1993 ϕ 507 Problems   Assigned: 2/26. Due: 3/5/93   \ Y67 file

(7)

(20) In probm (19), the Born Approxn (BA) provided cross-sections for scattering from a spherical well: $V(r)=(-)V_0,\ r<a;\ V(r)\equiv 0,\ r>a$. Evaluate the validity of the BA in this case, per class notes p. ScT 10, Eq.(22). Show that the BA can hold down to ~ zero incident energy, if the well is shallow enough. Discuss the shallowness condition on V_0 w.r.t. formation of possible bound states in the well.

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(21) [15 pts.]. Using the Born Approxn, find both the differential and total scattering cross-sections for the central potentials: (A) $V(r)=V_0 e^{-\alpha r}$, (B) $V(r)=V_0 e^{-\alpha^2 r^2}$, w/ α & V_0 = cnst. Now, with the range parameter α held the same for each $V(r)$, adjust the amplitudes 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. Finally, with this adjustment, intercompare and comment on the results for the $V(r)$'s in (A) & (B).

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(22) [15 pts]. Consider the scattering of an electron from a stationary charge distribution $\rho(\mathbf{r})$ which generates a potential ϕ per Poisson's eqtn: $\nabla^2\phi=-4\pi\rho$.

(A) The scattering potential is $V=-e\phi$. Show that in Born Approxn, the differential cross-section is: $\boxed{\frac{d\sigma}{d\Omega}=\left|\left(\frac{2me}{\hbar^2 q^2}\right)\int \rho(\mathbf{r})\, e^{i\mathbf{q}\cdot\mathbf{r}}\, d^3x\right|^2}$ w/ $\mathbf{q}=\mathbf{k}_{before}-\mathbf{k}_{after}$.

(B) Let $\rho(\mathbf{r})$ be due to an atomic ion w/ nucleus of charge Ze and N electrons distributed per their wavefcns ψ_k, i.e. $\rho(\mathbf{r})=Ze\,\delta(\mathbf{r})-e\sum_{k=1}^{N}|\psi_k(r)|^2$. The atom is randomly oriented, so only the radial dependence of ψ_k is kept; the norm is $\int_0^\infty |\psi_k(r)|\cdot 4\pi r^2 dr=1$. Show that $d\sigma/d\Omega$ of part (A) can be written: $\boxed{d\sigma/d\Omega=(4/a_0^2 q^4)\,|Z-F(q)|^2}$, w/ $a_0=\hbar^2/me^2$. $F(q)$ is the "form factor" for the atomic electrons. Find $F(q)$ and reduce it to a radial integral.

(C) Evaluate $F(q)$ for the single electron in the ground state of the H-atom [i.e. for $\psi(r)=(1/\sqrt{\pi a_0^3})\,e^{-r/a_0}$]. Then, write down the cross-section $(d\sigma/d\Omega)$, and compare it with Sakurai's result ["Modern QM" (Addison Wesley, 1985), p.448].

(20) Validity of Born Approx$^{\underline{n}}$ (BA) for scattering from a spherical well.

1. The BA validity criterion in Eq.(22), p. ScT10, requires evaluating:

$$\rightarrow J(k) = \int_0^\infty [e^{2ikr}-1]V(r)\,dr = \frac{V_0}{k}\int_0^{ka}(1-e^{2ix})\,dx, \text{ for a sph. well;}$$

$$\text{or}/\!/\quad \underline{J(k) = \frac{V_0}{k}[\phi - e^{i\phi}\sin\phi]}, \quad \text{w}/\!/\ \underline{\underline{\phi = ka}} \quad \left(\&\ \hbar k = \sqrt{2mE} = \begin{smallmatrix}\text{incident}\\ \text{momentum}\end{smallmatrix}\right). \qquad (1)$$

The validity condition is...

$$|J(k)|^2 \ll (\hbar\cdot\hbar k/m)^2 = (\hbar^2/ma)^2\phi^2$$

$$\text{or}/\!/\quad \left|(V_0 a)\left[1 - e^{i\phi}\left(\frac{\sin\phi}{\phi}\right)\right]\right|^2 \ll (\hbar^2/ma)^2\phi^2$$

$$\text{or}/\!/\quad \boxed{\phi^2 \gg Q^2\left[1 - 2\cos\phi\left(\frac{\sin\phi}{\phi}\right) + \left(\frac{\sin\phi}{\phi}\right)^2\right]} \int \begin{matrix}\phi = ka,\\ Q = mV_0a^2/\hbar^2.\end{matrix} \qquad (2)$$

For high energies, $\phi \gg 1$, this amounts to $\phi \gg Q$, and -- as usual -- is easily satisfied, so long as Q is not huge. The BA is always a good approxn for high energies.

