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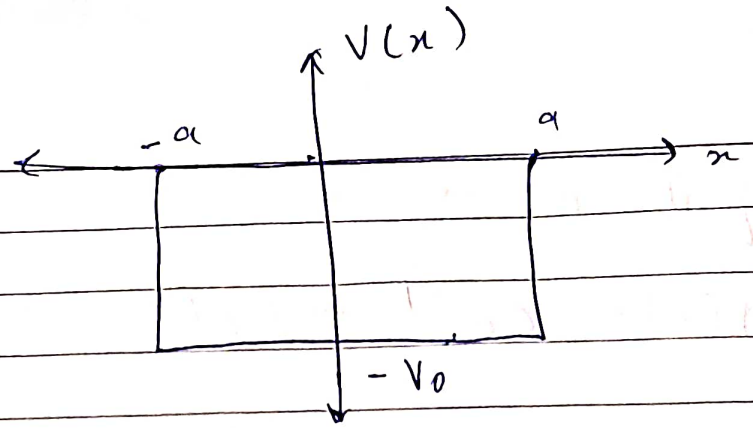
Ans 1)



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

For the case $E < 0 \rightarrow$ this gives rise to bound states

for $|x| < a \rightarrow$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} - V_0 \psi = E\psi = -|E|\psi$$

where $|E| = -E$

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

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \alpha^2 \psi = 0$$

where $\alpha^2 = \frac{2m(V_0 - |E|)}{\hbar^2}$

$|E| = -E \rightarrow$ Binding energy of the particle

$V_0 > |E| \Rightarrow \alpha^2$ is +ve

$$\psi(x) = A\sin\alpha x + B\cos\alpha x$$

for $|x| > a \rightarrow$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi = -|E|\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} - \beta^2 \psi = 0 \quad \& \text{ here } \beta^2 = \frac{2m|E|}{\hbar^2} \quad \text{— (1)}$$

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Sol^n of eq^n (1) is $\longrightarrow$

$$\psi(x) = Ce^{-\beta x} + De^{\beta x}$$

at $x \to \pm\infty \longrightarrow \psi(x) \neq \infty$

Hence at $x = -\infty$ for $x < -a$

$C = 0$

& for $x = \infty \longrightarrow$ for $x > a \longrightarrow$

$D = 0$

$$\Rightarrow \psi(x) = \begin{cases} De^{\beta x} & x < -a \\ A\sin\alpha x + B\cos\alpha x & -a < x < a \\ Ce^{-\beta x} & x > a \end{cases}$$

at $x = -a$ $\psi(x)$ and $\frac{d\psi(x)}{dx}$ should be continuous $\longrightarrow$

$$-A\sin\alpha a + B\cos\alpha a = De^{-\beta a} \quad \text{— (II)}$$

$$\alpha A\cos\alpha a + \beta\alpha\sin\alpha a = \beta De^{-\beta a} \quad \text{— (III)}$$

at $x = a$ $\psi(x)$ and $\frac{d\psi(x)}{dx}$ should be continuous $\longrightarrow$

$$A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a} \quad \text{— (IV)}$$

$$\alpha A\cos\alpha a - \beta\alpha\sin\alpha a = -\beta Ce^{-\beta a} \quad \text{— (V)}$$

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Taking eq^n (II) and (IV) and adding them

$$2\beta\cos\alpha a = (D+C)e^{-\beta a} \quad \text{— (VI)}$$

Taking eq^n (II) and (IV) and subtracting them →

$$2A\sin\alpha a = (C-D)e^{-\beta a} \quad \text{— (VII)}$$

Taking eq^n (III) and (V) and adding them →

$$2\alpha A\cos\alpha a = \beta D e^{-\beta a} - \beta C e^{-\beta a}$$

$$2\alpha A\cos\alpha a = \beta e^{-\beta a}(D-C) \quad \text{— (VIII)}$$

Taking eq^n (III) and (V) and subtracting them →

$$-2\beta\alpha\sin\alpha a = -\beta C e^{-\beta a} - \beta D e^{-\beta a}$$

$$2\beta\alpha\sin\alpha a = (C+D)\beta e^{-\beta a} \quad \text{— (IX)}$$

Dividing eq^n (VIII) / (VII) →

$A=0$ & $C=D$ → $\alpha\cot\alpha a = \dfrac{-\beta e^{-\beta a}(C-D)}{e^{-\beta a}(C-D)}$

$B=0$ & $C=-D$ → $\alpha\cot\alpha a = -\beta$ — (X)

