

4B5 solutions 2017  
Short answers

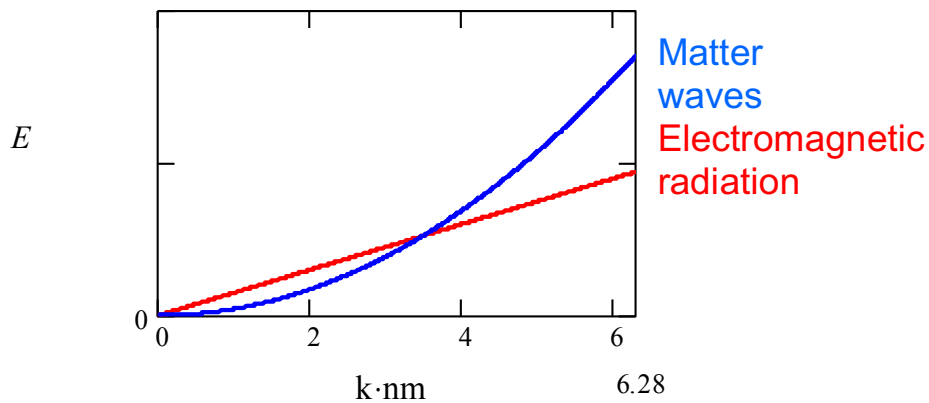
1(c) 2.23 nm

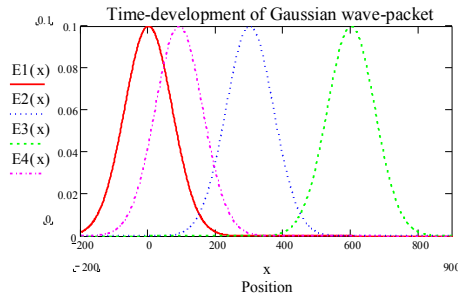
2(b) 8.9 meV, 1.33 meV

3(a) 0.988 eV

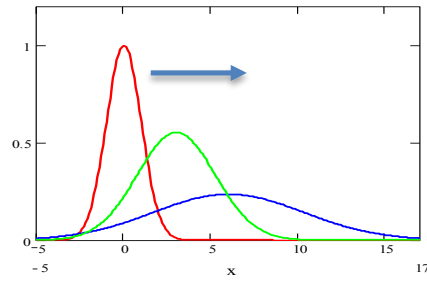
1.

- (a) We should consider electrons as wave-packets in situations where there are single electrons traversing a system at a time, i.e. when current levels are very low, typically sub femto Amp levels. When there are larger numbers of electrons, we can approximate them as a beam of electrons, which corresponds to a plane wave. Plane waves are monochromatic, so have a single value of energy and momentum, but have no spatial localization associated with them, whereas wavepackets comprise a range of energy and momentum values, and do exhibit localization, consistent with a single particle.
- (b) Wave-packets used to represent electromagnetic (EM) waves and matter have different dispersion properties, in that EM wavepackets exhibit no dispersion, and do not spread out over time, whereas matter wavepackets naturally disperse. The relationship between energy,  $E$  and momentum,  $k$  for EM wavepackets is  $E = \hbar kc$ , whereas for matter waves,  $E = \hbar^2 k^2 / 2m$ .





EM wavepacket



matter wavepacket

(c) Well,  $E = \hbar^2 k^2 / 2m$  which can be rearranged to be  $k = \frac{\sqrt{2mE}}{\hbar} = 2\pi/\lambda \Rightarrow \lambda = \frac{h}{\sqrt{2mE}}$

The numerical value of this is  $\frac{6.6 \times 10^{-34}}{\sqrt{2 \times 0.2 \times 9.1 \times 10^{-31} \times 1.5 \times 1.6 \times 10^{-19}}}$

