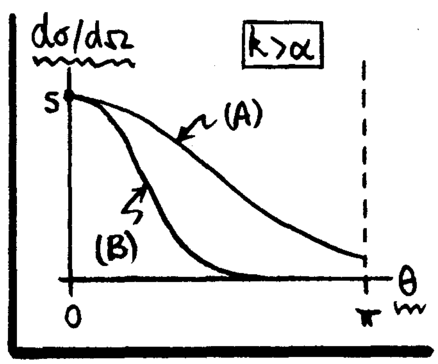
3. In above forms, we can intercompare the scattering effects of the long-range potential $V_A(r) = V_0^{(A)}\exp[-(\alpha r)]$ and the short-range $V_B(r) = V_0^{(B)}\exp[-(\alpha r)^2]$. The following points are relevant...

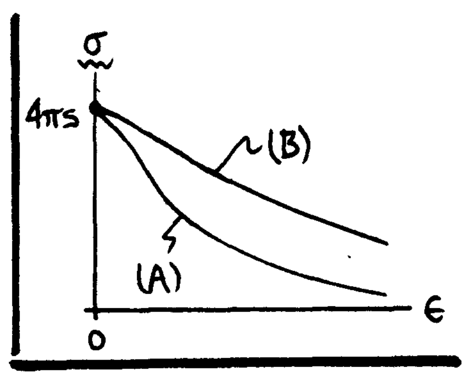
(1) Re $d\sigma/d\Omega$... (A) & (B) are the same at $\theta = 0$, but (for fixed k), (B) falls off much more rapidly as $\theta > 0$. If $k > \alpha$, there is much smaller chance of backscattering from the short-range potential (B).



(2) Re σ... (A) & (B) again start out the same at ~ zero energy ϵ, but now (A) falls off more rapidly:

$$\sigma_A \simeq \begin{cases} 4\pi S\{1-8\epsilon\}, & \text{as } \epsilon \to 0, \\ 4\pi S\{1/12\epsilon\}, & \text{for } \epsilon \gg 1; \end{cases} \quad (11)$$

$$\sigma_B \simeq \begin{cases} 4\pi S\{1-\frac{1}{2}\epsilon\}, & \text{as } \epsilon \to 0, \\ 4\pi S\{1/\epsilon\}, & \text{for } \epsilon \gg 1. \end{cases} \quad (12)$$



The short-range (well-localized) potential is relatively insensitive to the incoming particle energy -- it acts in the manner of a hard-sphere scatterer.

(45) [20pts]. Scattering via free particle approach (Feynman-Hellmann form$^{\underline{n}}$).

(A) 1. With the defining eqtns: (1) $\left(-i\frac{\partial}{\partial t'}-\mathcal{H}_0'\right)K(\xi,\xi')=i\,\delta(\xi-\xi')$, and (2) $\left(i\frac{\partial}{\partial t'}-\mathcal{H}_0'\right)\psi(\xi')=U(\xi')\psi(\xi')$, where $\hbar=1$, and we have interchanged primed & unprimed variables, the derivation of the integral eqtn proceeds the same way as in part (A) of problem (43). Only difference is that the potential term $V(\xi')$, previously attached to $\mathcal{H}_0'=-\frac{1}{2m}\partial^2/\partial\xi'^2$, now rides with the overall potential: $U(\xi')=V(\xi')$[binding]$+W(\xi')$[coupling]. Thus (1) & (2) imply:

$$\left[\begin{array}{l}\boxed{\psi(\xi)=\phi(\xi)-i\int d\xi'\,K_0(\xi,\xi')U(\xi')\psi(\xi')},\\ \text{w/}\ \phi(\xi)=\int d^3x'\,K_0(\mathbf{r},t;\mathbf{r}',0)\,\psi(\mathbf{r}',0),\ t>0;\ \int d\xi'=\int_0^t dt'\int_\infty d^3x'.\end{array}\right\} \quad (1)$$

This the counterpart of Eq. (5), part (A) of problem (43) solution. $t=0$ is chosen as the reference time when the whole interaction $U(\xi')$ is "turned on".

(B) 2. Construct K_0 from: $K(\xi,\xi')=\sum_n u_n(\mathbf{r})u_n^*(\mathbf{r}')e^{-i\omega_n(t-t')}$. For 1D planewaves:

$$\rightarrow u_n(x)\rightarrow\theta_k(x)=\frac{1}{\sqrt{2\pi}}e^{ikx},\quad \text{so}\ \int_{-\infty}^{\infty}\theta_k^*(x)\theta_{k'}(x)\,dx=\delta(k-k'), \quad (2)$$

Then energy $\omega_n\rightarrow k^2/2m$, and $\sum_n\rightarrow\int_{-\infty}^{\infty}dk$, so free particle K found from:

$$\rightarrow K_0(\xi,\xi')=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,e^{ik(x-x')-i(k^2/2m)(t-t')} \quad (3)$$

NOTE: when $t'\rightarrow t$, $K_0\rightarrow\delta(x-x')$, as is required by closure on the $\{\theta_k(x)\}$.