Dividing eq^n (IX) / (VI) →

$$\alpha\tan\alpha a = \beta \quad \text{— (XI)}$$

$\dfrac{XI}{X}$ → $\boxed{\tan^2\alpha a = -1}$

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$\tan^2 \alpha a = -1 \longrightarrow$ Not possible since α and a are +ve and real

$\Rightarrow$ We have 2 classes of sol^n $\rightarrow$

First class $\rightarrow$ $A = 0$, $C = D$

$\alpha \tan \alpha a = \beta$

Second class $\rightarrow$ $B = 0$ & $C = -D$

$\alpha \cot \alpha a = -\beta$

Solution for the first class $\rightarrow$

$$\psi(x) = \begin{cases} Ce^{\beta x} & x < -a \\ B\cos \alpha x & -a < x < a \\ Ce^{-\beta x} & x > a \end{cases}$$

Sol^n for the second class $\rightarrow$

$$\psi(x) = \begin{cases} Ce^{\beta x} & x < -a \\ A\sin \alpha x & -a < x < a \\ -Ce^{-\beta x} & x > a \end{cases}$$

For the energy levels $\rightarrow$

$\alpha \tan \alpha a = \beta$ — (XII)

$\alpha \cot \alpha a = -\beta$ — (XIII)

Multiply a on both sides of eq^n (XII) and (XIII) $\rightarrow$

$\alpha a \tan \alpha a = \beta a$

$\alpha a \cot \alpha a = -\beta a$

Substitute $\xi = \alpha a$ and $\eta = \beta a$

$$\Rightarrow \quad \left.\begin{aligned} \xi \tan \xi &= \eta \\ \xi \cot \xi &= \eta \end{aligned}\right\}$$

By solving these one can obtain the energy levels.

Q2 $\psi(x) = \frac{\sqrt{31}}{2a^{3/2}} \left(a^3 x^{3/2} - x^{5/2}\right)$

$$\hat{E} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

for $x < 0 \rightarrow V(x) = \infty \rightarrow$ $\psi(x)$ does not exist

for $x > \frac{3a}{2} \rightarrow V(x) = \infty \rightarrow$ $\psi(x)$ does not exist

$0 < x < \frac{3a}{2} \rightarrow \psi(x)$ exists

$$\langle \hat{E} \rangle = \int_0^{3a/2} \psi \underbrace{\hat{E}\,\psi}_{\text{solving}} \, dx$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[\frac{\sqrt{31}}{2a^{3/2}}\left(a^3 x^{3/2} - x^{5/2}\right)\right]$$

$$-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\frac{\sqrt{31}}{2a^{3/2}}\left[\frac{3}{2}a^3 x^{1/2} - \frac{5}{2}x^{3/2}\right]\right]$$

$$= -\frac{\hbar^2}{2m} \times \frac{\sqrt{31}}{2a^{3/2}}\left[\frac{3}{4}a^3 x^{-1/2} - \frac{15}{4}x^{1/2}\right]$$

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$$\Psi \hat{E} \Psi =$$

$$\frac{\sqrt{31}}{2a^{3/2}}\left[a^3x^{3/2} - x^{5/2}\right] \times \left(\frac{-\hbar^2}{2m}\right) \times \frac{\sqrt{31}}{2a^{3/2}} \times$$

$$\left[\frac{3}{4}a^3x^{-1/2} - \frac{15}{4}x^{1/2}\right]$$

$$\frac{31}{4a^3} \times \left(\frac{-\hbar^2}{2m}\right)\int_0^{3a/2}\left[\frac{3}{4}a^6x - \frac{3}{4}a^3x^2 - \frac{15}{4}x^2a^3 + \frac{15}{4}x^3\right]$$

$$= -\frac{31\hbar^2}{8a^3m}\left[\frac{3}{4}a^6 \times \frac{1}{2} \times x^2\Big|_0^{3a/2} - \frac{3}{4}\frac{a^3}{3}x^3\Big|_0^{3a/2} - \frac{15}{4}\frac{a^3}{3} \times x^3\Big|_0^{3a/2} + \frac{15}{4} \times \frac{1}{4}x^4\Big|_0^{3a/2}\right]$$

$$= -\frac{31\hbar^2}{8a^3m}\left[\frac{3}{8}a^6 \times \frac{9}{4}a^2 - \frac{1}{4}a^3 \times \frac{27}{8}a^3 - \frac{15}{4}a^3 \times \frac{27}{8}a^3 + \frac{15}{16} \times \frac{81}{16}a^4\right]$$

