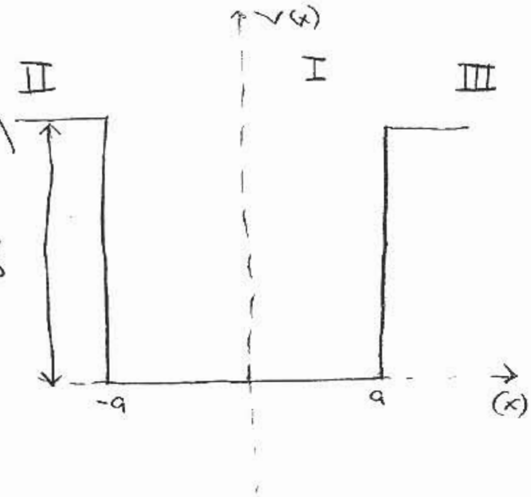
Solutions PS #3

1) (20 pts)



The time independent Schrödinger Equation in 1-D reads:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \left(V(x)-E\right)\psi(x) = 0$$

For the case of the finite square well:

$$V(x) = \begin{cases} 0, & \text{for } -a < x < a \\ V_0, & \text{for } |x| > a \end{cases}$$

In region I $V(x)=0$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) \Rightarrow \text{define } k = \frac{\sqrt{2mE}}{\hbar}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi(x)$$

The general solution is: $\psi(x) = A\cos kx + B\sin kx$

In region III $V(x) = V_0$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = -(V_0 - E)\psi(x)$$

$$\frac{d^2\psi}{dx^2} = \frac{2m(V_0-E)}{\hbar^2}\psi(x) \Rightarrow \text{define } l = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = l^2\psi(x)$$

The general solution is: $\psi(x) = Ce^{-\ell x} + De^{\ell x}$

we want $\psi(x) \to 0$ as $x \to \infty$, therefore

$\psi(x) = Ce^{-\ell x}$ is the only admissable solution for $x > a$.

In region 2 $V(x) = V_0$: $\frac{d^2\psi}{dx^2} = \ell^2 \psi(x)$

The only differance from region III is that we want

$\psi(x) \to 0$ as $x \to -\infty$, therefore $\psi(x) = De^{\ell x}$

-> The next step is to impose boundary conditions of ψ and $\frac{d\psi}{dx}$ continuous at $-a$ and a.

It is interesting to note that since the potential is an even function we can assume that the solutions to the problem are either even or odd. Therefore we only need to impose the boundary condition at one end $(x = a)$ and $\psi(-x) = \pm \psi(x)$.

=> For the even case:

$$\psi(x) = \begin{cases} Ce^{-\ell x} & x > a \\ A \cos kx & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

The wave function must be continuous across the boundary at

$x = a$; $$Ce^{-la} = A\cos ka \qquad (1)$$

Its derivative must also be continuous:

$$-lCe^{-la} = -kA\sin ka \qquad (2)$$

Divide Equation 2 by 1 to get:

$$l = k\tan ka \Rightarrow la = ka\tan ka$$

$$\Rightarrow \tan(2ka) = \frac{2\tan(ka)}{1-\tan^2(ka)} = \frac{2lk}{k^2-l^2}$$

$$\Rightarrow \tan\left[2a\sqrt{\frac{2mE}{\hbar^2}}\right] = \frac{2\sqrt{E(V_0-E)}}{2E-V_0}$$

It is straight forward to find the odd solutions:

$$l = -k\cot ka \Rightarrow la = -ka\cot ka$$

Find the roots of the above equations graphically:

I will adopt a nicer notation:

