Problem 1 (10.21) Problem Set 10

a. For $V(\vec{r}) = \frac{2\pi\hbar^2 b}{m} \sum_i \delta^3(\vec{r}-\vec{r}_i)$.

we'll use: $f(\theta,\phi) = -\frac{m}{2\pi\hbar^2} \int e^{i(\vec{k}'-\vec{k})\cdot\vec{r}'} V(\vec{r}')\, d\tau'$

$= -\frac{m}{2\pi\hbar^2} \cdot \frac{2\pi\hbar^2 b}{m} \sum_i e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_i}$

$= b \sum_i e^{-i\vec{q}\cdot\vec{r}_i}$ w/ $\vec{q} = \vec{k}-\vec{k}'$

then $D(\theta) = |f|^2 = b^2 \left| \sum_i e^{-i\vec{q}\cdot\vec{r}_i} \right|^2$.

b. Take $\vec{r}_i = a(l\hat{x} + m\hat{y} + n\hat{z})$, then

$$e^{-i\vec{q}\cdot\vec{r}_i} = e^{-iaq_x l} \cdot e^{-iaq_y m} e^{-iaq_z n}$$

we'll need: $S(n) = \sum_{j=0}^{n} e^{-i\theta j} = \sum_{j=0}^{n-1} e^{-i\theta j} + e^{-i\theta n} = S(n-1) + e^{-i\theta n}$ (*)

$$e^{i\theta} S(n) = \sum_{j=0}^{n} e^{-i\theta(j-1)} \underset{k=j-1}{=} \sum_{k=-1}^{n-1} e^{-i\theta k} = e^{i\theta} + S(n-1)$$

so

$$S(n) = 1 + e^{-i\theta} S(n-1) \qquad (\circ)$$

putting (*) & (o) together: $S(n) = 1 + e^{-i\theta}[S(n) - e^{-i\theta n}]$

$$S(n)(1-e^{-i\theta}) = 1 - e^{-i\theta(n+1)} \Rightarrow S(n) = \frac{1-e^{-i\theta(n+1)}}{1-e^{-i\theta}}$$

And our sums have $n = N-1$, + different values of "θ", for ex.

$$\sum_{l=0}^{N-1} e^{-iaq_x l} = \frac{1-e^{-iaq_x N}}{1-e^{-iaq_x}} = \frac{e^{-iaq_x N/2}\left(e^{+iaq_x N/2} - e^{-iaq_x N/2}\right)}{e^{-iaq_x/2}\left(e^{+iaq_x/2} - e^{-iaq_x/2}\right)}$$

$$= \left(\frac{e^{-iaq_x N/2}}{e^{-iaq_x/2}}\right) \frac{\sin(aq_x N/2)}{\sin(aq_x/2)}$$

so $\left| \sum_{l=0}^{N-1} e^{-iaq_x l} \right|^2 = \frac{\sin^2(aq_x N/2)}{\sin^2(aq_x/2)}$

Problem 1 (continued)

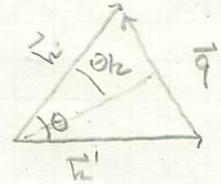
Then $\left|\sum_{\ell=0}^{N-1}\sum_{m=0}^{N-1}\sum_{n=0}^{N-1} e^{-iaq_x\ell}\cdot e^{-iaq_y m}\cdot e^{-iaq_z n}\right|^2$

$$= \frac{\sin^2(aq_x N/2)}{\sin^2(aq_x/2)}\cdot\frac{\sin^2(aq_y N/2)}{\sin^2(aq_y/2)}\cdot\frac{\sin^2(aq_z N/2)}{\sin^2(aq_z/2)}$$

$$\text{b } D(\theta,\phi) = b^2\,\frac{\sin^2(aq_x N/2)}{\sin^2(aq_x/2)}\cdot\frac{\sin^2(aq_y N/2)}{\sin^2(aq_y/2)}\cdot\frac{\sin^2(aq_z N/2)}{\sin^2(aq_z/2)}$$

c. see attached

d. We have $\vec{q} = \vec{k}-\vec{k}'$ w/ $\vec{k}=k\hat{r}$ & $\vec{k}'=k\hat{z}$:



so

$$q/2 = k\sin\theta/2 \Rightarrow q = 2k\sin\theta/2$$

& for $\vec{q}=\vec{G}_{\ell mn}$, $q = \frac{2\pi}{a}(\ell^2+m^2+n^2)^{1/2} = 2k\sin\theta/2$

so $\sin\theta/2 = \frac{\pi}{ak}(\ell^2+m^2+n^2)^{1/2} = \frac{\lambda}{2a}(\ell^2+m^2+n^2)^{1/2}$