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$$= \frac{-31\hbar^2}{8m}\left[\frac{27}{32}a^5 - \frac{27}{32}a^3 - \frac{135}{32}a^3 + \frac{1215}{256}a\right]$$

$$= \frac{-31\hbar^2}{8m}\left[\frac{27}{32}a^5 - \frac{162}{32}a^3 + \frac{1215}{256}a\right]$$

$$= \frac{-93\hbar^2}{32m}\left[\frac{9}{8}a^5 - \frac{54}{8}a^3 + \frac{405}{64}a\right]$$

$$= \left[\frac{-3.27}{m}a^5 + \frac{19.617}{m}a^3 - \frac{18.389}{m}a\right]\hbar^2$$

Q.3 Helium atom has two electrons. Let the regions of localization of the two electrons have dimensions r_1 & r_2. Then spread in momenta, & therefore, the minimum momenta, of the two electrons would be

$$p_1 \simeq \hbar/r_1 \ , \ p_2 \simeq \hbar/r_2$$

the kinetic energy of the system is

$$\simeq \frac{\hbar^2}{2m}\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)$$

where m is the mass of electron. The potential energy of the interaction of $\bar{e}$s with the nucleus of charge $2e$ is $\simeq -2e^2\left(\frac{1}{r_1}+\frac{1}{r_2}\right)$.

Finally, since the separation b/w the electrons is of order (r_1+r_2), the interaction energy b/w the $\bar{e}$s is

$$\simeq e^2/r_1+r_2 .$$

The total energy of the system is therefore

$$E \simeq \frac{\hbar^2}{2m}\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right) - 2e^2\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+\frac{e^2}{r_1+r_2}$$

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in ground State E is minimum. Therefore

$$\frac{dE}{dr_1} = -\frac{\hbar^2}{mr_1^3} + \frac{2e^2}{r_1^2} - \frac{e^2}{(r_1+r_2)^2} = 0$$

&

$$\frac{dE}{dr_2} = \frac{-\hbar^2}{mr_2^3} + \frac{2e^2}{r_2^2} - \frac{e^2}{(r_1+r_2)^2} = 0$$

Solving these eqns, we get

$$r_1 = r_2 = \frac{4}{7}\frac{\hbar^2}{me^2}$$

Substituting in the expression for E & Simplifying, the total energy in the ground state is

$$E \simeq \frac{-49}{16}\frac{me^2}{\hbar^2}$$

$$\boxed{E = -10.35\,eV}$$

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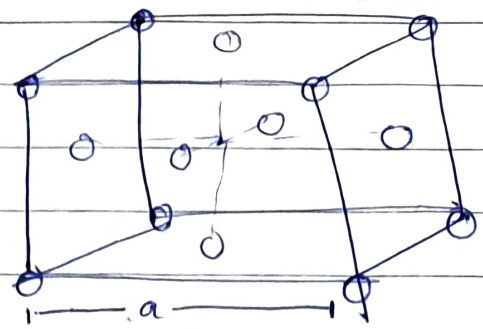
Ans 4) FCC →

~~direct~~ ~~primitive~~ lattice vectors →



$$\vec{a} = \frac{a}{2}(\hat{i}+\hat{j}) \; ; \; \vec{b} = \frac{a}{2}(\hat{j}+\hat{k}) \; ;$$

$$\vec{c} = \frac{a}{2}(\hat{k}+\hat{i})$$

Reciprocal lattice vectors →

0.5

$$\vec{a}^* = 2\pi \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

Volume of FCC $= \vec{a}\cdot(\vec{b}\times\vec{c})$

$$= \frac{a}{2}(\hat{i}+\hat{j})\cdot\left[\left(\frac{a}{2}\hat{j}+\frac{a}{2}\hat{k}\right)\times\left(\frac{a}{2}\hat{k}+\frac{a}{2}\hat{i}\right)\right]$$

$$= \frac{a}{2}(\hat{i}+\hat{j})\cdot\left[\frac{a^2}{4}\hat{i} - \frac{a^2}{4}\hat{k} + \frac{a^2}{4}\hat{j}\right]$$

$$= \frac{a}{2}(\hat{i}+\hat{j})\cdot\frac{a^2}{4}(\hat{i}+\hat{j}) = \frac{a^3}{4}$$

$$\Rightarrow \text{Now } \vec{a}^* = \frac{2\pi\left[\frac{a}{2}(\hat{j}+\hat{k})\times\frac{a}{2}(\hat{k}+\hat{i})\right]}{\frac{a^3}{4}}$$

$$\Rightarrow \vec{a}^* = \frac{2\pi}{a}(\hat{i}-\hat{k}+\hat{j})$$

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Similarly $\longrightarrow$ $\vec{b}^* = \dfrac{2\pi(\vec{c}\times\vec{a})}{\vec{a}\cdot(\vec{b}\times\vec{c})}$

