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Engineering Tripos, Part IIB 2012
Paper 4B5, Nanotechnology
Solutions

1. (a) Classical mechanics: deterministic, and dynamical variables (eg. Momentum & energy) vary smoothly – they are continuous.
Quantum mechanics: non-deterministic: don't always get the same value for a measurement, even though possible values can be calculated, as can the probability of any given value being measured. Also, the values of dynamical variables are discrete.
Some of the flaws in classical mechanics that led to the development of QM:
(i) The photoelectric effect. Briefly, this is the effect whereby light impinging on a surface can cause ejection of electrons from that surface, but only if the frequency, f is above some threshold value. Also, the energy of the emitted electrons does not depend on the intensity of light, as classical EM theory would suggest. In fact, changing intensity only changes the number of electrons emitted. It was shown that the kinetic energy of the ejected electrons varies as $hf - \phi$, where h is Planck's constant and ϕ is the work-function of the material. This shows that light exists in packets of energy, called *photons*.
(ii) Spectrum of light emitted from hot objects: shows black-body distribution (which is also quantum in origin) plus discrete colours – showing that energy is discretized in atoms.
(iii) Particle-wave duality: the answer should include a brief description on electron diffraction by crystals or the double-slit experiment.
(iv) Tunneling – could mention radioactive decay – Fermi calculated half-life for alpha decay using QM, with a knowledge of nuclear potential, and prediction was so accurate that gave QM a boost.

(b) Quantum systems are described by a wavefunction $\psi(r,t)$. The energy is given by: $E\,\psi(r,t) = i\hbar\, d\psi(r,t)/dt$
and the momentum is given by: $p\psi(r,t) = -i\hbar d\psi(r,t)/dr$

We use the Hamiltonian for the total energy: $H = KE + PE = \frac{1}{2} mv^2 + V(r) = p^2/2m + V(r) = E$

Replacing p & E by their respective operators (this is known as the correspondence principle), we get $H\psi(r,t) = E\,\psi(r,t)$

i.e. $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\psi(r,t) + V\psi(r,t) = i\hbar\frac{\partial}{\partial t}\psi(r,t)$

Now, if we use separation of variables and assume that $\psi(r,t) = \psi(r)T(t)$, we find that $T(t) = Ae^{-iEt/\hbar}$ and

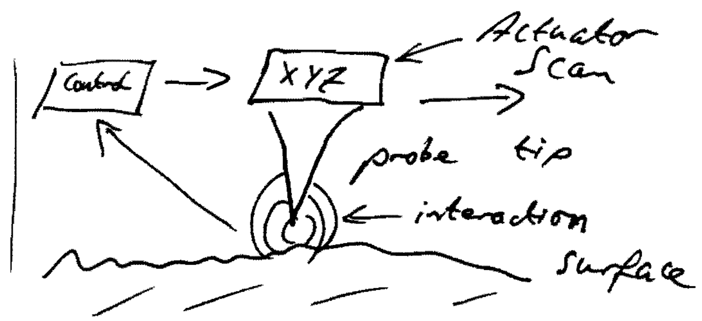
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\psi(r) + V\psi(r) = E\psi(r)$$

The conventional wave-equation is $\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial r^2}$

The key difference is that the solutions to Schrodinger's equation are always complex. These solutions, called wavefunctions, encode all the information about the system they describe. $|\psi(r)|^2$ represents the probability of finding they system at position r, assuming the wavefunction has been normalized.