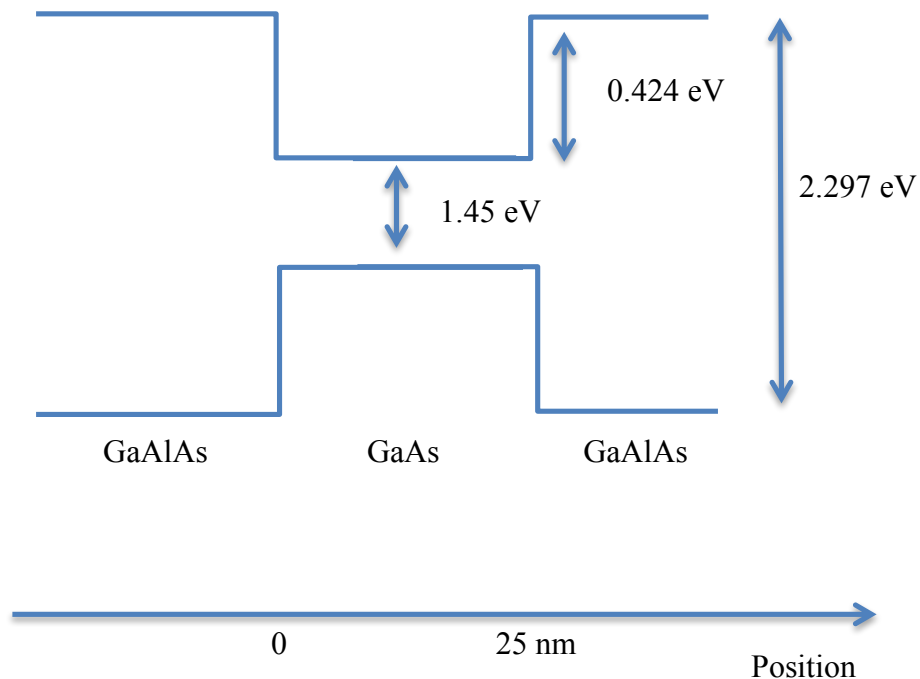
= 2.23 nm.

Given that the device size is around 14 times the electron wavelength, there is a strong chance quantum effects will be noticeable. The electron energy is much greater than the thermal energy  $k_B T$ , so these effects should not be smeared out. The current-voltage characteristics will display some oscillatory behavior due to interference between electrons scattered off both ends of the transistor.

As the transistor is reduced in size, the quantum effects will start to become more noticeable, and it will start to behave like a quantum well, with the effect that the current-voltage characteristics will start to deviate from those of a conventional transistor, with more pronounced oscillatory behavior. As well as this, as the wires to the transistor shrink, their resistance will continue to increase, and as their dimension shrinks below the electron mean free path, their resistivity will also increase. When they decrease below around 5 nm, the resistance will take on discrete values, again due to electron interference effects.

2.

(a) The material is  $\text{Ga}_{0.3}\text{Al}_{0.7}\text{As}$  and has a band gap of  $1.424 + 0.7 \times 1.247 = 2.297$  eV. This is split equally between the conduction and valence bands, and as the band gap of GaAs is 1.45 eV, this means the difference in bandgaps, which is  $(2.297 - 1.45)$  eV leads to quantum wells of depth  $(2.297 - 1.45)/2 = 0.424$  eV. Therefore, in the absence of any band-bending, the heterostructure has a band profile as shown:



(b) Assumptions:

- (i) The energy levels of interest are low enough that we can use the infinite well approximation. This is valid as long as they are less than  $1/10$  of the well depth.
- (ii) The electrons are non-interacting.
- (iii) There is no band-bending

The solution should include a derivation of the spectrum of energy levels associated with an electron of effective mass  $m^*$  in an infinitely deep well of width  $L$ :