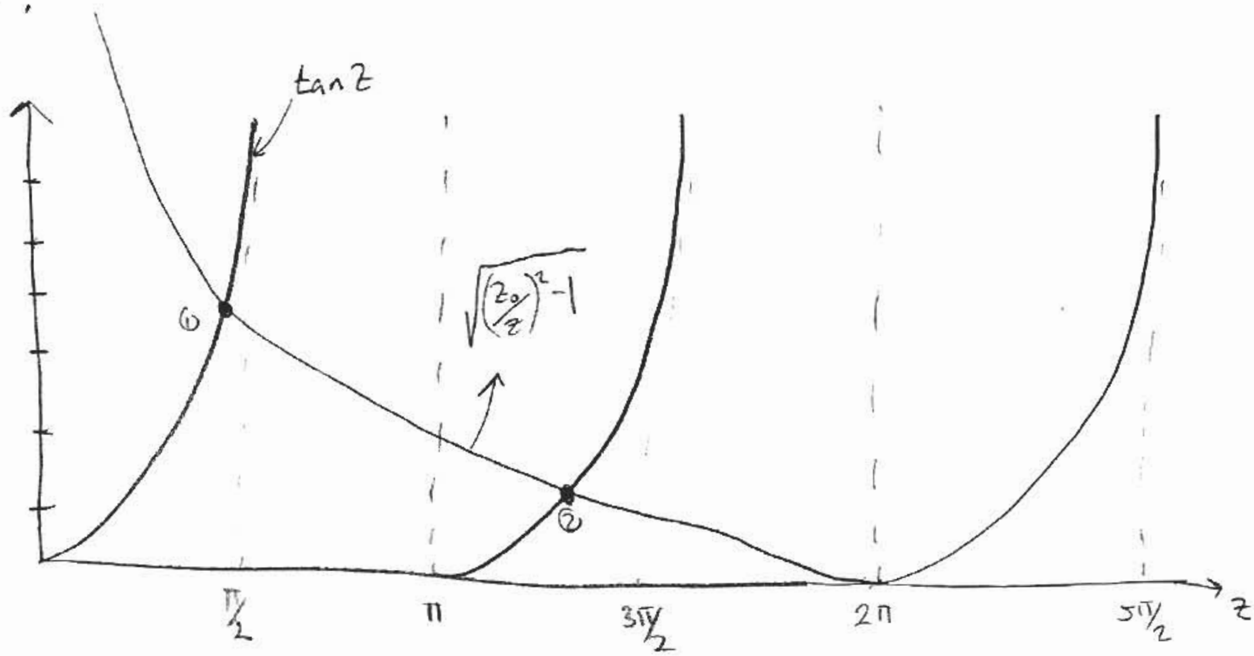
$$z \equiv la, \quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0} = \sqrt{36} = 6$$

we know $k^2 + \ell^2 = 2mV_0/\hbar^2$

so $ka = \sqrt{z_0^2 - z^2}$

$\Rightarrow \tan z = \sqrt{\left(z_0/z\right)^2 - 1}$

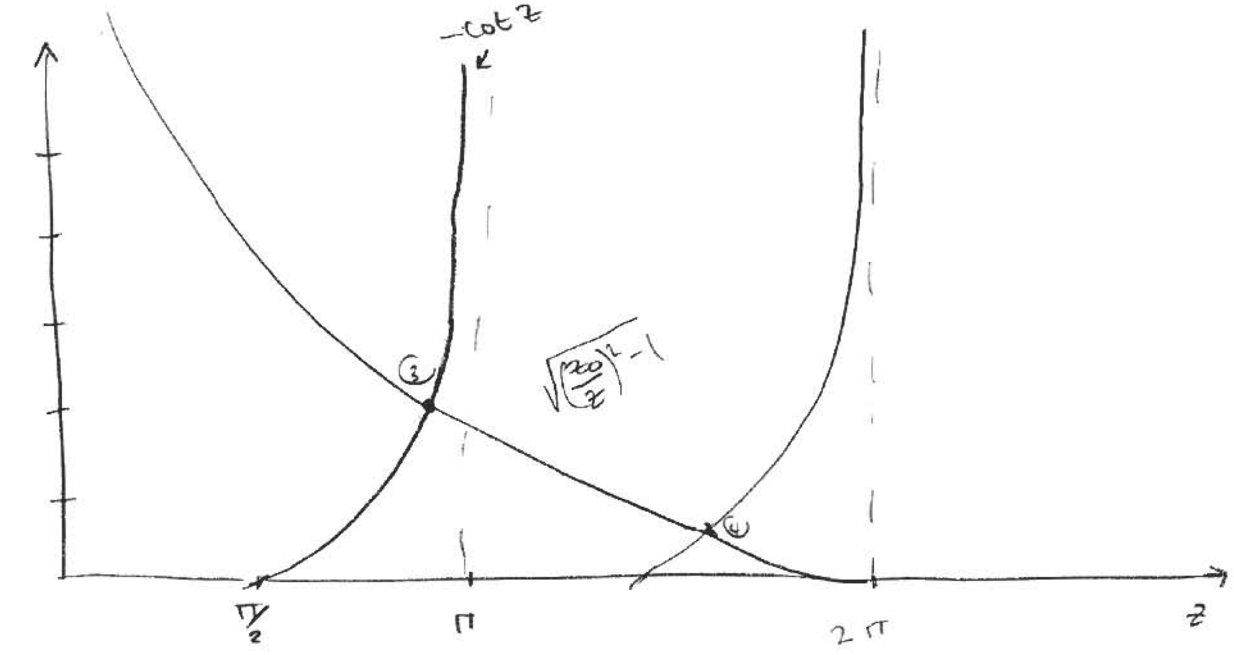
Plot: even case



① $z = 1.34 = \ell a = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$ $E = 0.36\,eV$