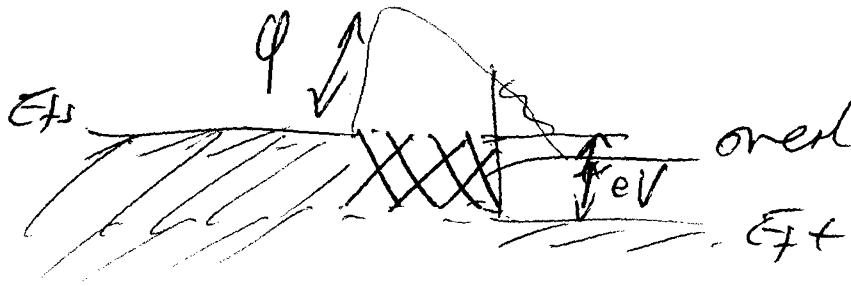
2. SPM in general first:

STm:



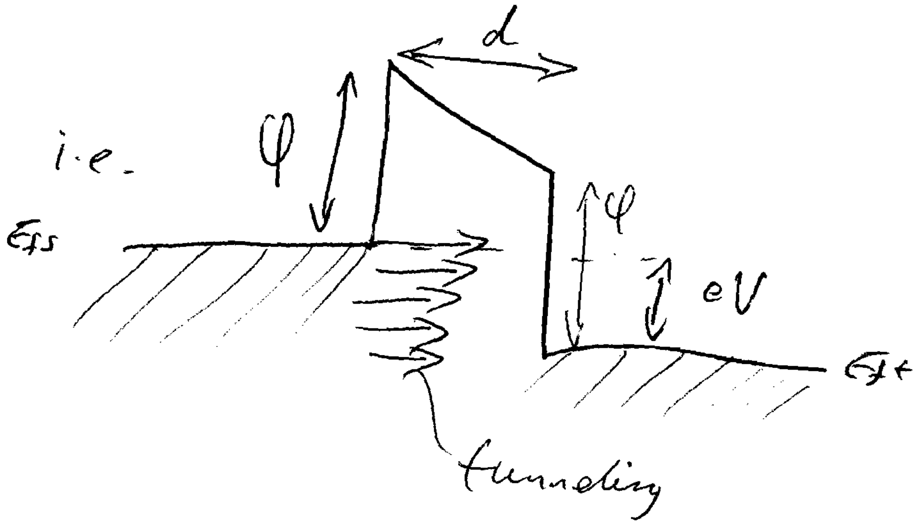
The tip raster scans above the surface whilst maintaining a constant interaction. For the STM, a bias voltage (typically 10 mV - 2V) is applied between the tip and sample, which must therefore be conductive. The z actuator moves the tip close to the sample until the set tunneling current is obtained (typically 0.1 - 1 nA) at which point the feedback control loop thereafter ensures this value is maintained. As the tip scans the surface, variations in conductivity and height are compensated for using the z actuator, and an image is formed by measuring the voltage sent to that actuator at each image point. An image can typically be taken in anything from a few seconds to several minutes, depending on the scan area and how rough it is.

When a bias, V is applied to the tip/sample, the Fermi level shifts:



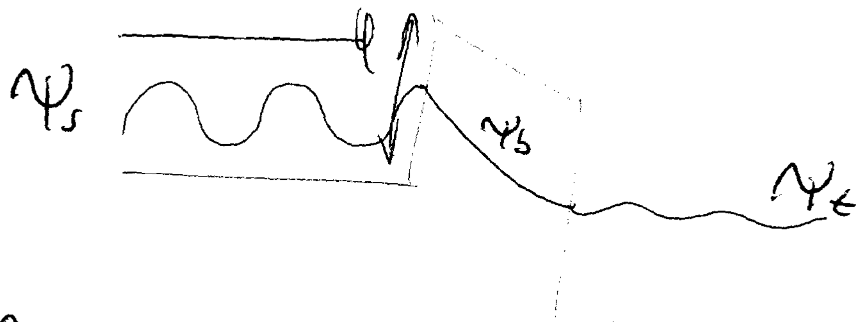
overlap between filled energy levels of sample & empty levels of tip
→ current can flow.

i.e.



barrier width, d ~ typically ≤ 1nm

(b) Using above figure, wave-function will be like:



$\Psi_s = \Psi$ in sample $= A_1 e^{ik_1x} + B_1 e^{-ik_1x}$

$\Psi_b = \Psi$ in barrier $= A_2 e^{k_2x} + B_2 e^{-k_2x}$

$\Psi_t = \Psi$ in tip $= A_3 e^{ik_3x}$

(63)

To a first approximation, we can say the $\psi_b \sim e^{-k_2 x}$, where $k_2 = \frac{\sqrt{2m(\phi - \epsilon)}}{\hbar}$

where ϵ = electron energy.

