Phys 492 Spring 2022

HW #7 Solution

Extra, Hund's rule $C = [He](2s)^2(2p)^2$

$l = 2, 1, 0 \quad s = 1, 0$

l	s	$(-1)^l$	Sym spin	j	Spectroscopic term	
0	0	+	−	0	$^1S_0$	
1	0	−	−	1	—	Pauli excluded
2	0	+	−	2	$^2D_2$	
0	1	+	+	1	—	
1	1	−	+	2, 1, 0	$^2P_2$, $^3P_1$, $^3P_0$	
2	1	+	+	3, 2, 1	—	

term is $^3P_0$: higest s, lowest j for $< \frac{1}{2}$ filled subsell.

Short cut: $p \rightarrow l = 1$

$m_l = 1$ ↑

0 ↑

-1 —

$s = \frac{1}{2} + \frac{1}{2} = 1$

$l = 1 \times 1 + 1 \times 0 = 1$

$j = |l - s| = 0$

$^3P_0$

Oxygen $= [He](2s)^2(2p)^4$

$m_l =$

$1 \quad \uparrow\downarrow$

$0 \quad \uparrow$

$-1 \quad \uparrow$

$s = \frac{1}{2} - \frac{1}{2} + \frac{1}{2} + \frac{1}{2} = 1$

$l = 2 \times 1 + 1 \cdot 0 + 1 \cdot (-1) = 1$

$j = l + s = 2$

$3P_2$

Maganese $Mn = [Ar](4s)^2(3d)^5$

m_l

$2 \quad \uparrow$

$1 \quad \uparrow$

$0 \quad \uparrow$

$-1 \quad \uparrow$

$-2 \quad \uparrow$

$S = 5/2 \qquad 2S+1 = 6$

$l = 2 + 1 + 0 - 1 - 2 = 0$

$j = 5/2$

${}^6S_{5/2}$

12.10

Eigenvalue of $\hat{H}$ for Hydrogen molecular ion.

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle \quad \text{with } |c_1|^2 + |c_2|^2 = 1$$

$$\langle\psi|\psi\rangle = (c_1^*, c_2^*) \begin{pmatrix} 1 & \Delta \\ \Delta & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

with $\Delta = \langle 1|2\rangle = \langle 2|1\rangle$ overlap

From $\langle\psi|\hat{H}|\psi\rangle = E\langle\psi|\psi\rangle$

We see that the eigenvalue equation is:

$$\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} 1 & \Delta \\ \Delta & 1 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\det \begin{vmatrix} E_0 - E & -A - E\Delta \\ -A - E\Delta & E_0 - E \end{vmatrix} = 0$$

Solutions:

$$E_I = \frac{1}{1+\Delta}(E_0 - A) \; ; \; |I\rangle = \frac{1}{\sqrt{2+2\Delta}}\left(|1\rangle + |2\rangle\right)$$

$$E_{II} = \frac{1}{1-\Delta}(E_0 + A) \; ; \; |II\rangle = \frac{1}{\sqrt{2+2\Delta}}\left(|1\rangle - |2\rangle\right)$$

HW # 7 Solutions

13.2 $\psi_{sc} \xrightarrow[r\to\infty]{} A f(\theta,\phi) \dfrac{e^{ikr}}{r}$

$$\vec{J} = \frac{\hbar}{\mu} \mathrm{Im}\left(\psi^* \vec{\nabla}\psi\right)$$

$$\vec{\nabla}\psi = A f \hat{r} \frac{\partial}{\partial r}\left(\frac{e^{ikr}}{r}\right) + A \frac{e^{ikr}}{r}\left(\frac{1}{r}\right)\left[\hat{\theta}\frac{\partial f}{\partial \theta} + \frac{\hat{\phi}}{\sin\theta}\frac{\partial f}{\partial \phi}\right].$$

$$\xrightarrow[r\to\infty]{} A \frac{f \hat{r}}{r}(ik) e^{ikr} \quad \left(\text{dropping } \tfrac{1}{r^2} \text{ terms}\right)$$

$$\vec{J} \xrightarrow[r\to\infty]{} \frac{\hbar k}{\mu r^2} |A|^2 |f|^2 \hat{r}$$