② $z = 3.968 = \ell a = \dfrac{\sqrt{2m(V_0-E)}}{\hbar}$ $E = 2.64\,eV$

For odd case:

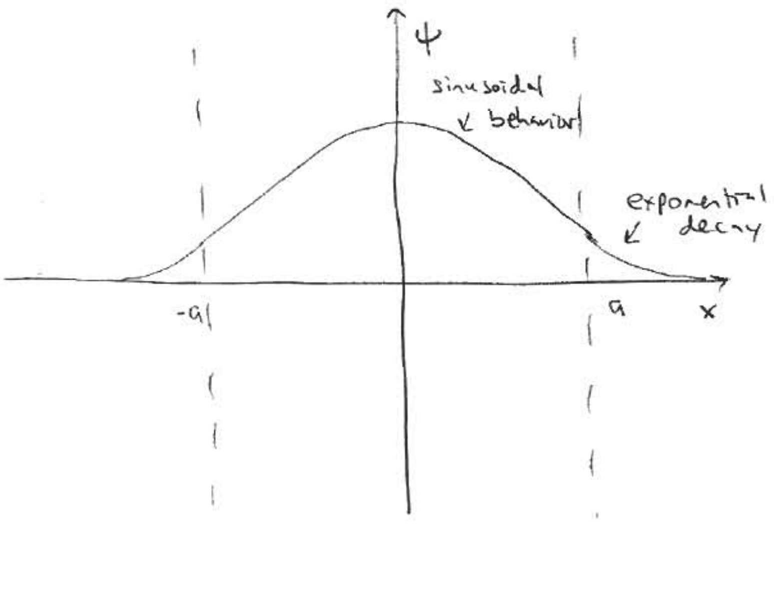


③ $z = 2.69 = la = \dfrac{\sqrt{2m(V_0-E)}}{\hbar}$ $\quad E = 1.2\,\text{eV}$

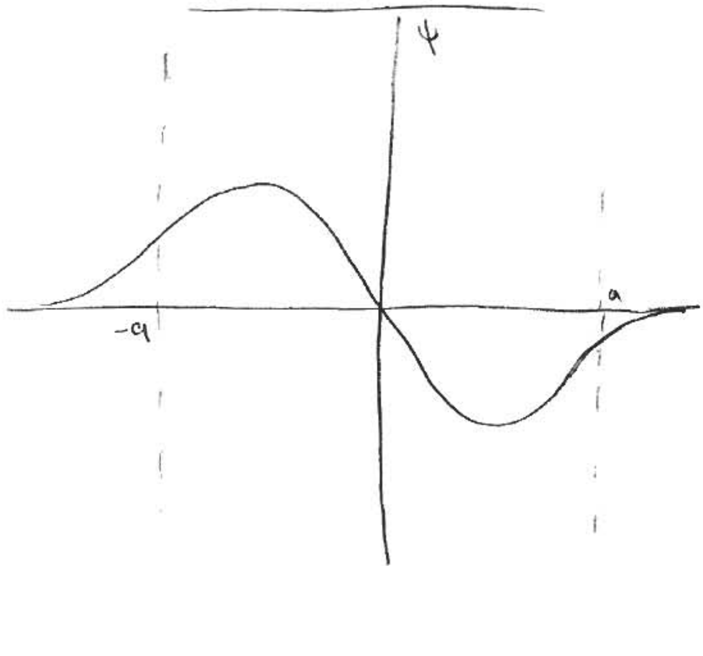
④ $z = 5.23 = la = \dfrac{\sqrt{2m(V_0-E)}}{\hbar}$ $\quad E = 4.62\,\text{eV}$

Wave functions:

ground state



1st excited state



2) (20 pts) For the deuteron problem we derived the transcendental equation:

$$\chi b \cot \chi b = -\alpha b$$

$$\chi = \sqrt{\frac{M(V_0 - B)}{\hbar}}, \quad \alpha = \sqrt{\frac{MB}{\hbar}} = 0.232\ (\text{fm})^{-1}$$

$b \leq 3\,\text{fm} \qquad V_0 = 38.5\ \text{MeV}$

$$\left.\begin{aligned} (\chi b)^2 &= \frac{b^2 M (V_0 - B)}{\hbar^2} \\ (\alpha b)^2 &= \frac{b^2 MB}{\hbar^2} \end{aligned}\right\} \quad \begin{aligned} (\chi b)^2 + (\alpha b)^2 &= \frac{b^2 M V_0}{\hbar^2} \\ \alpha b &= \sqrt{\frac{b^2 M V_0}{\hbar^2} - (\chi b)^2} \end{aligned}$$