$\therefore$ the value of ψ after traversing the width, d, of the barrier $\sim e^{-k_2 d}$

$\therefore$ The transmission probability $\sim e^{-2k_2 d}$ ($T \propto |\psi|^2$)

Now, the current also depends on the voltage and the density of states of sample & tip ρ_s & ρ_t.

We can write $I \propto \int_{eV}^{0} \rho_s \rho_t T \, dE$

$$= \int_{eV}^{0} \rho_s \rho_t e^{-2k_2 d} \, dE$$

$$\therefore I \propto \int_{eV}^{0} \rho_s \rho_t e^{-\frac{2d\sqrt{2m(\phi-\epsilon)}}{\hbar}} \, dE$$

clearly if this approx is used then $I \propto V$
and $I \propto e^{-d}$

where d is the tip sample distance.

If we assume ~~$\frac{e}{}$~~ V is constant, as is $T(\epsilon)$, ρ_s dk, then the ratio of currents for two different values of distance are:

$$\frac{I_2}{I_1} = e^{-2k_2(d_2-d_1)}$$

now; $k_2 = \frac{\sqrt{2m(\phi-\epsilon)}}{\hbar}$ ϕ = 4eV above E_f $\Rightarrow \phi - \epsilon = 4eV$.

$$\Rightarrow k_2 = \frac{\sqrt{2\times 9.1\times10^{-31}\times 4\times 1.6\times10^{-19}}}{1.05\times10^{-34}} = 10.3\times10^{9}$$

and $d_2 - d_1 = 0.01\times10^{-9}$ m $= 10^{-11}$ m

$$\Rightarrow \frac{I_2}{I_1} = e^{-2\times10.3\times10^{9}\times10^{-11}} = e^{-0.2} = 0.82$$

i.e. if the tip sample distance is reduced by 0.01 nm, the current will increase by nearly 20%.

(C) Vibration isolation - need to get to better than 0.01 nm or will be too noisy and unable to maintain feedback.

design of STM: should be small & compact, to minimize effect of floor vibrations (typically ~ 0.1-10 Hz).

Should have vibration isolation to minimize noise, can be multi-stage - typically STM is on a spring-suspens. eddy-current damped stage, in a UHV chamber which is typically supported by air-legs.

Discussion can mention UHV for cleanliness, low temperature for stability, low-noise, high speed electronics.

(d) We saw earlier that

$$I \propto \int_{eV}^{0} \rho_s \rho_t T \, dE$$

if we use a tip for which $\rho_t \sim$ Constant (W or Pt(Ir)) over a wide range of E, and if $T \sim$ Constant, then

$$I = CT \int_{eV}^{0} \rho_s \, dE \qquad \text{where } C \text{ is a Constant.}$$

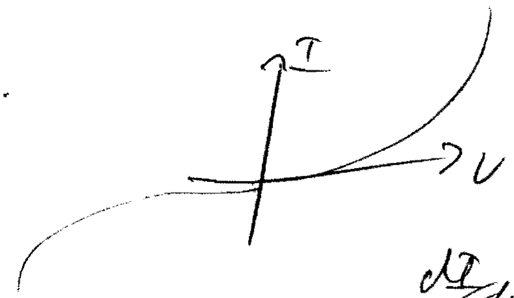
$$\Rightarrow \frac{dI}{dV} = CT\rho_s V \quad \propto \rho_s.$$