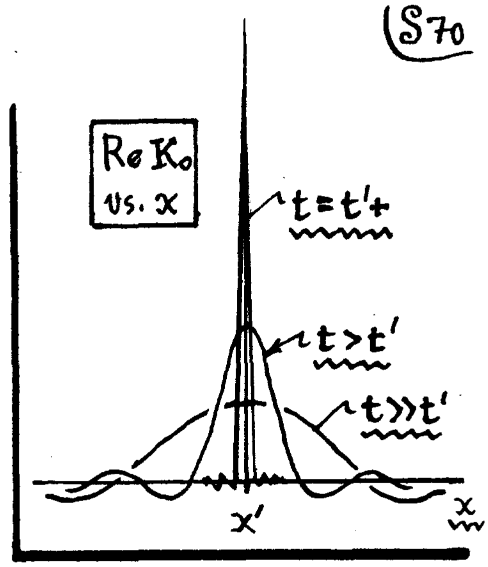
Now write Eq. (3) as...

$$K_0(\xi,\xi')=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-qk^2+ikr}\,dk \quad \text{w/}\ r=(x-x'),\ q=\frac{i}{2m}(t-t'). \quad (4)$$

The integral converges when a small $\mathrm{Re}\,q\rightarrow 0+$ is inserted. Then -- consulting tables [e.g. Gradshteyn & Ryzhik, #(3.323.2)] -- we find

$K_0(\xi,\xi') = \frac{1}{2\pi}\sqrt{\pi/q}\; e^{-r^2/4q}$, or -- as desired:

or $\boxed{K_0(\xi,\xi') = \left(\frac{m/2\pi i}{t-t'}\right)^{\frac{1}{2}} \exp\left\{\frac{im}{2}(x-x')^2/(t-t')\right\}}$ (5)



This is in 1D. Generalization to 3D: just multiply three independent 1D K_0's to get...

$$\left[\!\left[K_0(\xi,\xi') = \left(\frac{m/2\pi i}{t-t'}\right)^{\frac{3}{2}} \exp\left\{\frac{im}{2}|\mathbf{r}-\mathbf{r}'|^2/(t-t')\right\} \right]\!\right] \quad (6)$$

The evolution in x & t for the 1D K_0 is sketched. Initially ($t=t'+$) $K_0 \sim \delta(x-x')$ is well-localized at $x=x'$. As time goes on, K_0 "diffuses" away from x', eventually reaching all space-time points $\xi=(x,t)$.

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3. Absorb the i in Eq. (1) by defining the Green's fcn: $\underline{G_0(\xi,\xi') = -i\,K_0(\xi,\xi')}$.

(c) Then: $\psi(\xi) = \phi(\xi) + \int d\xi_1\, G_0(\xi,\xi_1)\,U(\xi_1)\,\psi(\xi_1)$. First Born Approxn is:

$\rightarrow \psi^{(1)}(\xi) = \phi(\xi) + \int d\xi_1\, G_0(\xi,\xi_1)\,U(\xi_1)\,\phi(\xi_1)$, first Born Approxn, (7)

obtained by replacing $\psi(\xi_1)$ by $\phi(\xi_1)$ in the integral. The iteration continues by defining the n^{th} Born Approxn via [see Eq. (36), p. ScT 15, of class notes]

$\rightarrow \underline{\psi^{(n)}(\xi) = \phi(\xi) + \int d\xi_1\, G_0(\xi,\xi_1)\,U(\xi_1)\,\psi^{(n-1)}(\xi_1)}$, w/ $\psi^{(0)}(\xi) = \phi(\xi)$. (8)

At step n, this procedure yields [see Eq. (37), p ScT 16, of notes]:

$$\left[\!\left[\begin{array}{l} \psi^{(n)}(\xi) = \psi^{(n-1)}(\xi) + \int d\xi_1 \int d\xi_2 \cdots \int d\xi_n\, P_n(\xi;\xi_n,\ldots,\xi_1)\,\phi(\xi_1), \\ \text{w/ } P_n(\xi;\xi_n,\ldots,\xi_1) = G_0(\xi,\xi_n)U(\xi_n)G(\xi_n,\xi_{n-1})U(\xi_{n-1})\cdots G_0(\xi_2,\xi_1)U(\xi_1). \end{array} \right.\right. \quad (9)$$

This is a solution for $\psi(\xi)$ after n "scattering" encounters with $U(\xi)$. $\phi(\xi)$ is the free propagation (via G_0, see Eq. (1)) of the initial state to ξ_1. If $\phi(\xi)$ is referred to $t=-\infty$ (when m was free), we have an overall free-particle soln for ψ.