If I adopt a similar notation as in pb. 1:

$$z \equiv \chi b \qquad z_0 = \frac{b}{\hbar}\sqrt{M V_0} \Rightarrow \alpha b = \sqrt{z_0^2 - z^2}$$

$$\Rightarrow -\cot z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

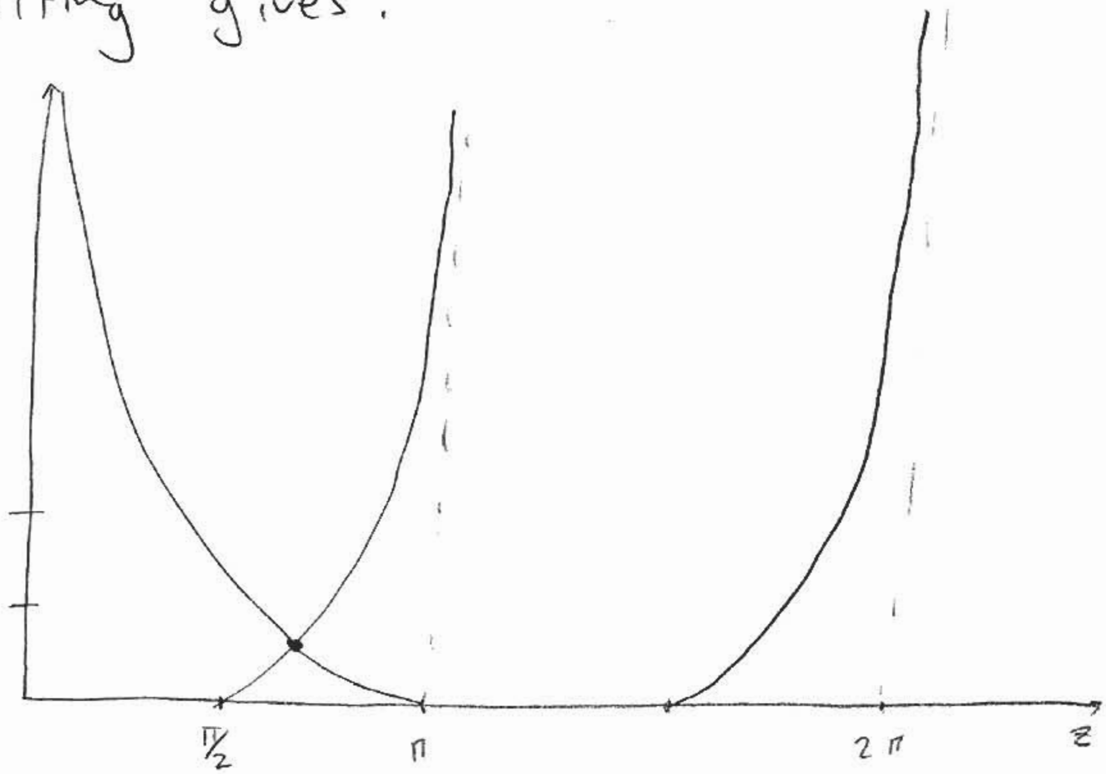
Plot this equation to find the roots:

All we need to do is define z_0

$$z_0 = \frac{3\times10^{-15}\,\text{m}}{1.05457\times10^{-34}\,\text{J}\cdot\text{s}}\sqrt{1.67\times10^{-27}\,\text{kg}\,(6.16\times10^{-12}\,\text{J}} = 2.887$$

$$\Rightarrow \quad -\cot z = \sqrt{\left(\frac{2.887}{z}\right)^2 - 1}$$

Plotting gives:



Only one state is possible for this potential well.

3) Hamiltonian of 1-D harmonic oscillator:

(10 pts)

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

The ground state wave function is:

$$\psi_0(x) = \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\frac{1}{2}\beta x^2} \quad , \quad \beta = \frac{m\omega}{\hbar}$$