$$E_n = \frac{h^2 n^2}{8m^* L^2}$$

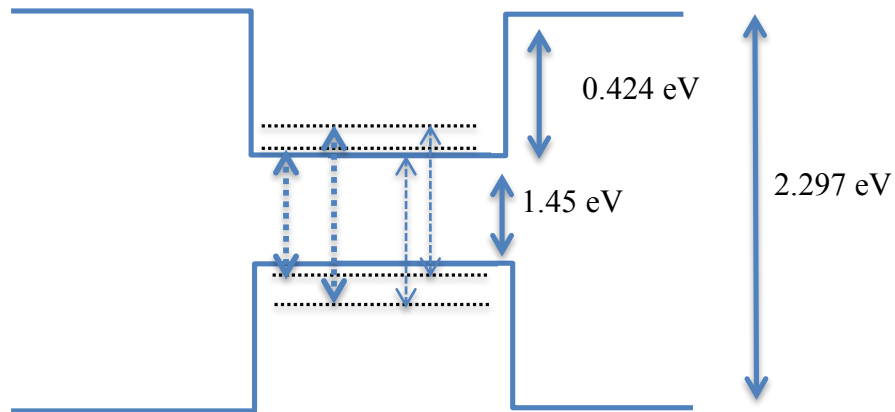
From which we find that the electron energies are  $E_n^e = 8.9 n^2 \text{ meV}$

and the hole energies are  $E_n^h = 1.33 n^2 \text{ meV}$

The electron ground state energy ( $n = 1$ ) is around 1/50 of the well depth, so our estimate will be accurate, as will the hole ground state energy which is around 1/100 of the well depth.

Therefore, the ground state energies are :  $E_n^e = 8.9^2 \text{ meV}$ ,  $E_n^h = 1.33 \text{ meV}$ , leading to a transition energy of  $1.45 + 0.0089 + 0.00133 \text{ eV} = 1.46 \text{ eV}$

(c) Sketch of optical density and it's origin:



Examiner's note: a few candidates forgot to include the fact that the change in band gap was shared equally between the conduction and valence bands, and a few also assumed the transition energy was just the difference between the energy levels, leaving out the 1.45 eV band gap. Also it is worth mentioning that the transitions between states of equal symmetry (the thicker lines above) are more favourable, so have higher intensity.

3(a)

The potential energy of the system is  $V$ , where

$$V = 1/2 \kappa x^2 = 1/2 m \omega_c^2 x^2$$

Schrödinger's equation for this system is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{1}{2} m \omega_c^2 x^2 \psi = \mathcal{E} \psi.$$

This problem can be simplified if we employ a change of variables from  $x$  to  $y$ , where  $y = x \sqrt{m \omega_c / \hbar}$ , and define  $\alpha = 2E / \hbar \omega_c$

Schrödinger's equation is now:

$$\frac{d^2 \psi}{dy^2} + (\alpha - y^2) \psi = 0.$$

The solution of which is known to be  $\psi(y) = F(y) e^{-y^2/2}$ .

*(To see where this comes from, look at the asymptotic solution when  $y \gg a$ , which is of the form  $y = y^n \exp(-y^2/2)$ .)*

Substituting this form of  $\psi(y)$  into the above equation, we find

$$F'' - 2yF' + (\alpha - 1)F = 0.$$

We should now assume a power series solution for  $F(y)$ ;

$$F = \sum_{p=0}^{\infty} a_p y^p.$$

From which it can be seen that:

$$F' = \sum_{p=0}^{\infty} p a_p y^{p-1} \quad \text{and} \quad F'' = \sum_{p=0}^{\infty} p(p-1) a_p y^{p-2}.$$

An important point here is that  $y$  can never have a negative power, as that would lead to an infinity at  $y = 0$  which would be unphysical ( $\psi$  must always be finite, as  $|\psi(x)|^2$  represents the probability of the particle being located at position  $x$ ). The first two terms of  $F''$  therefore must equal 0, so we must put  $p = p+2$  in the above expression for  $F''$ .

Substituting for  $F$ ,  $F'$  and  $F''$  into Schrödinger's equation leads to the following:

$$\sum_{p=0}^{\infty} [(p+2)(p+1)a_{p+2} - (2p+1-\alpha)a_p] y^p = 0.$$

For a non-trivial solution, the coefficient of each power of  $y$  must vanish, leading to the following recursion relationship:

$$\frac{a_{p+2}}{a_p} = \frac{(2p+1-\alpha)}{[(p+1)(p+2)]}.$$

However, the resulting power series tends to infinity with increasing  $y$  (the limit of  $a_{p+2}/a_p$  tends to  $1/p$ , the sum of which is infinity), so we must truncate the power series.

