

## ENGINEERING TRIPOS PART IIB 2020/21

### CRIBS FOR MODULE 4B5

1.(a) The need for quantum mechanics arose from the turn of the 20<sup>th</sup> century, necessitated by a number of experimental irregularities. For instance, on the basis of the understanding of nature at the time, the very existence of atoms was puzzling. It was known that atoms consisted of negatively charged electrons orbiting positively charged nuclei. From conventional electromagnetism, we know that any accelerating charged particle will emit electromagnetic radiation and hence lose energy. Therefore, if an electron orbits a nucleus, by the very fact that it is moving around the nucleus, it is accelerating, and we would expect it to radiate, lose energy and eventually spiral in towards the nucleus. This clearly does not happen, so a theory was needed to explain why not, as Maxwell's theory of electromagnetism had very successfully been able to explain very many other phenomena and was widely accepted.

Another problem was the phenomenon of photoemission – the effect whereby incident electromagnetic radiation causes electrons to be ejected from metal surfaces. It was observed that electrons are only ejected once the frequency of the light reaches some threshold value, their energy scales linearly with frequency and the number of electrons ejected increases as the light intensity increases. This is at odds with classical electromagnetism which predicts that (i) the frequency should not make any difference whatsoever and (ii) the energy of the ejected electrons should only depend on the intensity of the light (Energy per unit volume of light is  $\frac{1}{2} \epsilon_0 E^2$ , and intensity is energy per unit area). There is no reason classically for the number of electrons ejected to depend on intensity. The explanation for this effect within the framework of quantum mechanics is that light consists not only of waves, but also of particles called *photons*, which contain distinct amounts of energy depending linearly of frequency. The proportionality constant is Planck's constant,  $h$ . Electrons are bound to the metal by an energy called the work function and until the frequency of light is high enough, individual photons don't have enough energy to free them. Above this threshold frequency, electrons are emitted, and the excess energy is taken up as the electron's kinetic energy. The number of electrons ejected then scales as the number of photons, which depends on the intensity. Another turning point was the observation of electron diffraction – clear evidence that particles have a wave-like character.

Other experimental evidence was for instance the inability of Physics to explain (i) why some materials are conductors and others are insulators, (ii) the origin of electrical resistance, (iii) the observed dependence of specific heat capacity on temperature and (iv) the origin of discrete spectra from heated materials, e.g. the sun.

(b) Wavepackets are used to represent localised entities such as particles. To construct a wavepacket, add two sinewaves,  $E = E_0[\cos(\omega_1 t - k_1 x) + \cos(\omega_2 t - k_2 x)]$ . This can be rewritten as  $E = 2E_0 \sin(\omega_{\pm} t - k_{\pm} x) \cos(\omega_{\mp} t - k_{\mp} x)$ , where  $\omega_{\pm} = (\omega_1 \pm \omega_2)/2$  and  $k_{\pm} = (k_1 \pm k_2)/2$ . This represents a sinewave of frequency  $\omega_{\pm}$  which has its amplitude modulated at the frequency  $\omega_{\mp}$ .

to produce beats. This therefore exhibits localised areas of enhanced field strength which may be used to represent particles. These localised areas that we call wavepackets propagate through space at the group velocity  $d\omega/dk = c$  (the speed of light). In the absence of dispersion, these wavepackets will propagate without changing shape, but if there is dispersion, they will spread out.

The phase velocity is  $\omega/k = \omega_2/k_2 = c$ . The group velocity can in principle vary, but up to a maximum limit of  $c$ . We could refine/modify the wavepacket by summing together an infinite number of sinwaves with e.g. a Gaussian spectral function. This will increase the degree of localisation.

(c) Construct a wavepacket as follows:

$$E = E_0 \int_{-\infty}^{\infty} f(k) e^{-i(kx - \omega t)} dk \quad (1)$$

Where  $f(k)$  is the *spectral function*, which is a Gaussian of width  $\delta$ :

$$f(k) = \frac{1}{\sqrt{2\pi}\delta} e^{-\frac{k^2}{2\delta^2}}$$

Therefore, we can write (1) as :

$$E = E_0 \frac{1}{\sqrt{2\pi}\delta} \int_{-\infty}^{\infty} e^{-\frac{k^2}{2\delta^2}} e^{-ik(x - ct)} dk$$

Where we have used the relationship that  $\omega = ck$ .