2. For low energies, $\phi \ll 1$, and the [ ] in Eq. (2) has the expansion...

$$\left[1 - 2\cos\phi\left(\frac{\sin\phi}{\phi}\right) + \left(\frac{\sin\phi}{\phi}\right)^2\right] = \phi^2\left[1 - \tfrac{2}{9}\phi^2 + \dots\right]$$

$$\text{So}/\!/\quad 1 \gg Q^2\left[1 - \tfrac{2}{9}\phi^2\right], \quad \text{or}/\!/\quad \underline{\underline{Q \ll 1 + \tfrac{1}{9}(ka)^2}}, \text{ as } k\to 0. \qquad (3)$$

This low energy validity condition can be satisfied even when $k\to 0$, if the well is shallow enough so that $Q = mV_0a^2/\hbar^2 \ll 1$, i.e. if...

$$\boxed{V_0 \ll \hbar^2/ma^2} \longleftrightarrow \text{for validity of BA down to} \sim \text{zero incident } E. \qquad (4)$$

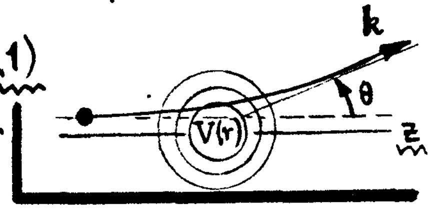
This well is so shallow it cannot even bind the particle in a single state. For if the particle were localized in the well, its momentum would be $p \sim \hbar/a \Rightarrow$ energy $E = p^2/2m \sim \hbar^2/2ma^2 \gg V_0$; V_0 in (4) is insufficient to bind.

(21) [15 pts]. $\frac{d\sigma}{d\Omega}$ & σ in Born Approxn 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 :

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

(momentum transfer).



for spherically symmetric potentials. So...

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

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

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...

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

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

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

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

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

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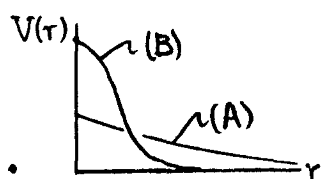
2. Adjust the coefficients V_0 in parts (A) & (B) to same "volume" Λ...

(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:

$$\rightarrow \left(\frac{d\sigma}{d\Omega}\right)_A = \frac{S}{[1+(q^2/\alpha^2)]^4}, \quad \left(\frac{d\sigma}{d\Omega}\right)_B = S\,e^{-\frac{1}{4}q^2/\alpha^2}; \quad q = 2k\sin\frac{\theta}{2}; \tag{9}$$

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

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

$$\rightarrow \sigma_A = 4\pi S\left\{\frac{1+4\epsilon+(16/3)\epsilon^2}{(1+4\epsilon)^3}\right\}, \quad \sigma_B = 4\pi S\left\{\frac{1}{\epsilon}(1-e^{-\epsilon})\right\}; \tag{10}$$

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

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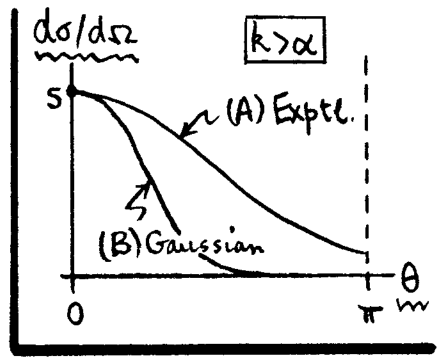
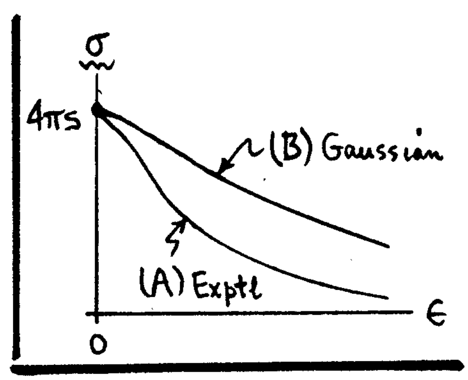
3. In above forms, we can intercompare the scattering effects of the long-range potential $V_A(r) = V_0^{(A)}\exp[-(\alpha r)]$ and the short-range $V_B(r) = V_0^{(B)}\exp[-(\alpha r)^2]$. The following points are relevant...