The solution can be re-written as two power series, each containing either all even or odd powers of  $y$ . Using the recursion relation above, all coefficients can be expressed in terms of either  $a_0$  or  $a_1$ . Then we need to choose some value for  $p$ , say,  $n$ , such that  $2p+1-\alpha=0$ . That power series will end there, and we need to neglect the other power series.

Both of these conditions lead to the following:

$$\begin{aligned} \alpha &= 2n+1 \text{ for } n = 0, 1, 2, \dots \\ a_1 &= 0 \text{ for } n \text{ even, } a_0 = 0 \text{ for } n \text{ odd} \end{aligned}$$

From our definition of  $\alpha = 2E/\hbar\omega_c$  we have for the energy eigenstates of the quantum simple harmonic oscillator:

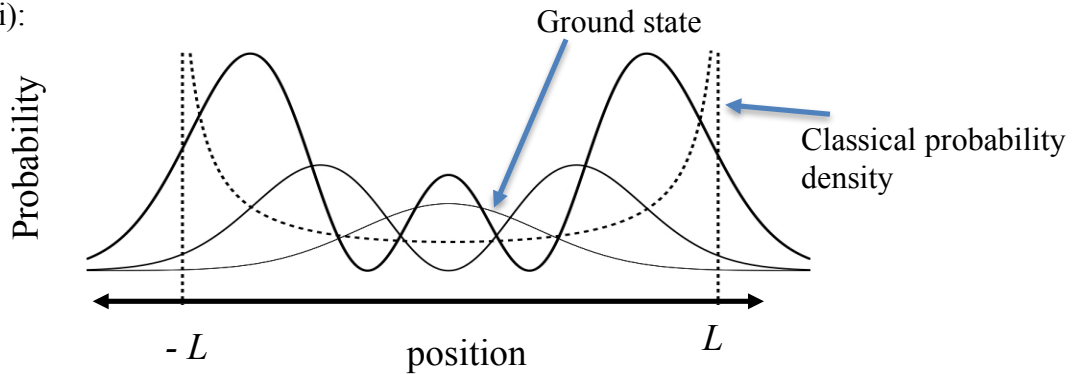
$$E_n = (n+1/2)\hbar\omega_c.$$

So, for our specific problem, we do not know  $\omega_c$  but we do know  $k$  and  $m$ . The relationship between these parameters is  $\omega_c = \sqrt{\frac{k}{m}} = 1.59 \times 10^{14}$  rad/s. Therefore, the ground state energy, where  $n = 0$  is  $\hbar\omega_c/2 = 8.3 \times 10^{-21}$  J = 0.988 eV.

(b)

In the ground state, the most probable position is in the centre, whereas for higher levels, the probability oscillates quickly.

(i) & (ii):



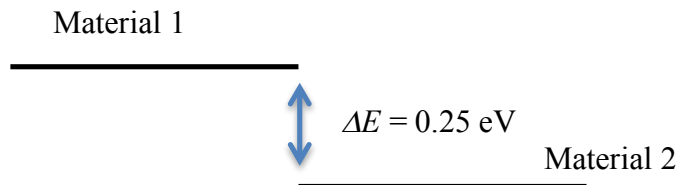
The differences between the classical and quantum harmonic oscillator are that for the ground state, the classical oscillator is most likely to be found at the extremes, whereas the quantum oscillator is most likely to be found at the centre. Also, the quantum oscillator has a finite probability of being found beyond the classical extremes of motion. For highly excited states (large values of  $n$ ), the quantum and classical agree. This is indicated above where we have also drawn the probability density for  $n=2$  and  $n=3$ , and we can see that by the time we get to  $n=3$ , the peak probability is shifting towards the extremes.

Examiner's note: almost all were able to derive the correct expression for  $E_n$ , but a few though the ground state was  $n = 1$  rather than  $n = 0$ . Most candidates did not mention that the quantum and classical probabilities converge for high values of  $n$ .