$$\vec{b}^* = \frac{2\pi\left[\frac{a}{2}(\hat{k}+\hat{i})\times\frac{a}{2}(\hat{i}+\hat{j})\right]}{\frac{a^3}{4}}$$

$$= \frac{2\pi}{a}\left(-\hat{i}+\hat{j}+\hat{k}\right)$$

$$\vec{c}^* = \frac{2\pi(\vec{a}\times\vec{b})}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

$$= \frac{2\pi\left[\frac{a}{2}(\hat{i}+\hat{j})\times\frac{a}{2}(\hat{j}+\hat{k})\right]}{\frac{a^3}{4}}$$

$$\vec{c}^* = \frac{2\pi}{a}(\hat{i}-\hat{j}+\hat{k}) \quad \text{—— (1)}$$

Translation vectors in Reciprocal Lattice $\longrightarrow$

$$\vec{G} = ha^* + kb^* + lc^*$$

$$\vec{G} = \frac{2\pi}{a}(\hat{i}+\hat{j}-\hat{k}).h + \frac{2\pi}{a}(-\hat{i}+\hat{j}+\hat{k}).k + \frac{2\pi}{a}(\hat{i}-\hat{j}+\hat{k}).l$$

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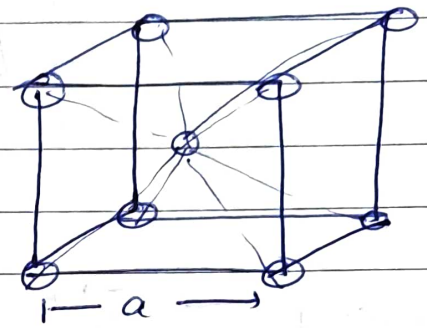
$$\vec{G} = \frac{2\pi}{a}\left[(h-k+l)\hat{i} + (h+k-l)\hat{j} + (-h+k+l)\hat{k}\right]$$ — 1

Reciprocal lattice for BCC crystal structures



Direct translation vectors →

$$\vec{a} = \frac{a}{2}(\hat{i}+\hat{j}-\hat{k})$$

$$\vec{b} = \frac{a}{2}(-\hat{i}+\hat{j}+\hat{k})$$

$$\vec{c} = \frac{a}{2}(\hat{i}-\hat{j}+\hat{k})$$

Volume $= \vec{a}.(\vec{b}\times\vec{c})$

$$= \frac{a}{2}(\hat{i}+\hat{j}-\hat{k}).\left[\frac{a^2}{4}\left[(-\hat{i}+\hat{j}+\hat{k})\times(\hat{i}-\hat{j}+\hat{k})\right]\right]$$

$$= \frac{a}{2}(\hat{i}+\hat{j}-\hat{k}).\frac{a^2}{4}\left[(\hat{k}+\hat{j}-\hat{k}+\hat{i}+\hat{j}+\hat{i})\right]$$

$$= \frac{a}{2}(\hat{i}+\hat{j}-\hat{k}).\frac{a^2}{4}(2\hat{i}+2\hat{j})$$

$$= \frac{a^3}{8}(2+2) = \frac{a^3}{2}$$ — $\boxed{0.5}$

$$\Rightarrow \vec{a}^* = 2\pi\frac{\vec{b}\times\vec{c}}{\vec{a}.(\vec{b}\times\vec{c})}$$

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$$\vec{a}^* = \frac{2\pi \frac{a}{2}\left(-\hat{i}+\hat{j}+\hat{k}\right) \times \frac{a}{2}\left(\hat{i}-\hat{j}+\hat{k}\right)}{\frac{a^3}{2}}$$

$$= \frac{\pi}{a}\left[\hat{k}+\hat{j}-\hat{k}+\hat{i}+\hat{j}+\hat{i}\right]$$

$$= \frac{\pi}{a}\left[2\hat{j}+2\hat{k}\right]$$

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$$\vec{b}^* = \frac{2\pi(\vec{c}\times\vec{a})}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

$$= \frac{2\pi}{\frac{a^3}{2}} \times \left[\frac{a}{2}(\hat{i}-\hat{j}+\hat{k}) \times \frac{a}{2}(\hat{i}+\hat{j}-\hat{k})\right]$$

$$= \frac{\pi}{a}(\hat{i}-\hat{j}+\hat{k}) \times (\hat{i}+\hat{j}-\hat{k})$$

$$= \frac{\pi}{a}(\hat{k}+\hat{j}+\hat{k}+\hat{i}+\hat{j}-\hat{i})$$

$$= \frac{\pi}{a}(2\hat{k}+2\hat{j})$$

$$\vec{c}^* = \frac{2\pi(\vec{a}\times\vec{b})}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