13.4 Born approximation in 1D:

(a) the 1D Schrödinger equation is

$$\frac{d^2\psi}{dx^2} + k^2\psi = V\psi \quad , \quad k = \frac{\sqrt{2mE}}{\hbar}$$

defining $G(x,x')$ as the Green's function,

$$\frac{\partial^2}{\partial x^2} G(x,x') + k^2 G(x,x') = \delta(x,x')$$

then by substitution we can check that the integral equation is,

$$\psi(x) = e^{ikx} + \int dx' \, G(x,x') \frac{2m}{\hbar^2} V(x') \psi(x')$$

(b) the Green's function $G(x,0)$ may be found by fourier transforming: not asked to do contour integral in problem, only to show that it satisfies Green's equation

$$G(x,0) = \frac{1}{\sqrt{2\pi}} \int dk' \, e^{ik'x} \tilde{G}(k')$$

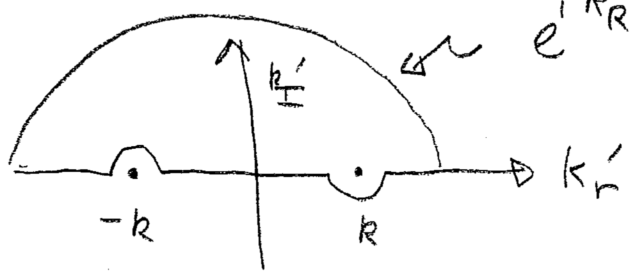
$$\delta(x) = \frac{1}{2\pi} \int dk \, e^{ikx}$$

$$\Rightarrow \tilde{G}(k') = \frac{1}{\sqrt{2\pi}} \; \frac{1}{k^2 - k'^2} \quad \text{and}$$

$$G(x,0) = \frac{-1}{2\pi} \int_{-\infty}^{\infty} \frac{dk' \, e^{ik'x}}{(k'-k)(k'+k)}$$

which can be evaluated by contour integration.

for $x>0$ the contour can be closed in the upper half plane:



$$e^{ik_R x}\, e^{-k_I x} \xrightarrow[k_I \to \infty]{} 0$$

$$G(x,0) = \left(\frac{-1}{2\pi}\right) 2\pi i \left(\frac{e^{ikx}}{2k}\right) = \frac{1}{2ik}\, e^{ikx} \quad (x>0)$$

and similarly, for $x<0$ closing in the lower half plane,

$$G(x,0) = \frac{1}{2ik}\, e^{-ikx} \quad (x<0)$$

thus $$\boxed{G(x,0) = \frac{1}{2ik}\, e^{ik|x|}}$$

Integrating the diff. eq. for $G(x,0)$ we find

$$\left.\frac{\partial G}{\partial x}\right|_{0+} - \left.\frac{\partial G}{\partial x}\right|_{0-} = 1$$

which the above G clearly satisfies.

(c) Using our G;

$$\psi(x) = e^{ikx} + \int dx' \left(\frac{2m}{2ik\hbar^2}\right) e^{ik|x-x'|} V(x')\,\psi(x')$$

the Born approximation is,

$$\psi(x) = e^{ikx} + \frac{m}{ik\hbar^2} \int_{-\infty}^{\infty} dx'\, e^{ik|x-x'|}\, e^{ikx'}\, V(x')$$

the integral becomes,

$$\int_{-\infty}^{x} dx'\, e^{+ik(x-x')}\, e^{ikx'}\, V(x') + \int_{x}^{\infty} dx'\, e^{-ik(x-x')}\, e^{ikx'}\, V(x')$$

in the limit $x \to -\infty$, the first piece is zero and the second is

$$e^{-ikx} \int_{-\infty}^{\infty} dx'\, e^{2ikx'}\, V(x')$$

The reflection coefficient is thus the square of the reflected wave amplitude,

$$R = \frac{m^2}{k^2\hbar^4} \left| \int_{-\infty}^{\infty} dx'\, e^{2ikx'}\, V(x') \right|^2$$