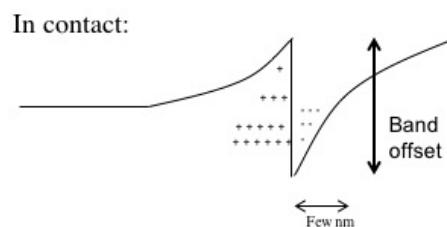


4. (a)

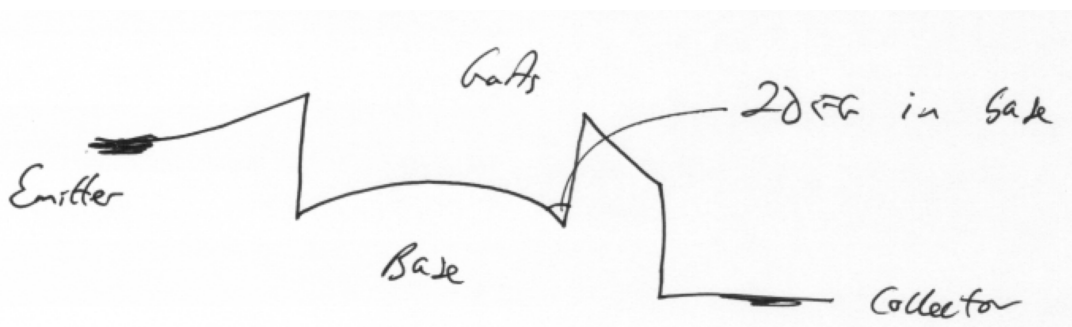
Consider the two materials independently: they have different band-gaps, where the difference between them both is the band offset,  $\Delta E$ . Before allowing band-bending:



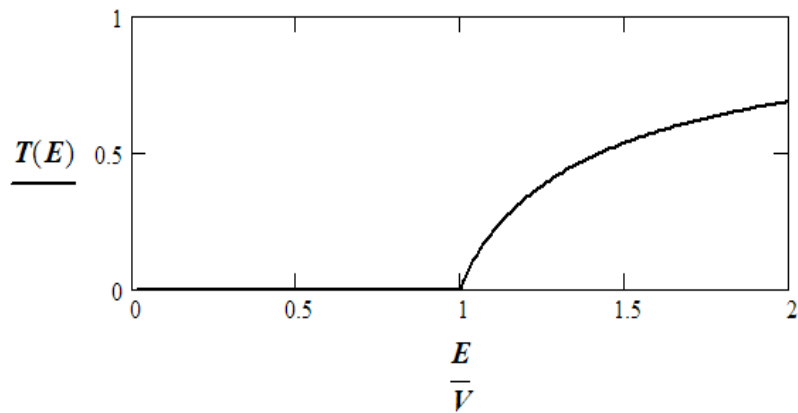
When the materials are placed together, electrons will diffuse down the potential step from the GaAlAs where there is a higher concentration of electrons, and go to the GaAs where there are fewer electrons. Likewise, holes will diffuse to the left. The net effect of this is that a dipole layer of charge is formed just at the interface, which causes the bands to electrostatically bend, resulting in the following band structure:



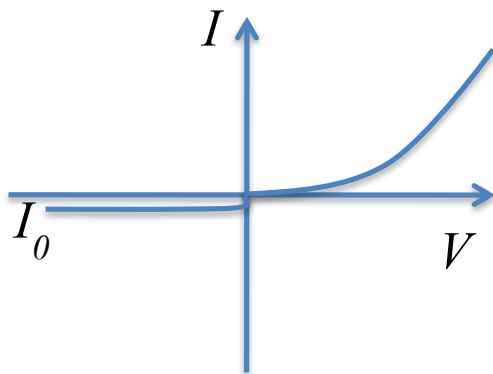
(b) 2DEGs have a very high mobility – they are a way to greatly increase the carrier density in a semiconductor without having to dope it, hence reducing the scattering of electrons as they traverse the material. An example of a device incorporating a 2DEG is a bipolar transistor as shown below:



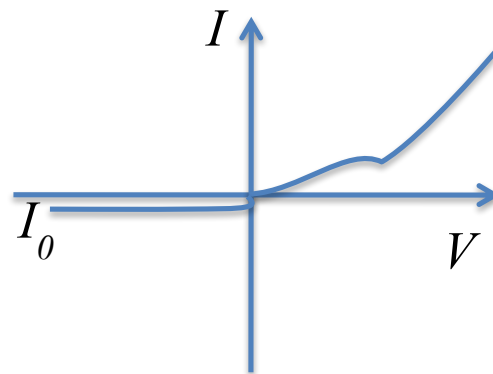
- (c) As electrons flow across this junction, we would expect the I/V characteristics to be mostly determined by the transmission probability,  $T$ . This is a potential step, so will have a  $T$  which varies as follows:



$T$  asymptotically approaches 1, so once the voltage is high enough,  $I$  will vary linearly with  $V$ , but until then, it will have a dependence more like that shown above. The expected characteristics will vary as shown below, akin to a diode. When there is band-bending, that results in more noticeable diode-like characteristics, also shown below:



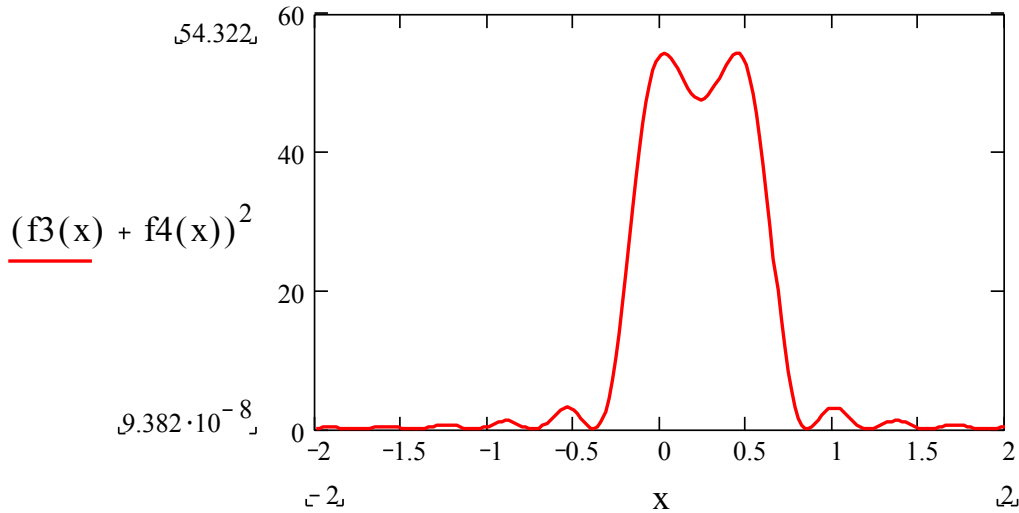
No band-bending



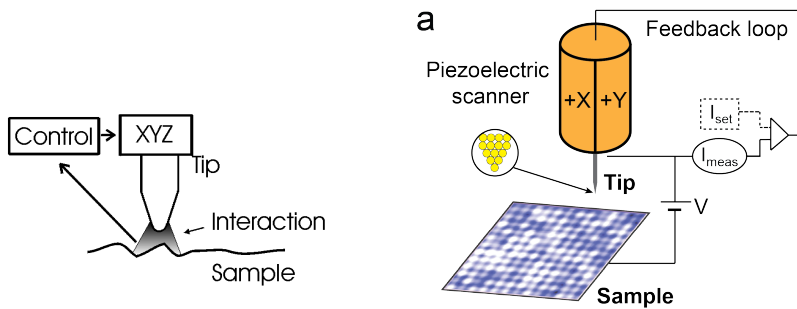
Band-bending

5.

(a) The Rayleigh criterion states that the closest spacing between two point objects that can be resolved is of the order  $0.8\lambda$ . At this point, the dip in intensity at the midpoint between the images is 20%. For light of wavelength 500 nm, that corresponds to a spacing of  $0.8 \times 500 \text{ nm} = 400 \text{ nm}$ .