$\uparrow k = 2\pi/\lambda$

$$\theta = 2\sin^{-1}\left(\frac{\lambda}{2a}(\ell^2+m^2+n^2)^{1/2}\right)$$

the lowest values of $\ell^2+m^2+n^2$ are 1, 2, & 3, so, for $\lambda = a$

$$\theta_1 = 2\sin^{-1}(1/2) = \pi/3,\ \theta_2 = 2\sin^{-1}\left(\tfrac{1}{2}\sqrt{2}\right) = \pi/2,\ \theta_3 = 2\sin^{-1}\left(\tfrac{1}{2}\sqrt{3}\right) = \tfrac{2\pi}{3}.$$

Problem 1.c

In[1]:=
```
n = 1;
G1 = Plot[Sin[n y / 2] ^2 / Sin[y / 2] ^2, {y, -Pi, Pi}] ;
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In[3]:=
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n = 5;
G5 = Plot[Sin[n y / 2] ^2 / Sin[y / 2] ^2, {y, -Pi, Pi}] ;
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In[5]:=
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n = 10;
G10 = Plot[Sin[n y / 2] ^2 / Sin[y / 2] ^2, {y, -Pi, Pi}, PlotRange → All] ;
```

In[7]:=
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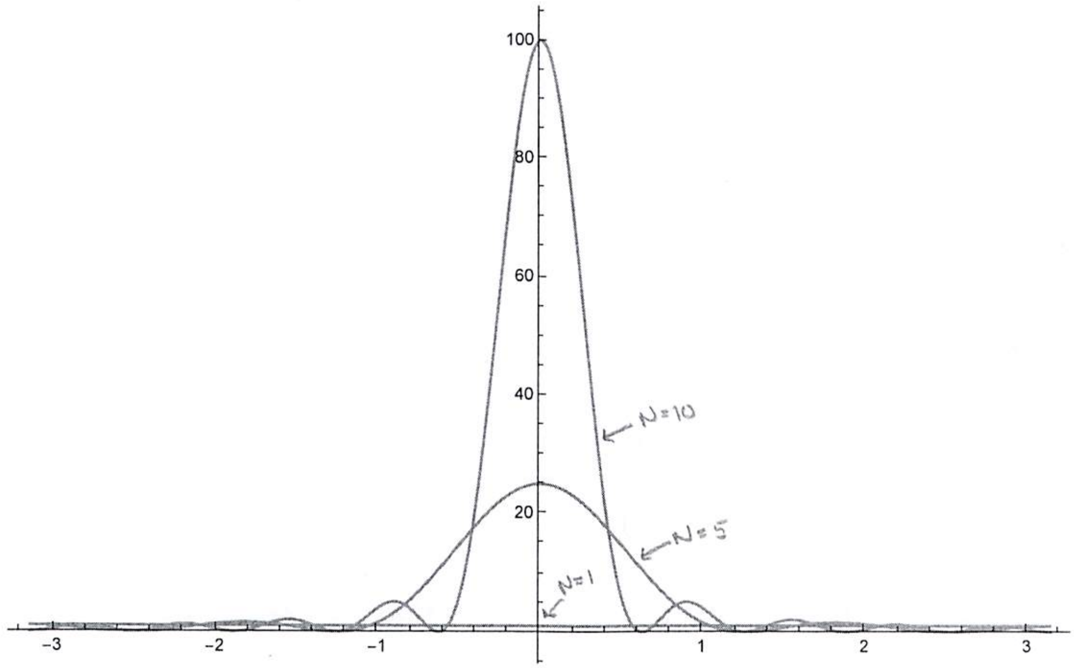
Show[{G1, G5, G10}, PlotRange → {0, 100}]
```

Out[7]=



Problem 3

In $D=2$, we have: $\nabla^2 V = -\rho/\epsilon$, & $\vec{E} = -\nabla V$ means that V has units of

$$|V| = N/C\cdot m, \text{ then } |\nabla^2 V| = \frac{N}{Cm}, \text{ so } |\epsilon| = \frac{|\rho|}{|\nabla^2 V|} = \frac{C/m^2}{N/Cm} = \frac{C^2}{Nm}$$

For a point charge, w/ $\rho = q\,\delta^2(\vec r)$, we have $V(\vec r) = V(r)$ ("spherical symmetry), then:

$$\nabla^2 V = -q\delta^2(\vec r)/\epsilon \Rightarrow \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V}{\partial r}\right) = -q/\epsilon\,\delta^2(\vec r)$$

for pts away from the origin, $\frac{1}{r}\frac{\partial}{\partial r}(rV') = 0 \Rightarrow rV' = \alpha \Rightarrow V = \alpha\log(r/r_0)$

To set α, integrate $\nabla^2 V = -q/\epsilon\,\delta^2(\vec r)$ over "ball" of radius r centered at the origin:

$$\oint \nabla V\cdot d\vec a = -q/\epsilon \Rightarrow \frac{\alpha}{r}\int_0^{2\pi} r\,d\phi = -q/\epsilon \Rightarrow \alpha = \frac{-q}{2\pi\epsilon}.$$

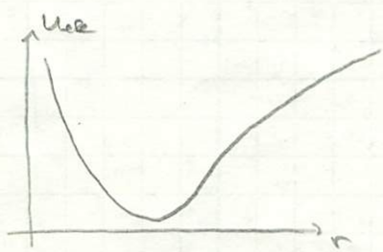
so $V(r) = -\frac{q}{2\pi\epsilon}\log(r/r_0)$

The Hamiltonian is: $H = \frac{p^2}{2m} + qV(r) = \frac{1}{2m}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right) + qV(r)$

