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1968 (8)

1993 Φ 507 Problems Assigned: 3/5. Due: 3/12/93.

(23) In problem (22), you showed that for an electron scattering from a charge distribution $\rho(\mathbf{r})$, the transform of the scattering potential important for the Born Approx^n was: $\tilde{V}(\mathbf{q}) = -(4\pi e/q^2)\int \rho(\mathbf{r})\, e^{i\mathbf{q}\cdot\mathbf{r}}\, d^3x$, w/ $\mathbf{q} = \mathbf{k}(\text{before}) - \mathbf{k}(\text{after})$, the momentum transfer.

(A) Put: $\rho(\mathbf{r}) = e\,\delta(\mathbf{r}) - e|\psi(r)|^2$, for e-scattering from a neutral H-atom, with the bound electron in a spherically symmetric eigenstate $\psi(r)$. By inverting the transform $\tilde{V}(\mathbf{q})$, first show that the actual scattering potential can be written as: [10 pts.]

$$V(\mathbf{r}) = -e^2\left[\frac{1}{r} - \int \frac{d^3x'}{|\mathbf{r}-\mathbf{r}'|}|\psi(r')|^2\right].$$

Interpret. Then, for the H-atom ground state: $\psi(r') = (1/\sqrt{\pi a_0^3})\, e^{-r'/a_0}$, w/ $a_0 = \hbar^2/me^2$, find $V(\mathbf{r})$. Show: $V(r) = -\frac{e^2}{a_0}\left(1+\frac{1}{\rho}\right)e^{-2\rho}$, w/ $\rho = r/a_0$. HINT: use the expansion for $1/|\mathbf{r}-\mathbf{r}'|$ per Jackson's Eq. (3.38).

(B) For the $V(r)$ in part (A), evaluate the Born Approx^n "validity criterion" (see class notes: Eq. (22), p. ScT 10). It is convenient to use the dimensionless energy parameter $\lambda = k^2a_0^2 = E/E_H$ (E = incident electron energy; $E_H = e^2/2a_0$ = H-atom ionization). Show that the Born Approx^n fails at low energies, $\lambda \to 0$. Estimate a lower bound for λ, above which the Born Approx^n ~ OK. [10 pts.]

(C) Assume Sakurai's version of the differential cross-section for e→H-atom scattering (as quoted in prob. (22)) is correct: $\frac{d\sigma}{d\Omega} = (4a_0^2/Q^4)\left[1-16/(Q^2+4)^2\right]^2$, w/ $Q = qa_0$, & $q = 2k\sin\frac{\theta}{2}$, θ = scattering ∡. From this, find the total cross-section $\sigma(\lambda)$. [HINT: develop and use the relation: $d\Omega = (2\pi/k^2a_0^2)\,Q\,dQ$]. Find limiting forms for σ for low & high energies. Compare with: $\sigma(\lambda\to 0) = (30\pm 5)\pi a_0^2$, measured; $\sigma(\lambda \gg 1) \simeq 7\pi/3k^2$, per Landau & Lifshitz "QM" (Addison Wesley, 2nd ed. 1965), p. 535. Comments? [10 pts.]

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(24) Consider scattering of an electron from a screened Coulomb potential: $V(r) = -(Ze^2/r)\,e^{-\alpha r}$, by means of partial wave analysis. Using Eq. (32), p. PW 9 of class notes, show that the l^{th} partial wave phase shift $\delta_l(k)$ is given by: $\tan\delta_l(k) = \frac{Z}{ka_0}\,Q_l\left(1+\frac{\alpha^2}{2k^2}\right)$, w/ $a_0 = \hbar^2/me^2$, $k = \sqrt{2mE/\hbar^2}$, and $Q_l(z)$ = Legendre fcn of 2nd kind. Write $\tan\delta_0(k)$ explicitly, and find its limit for $k\to\infty$ & $\alpha > 0$. What happens to the analysis when $\alpha \to 0$?

③ [30 pts]. Born Approxn: total cross-section for electron-H atom scattering.