We tend to use Gaussian spectral functions as they provide the best agreement with experiment. This is known as a *Gaussian integral* and the easiest way to solve is to change the variables as follows:

Let  $k' = k - ib/2a$  where  $a = 1/2\delta^2$  and  $b = x - ct$ . This gives us:

$$E = E_0 \frac{1}{\sqrt{2\pi}\delta} e^{-\frac{b^2}{4a}} \int_{-\infty}^{\infty} e^{-ak'^2} dk'$$

This integral is known to be equal to  $\sqrt{\pi/a}$ , with the net result therefore being that:

$$E = E_0 \sqrt{\delta} e^{-\frac{\delta^2}{2}(x - ct)^2}$$

$$E = E_0 \sqrt{\delta} e^{-\frac{\delta^2}{2}(x - ct)^2} \cos(\omega t - kx)$$

Heisenberg's uncertainty principle states that  $\Delta x \Delta p \geq \frac{\hbar}{2}$ . To see where this comes from, consider that the spectral function has a width (in  $k$  - space) of  $\Delta k = \delta$ . By inspection, the solution for  $E(x)$  has a spatial width  $\Delta x = 1/\delta$ . Therefore, by inspection,  $\Delta x \Delta k = 1$ . Given that momentum,  $p = \hbar k$ , it follows that  $\Delta x \Delta p = \hbar$ . This is just a lower bound on the uncertainty, hence the inequality in Heisenberg's uncertainty principle. What this all means physically is that we can never simultaneously know absolutely both the position and momentum of a particle, and the more accurately we know one, the less we can know about the other.

***Principal Assessor's comments:***

*This question was reasonably well answered. All candidates were able to answer the first part which was a description of two areas where quantum theory was needed to explain an anomalous result. Some students gave very brief answers whereas others recognized that being worth 30% of the marks, it warranted a more fulsome answer, as it was somewhat open-ended. The rest was generally well answered and most students demonstrated an understanding of the difference between group and phase velocity, although only a few students were then able to rationally explain the origin of the uncertainty principle.*

2. (a)

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

To answer the question, in principle only this equation needs to be written down – the derivation is not necessary. The trick is in applying it correctly. By definition,  $\omega_c = \sqrt{\frac{k}{m}}$ , so we need to know the mass of the atoms. We know that  $k = 520$  N/m and  $m = 10^{-26}$  kg, so we can determine that  $\omega_c = \sqrt{\frac{520}{10^{-26}}} = 228 \times 10^{12}$  rad/s. Therefore, the spectrum of energy levels is  $(n + 1/2) 1.05 \times 10^{-34} \times 228 \times 10^{12} / 1.6 \times 10^{-19}$  eV.

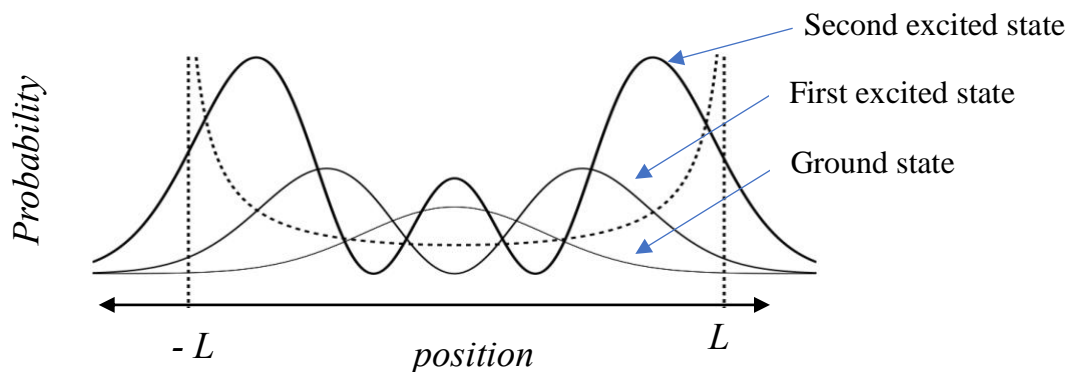
This reduces down to  $149.6(n + 1/2)$  meV.