(d) for $V(x) = \begin{cases} V_0 & 0 < x < a \\ 0 & \text{elsewhere} \end{cases}$

The Born approximation gives:

$$V_0 \int_0^a dx\, e^{2ikx} = \frac{V_0}{2ik}\left(e^{2ika} - 1\right)$$

$$= \frac{V_0}{k} e^{ika} \sin(ka)$$

then $$R_B = \frac{m^2}{k^2\hbar^4} \frac{V_0^2}{k^2} \sin^2(ka)$$

$$= \frac{m^2}{4m^2E^2} V_0^2 \sin^2(ka) = \frac{V_0^2}{4E^2} \sin^2 ka$$

In the limit $E \gg V_0$ the exact Transmission coefficient becomes

$$T^{-1} = 1 + \frac{V_0^2}{4E(E-V_0)} \sin^2\left[\sqrt{\frac{2m}{\hbar^2}(E-V_0)}\, a\right]$$

$$T \approx 1 - \frac{V_0^2}{4E^2} \sin^2 ka$$

$$R = 1 - T = R_B$$

13.5 For the Rutherford experiment, over what angle should Rutherford scattering be expected to hold?

the condition is $4k^2 \sin^2(\theta/2) >> m_0^2$

where $r_0 = 1/m_0$ is the range of the effective Coulomb scattering.

Scattering off of a Gold foil, the range $r_0 \approx 1\text{Å}$, the atomic spacing in the foil.

$$\text{then} \quad \sin\left(\frac{\theta}{2}\right) >> \frac{m_0}{2k} = \frac{1}{2k r_0}$$

$$k = \frac{\sqrt{2m_\alpha E}}{\hbar} = \frac{\sqrt{2m_\alpha c^2 E}}{\hbar c} = \frac{\sqrt{2(4\times 1000\,\text{MeV})5\,\text{MeV}}}{200\,\text{MeV}\cdot\text{fm}}$$

$$= \frac{200\,\text{MeV}}{200\,\text{MeV}\cdot\text{fm}} = \frac{1}{10^{-5}\text{A}^0}$$

$$\sin\left(\frac{\theta}{2}\right) >> \frac{1}{2}\times 10^{-5} \Rightarrow \theta >> 10^{-5}\ \text{Rad.}$$

13.7 $\quad V(r) = V_0 e^{-r/a}$

The Born approximation for a spherically symmetric potential is,

$$f_B = \frac{-2\mu}{\hbar^2 q} \int_0^\infty r\,dr \sin(qr) V(r)$$

where $q = |\vec{k} - \vec{k}'| = 2k^2(1-\cos\theta) = 4k^2 \sin^2\frac{\theta}{2}$

Then in this case:

$$f_B = \frac{-2\mu}{\hbar^2 q} V_0 \int_0^\infty dr\, r e^{-r/a} \sin(qr) = \frac{-2\mu}{\hbar^2 q} \frac{1}{a^2} \int_0^\infty dx\, x e^{-x} \sin(qax)$$

$$= \frac{-2\mu}{\hbar^2 q} V_0 a^2 \int_0^\infty dx\, x \left(\frac{1}{2i}\right) \left[e^{-x(1-iqa)} - e^{-x(1+iqa)} \right]$$

$$= -\frac{2\mu}{\hbar^2 q} V_0 a^2 \left(\frac{1}{2i}\right) \left[\left(\frac{1}{1-iqa}\right)^2 - \left(\frac{1}{1+iqa}\right)^2 \right]$$

$$= -\frac{2\mu}{\hbar^2 q} V_0 a^2 \left(\frac{1}{2i}\right) \frac{4iqa}{(1+(qa)^2)^2}$$

$$= -\frac{4\mu V_0 a^3}{\hbar^2} \left[\frac{1}{1+(qa)^2} \right]$$

$$\frac{d\sigma}{d\Omega} = |f_B|^2 = \frac{16\mu^2 V_0^2}{\hbar^4} a^6 \left[\frac{1}{4k^2 a^2 \sin^2\frac{\theta}{2} + 1} \right]^4$$