Kinetic energy operator $\Rightarrow \dfrac{-\hbar^2}{2m}\dfrac{d^2}{dx^2}$

Potential energy operator $\Rightarrow \frac{1}{2} m\omega^2 x^2$

The expectation value is defined as $\langle V \rangle = \int_{-\infty}^{\infty} \psi^* V \psi \, dx$

$$\Rightarrow \langle V \rangle = \int_{-\infty}^{\infty} \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\frac{1}{2}\beta x^2} \frac{1}{2} m\omega^2 x^2 \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\frac{1}{2}\beta x^2} dx$$

$$= \sqrt{\frac{\beta}{\pi}} \frac{1}{2} m\omega^2 \underbrace{\int_{-\infty}^{\infty} x^2 e^{-\beta x^2} dx}_{\text{look up in table}}$$

$$= \frac{1}{4}\hbar\omega$$

We "expect" the total Energy $\langle E \rangle = \frac{1}{2}\hbar\omega$

$$\Rightarrow \langle E \rangle = \langle T \rangle + \langle V \rangle \quad , \quad \langle T \rangle = \langle E \rangle - \langle V \rangle = \boxed{\frac{1}{2}\hbar\omega}$$

$$\Rightarrow \boxed{\langle T \rangle = \langle V \rangle}$$

4) The Hamiltonian for a Hydrogen-like system:
(10 pts)

$$H = T + V = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

The ground state wave function is:

$$\psi_0(x) = \sqrt{\frac{Z^3}{\pi a_b^3}}\, e^{-Zr/a_b}, \quad a_b = \frac{\hbar^2}{me^2}, \quad E_0 = -\frac{Z^2 m e^4}{2\hbar^2}$$

As in pb. 3

$$\langle V\rangle = \int_{-\infty}^{\infty} \psi^* V \psi \, dx = \int_{-\infty}^{\infty} \sqrt{\frac{Z^3}{\pi a_b^3}}\, e^{-Zr/a_b}\left(-\frac{Ze^2}{r}\right)\sqrt{\frac{Z^3}{\pi a_b^3}}\, e^{-Zr/a_b}\, dr$$

this integral is over all space so:

$$\langle V\rangle = \frac{-Z^4 e^2}{\pi a_b^3}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} \frac{1}{r} e^{-2Zr/a_b}\, r^2\, dr$$

$$= \frac{-Z^4 e^2}{\pi a_b^3}(2\pi)(2)\int_0^{\infty} r e^{-2Zr/a_b}\, dr$$

$$= \frac{-\cancel{4} Z^{\cancel{4}\,2} e^2}{a_b^{\cancel{3}}}\left(\frac{\cancel{a_b^2}}{\cancel{4}\cancel{Z^2}}\right) = \frac{-Z^2 e^2}{a_b} = -\frac{Z^2 m e^4}{\hbar^2} = 2E_0$$

$$\Rightarrow \langle T\rangle = \langle E\rangle - \langle V\rangle = \boxed{E_0 - 2E_0 = -E_0 = -\tfrac{1}{2}\langle V\rangle}$$

5) The momentum operator is given by:
(20pts)

$$\hat{p} = -i\hbar \frac{1}{r}\frac{\partial}{\partial r} r \quad \text{in polar coordinates}$$

The commutator $[x, y] = xy - yx$

$\Rightarrow [\hat{r}, \hat{p}] = \hat{r}\hat{p} - \hat{p}\hat{r}$ → since these are operators we need

a test function to keep the math straight:

$$[\hat{r}, \hat{p}]\psi = [\hat{r}\hat{p} - \hat{p}\hat{r}]\psi = \hat{r}\hat{p}\psi - \hat{p}\hat{r}\psi \quad \rightarrow \hat{r} = r$$

$$= \cancel{r}\left[-i\hbar \frac{1}{\cancel{r}}\frac{\partial}{\partial r}(r\psi)\right] + i\hbar \frac{1}{r}\frac{\partial}{\partial r}(r^2\psi)$$

$$= -i\hbar \frac{\partial}{\partial r}(r\psi) + i\hbar \frac{1}{r}\left(r^2 \frac{\partial \psi}{\partial r} + \psi r + \psi r\right)$$

$$= \cancel{-i\hbar r \frac{\partial \psi}{\partial r}} \cancel{- i\hbar\psi} + \cancel{i\hbar r \frac{\partial \psi}{\partial r}} + \cancel{i\hbar\psi} + i\hbar\psi$$

$$= i\hbar\psi$$

Drop the test function $\Rightarrow \boxed{[\hat{r}, \hat{p}] = i\hbar}$

$$\hat{p}\psi = -i\hbar \frac{1}{r}\frac{\partial}{\partial r}(r\psi) = -i\hbar \frac{1}{r}\left(r\frac{\partial \psi}{\partial r} + \psi\right) = -i\hbar \frac{\partial \psi}{\partial r} - i\hbar \frac{\psi}{r}$$

$$\hat{p}(\hat{p}\psi) = -i\hbar \frac{1}{r}\frac{\partial}{\partial r}\left(r\left[-i\hbar \frac{\partial \psi}{\partial r} - i\hbar \frac{\psi}{r}\right]\right.$$

$$-\hbar^2 \frac{1}{r}\frac{\partial}{\partial r} r\left(\frac{\partial \psi}{\partial r} + \frac{\psi}{r}\right) = -\hbar^2 \frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial \psi}{\partial r} + \psi\right]$$

$$= -\hbar^2 \frac{1}{r}\left[r\frac{\partial^2 \psi}{\partial r^2} + 2\frac{\partial \psi}{\partial r}\right]$$