(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:

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

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

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

㉒ [15 pts]. Electron-Atom Scattering: Born-Approxn $\leftrightarrow$ Form-Factor approach.

(A) 1. If: $\tilde{\phi}(\mathbf{q}) = \int \phi(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3x$, then the inverse is: $\phi(\mathbf{r}) = \frac{1}{(2\pi)^3}\int \tilde{\phi}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3q$, and $\nabla^2\phi = (1/2\pi)^3 \int [-q^2\tilde{\phi}] e^{-i\mathbf{q}\cdot\mathbf{r}} d^3q$. The Fourier-transformed version of Poisson's Eqtn $\nabla^2\phi = -4\pi\rho$ then yields

$$\rightarrow \cancel{\frac{1}{(2\pi)^3}} \int [-q^2\tilde{\phi}] e^{-i\mathbf{q}\cdot\mathbf{r}} d^3q = -4\pi \cdot \cancel{\frac{1}{(2\pi)^3}} \int [\tilde{\rho}] e^{-i\mathbf{q}\cdot\mathbf{r}} d^3q$$

or/ $q^2\tilde{\phi} = 4\pi\tilde{\rho}$, i.e./ $\underline{\underline{\tilde{\phi}(\mathbf{q}) = \frac{4\pi}{q^2}\int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3x}}$ $\int \mathbf{q} = \mathbf{k}_b - \mathbf{k}_a$, $q = 2k\sin(\theta/2)$. (1)

Back in Born's differential scattering cross section, this gives...*

$$\boxed{\frac{d\sigma}{d\Omega} = \left|\left(\frac{me}{2\pi\hbar^2}\right)\tilde{\phi}(\mathbf{q})\right|^2 = \left|\left(\frac{2me}{\hbar^2 q^2}\right)\int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3x\right|^2}. \quad (2)$$

(B) 2. If, for an atom $\left(\begin{smallmatrix}\text{nuclear charge } Ze\\ \text{and } k = 1\rightarrow N \text{ electrons}\end{smallmatrix}\right)$: $\rho(\mathbf{r}) = Ze\,\delta(\mathbf{r}) - e\sum_{k=1}^{N}|\psi_k(r)|^2$, then

$$\rightarrow \int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3x = Ze - e\sum_{k=1}^{N}\int |\psi_k(r)|^2 e^{i\mathbf{q}\cdot\mathbf{r}} d^3x$$

so/
$$\left[\begin{aligned} &\frac{d\sigma}{d\Omega} = (4/a_0^2 q^4)\left|Z - F(q)\right|^2, \quad \text{w/ } \underline{\underline{a_0}} = \hbar^2/me^2 = \text{Bohr radius},\\ &\text{where: } F(q) = \sum_{k=1}^{N}\int |\psi_k(r)|^2 e^{i\mathbf{q}\cdot\mathbf{r}} d^3x \leftarrow \text{"form factor" for atomic electrons}\end{aligned}\right\} \quad (3)$$

The $\measuredangle$ integration in $F(q)$ can be done as in class notes, Eq. (31), p. ScT 13...

so/ $\underline{\underline{F(q) = \frac{4\pi}{q}\sum_{k=1}^{N}\int_0^\infty r|\psi_k(r)|^2 \sin qr\, dr.}}$ (4)

(C) 3. For H-atom ground state, $N=1$ & $\psi(r) = (1/\sqrt{\pi a_0^3})e^{-r/a_0}$. Then, with $\rho = r/a_0$ & $Q = qa_0$, Eq. (4) $\Rightarrow$ $F(q) = \frac{4}{Q}\cdot\int_0^\infty \rho e^{-2\rho}\sin Q\rho\, d\rho = 1/(1+\frac{Q^2}{4})^2$. So (3) gives:

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{4a_0^2}{Q^4}\left[1 - \frac{16}{(Q^2+4)^2}\right]^2} \int q = 2k\sin\frac{\theta}{2}, \; Q = qa_0 \;\&\; a_0 = \frac{\hbar^2}{me^2}. \quad (5)$$

This is $\equiv$ Sakurai's result as cited.

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* $\nabla^2\phi = -4\pi\rho$ gives the potential. The interaction is $-e\phi$ for an incident electron.