$$= \frac{2\pi}{\frac{a^3}{2}} \times \left[\frac{a}{2}(\hat{i}+\hat{j}-\hat{k}) \times \frac{a}{2}(-\hat{i}+\hat{j}+\hat{k})\right]$$

$$= \frac{\pi}{a}\left[\hat{k}-\hat{j}+\hat{k}+\hat{i}+\hat{j}+\hat{i}\right]$$

$$= \frac{2\pi}{a}[\hat{i}+\hat{k}] \quad \text{—— (1)}$$

Reciprocal lattice vectors →

$$G = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

$$h\left[\frac{2\pi}{a}(\hat{i}+\hat{j})\right] + k\left[\frac{2\pi}{a}(\hat{j}+\hat{k})\right] + l\left[\frac{2\pi}{a}(\hat{i}+\hat{k})\right]$$

$$= \frac{2\pi}{a}\left[(h+l)\hat{i} + (h+k)\hat{j} + (k+l)\hat{k}\right] \quad \text{—— (II)}$$

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Q.5

$$T = \left[1 + \frac{V_0^2 \sinh^2(ka)}{4E(V_0 - E)}\right]^{-1}$$

for a broad high barrier

$$T \simeq 16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right) e^{-2ka}$$

where $k = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar}$

This gives

$$e^{2ka} = \frac{16}{T}\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)$$

or

$$a = \frac{1}{2k}\left[2.303 \log_{10}\left\{\frac{16}{T}\left(\frac{E}{V_0}\right)\left(1 - E/V_0\right)\right\}\right]$$

Now

$$k = \sqrt{\frac{2 \times 6.68 \times 10^{-27} (30 - 10) \times 10^{6} \times 1.6 \times 10^{-19}}{1.054 \times 10^{-34}}}$$

$$= 19.62 \times 10^{14}$$

$\therefore$

$$\boxed{a = 1.91 \times 10^{-15}\ m}$$

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Alternate

5.5

$E = 10\ MeV, \quad V = 30\ MeV$

$T = 2 \times 10^{-3}$

$$T = \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}\,dx\right.$$

here $x_1 = 0$

$x_2 = a$

$V(x) =$ Constant

$$T = \exp\left[-\frac{2}{\hbar}\int_0^a \sqrt{2m(V-E)}\,dx\right]$$

$$T = \exp\left[-\frac{2a}{\hbar}\cdot\sqrt{2m(V-E)}\right]$$

Now

$$2 \times 10^{-3} = \exp\left[\frac{-2a}{1.054 \times 10^{-34}}\sqrt{2 \times 6.60 \times 10^{-27} \times 20 \times 10^{6}\ eV}\right.$$

Taking ln on b/s

$$\ln(2 \times 10^{-3}) = \frac{-2a}{1.054 \times 10^{-34}}\sqrt{2 \times 6.60 \times 10^{-27} \times 20 \times 10^{6}\ eV}$$

$$\boxed{a = 1.584 \times 10^{-15}\ m}$$

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Ans 6)

Tunneling prob $\rightarrow$ $T = e^{-2\gamma}$

where $\gamma = \int_0^L \sqrt{\frac{2m(V(x)-E)}{\hbar^2}}\, dx$

$\boxed{0.5}$

For Barrier A $\rightarrow$ $\gamma = \frac{1}{\hbar}\int_0^b \sqrt{2m\left(\frac{V_0}{2} - \frac{V_0}{100}\right)}\, dx$

$\gamma = \frac{1}{\hbar}\sqrt{2m(0.49)(V_0)}\,(b)$

$\gamma = \sqrt{\frac{0.98\, V_0 m\, b^2}{\hbar^2}}$

$T_A = e^{-\frac{2b}{\hbar}\sqrt{0.98 V_0 m}}$

$\boxed{1.5}$

For barrier B $\rightarrow$ $\gamma = \frac{1}{\hbar}\int_0^b \sqrt{2m\left(3V_0 - \frac{V_0}{100}\right)}\, dx$

$\gamma = \frac{1}{\hbar}(b)\sqrt{2m(2.99)(V_0)}$

$= \sqrt{\frac{5.98\, V_0 m\, b^2}{\hbar^2}}$

$T_B = e^{-\frac{2b}{\hbar}\left(\sqrt{5.98\, V_0 m}\right)}$

$\boxed{1.5}$

$\frac{T_A}{T_B} = e^{\frac{2b\sqrt{V_0 m}}{\hbar}\left(\sqrt{5.98} - \sqrt{0.98}\right)}$

$\boxed{1.5}$