It can be shown that $\hat{p}^2 \psi = -\hbar^2 \frac{1}{r}\left[r\frac{\partial^2 \psi}{\partial r^2} + 2\frac{\partial \psi}{\partial r}\right]$

if $\hat{p}^2 = -\hbar^2 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right)$

$\Rightarrow$ our derivation above shows

$$\boxed{\hat{p}_r^2 \psi = -\hbar^2 \frac{1}{r}\left[r\frac{\partial^2 \psi}{\partial r^2} + 2\frac{\partial \psi}{\partial r}\right]}$$

The kinetic Energy operator is given as:

$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right)$ in the r direction

$$\Rightarrow \langle T\rangle = -\frac{\hbar^2}{2m}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta \, d\theta \int_0^{\infty} \psi_0(r)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right) r^2 \, dr$$

$$= -\frac{\hbar^2 4\pi}{2m}\int_0^{\infty} \psi_0(r)\frac{1}{\cancel{r^2}}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right)\cancel{r^2}\, dr$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\sqrt{\frac{Z^3}{\pi a_b^3}}\, e^{-\frac{Zr}{a_b}}\right) = \frac{\partial}{\partial r} r^2 \frac{-Z}{a_b}\sqrt{\frac{Z^3}{\pi a_b^3}}\, e^{-\frac{Zr}{a_b}}$$

$$= \frac{-Z}{a_b}\sqrt{\frac{Z^3}{\pi a_b^3}} \frac{\partial}{\partial r} r^2 e^{-\frac{Zr}{a_b}} \quad = \frac{-Z}{a_b} r^2 e^{-Zr/a_b} + 2e^{-Zr/a_b} r$$

$$= \frac{\cancel{-Z}}{a_b}\sqrt{\frac{\cancel{Z^3}}{\pi a_b^3}}\left(\frac{\cancel{-Z}}{a_b} r^2 e^{-\cancel{Z}r/a_b} + 2e^{-\cancel{Z}r/a_b} r\right) \quad Z=1$$

$$= \frac{-1}{a_b}\sqrt{\frac{1}{\pi a_b^3}}\, e^{-r/a_b}\left(2r - \frac{r^2}{a_b}\right)$$

$$\Rightarrow +\frac{\hbar^2 2\cancel{\pi}}{m}\frac{1}{a_b}\frac{1}{\cancel{\pi} a_b^3}\int_0^\infty e^{-2r/a_b}\left(2r - \frac{r^2}{a_b}\right) dr$$

$$\frac{-\hbar^2 2}{m a_b^4}\int_0^\infty e^{-2r/a_b}\left(2r - \frac{r^2}{a_b}\right) dr$$

integrate and get,

$$\frac{\hbar^2}{2 m a_b^2} = \boxed{\frac{m e^4}{2\hbar^2}}$$

c) Recall that the variance of a distribution j is given as $\overline{(\Delta j)^2} = \langle j^2 \rangle - \langle j \rangle^2$

$$\Rightarrow \quad \overline{(\Delta r)^2} = \langle r^2 \rangle - \langle r \rangle^2$$

$$\overline{(\Delta P_r)^2} = \langle \hat{P}_r^2 \rangle - \langle \hat{P}_r \rangle^2$$

Blasting through the integration...

$$\langle r \rangle = \int_0^\infty \psi_0^* \hat{r} \psi \, 4\pi r^2 dr$$

$$= \frac{3a_0}{2Z}$$

$$\langle r^2 \rangle = \int_0^\infty \psi_0^* \hat{r}^2 \psi \, 4\pi r^2 dr$$

$$= \frac{3a_0^2}{Z^2}$$

$$\Rightarrow (\Delta r)^2 = \frac{3a_0^2}{Z^2} - \left(\frac{3a_0}{2Z}\right)^2 = \frac{3a_0^2}{4Z^2}$$

$$\langle P_r \rangle = \int_0^\infty \psi_0^* \left(-i\hbar \frac{1}{r} \frac{\partial}{\partial r} r \psi\right) 4\pi r^2 dr$$