If we scale this by I/V

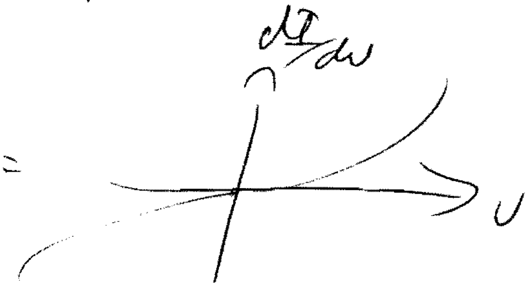
i.e. ~~dI~~ $\boxed{\frac{dI}{dV} \times \frac{V}{I} \propto \rho_s}$, this

removes the exponential nature of I

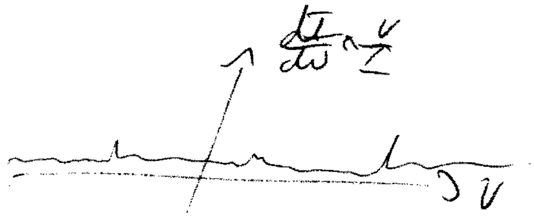
i.e.



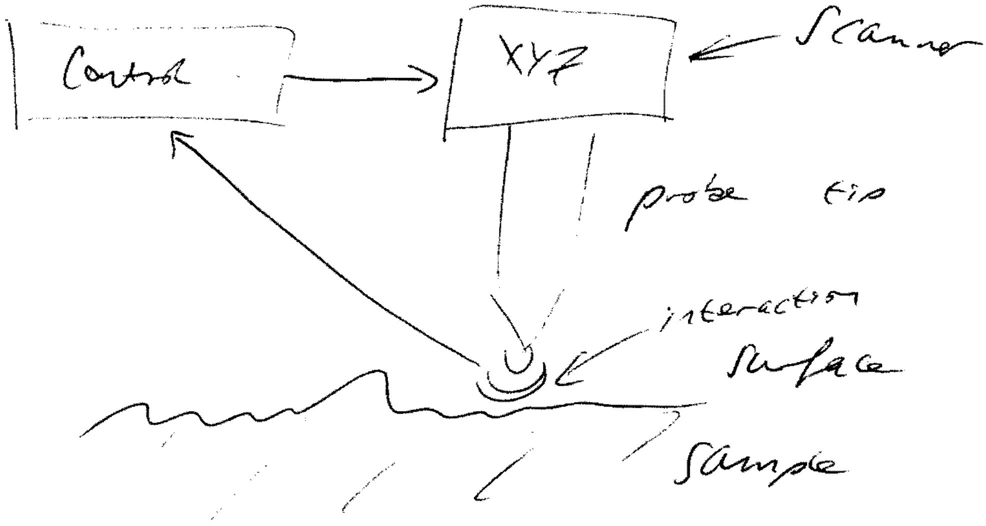
$\rightarrow \quad \frac{dI}{dV} =$



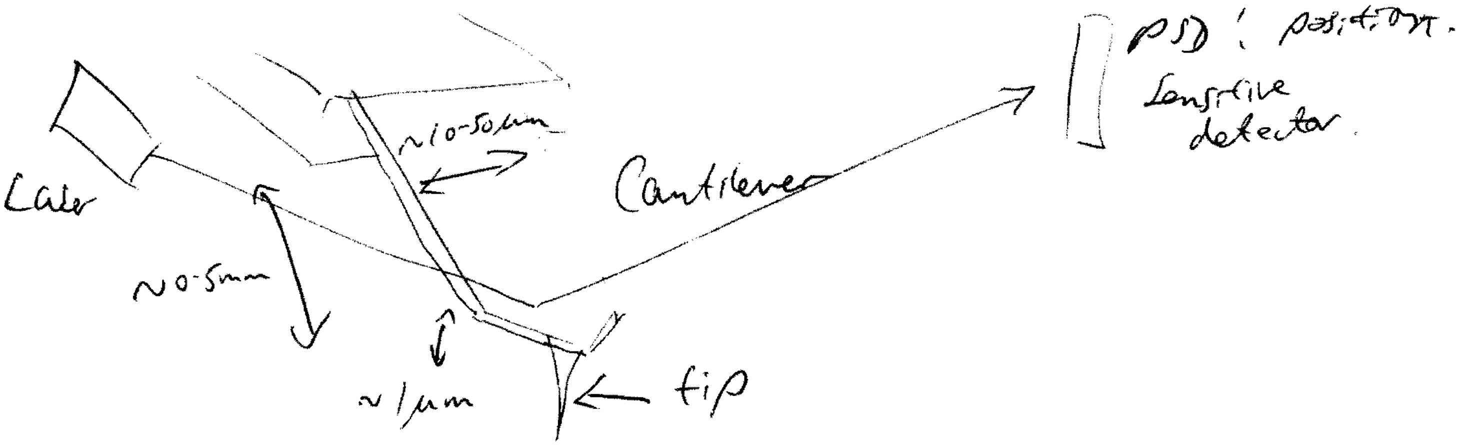
$\frac{dI}{dV} \times \frac{V}{I} =$



3. Start with SPM principle:



Principle of AFM:



The deflection of the cantilever (typically Si or Si_3N_4) is measured using an optical lever: light from a laser is focused on the cantilever near the apex, and the position of the reflected beam is measured using a PSD. Can ~~____~~ measure deflections ~ 0.1 Å in this way.

The three modes of operation are contact, non-contact and intermittent contact (tapping). Answer should show a plot of deflection vs distance for each and discuss what causes the deflection.

(1)

Non-contact: V. high resolution in UHV, for MEMS & FZm.

Contact: for electrical measurements and for imaging very soft samples under liquid, or hard samples in air.

tapping-mode: most common mode for most applications. Does not work well in liquid. Tip is oscillating by 10s of nm.

P.S. mention that in non-contact tip is oscillating by ~ 1nm.