(b) Principle of operation:

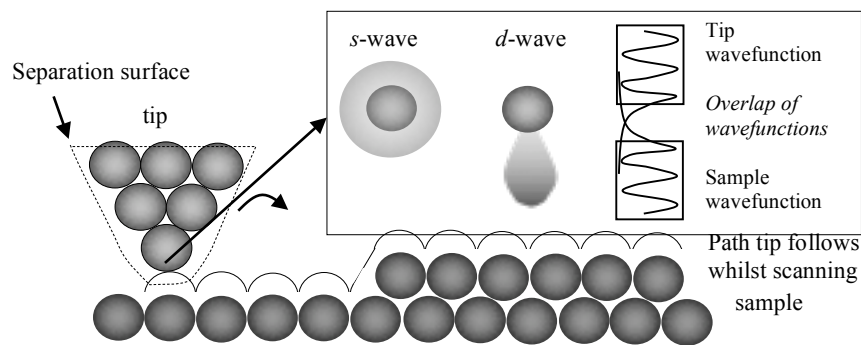


A bias voltage is applied between the tip and the sample, both of which must be conducting. When the distance between them is less than  $\sim 1 \text{ nm}$ , a tunnel current flows, which is typically in the range  $1 \text{ pA} - 1 \text{ nA}$  for a bias voltage  $0.1 - 1 \text{ V}$ . The tip is mounted on an xyz actuator which scans it over the surface, and a feedback loop controls the z-height in order to maintain a constant tunnel current. The image thus obtained, of z-height as a function of xy position, is essentially a map of the local density of electronic states of the sample. The tunnel current varies exponentially with tip-sample distance, in accordance with the transmission probability varying as  $T \sim e^{-2ka}$ , where  $k$  is the wave-vector of electrons in the tunnel gap. More exactly, the current varies as :

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

where  $\rho_s$  and  $\rho_t$  are the density of electronic states in both the tip and the sample.

For typical materials, this leads to a variation of the tunnel current by around an order of magnitude for each Å variation in tip-sample distance. This means that the mechanical construction of the STM must lead to very low external noise being coupled into the microscope.



Principle of operation of STM. Insert shows two possible tip states, i.e. where the apex atom has its outer electrons in *s* or *d* orbitals. On the right, we have indicated the overlap between tip and sample wavefunctions, which gives rise to tunneling.

To estimate the lateral resolution of STM, we make use of the fact that the tunnel current depends exponentially on the tip-sample distance. If the STM tip has a radius of  $R$  nm, and the minimum tip-sample distance is  $s$ , then the distance between the tip surface and the sample varies with  $x$  as  $z = s + x^2/2R$ , as shown in Fig 4.3.

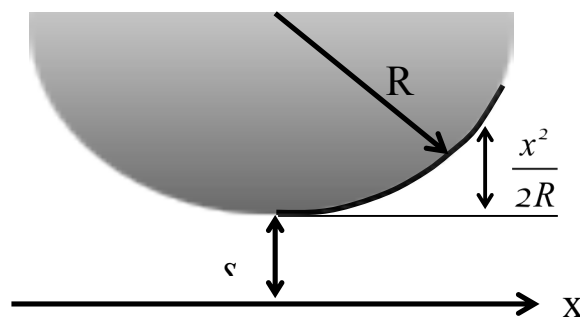


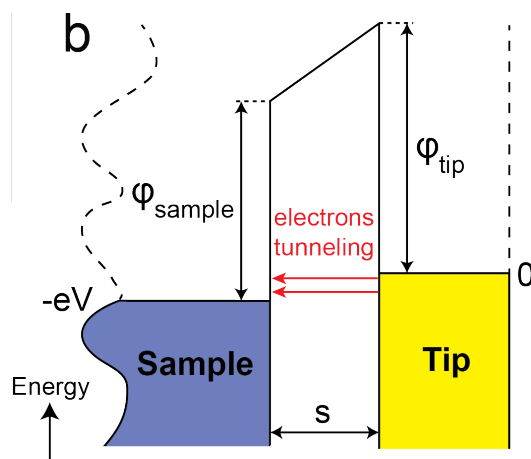
Fig. 4.3. STM tip of radius  $R$  a distance  $s$  away from a surface showing the variation in distance from the tip away from the apex.