(b)

Therefore, only discrete values of energy are allowed, which is a characteristic of all quantum systems and arises due to the boundary conditions we are imposing. If we visualise the potential within a QSHO, it is a parabolic well so only those quantum states whose corresponding wavelength is a half-integer divisor of the well extent are allowed. The main disparity between quantum and classical is that they both seem to predict the opposite behaviour – the ground state wavefunction has its maximum at the centre of the well, whereas a classical oscillator spends most time at the extremes (where it is travelling slowest). However, higher energy levels in the QSHO have probability densities that approach this, and eventually the quantum and classical models converge. This is commonly seen in quantum

systems – apparently very different behaviour for low energy levels and agreement with classical expectations for highly excited states – this is known as the *correspondence principle*. The consequence of the ground state having nonzero energy is that according to quantum mechanics, no system is ever fully at rest – there is always some vibration. This is essentially another way of demonstrating the uncertainty principle.

(c) The probability density of the ground state and the first two excited states are shown below:



Where  $L$  is the classical extent of the oscillating system (e.g. if it is a mass on a spring, it is the initial amount by which the spring is extended or compressed before being released and allowed to oscillate) and the dotted curve is the classically expected probability (determined by plotting  $1/\text{velocity}$ ).

***Principal Assessor's comments:***

*This question was very well answered. Some students were a little uncertain about the level of detail required as the appropriate formula was in the formula sheet, but some went and derived it anyway. The key point was that all students recognized the relationship between the classical and quantum harmonic oscillator, and most obtained the correct energy levels. Very few students were able to succinctly explain why energy levels are quantized and thought it was to do with electron wavelengths, rather than recognizing it is a direct consequence of the boundary conditions. Most got the point about classical and quantum mechanics converging for highly excited states.*

3. (a) Wavefunctions represent the probability distribution of the quantum particles to which they pertain. If we have a particle described by the wavefunction  $\psi(r,t)$ , then  $|\psi(r,t)|^2$  is the probability of finding the particle at position  $r$  at time  $t$ . The rules for determining  $\psi(r,t)$  in boundary-value problems are that  $\psi(r,t)$  and its first derivative are continuous at all boundaries. Physically this means that the wavefunctions are single-valued, i.e. there is only one value for the probability of finding the particle at any point in space. Also, the energy of a quantum particle is proportional to  $\frac{d^2\psi}{dr^2}$ , so if there were any discontinuities, that would correspond to infinite energy which is unphysical.

(b) We expect that as the electrons have more energy than the cylinder, they will have sufficient energy to pass through. On the basis of classical mechanics, we would expect that they will simply slow down, with a net kinetic energy before of 50 eV and inside of 10 eV, hence the slower motion. However, quantum mechanically, given that the electron beam is described by waves, it will partly reflect as it experiences a discontinuity. Schrödinger's equation can be written in the regions before (region I) and in the cylinder (region II) as

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_I}{dx^2} = E\psi_I$$

And

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}}{dx^2} + V\psi_{II} = E\psi_{II}$$

Where  $E = 50$  eV &  $V = 40$  eV.

The solutions to these equations are:

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

And

$$\psi_{II}(x) = A_2 e^{-ik_2 x}$$

Where  $k_1 = \sqrt{\frac{2mE}{\hbar}}$  and  $k_2 = \sqrt{\frac{2m(E-V)}{\hbar}}$

Invoking our boundary conditions, i.e. that the wavefunctions and their first derivatives are continuous at the boundary ( $x = 0$ ), we determine the following relationships:

$$A_1 + B_1 = A_2$$

$$ik_1A_1 - ik_1B_1 = -ik_2A_2$$

From which we have that  $\frac{B_1}{A_1} = \frac{(k_1-k_2)}{(k_2+k_1)}$ , from which we determine that the reflection probability,

$$R = \left| \frac{(k_1-k_2)}{(k_2+k_1)} \right|^2 = 0.144$$

(c) Now that the cylinder is finite in extent, there is an additional boundary, at a position we are calling  $x = L$ , where  $L = 1$  nm. The extra boundary arises as we now have the regions before and after the cylinder (regions I and III, respectively) as well as inside the cylinder (region II).