1. For the density $\rho(\mathbf{r}) = e\,\delta(\mathbf{r}) - e|\psi(r)|^2$, the scattering pot$^{\underline{l}}$ transform is:

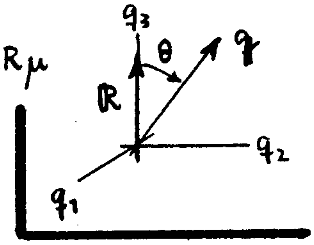
(A) [10 pts]
$$\rightarrow \tilde{V}(\mathbf{q}) = -\frac{4\pi e}{q^2}\int \rho(\mathbf{r})\, e^{i\mathbf{q}\cdot\mathbf{r}} d^3x = -\frac{4\pi e^2}{q^2}\left[1 - \int |\psi(r')|^2 e^{i\mathbf{q}\cdot\mathbf{r}'} d^3x'\right]. \quad (1)$$

The inverse $V(\mathbf{r}) = \frac{1}{(2\pi)^3}\int \tilde{V}(\mathbf{q})\, e^{-i\mathbf{q}\cdot\mathbf{r}} d^3q$ is the desired potential itself, i.e.

$$\rightarrow V(\mathbf{r}) = -\frac{4\pi e^2}{(2\pi)^3}\int d^3q \left(\frac{e^{-i\mathbf{q}\cdot\mathbf{r}}}{q^2}\right)\left[1 - \int e^{i\mathbf{q}\cdot\mathbf{r}'} |\psi(r')|^2 d^3x'\right] \quad (2)$$

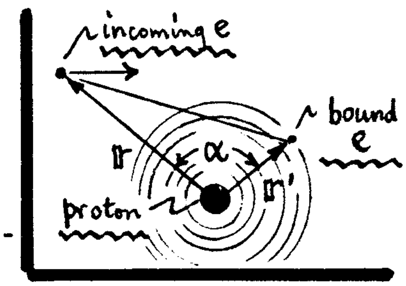
A key integral here is $J(R) = \int d^3q\, (e^{i\mathbf{q}\cdot\mathbf{R}}/q^2)$. In sph. cds. in $\mathbf{q}$-space:

$$\left[\!\left[\; \begin{aligned} J(R) &= \int_0^\infty 2\pi q^2\, dq \int_0^\pi \sin\theta\, d\theta \left(\frac{e^{iqR\cos\theta}}{q^2}\right) = 2\pi \int_0^\infty dq \int_{-1}^{+1} d\mu\, e^{iqR\mu} \\ &= \frac{4\pi}{R}\int_0^\infty dq \left(\frac{\sin qR}{q}\right) = \frac{2\pi^2}{R}, \quad \text{w/ } R = |\mathbf{R}|. \quad (3) \end{aligned} \right.$$



Use of this result in Eq. (2) shows that...

$$V(\mathbf{r}) = -e^2\left[\frac{1}{r} - \int \frac{|\psi(r')|^2}{|\mathbf{r}-\mathbf{r}'|} d^3x'\right]. \quad (4)$$



The first term RHS in (4) is evidently the Coulomb interaction between the incoming e and the proton; the 2nd term is the coupling between the incoming e and the bound e considered as a distribution.

2. To evaluate the integral in (4), expand: $\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^l P_l(\cos\alpha)$, w/ $\alpha = \measuredangle(\mathbf{r}, \mathbf{r}')$ & $P_l(\cos\alpha)$ = Legendre polynomials; this is for $0 \leq r' < r$... when $r < r'$, interchange r & r'.* Since $|\psi(r')|^2$ is spherically symmetric, then in the $\int d^3x'$ integration, all but the $l=0$ terms drop out, so: $1/|\mathbf{r}-\mathbf{r}'| = \frac{1}{r}$, $0 \leq r' < r$, and: $1/|\mathbf{r}-\mathbf{r}'| = \frac{1}{r'}$, $r < r'$. Also $\int d^3x' \rightarrow 4\pi\int_0^\infty r'^2 dr'$. Thus the integral in (4) is

$$\rightarrow \int \frac{|\psi(r')|^2}{|\mathbf{r}-\mathbf{r}'|} d^3x' = 4\pi\left\{\int_0^r \frac{1}{r}|\psi(r')|^2 r'^2 dr' + \int_r^\infty \frac{1}{r'}|\psi(r')|^2 r'^2 dr'\right\}$$

$$= \frac{1}{r} - \frac{e^2}{a_0}\left(1 + \frac{1}{\rho}\right)e^{-2\rho}, \quad \rho = r/a_0. \quad (5)$$

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* Expansion is done in Jackson "Classical Electrodynamics", Eq. (3.38), p. 92.