(b) Fast scanning – many commercial systems can now scan at line rates of ~ 1kHz – use small levers with v. high resonance frequencies (several 100 kHz) for tapping-mode. If feedback loop is fast, can ensure tip-sample distance is maintained even during each oscillation cycle (a few μs). ~~Also~~

Parallel scanning – use multiple tips, each of which scans a small area.

Mention: dip pen nanolithography

Step and scan – automated scanning of multiple areas.

(c) $\frac{1}{2}k_BT = \frac{1}{2}kx^2$ $\Rightarrow \langle x\rangle = \sqrt{\frac{k_BT}{k}}$

Thermal energy = Elastic energy

$= 2.04\,nm$ when $k = 1\,mN\,m^{-1}$

If $k = 50\,N\,m^{-1}$; $\langle x\rangle = 9\times10^{-12}\,m \sim 9\,pm$

Even though the deflection is very large for the soft cantilever, most contact-mode cantilevers have a stiffness of ~ 0.1 N.m⁻¹, so the deflection ~ 0.2 nm.

Also, when a cantilever is in contact with a surface, the lever's effective stiffness ~~[illegible]~~ increases, causing the rms noise to decrease. The thermal noise in most cases is then around 0.1 nm, which is smaller than most atomic step heights, so the AFM will be able to resolve them, which is perfectly adequate for most cases. In some systems, the measurement requires the tip to be in ~~sample~~ contact with the sample.