The solutions to Schrödinger's equation in these regions are:

$$\psi_I(x) = A_1e^{ik_1x} + B_1e^{-ik_1x}$$

$$\psi_{II}(x) = A_2e^{ik_2x} + B_2e^{-ik_2x}$$

And

$$\psi_{III}(x) = A_3e^{-ik_1x}$$

$$\text{Where } k_1 = \sqrt{\frac{2mE}{\hbar}} \text{ and } k_2 = \sqrt{\frac{2m(E-V)}{\hbar}}$$

Invoking our boundary conditions as before, at the first boundary where  $x = 0$ , we find that

$$A_1 + B_1 = A_2 + B_2$$

$$ik_1A_1 - ik_1B_1 = ik_2A_2 - ik_2B_2$$

From this, we can say that

$$\frac{B_1}{A_1} = \frac{A_2(k_1-k_2) + B_2(k_1+k_2)}{A_2(k_1+k_2) + B_2(k_1-k_2)}$$

At the right boundary (where  $x = L$ ), we find that

$$A_2 = \frac{A_3e^{ik_1L}[k_2 + k_1]e^{-ik_2L}}{2k_2}$$

And

$$B_2 = \frac{A_3 e^{ik_1 L} [k_2 - k_1] e^{ik_2 L}}{2k_2}$$

Substituting into the above expression for  $B_1/A_1$ , we arrive at the following expression:

$$R = \left| \frac{B_1}{A_1} \right|^2 = \frac{(k_2^2 - k_1^2) \text{Sinh}(k_2 L)}{2k_1 k_2 \text{Cosh}(k_2 L) - (k_2^2 + k_1^2) \text{Sinh}(k_2 L)}$$

For our particular situation,  $R = 0.1$

***Principal Assessor's comments:***

*All students managed to explain what wave-functions are and what they represent, and most were able to explain their properties in the context of boundary-value problems. A few were a bit brief and stated the boundary conditions rather than explaining what they mean, which is what the question was asking for. The next bit, looking at quantum scattering from a potential step was straightforward, but a few students did not answer the question asked – we were looking for the reflection probability, whereas some gave the transmission probability. A few also mixed up reflection coefficient and reflection probability. The last part of the question, which considered a potential step rather than a barrier, was less well answered, and a few students simply stated a formula they had clearly memorized, and which was the incorrect one anyway as it was only valid for the case of tunneling.*

4. (a) The potential is shown below. In regions I & III, the potential is infinite, which means there is no probability of finding the particle there so it must be confined within region II. Therefore, the problem reduces down to simply solving Schrödinger's equation in region II, which is of the form:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

The simplest solution to this equation is:

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

Where  $k = \sqrt{\frac{2mE}{\hbar}}$

As the wavefunction must be zero outside the well, it must also be zero at the boundaries for continuity.

Matching at the left side ( $x = 0$ ):  $A + B = 0 \Rightarrow A = -B$

i.e. we can rewrite the wavefunction as

$$\psi(x) = Ae^{ik_1x} - Ae^{-ik_1x} = C\sin(kx)$$

Matching at the right side,  $C\sin(kL) = 0 \Rightarrow k = \frac{n\pi}{L}$ , where  $n = 1, 2, \dots$

Therefore, the wavefunction for an electron in an infinitely deep potential well is of the form

$$\psi(x) = C\sin\left(\frac{n\pi}{L}x\right)$$

To find the value of  $C$ , we need to normalise, i.e.

$$\int_0^L |\psi(x)|^2 dx = 1 \Rightarrow \int_0^L C^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

Which gives us a value of  $C = \sqrt{\frac{2}{L}}$

To determine the energy levels, remember that the energy of the electrons within the well is purely kinetic and is given by  $E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$



As  $k$  has quantised values as dictated by the boundary conditions above, the consequence of this is that the energy levels are also quantised. Substituting for  $k$  into the expression for energy above, we find that:

$$E = \frac{\hbar^2 \left(\frac{n\pi}{L}\right)^2}{2m} = \frac{h^2 n^2}{8mL^2}$$

To answer the question, all that is actually needed is to write the following:

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$$

So, we can write the wavefunction as

$$\psi(x) = \sqrt{\frac{2}{20 \times 10^{-9}}} \sin\left(\frac{n\pi}{20 \times 10^{-9}} x\right) = 10^4 \sin\left(\frac{n\pi}{20 \times 10^{-9}} x\right) = 10^4 \sin(0.157nx) \text{ where } x \text{ is in nm.}$$