The last result follows from inserting $\psi(r') = e^{-r'/a_0}/\sqrt{\pi a_0^3}$, w/ $\int_0^\infty |\psi(r')|^2 \cdot 4\pi r'^2 dr = 1$, and performing several elementary integrations. Used in (4), this result gives:

$$\boxed{V(r) = -\frac{e^2}{a_0}\left(1+\frac{1}{\rho}\right)e^{-2\rho}} \quad \rho = r/a_0, \; a_0 = \hbar^2/me^2. \tag{6}$$

as the effective e–H atom scattering potential. As $\rho\to 0$, $V\sim -e^2/r$ shows the usual e-p Coulomb singularity. But as $\rho\to\infty$, V is Yukawa-like, due to screening.

(B) [10 pts] **3.** The Born Approx^n validity condition [Eq. (22), p. ScT 10, class notes] reads in this case:

$$\rightarrow \left|\int_0^\infty [e^{2ika_0\rho}-1]\frac{1}{\rho}(1+\rho)e^{-2\rho}\,d\rho\right|^2 \ll \lambda, \text{ w/ } \underline{\lambda} = k^2a_0^2 = E/(\hbar^2/2ma_0^2),$$

or/ $$\frac{\lambda}{4} \gg \left|\int_0^\infty (1+\rho)e^{-b\rho}\left[\frac{\sin ka_0\rho}{\rho}\right]d\rho\right|^2, \text{ w/ } \underline{b} = 2-ika_0. \tag{7}$$

The integrals are tabulated [Dwight # (861.01) & # (860.80)], with result:

$$\left[\!\left[\frac{1}{4} \gg \left|\frac{1}{ka_0}\tan^{-1}\left(\frac{ka_0}{b}\right)+\frac{1}{b^2+\lambda}\right|^2 = \left|\frac{1}{2i\sqrt{\lambda}}\ln\left(\frac{2+\lambda-i\sqrt{\lambda}}{2+i\sqrt{\lambda}}\right) - \frac{1}{4}\left(\frac{1+i\sqrt{\lambda}}{1+\lambda}\right)\right|^2. \right.\right. \tag{8}$$

For low energy, $\lambda = k^2a^2\to 0$, the inequality requires: $\frac{1}{4} \gg \left|\frac{1}{\sqrt{\lambda}}\tan^{-1}\left(\frac{\sqrt{\lambda}}{2}\right)+\frac{1}{4}\right|^2 \to \frac{9}{16}$, which is certainly not satisfied. For high energies, $\lambda\to$ large, and we need:

$$\rightarrow \frac{1}{4} \gg \left|\frac{1}{2i\sqrt{\lambda}}\ln(\lambda/i\sqrt{\lambda}) - \frac{1}{4}\left(\frac{i\sqrt{\lambda}}{\lambda}\right)\right|^2, \text{ or/ } \underline{4\lambda \gg |(\ln\lambda+1)-i\pi|^2}. \tag{9}$$

The inequality here is fairly flabby... it begins to be obeyed at $\lambda\simeq 4$, and when $\lambda=5$, it reads: $20 \gg 16.7$; $\lambda=10 \Rightarrow 40\gg 20.8$; $\lambda=20\Rightarrow 80\gg 25.8$.

$\underline{\lambda > 10 \text{ is probably a reasonable low-energy bound}}$ for the Born Approx^n to work.

In Eq. (7)'s def^n of λ, note that: $\hbar^2/2ma_0^2 = e^2/2a_0 = E_H$, is the H-atom ionization energy (13.6 eV). So: $\boxed{\lambda = E/E_H}$, and the low-energy bound $\lambda > 10$ means the incident electron energy should be $E > 136$ eV, or so.