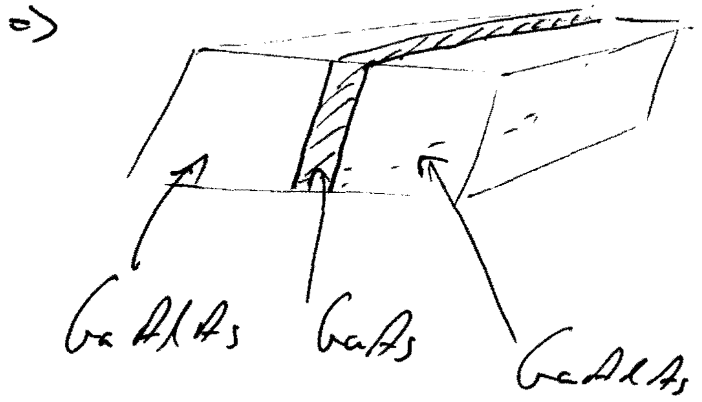
4

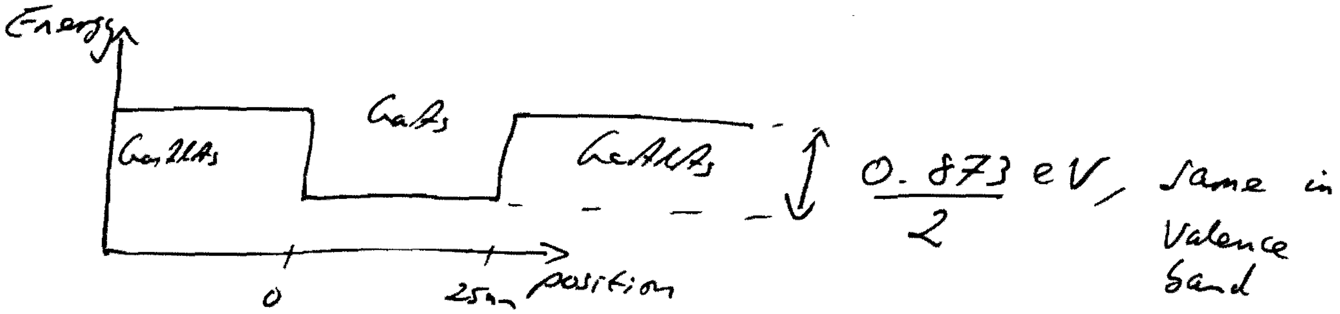
(a) $Ga_{0.3}Al_{0.7}As$ has a band gap of

$1.247 \times 0.7 + 1.424 = 2.2969$ eV.

Difference between this and GaAs is 0.873 eV

=>





(b)

Assumptions: (i) Half energy difference appears in Conduction band, the other half in the valence band

(ii) Ground-state energy is low enough that we can use the infinite well approximation.

Derive the spectrum of energy levels:

$$E = \frac{\hbar^2 k^2}{2m}.$$ From boundary conditions,

$$k = \frac{n\pi}{\ }$$

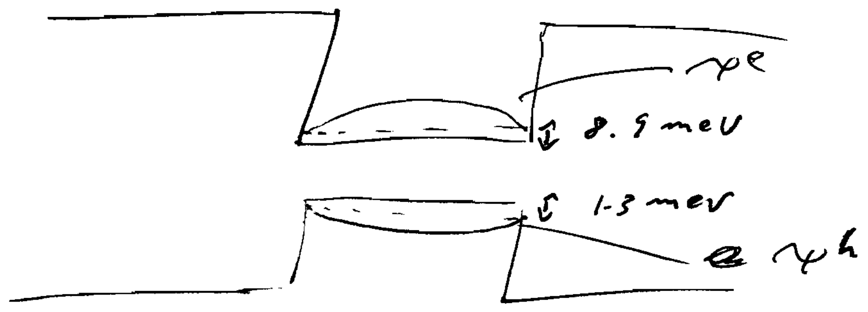
$$\Rightarrow \quad E^e = \frac{n^2 h^2}{8 m_e^* L^2} \quad ; \quad E^h = \frac{n^2 h^2}{8 m_h^* L^2}$$

$m^* \rightarrow$ effective mass.