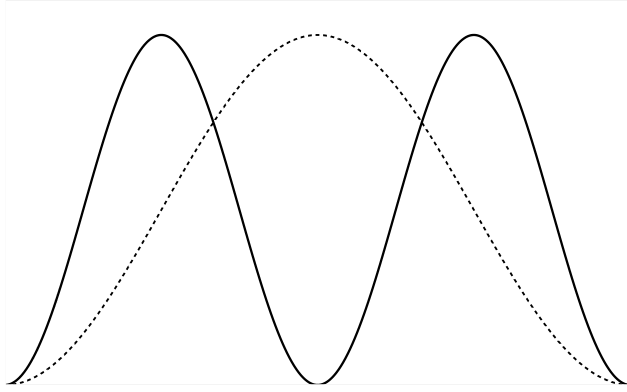
For the energies in eV,  $E = \frac{h^2 n^2}{8mL^2} = \frac{(6.6 \times 10^{-34})^2 n^2}{8 \times 0.1 \times 9.1 \times 10^{-31} \times (20 \times 10^{-9})^2} \times \frac{1}{1.6 \times 10^{-19}} = 9.3n^2 \text{ meV}$

(b) Quantum wells are fabricated using what is known as *band-gap engineering*. The technique used to fabricate them is generally MBE (molecular beam epitaxy). The materials used are semiconductors, as they can be doped controllably to produce specific band profiles. In infinite wells, wavefunctions exist only within the well, and there is zero probability of finding them outside the well. In finite wells, there is a probability of locating the particle outside the well. This probability increases as (i) the energy levels ( $n$ ) increase, (ii) the well-width decreases or (ii) the confining potential (the depth of the well) decreases.

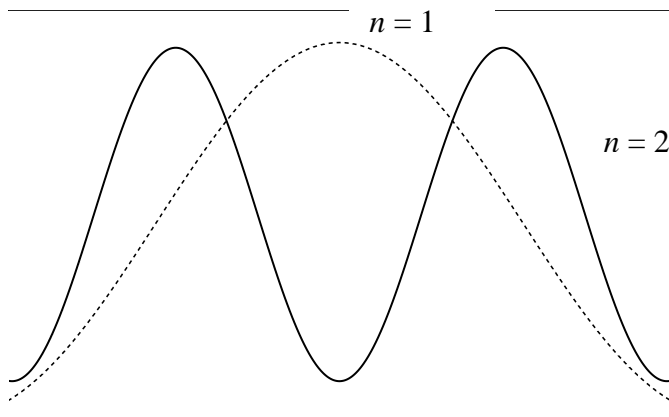
A finite well can be approximated as an infinite one if it is not too shallow, i.e. if the depth of the well is larger than the first bound state of the corresponding infinite well of the same width. A common example of a quantum well is a semiconductor laser. These are typically 10-20 nm wide, and fabricated from direct band-gap materials such as GaAs and GaAlAs. The depth of such wells tends to be in the range 0.1-0.3 eV. For the semiconductor laser, the operation is based on transitions between electron states in the conduction band and same-symmetry hole states in the valence band. The energy of these transitions is dictated by the bandgap plus the confinement energies of the corresponding states.

(c) Probability density for an electron in an infinitely deep well, ground state ( $n = 1$ ) and first excited state ( $n = 2$ ).

$$n = 1 \qquad n = 2$$



Probability density for an electron in a finite depth well, ground state ( $n = 1$ ) and first excited state ( $n = 2$ ).



For the infinite well, the wavefunctions are zero outside the well, whereas for a finite well, this is not the case. As the well is made narrower or higher energy levels are looked at, the wavefunctions extend more into the region outside the well. As we reduce the depth of a well, the energy levels also reduce.

(d) The uncertainty principle tells us that the minimum product of the uncertainty of the momentum and position,  $\Delta x \Delta p = \frac{\hbar}{2}$ . If we assume that  $\Delta x = 2$  nm, the width of the well, and the energy is  $\frac{\Delta p^2}{2m}$ , we can determine that  $\Delta p = \frac{\hbar}{2\Delta x} \Rightarrow E = \frac{\hbar^2}{8m\Delta x^2}$ .

By comparison with the above, this energy is a factor of  $\pi^2$  smaller than the exact calculation. We could obtain a more accurate estimate by recognising that the uncertainty in position is in fact smaller than the size of the well, and if we use the correct forms for uncertainty of position and momentum, we recover the exact value of energy.