If we define the resolution as the lateral distance at which the current drops to around 10% of its maximum value, we get a value for  $x$  of around  $(0.1/2R)^{0.5}$ . This means that in order to achieve atomic resolution (i.e.  $x \sim 0.1$  nm) the tip radius should be no

larger than 5 nm. In actual fact, the tip radius is often much larger than this, and atomic resolution is still achieved, indicating that there must be an asperity, possibly even a single atom at the end of most STM tips. In many cases, this single atom can come from the sample itself. The nature of this apex atom will determine the resolution, image contrast and spectroscopy data obtained in any given STM experiment, so extensive cleaning is often carried out on STM tips in order to improve repeatability.

STM has been demonstrated time and time again to be capable of atomic resolution on surfaces. However, apart from the case of HOPG (graphite), this comes at a price — UHV (Ultra-High Vacuum). UHV conditions (i.e. base pressure of  $10^{-10}$  mbar or lower) are required in order to maintain a clean STM tip and sample surface for a number of hours. Under ambient conditions, all surfaces are coated with several monolayers of adsorbed “contamination” — mostly water and hydrocarbons that are naturally present in air. In order to probe the underlying surface, samples need to be cleaned, and the amount of time for which they remain clean will depend on the pressure of their local environment. Under ambient conditions, any surface will remain clean for only a fraction of a second, and under deep UHV conditions ( $\sim 10^{-11}$  mbar) this can be extended to several days. In a typical STM experiment, the tip (usually etched W or mechanically cut Pt/Ir tips are used) and sample are cleaned immediately prior to imaging, usually by repeated cycles of thermal annealing and ion sputtering. Vibration isolation is paramount, as the floor in a typical building will be vibrating at several Hz, with an amplitude of several  $\mu\text{m}$ . These vibrations must be damped to around 1 pm or below for the STM to work effectively. There are many different ways of achieving this level of isolation: (i) the STM head can be made small and stiff with natural resonance frequencies in the kHz range, or (ii) the STM can be mounted on vibration isolators. For ease of use, many researchers have gone for the second option, as small STMs can be rather difficult to use, especially under UHV conditions.

(c) The potential as seen by an electron.  $S$  is the gap, which in this case is 1 nm.



**Q1 Wave-particle duality & the structure of atoms**

This question was mostly well answered, with good descriptions of the differences between plane waves and wave packets in the context of quantum mechanics. The last section on calculating the wavelength of an electron in a transistor was also well handled with some insightful discussions.

**Q2 Band Engineering & Quantum wells**

This question was very well answered. The majority of candidates who attempted it obtained the correct energy levels and were able to describe the optical density of a 1D quantum well.

**Q3 Quantum harmonic oscillator**

This was very well answered. Most candidates were able to solve the Schrödinger equation for the quantum harmonic oscillator, and derived the correct spectrum of energy levels, with the result that most calculated the ground state vibration energy of the given molecule. A few candidates mistakenly thought the ground state was for  $n = 1$  rather than  $n = 0$ . Most were conceptually correct regarding the differences between the probability distribution and the classically expected one, but only a handful of candidates went on to describe how the classical and quantum results converge for high values of  $n$ .

**Q4 Semiconductor heterostructures and 2D electron gasses**

This was not well-answered in general, perhaps as it involved some lateral thinking and was about a heterostructure not encountered before. The aim was to apply the principles learned in lectures to this new setup to predict the overall shape of the current-voltage characteristics. All answers correctly drew the band structure and knew the relationship between Transmission probability and current but struggled to put it all together. As regards the last part, only one candidate mentioned that the 2DEG is desirable as it is a way of increasing the charge density within an intrinsic semiconductor, so will have a very high mobility, as opposed to the case when we dope a semiconductor which results in lower mobility.

**Q5 Microscopy**

This question was well-answered. A few candidates forgot to add the fact that in order for an electron to flow from the tip to the sample, there needs to be a potential difference, and 2 candidates described the AFM rather than the STM, but otherwise it was well done.