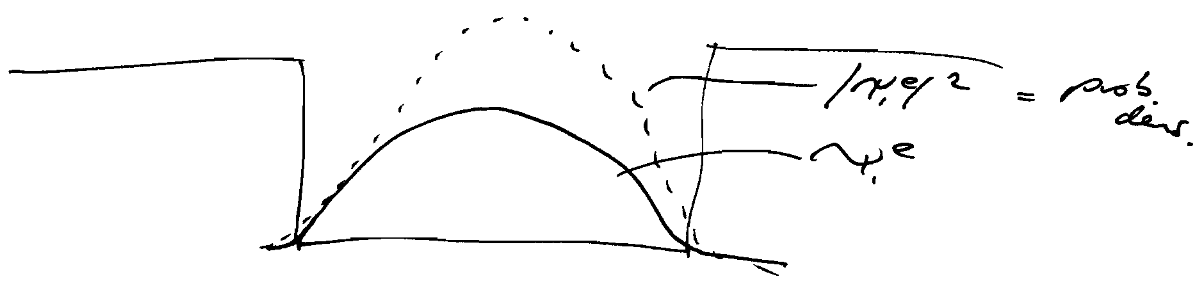
This gives the electron & hole ~~effective~~ ~~mass~~ energies as 8.9 meV and 1.3 meV, respectively.

As both of these energies are much less than the height of the well, the assumption that ~~it~~ is infinite is justified.

i.e.



(c)



The characteristic decay length $= \frac{1}{k_2}$

$$k_2 = \sqrt{2m_e^*(V-E_1^e)} \Big/ \hbar$$

$$= \frac{\sqrt{2\times 0.067\times 9.1\times10^{-31}\times\left(\frac{0.873}{2} - 0.0089\right)\times 1.6\times10^{-19}}}{1.05\times10^{-34}}$$

$$\frac{1}{k_2} = 1.15\ nm$$

To determine the probability of finding the particle outside the well, we can numerically determine E_1, and use this to find k_1 inside the well. We can then use the wavefunctions and boundary conditions to determine coefficients A_i, B_i of wavefunctions. After normalising we can then simply integrate outside the well to find probability; P.

$$\text{i.e. } P = \int_{-\infty}^{0} A_1^2 e^{+2k_2 x}\,dx + \int_{a}^{\infty} A_3^2 e^{-2k_2 x}\,dx$$

5.

In region I;

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_1(x)}{\partial x^2} = E\psi_1(x)$$

Solution :

$$\psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

$$k_1 = \cancel{\frac{\sqrt{2m(E-0)}}{\hbar}} = \frac{\sqrt{2mE}}{\hbar}$$

In region II,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_2(x)}{\partial x^2} + V\psi_2(x) = E\psi_2(x)$$

Solution :

$$\psi_2(x) = A_2 e^{ik_2 x} + \cancel{B_2}$$

where $k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$

probability flux for incident wave

$$= \cancel{|\psi_1|^2 \frac{\hbar k}{m}}$$
$$A_1^2 \hbar k_1$$

~~ref~~ transmitted wave

$$= |\psi_2|^2 \frac{\hbar k_2}{m}$$

$$\Rightarrow T = \frac{|A_2|^2}{|A_1|^2} \frac{k_2}{k_1}$$

@ $x = 0$; $\psi_1 = \psi_2$

$$\Rightarrow A_1 + B_1 = A_2 + \cancel{B_2} \quad \ldots (1)$$

$$\psi_1' = \psi_2'$$

$$\Rightarrow A_1 ik_1 - B_1 ik_1 = A_2 ik_2$$

$$\Rightarrow A_1 k_1 - B_1 k_1 = A_2 k_2 \quad \ldots (2)$$

$\times (1)$ by k_1

$$\Rightarrow A_1 k_1 + B_1 k_1 = A_2 k_1$$

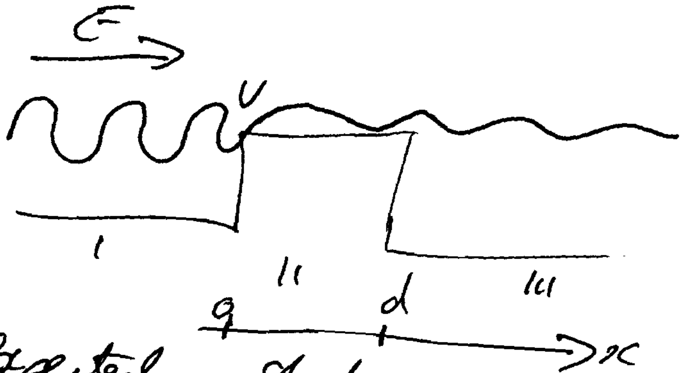
Combine with (2) $\Rightarrow A_1 k_1 - B_1 k_1 = A_2 k_2$