***Principal Assessor's comments:***

*This question was well-answered across the board. Almost all students calculated the correct wave-function and most got the correct energy levels. Given that the formula for the spectrum of energy levels was in the formula sheet, it highlighted that some students were a bit careless when applying it and obtained incorrect values. The next part of the question on how quantum wells are created and a description of the use of a device incorporating one was well-answered. It was quite open-ended, and some students went into a lot of detail, which was a pleasure to read through. The next part, looking at the differences between finite and infinite quantum wells was answered well by all. The last part of the question was somewhat inconsistently answered. Some students applied the uncertainty principle appropriately and obtained sensible energy levels, whereas others were uncertain as to what to do. This turned out to be a more probing part of the question than anticipated.*

5. (a) Quantum supremacy is that point at which a quantum computer can solve problems that are beyond the capability of conventional devices/computers. Answer should include a mention of different types of qubit, with particular reference to superconducting Josephson junctions as the most promising.

(b) Answer should discuss some of the following: quantum computing can efficiently solve some hard problems that are intractable with conventional computers, a standard example is Shor's efficient quantum algorithm for factoring, which is a hard problem studied by mathematicians for centuries and is also the foundation of security of standard RSA cryptosystem.

-if a quantum computer is ever built, much of conventional cryptography will fall apart!

-quantum mechanics can be used to make codes as well as breaking them. Indeed, quantum cryptography (the art of code-making), in principle, allows perfectly secure communication between two parties in the presence of a technologically arbitrarily advanced eavesdropper,

-quantum mechanics has the potential to revolutionize both code- making and code-breaking,

-quantum information processing also allows other novel types of information processing. For instance, in a process called "quantum teleportation", a quantum state is decomposed locally in one spatial location and remotely reconstructed in another location through the communication of a classical message and the prior sharing of some quantum resource called "entanglement".

**What QIP cannot do**

There are tasks that even quantum information processing cannot do:

- The first example is to compute a "non-computable function" defined in the standard Church-Turing model.

So, while quantum computing can speed up (sometimes dramatically) some computations, it can always be simulated by a classical computer—but perhaps with an exponential overhead in some resource—time or space or resolution.

- A second example is a cryptographic task called quantum bit commitment.
  - A first major challenge of QIP is to discover new tasks where QIP gives a dramatic advantage. For instance, invent a useful new quantum algorithm. One important open problem is the graph isomorphism problem.
  - A second major challenge of QIP is to construct a large-scale quantum information processing in the real world. While writing equations on paper is easy, building a real large-scale quantum information processing is a major technological challenge that many groups in the world have been working very hard on.
  - A third major challenge of QIP is to solve some of the well-known open problems in the subject. An example is to find an efficient way to compute the various quantum channel capacities defined in the literature.
  - A fourth major challenge of QIP is to continue the quantization program and apply it to other subjects. If one takes the quantization program seriously, one would believe that it is meaningful to pick almost any scientific subject and ask if and how it can be combined with quantum mechanics. For instance, one can start with control theory and ask how quantum control theory can be formulated.
  - A fifth major challenge is to use QIP as a proof technique to tackle problems strictly in classical information theory. The power and limitation of such a proof technique deserves investigations.

(c)

- The theoretical developments concerning quantum complexity and quantum error correction have been accompanied by a burgeoning experimental effort to process coherent quantum information.
- To build hardware for a quantum computer, we'll need technology that enables us to manipulate qubits. The hardware will need to meet some stringent specifications:
  1. Storage: We'll need to store qubits for a long time, long enough to complete an interesting computation.
  2. Isolation: The qubits must be well isolated from the environment, to minimize decoherence errors.
  3. Readout: We'll need to measure the qubits efficiently and reliably.
  4. Gates: We'll need to manipulate the quantum states of individual qubits, and to induce controlled interactions among qubits, so that we can perform quantum gates.

5. Precision: The quantum gates should be implemented with high precision if the device is to perform reliably.

***Principal Assessor's comments:***

*This question was on a new part of the course on quantum computing and was the most open-ended question on the paper, also being largely descriptive and explanation – based. It was therefore very surprising that only two candidates attempted it. Both answers were reasonably good, of a roughly II.1 standard and demonstrated a good understanding of the core concepts. I suspect students stayed with the more tried and tested parts of the course for examination, and moving forward, I will ensure more emphasis is given to this area.*