(C) [10 pts] **4.** The quoted cross-section $(d\sigma/d\Omega)$ can be written in the form...

$$\rightarrow \frac{d\sigma}{d\Omega} = 4a_0^2\left[(Q^2+8)/(Q^2+4)^2\right]^2, \quad Q = qa_0 = 2ka_0\sin\frac{\theta}{2}. \tag{10}$$

NOTE: $d\sigma/d\Omega$ finite for all Q.

By the hint, develop the solid $\measuredangle$ element $d\Omega$ in terms of Q...

$$\rightarrow d\Omega = 2\pi \sin\theta \, d\theta = 8\pi \sin\frac{\theta}{2}\, d\sin\frac{\theta}{2} = \frac{2\pi}{k^2} q\, dq = \frac{2\pi}{k^2 a_0^2} Q\, dQ. \quad (11)$$

So

$$\sigma(k) = \int_{4\pi} (d\sigma/d\Omega)\, d\Omega = \int_{Q=0}^{Q=2ka_0} 4\cancel{a_0^2}\left[(Q^2+8)/(Q^2+4)\right]^2 \cdot \frac{\pi}{k^2 \cancel{a_0^2}}\, dQ^2$$

or

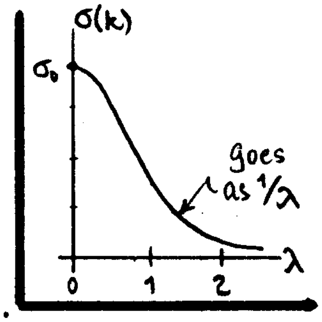
$$\sigma(k) = \frac{4\pi}{k^2}\int_{Q=0}^{Q=2ka_0} \left[(Q^2+8)^2/(Q^2+4)^4\right] dQ^2. \quad (12)$$

Change integration variables in (12) to: $u = \frac{Q^2}{4} + 1$, and put $\underline{\lambda = k^2 a_0^2}$ as in (7)...

$$\rightarrow \sigma(k) = \frac{\pi}{k^2}\int_{u=1}^{1+\lambda} \frac{du}{u^4}(u+1)^2 = \frac{\pi}{k^2}\left(\int \frac{du}{u^2} + 2\int\frac{du}{u^3} + \int\frac{du}{u^4}\right)\Bigg|_{u=1}^{u=1+\lambda}$$

$$= \frac{\pi}{k^2}\left(\frac{1}{u} + \frac{1}{u^2} + \frac{1}{3u^3}\right)\Bigg|_{u=1+\lambda}^{u=1} = \ldots \text{ etc. Finally...}$$

$$\boxed{\sigma(\lambda) = \frac{\pi a_0^2}{3(1+\lambda)^3}\left[12 + 18\lambda + 7\lambda^2\right]}, \text{ w/ } \underline{\underline{\lambda}} = k^2 a_0^2 = E/E_H. \quad (13)$$



σ(k) is finite for all λ, and has the general shape as sketched. In the low and high energy limits, we find...

$$\left.\frac{\text{LOW ENERGY}}{(\lambda \to 0)}\right\}\ \underline{\underline{\sigma(\lambda) \simeq \sigma_0\left(1 - \tfrac{3}{2}\lambda\right)}}, \text{ w/ } \underline{\underline{\sigma_0}} = 4\pi a_0^2; \quad (14)$$

$$\left.\frac{\text{HIGH ENERGY}}{(\lambda \gg 1)}\right\}\ \underline{\underline{\sigma(\lambda) \simeq \frac{7\pi a_0^2}{3\lambda}\left[1 - \left(\tfrac{3}{7}\right)\tfrac{1}{\lambda}\right]}}, \ \underline{\underline{\lambda}} = E/E_H \gg 1. \quad (15)$$

The high energy limit: $\sigma(k) \simeq (7\pi/3k^2)[1 - \ldots]$, agrees exactly with the citation in Landau & Lifshitz. This is where the Born Approx$^{\underline{n}}$ works best. The low energy limit: $\sigma \to \sigma_0 = 4\pi a_0^2$, is significantly below the exptal value: $\sigma_0(\text{expt.}) = (30 \pm 5)\pi a_0^2$. This where the Born Approx$^{\underline{n}}$ is expected to fail -- by the analysis of part (B). And fail it does!