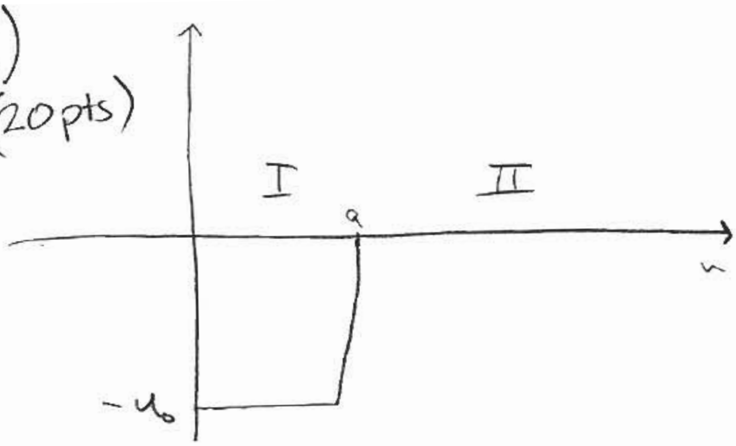
$$= 0$$

$$\langle \hat{p}_r^2 \rangle = 2m\langle T \rangle = \frac{Z^2\hbar^2}{a_b^2}$$

$$(\Delta P_r)^2 = \frac{Z^2\hbar^2}{a_b^2}$$

$$\sqrt{(\Delta r)^2 (\Delta P_r)^2} = \sqrt{\left(\frac{3a_b^{\cancel{2}}}{4\cancel{Z^2}}\right)\left(\frac{\cancel{Z^2}\hbar^2}{\cancel{a_b^2}}\right)} = \boxed{\frac{\sqrt{3}}{2}\hbar}$$

6)
(20pts)



a) Radial part of Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla_r^2 R(r) + V(r)R(r) = E\,R(r)$$

b) Make a transformation by $R(r) = \frac{u(r)}{r}$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\frac{u(r)}{r} + V(r)\frac{u(r)}{r} = E\,\frac{u(r)}{r}$$

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\cancel{r^2}\left(\frac{r\frac{\partial u}{\partial r} - u(r)}{\cancel{r^2}}\right) + V(r)\frac{u(r)}{r} = E\,\frac{u(r)}{r}$$

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\left(r\frac{\partial^2 u}{\partial r^2} + \cancel{\frac{\partial u}{\partial r}} - \cancel{\frac{\partial u}{\partial r}}\right) + V(r)\frac{u(r)}{r} = E\,\frac{u(r)}{r}$$

$$-\frac{\hbar^2}{2m}\frac{1}{\cancel{r}}\frac{\partial^2 u}{\partial r^2} + V(r)\frac{u(r)}{\cancel{r}} = E\,\frac{u(r)}{\cancel{r}}$$

$$\Rightarrow \boxed{\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left(E - U\right)u(r) = 0}$$

c) $u(r) = \begin{cases} 0 \; ; \; r > a & (\text{II}) \\ -u_0 \; r \leq a & (\text{I}) \end{cases}$

$\Rightarrow$ in region I

Schrödinger equation reads:

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}(u_0 - \varepsilon)u(r) = 0$$

$$u'' = -\alpha^2 u \quad , \quad \alpha = \frac{\sqrt{2m(u_0-\varepsilon)}}{\hbar} > 0$$

general solution

$$\underset{r \to 0}{u(r)} = A\cos\cancel{\alpha r} + B\sin\alpha r \to \frac{0}{0} \Rightarrow \text{resolvable using L'Hopital}$$

singular in $R(r)$

in $R(r)$

$$\Rightarrow u_{\text{I}}(r) = B\sin\alpha R$$

In region II

$$u'' = \beta u \qquad \beta = \frac{\sqrt{2M\varepsilon}}{\hbar} > 0$$

general solution:

$$u(r) = \cancel{Ce^{\beta r}} + Ce^{-\beta r} \quad \text{as } r \to \infty$$

$$u_{\text{II}}(\infty) = 0$$

$U(r)$ continuous at a;

$$B \sin \alpha a = C e^{-\beta a} \quad (1)$$

Its derivatives are also continuous at a;