& we know that: $p_r = m\dot r$, $\dot p_\phi = -\frac{\partial H}{\partial \phi} = 0 \Rightarrow p_\phi = L_z$, so

$$E = \tfrac{1}{2} m\dot r^2 + \underbrace{\left(\frac{L_z^2}{2mr^2} + \frac{q^2}{2\pi\epsilon}\log(r/r_0)\right)}_{\equiv U_{eff}}$$

The effective potential energy looks like:



As $r\to 0$, $U_{eff}\to\infty$, & as $r\to\infty$, $U_{eff}\to\infty$

The electron *cannot* be removed – there are no scattering states here

Problem 4

We have: $-\frac{\hbar^2}{2m}\nabla^2\psi_a + U\psi_a = E_a\psi_a$ & $-\frac{\hbar^2}{2m}\nabla^2\psi_b^* + U\psi_b^* = E\psi_b^*$

mult. the 1st eqn by ψ_b^*, the 2nd by ψ_a, & integrate over all space:

$$-\frac{\hbar^2}{2m}\int \psi_b^*\nabla^2\psi_a\,d\tau + \int U\psi_b^*\psi_a\,d\tau = E_a\int\psi_b^*\psi_a\,d\tau \quad \&$$

$$-\frac{\hbar^2}{2m}\int \psi_a\nabla^2\psi_b^*\,d\tau + \int U\psi_b^*\psi_a\,d\tau = E_b\int\psi_b^*\psi\,d\tau$$

subtract the two to get:

$$-\frac{\hbar^2}{2m}\underbrace{\int\left[\psi_b^*\nabla^2\psi_a - \psi_a\nabla^2\psi_b^*\right]d\tau}_{\text{int. by parts, w/ } \psi_{a,b}\to 0 \text{ at spatial } \infty} = (E_a - E_b)\int\psi_b^*\psi_a\,d\tau$$

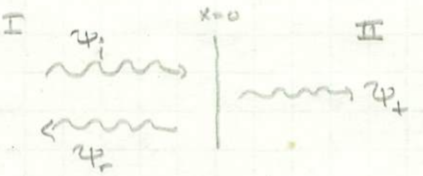
Problem 4 (continued)

$$\frac{\hbar^2}{2m}\underbrace{\int\left[\nabla\psi_b^*\cdot\nabla\psi_a - \nabla\psi_a\cdot\nabla\psi_b^*\right]d\tau}_{0} = (E_a - E_b)\int\psi_b^*\psi_a\,d\tau$$

If $E_a \neq E_b$, we must have $\int\psi_b^*\psi_a\,d\tau = \langle\psi_b|\psi_a\rangle = 0$ ✓

Problem 5

We have



w/ incident $\psi_i = Ae^{ikx}$, $\psi_r = Be^{-ikx}$, $\psi_t = Ce^{i\bar{k}x}$

w/ $k^2 = 2mE$, $\bar{k}^2 = 2m(E - U_0)$

then $\psi_I = \psi_i + \psi_r = Ae^{ikx} + Be^{-ikx}$ & $\psi_{II} = \psi_t = Ce^{i\bar{k}x}$

so the time-dependent solutions are

$$\Psi_I = e^{-iEt/\hbar}(Ae^{ikx} + Be^{-ikx}) \qquad \Psi_{II} = e^{-iEt/\hbar}\,Ce^{i\bar{k}x}$$

w/

$$\rho_I = \Psi_I^*\Psi_I = (A^*e^{-ikx} + B^*e^{ikx})(Ae^{ikx} + Be^{-ikx})$$
$$= (|A|^2 + A^*Be^{-i2kx} + B^*e^{i2kx} + |B|^2)$$

$$\rho_{II} = \Psi_{II}^*\Psi_{II} = |C|^2$$

The integral form of the conservation law is:

$$\frac{d}{dt}\int_\Omega \rho\,d\tau = -\oint_{\partial\Omega}\vec{J}\cdot d\vec{a}$$

& ρ is time-independent, so the left hand side is zero