$$\Rightarrow 2A_1 k_1 = A_2 (k_1 + k_2)$$

$$\Rightarrow \frac{A_2}{A_1} = \frac{2k_1}{k_1 + k_2}$$

$$\Rightarrow T = \frac{4k_1^2}{(k_1+k_2)^2} \times \frac{k_2}{k_1} = \frac{4k_1 k_2}{(k_1+k_2)^2}$$

(5)



expected solutions:

here, $E > V$

$\Rightarrow$ waves in all regions, no tunneling

region $\underline{I}$:

$$\psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

region $\underline{II}$:

$$\psi_2 = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}$$

region $\underline{III}$:

$$\psi_3 = A_3 e^{ik_3 x}$$

$$k_1 = k_3 = \frac{\sqrt{2mE}}{\hbar} \quad ; \quad k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$$

@ $x = 0$, $\psi_1 = \psi_2$ & $\psi_1' = \psi_2'$

$$\Rightarrow A_1 + B_1 = A_2 + B_2 \qquad (1)$$

$$ik_1 A_1 - ik_1 B_1 = ik_2 A_2 - ik_2 B_2 \qquad (2)$$

@ $x = d$, $\psi_2 = \psi_3$, $\psi_2' = \psi_3'$

$$\Rightarrow A_2 e^{ik_2 d} + B_2 e^{-ik_2 d} = A_3 e^{ik_3 d} \qquad (3)$$

$$ik_2 A_2 e^{ik_2 d} - ik_2 B_2 e^{-ik_2 d} = ik_3 A_3 e^{ik_3 d} \qquad (4)$$

from (3) & (4):

$$k_2 e^{ik_2 d} A_2 + k_2 B_2 e^{-ik_2 d} = k_2 e^{ik_1 d} A_3 \quad (k \times (3))$$

$$(4) \Rightarrow k_2 e^{ik_2 d} A_2 - k_2 e^{-ik_2 d} B_2 = k_1 e^{ik_1 d} A_3$$

$$\Rightarrow 2k_2 e^{ik_2 d} A_2 = A_3 e^{ik_1 d}(k_1 + k_2)$$

$$\Rightarrow A_2 = \frac{A_3 e^{ik_1 d}(k_1 + k_2)}{2k_2 e^{ik_2 d}}$$

and; $$B_2 = \frac{A_3 e^{ik_1 d}(k_2 - k_1)}{2k_2 e^{-ik_2 d}}$$

Substituting, we obtain

$$T = \left|\frac{A_3}{A_1}\right|^2 = \frac{1}{1 + \left(\frac{k_1^2 - k_2^2}{2k_1 k_2}\right)^2 \sin^2(k_2 d)}$$

Value for $k_1 = \dfrac{\sqrt{2 \times 9.1 \times 10^{-31} \times 5 \times 1.6 \times 10^{-19}}}{1.05 \times 10^{-34}} = 1.15 \times 10^{10}\ \text{nm}^{-1}$

$k_2 = \dfrac{\sqrt{2 \times 9.1 \times 10^{-31} \times \cancel{5}\, 1 \times 1.6 \times 10^{-19}}}{1.05 \times 10^{-34}} = 0.51 \times 10^{10}\ \text{nm}^{-1}$

$$\Rightarrow T = \frac{1}{1 + 0.82 \times \sin^2\left(\underbrace{0.51 \times 10^{10} \times 1 \times 10^{-9}}_{\text{make sure this is in radians}}\right)}$$

$$= \underline{\underline{0.58}}$$

<u>end</u>