$$B\alpha \cos \alpha a = -C\beta e^{-\beta a} \quad (2)$$

Divide (2) by (1) $\Rightarrow$ $\alpha \cot \alpha a = -\beta$

$$\Rightarrow \boxed{\alpha a \cot \alpha a = -\beta a}$$

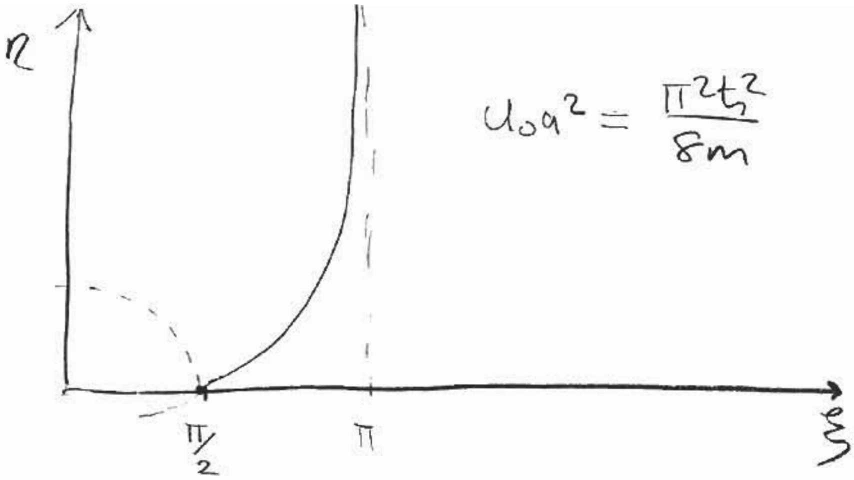
$$\xi = \alpha a \quad , \quad \eta = \beta a$$

$$\Rightarrow \eta = -\xi \cot \xi$$

$$\xi^2 + \eta^2 = (\alpha a)^2 + (\beta a)^2 = \frac{2m(U_0 - \varepsilon)a^2}{\hbar^2} + \frac{2m\varepsilon a^2}{\hbar^2} = \frac{2mU_0 a}{\hbar^2}$$

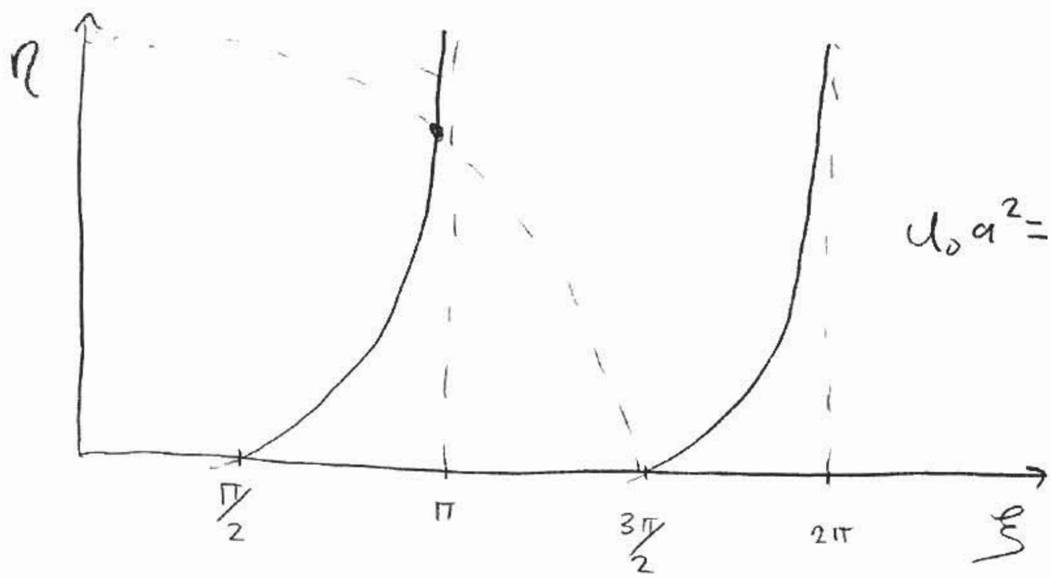
Plot equations for specific cases;

if $U_0 a^2 \leq \frac{\pi^2 \hbar^2}{8m}$, $\xi^2 + \eta^2 = \frac{2\cancel{m} \pi^2 \cancel{\hbar^2}}{8\cancel{m}\cancel{\hbar^2}} = \frac{\pi^2}{4} = 2.467$



$$u_0 a^2 = \frac{\pi^2\hbar^2}{8m}$$

If $u_0 a^2 = \dfrac{9\pi^2\hbar^2}{8m}$, $\xi + \eta^2 = \dfrac{2\cancel{m}\,9\pi^2\cancel{\hbar^2}}{8\cancel{m}\,\cancel{\hbar^2}} = \left(\dfrac{3}{2}\pi\right)^2$



$$u_0 a^2 = \frac{9\pi^2\hbar^2}{8m}$$

If $u_0 a^2 = \dfrac{25\pi^2\hbar^2}{8m}$, $\xi + \eta^2 = \dfrac{2\cancel{m}\,25\pi^2\cancel{\hbar^2}}{8\cancel{m}\,\cancel{\hbar^2}} = \left(\dfrac{25}{4}\pi\right)^2$