$$\vec{J}_I = \frac{i\hbar}{2m}(\Psi_I\nabla\Psi_I^* - \Psi_I^*\nabla\Psi_I)$$
$$= \frac{i\hbar}{2m}\left[(Ae^{ikx} + Be^{-ikx})\,ik\hat{x}(-A^*e^{-ikx} + B^*e^{ikx}) - (A^*e^{-ikx} + B^*e^{ikx})\,ik\hat{x}(Ae^{ikx} - Be^{-ikx})\right]$$
$$= \frac{i\hbar}{2m}ik\hat{x}\left[-|A|^2 + \cancel{AB^*e^{i2kx}} - \cancel{BA^*e^{-i2kx}} + |B|^2 - |A|^2 + \cancel{A^*Be^{-i2kx}} - \cancel{B^*Ae^{i2kx}} + |B|^2\right]$$
$$= -\frac{\hbar k}{2m}\hat{x}\left[-2|A|^2 + 2|B|^2\right] = \frac{\hbar k}{m}\hat{x}\left[|A|^2 - |B|^2\right]$$

$$\vec{J}_{II} = \frac{i\hbar}{2m}(\Psi_{II}\nabla\Psi_{II}^* - \Psi_{II}^*\nabla\Psi_{II}) = \frac{i\hbar}{2m}\left[Ce^{i\bar{k}x}(-C^*i\bar{k})e^{-i\bar{k}x} - C^*e^{-i\bar{k}x}(i\bar{k}Ce^{i\bar{k}x})\right]\hat{x}$$
$$= \frac{\hbar\bar{k}}{m}\hat{x}|C|^2$$

Problem 5 (continued)

The prob. cons. eqn. reads:

$$0 = \oint \vec{J}\cdot d\vec{a} = J_I(-a) + J_{II}(a) = \frac{\hbar k}{m}\left(|B|^2 - |A|^2\right)\cdot a + \frac{\hbar \bar{k}}{m}|C|^2 a$$

this gives: $k\left(\frac{|B|^2}{|A|^2} - 1\right) + \bar{k}\frac{|C|^2}{|A|^2} = 0 \Rightarrow \underbrace{\frac{|B|^2}{|A|^2}}_{R} + \underbrace{\frac{\bar{k}}{k}\frac{|C|^2}{|A|^2}}_{T} = 1$

$$R + T = 1$$

the reflection coefficient is $R = \frac{|B|^2}{|A|^2}$, $T = \frac{\bar{k}}{k}\frac{|C|^2}{|A|^2}$

w/ $\frac{\bar{k}}{k} = \left(\frac{2m(E-U_0)}{2mE}\right)^{1/2} = \sqrt{1 - \frac{U_0}{E}}$.

Problem 2

We want the matrix elts of z w/ the states: $|100\rangle$ and: $|200\rangle$, $|21-1\rangle$, $|210\rangle$, $|211\rangle$.
we know that

$$\langle n'l'm'|z|nlm\rangle = 0 \text{ unless } m' = m$$

so only $\langle 100|z|210\rangle$ is non-zero.

We have: $\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$ + $\psi_{210} = \frac{1}{\sqrt{32\pi a^3}}\left(\frac{r}{a}\right)e^{-r/2a}\cos\theta$

$$\langle 100|z|210\rangle = \int_0^\infty \int_0^{2\pi}\int_0^\pi \frac{1}{\pi a^3}\frac{1}{\sqrt{32}}\frac{r}{a}e^{-3r/2a}\cos\theta \cdot \underbrace{r\cos\theta}_{z} \cdot r^2\sin\theta\, d\theta\, d\phi\, dr$$

$$= \frac{1}{\sqrt{32}}\frac{1}{a^4}\frac{1024 a^5 \pi}{243}$$

so $\langle 100|eEz|210\rangle = \frac{1024\pi}{\sqrt{32}\,243} aeE$ all $\langle nlm|\vec{p}|nlm\rangle = 0$ (Laporte's rule)