13.10 For the hard sphere potential,

the particle is free for $r > a$ so the radial wave function is,

$$R = A j_1(kr) + B n_1(kr)$$

with Boundary condition $R(a) = 0$ we have

$$\frac{B}{A} = -\frac{j_1(ka)}{n_1(ka)}$$

To extract the phase shift we look at the asymptotic form,

$$R \xrightarrow[r\to\infty]{} \frac{1}{kr}\left[A \sin(kr - \pi/2) - B \cos(kr - \pi/2)\right)$$

$$= \frac{C_1}{kr} \sin(kr - \pi/2 + \delta_1)$$

$$= \frac{C_1 \cos\delta_1}{kr}\left[\sin(kr - \pi/2) + \tan\delta_1 \cos(kr - \pi/2)\right]$$

from which we find $\tan\delta_1 = \frac{-B}{A} = +\frac{j_1(ka)}{n_1(ka)}$

putting in the explicit form for j_1, n_1,

$$\tan\delta_1 = \frac{(\sin(ka) - ka\cos ka)/(ka)^2}{-(\cos ka + ka \sin ka)/(ka)^2} = \frac{-\tan(ka) + ka}{1 + ka\tan(ka)}$$

with $\tan\theta \simeq \theta + \frac{\theta^3}{3}$, $\delta_1 \cong -\frac{1}{3}(ka)^3 \ll \delta_0$

3.11 For scattering from the potential

$$V(r) = \begin{cases} -V_0 & r<a \\ 0 & r>a \end{cases}$$

the Born amplitude is:

$$f_B = -\frac{2\mu}{\hbar^2}\frac{1}{q}\int_0^\infty r\,dr\,\sin(qr)V(r) = \frac{2\mu}{\hbar^2}\frac{V_0}{q}\int_0^a r\,dr\,\sin qr$$

$$= \frac{2\mu}{\hbar^2}\frac{V_0}{q^3}\int_0^{qa} x\,dx\,\sin x$$

$$= \frac{2\mu}{\hbar^2}\frac{V_0}{q^3}\left[\sin qa - qa\cos qa\right]$$

where $q = 2k\sin(\theta/2)$
at low energy, $ka \ll 1$ and

$$\sin qa - qa\cos qa \approx qa - \frac{1}{3!}(qa)^3 - (qa)\left(1-\frac{1}{2}(qa)^2\right) = \frac{1}{3}(qa)^3$$

$$f_B \approx -\frac{2\mu}{\hbar^2}\frac{V_0\,\cancel{q^3}a^3}{\cancel{q^3}\,6} = \frac{2\mu}{\hbar^2}\frac{V_0 a^3}{3}$$

which is independent of k as it should be at low energy.

$$\sigma_B = \left(\frac{2\mu V_0 a^2}{\hbar^2}\right)^2 \frac{4\pi a^2}{9}$$

The total s-wave cross section is

$$\sigma_0 = 4\pi a^2 \left(\frac{\tan k_0 a}{k_0 a} - 1 \right)^2$$

where $k_0 a = \sqrt{(k a)^2 + \frac{2\mu V_0 a^2}{\hbar^2}}$

for $ka \ll 1$, $k_0 a \cong \sqrt{\frac{2\mu V_0 a^2}{\hbar^2}}$

The condition for the validity of the Born approximation at low energy is,

$$\frac{\mu V_0 a^2}{\hbar^2} \ll 1$$

in which case $\frac{\tan k_0 a}{k_0 a} - 1 \simeq -\frac{1}{3} (k_0 a)^2$

$$\sigma_0 = 4\pi a^2 \left(\frac{2\mu V_0 a^2}{\hbar^2} \right)^2 \frac{1}{9} = \sigma_B$$