Question: does $V(r)$ of Eq. (4) really make sense? We could make an argument for: $V(r) = -\frac{e^2}{r} + \frac{e^2}{r}\int_0^r |\psi(r')|^2 d^3x' = -\frac{e^2}{a_0}\left[\frac{1}{\rho}(1 + 2\rho + \rho^2)e^{-2\rho}\right]$. Etc.

(24) Analyse phase shifts for scattering from a screened Coulomb potential.

1. Put $V(x) = -(Ze^2/x)\,e^{-\alpha x}$ into the phase shift formula of Eq. (32), p. PW 9 of class notes. Change integration variable to $u = kx$, so that...

$$\rightarrow \tan\delta_l(k) \simeq (2mZe^2/\hbar^2 k)\int_0^\infty e^{-\beta u}\,u\,[j_l(u)]^2\,du, \text{ w/ } \underline{\beta} = \alpha/k. \quad (1)$$

Recall that the spherical Bessel fcns: $j_l(u) = \sqrt{\frac{\pi}{2u}}\,J_{l+\frac{1}{2}}(u)$, w/ J_ν = ordinary Bessel fcn. Then (1) becomes...

$$\rightarrow \tan\delta_l(k) \simeq (\pi m Ze^2/\hbar^2 k)\int_0^\infty e^{-\beta u}[J_\nu(u)]^2\,du, \; \underline{\underline{\nu}} = l + \tfrac{1}{2}. \quad (2)$$

Such integrals are tabulated -- see e.g. Gradshteyn & Ryzhik #(6.612,3), p. 709. Where $Q_l(z)$ = Legendre fcn of the second kind, the result is

$$\boxed{\tan\delta_l(k) \simeq \frac{mZe^2}{\hbar^2 k}\,Q_l\left(1 + \frac{\alpha^2}{2k^2}\right)}, \; l = 0, 1, 2, \ldots \quad (3)$$

NOTE: $me^2/\hbar^2 = 1/a_0$ w/ a_0 = Bohr radius.

2. Information on the Q_l can be found in G&R Secs. (8.82)-(8.83), or the NBS Handbook, Ch. (8). E.g. $Q_0(z) = \frac{1}{2}\ln\left(\frac{z+1}{z-1}\right)$ so the S-wave phase shift for a screened Coulomb potential goes as

$$\underline{\underline{\tan\delta_0(k) \simeq \frac{mZe^2}{2\hbar^2 k}\ln\left(1 + \frac{4k^2}{\alpha^2}\right)}} \rightarrow \frac{mZe^2}{\hbar^2 k}\ln(2k/\alpha) \quad \text{high energy: } k \gg \alpha > 0. \quad (4)$$

Evidently $\delta_0(k) \rightarrow 0$ as $k \rightarrow \infty$, so long as $\alpha > 0$. When $\alpha \rightarrow 0$, $\tan\delta_0(k) \rightarrow \infty$.

3. In general, all the $Q_l(z)$ have the logarithmic singularity just noted, as $z \rightarrow 1$ (i.e. as the screening cnst $\alpha \rightarrow 0$).* So, when $\alpha \rightarrow 0$, (3) reads...

$$\underline{\tan\delta_l(k) \simeq \frac{Z}{ka_0}\ln(2k/\alpha)}, \text{ as } \alpha \rightarrow 0 \; (\text{w/ } a_0 = \hbar^2/me^2 = \text{Bohr rad.}). \quad (5)$$

At $\alpha = 0$, all the phase shifts $\delta_l(k) \rightarrow \frac{\pi}{2}$. The scattering amplitude $f_k(\theta)$ [Eq. (6), p. PW 2] diverges, and the analysis breaks down ($\sigma \rightarrow \infty$, etc.).

*See G&R #(8.831,2): $Q_n(z) = \frac{1}{2}P_n(z)\ln\left(\frac{z+1}{z-1}\right) - \sum_{\lambda=1}^{n}\frac{1}{\lambda}P_{\lambda-1}(z)P_{n-\lambda}(z)$, w/ $P_\nu(1) = 1$.