

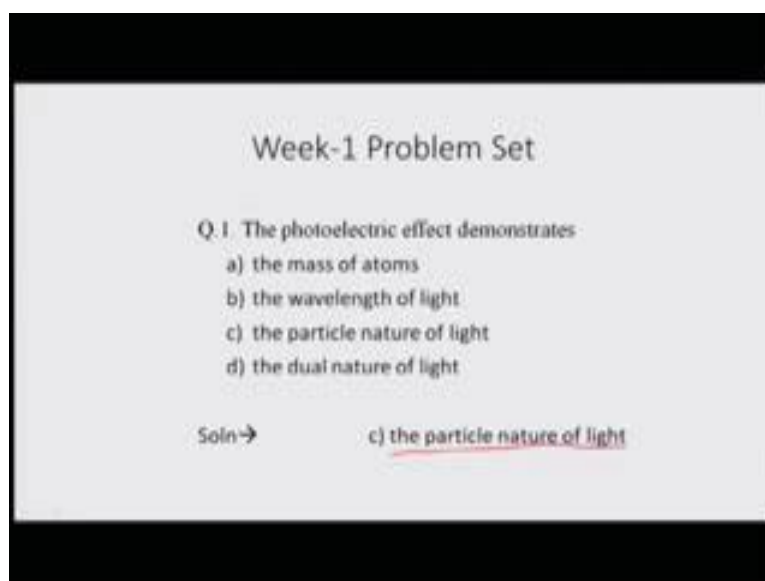
Implementation Aspects of Quantum Computing
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Lecture - 22
Solution to problem set – 1

In the last lecture we looked at the levels of implementation that you can do with optical approaches to quantum computing. And there may be several more of it, but what we will do now is that we will look at those kinds of implementations with other aspects as we mentioned in the last class also. That there are other aspects like Spintronics, where optics and other kinds of optical implementations as well as teleportation, we have looked at it before all those become very interesting and important. Those we will deal with it as we look at those particular kinds of implementations.

From today's lecture onwards for this week, for the rest of this week, we will be solving the assignment problems that we have been giving you for the last 6 weeks. And, maybe I will not be able to do it in the last week, but generally as much as possible we will try to do because while doing these assignment problems we will also revisit and refresh some of the problems and some of the aspects that we were been looking into in this area of implementation of quantum computing. We will also link you at every time while we do the problems to the key concepts that we are looking at while we are doing this.

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Week-1 Problem Set

Q.1 The photoelectric effect demonstrates

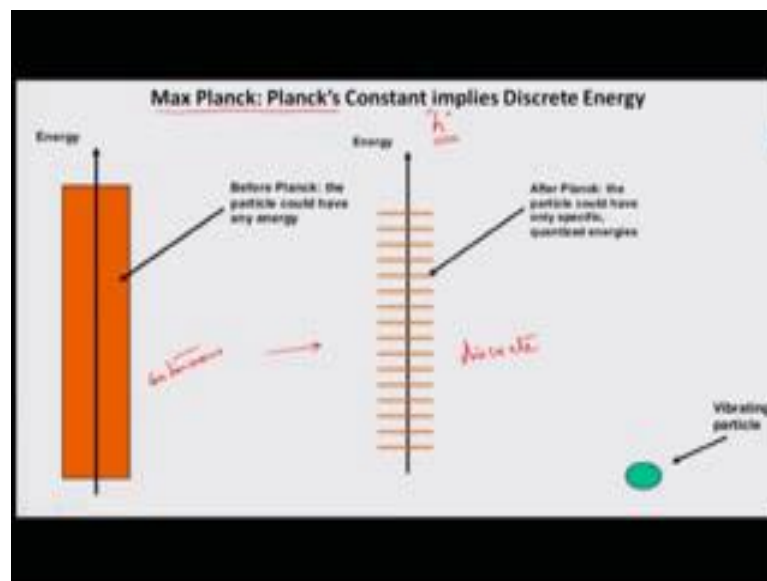
- a) the mass of atoms
- b) the wavelength of light
- c) the particle nature of light
- d) the dual nature of light

Soln -> c) the particle nature of light

Let us now look at this principle of solving the problems. The first problem set is the one which we had given to you in the very first week, and the first question in that problem is as we mentioned here and the solution had been given to you. But the basic concept that we were discussing and looking for in that problem was the principle of the particle nature of light.

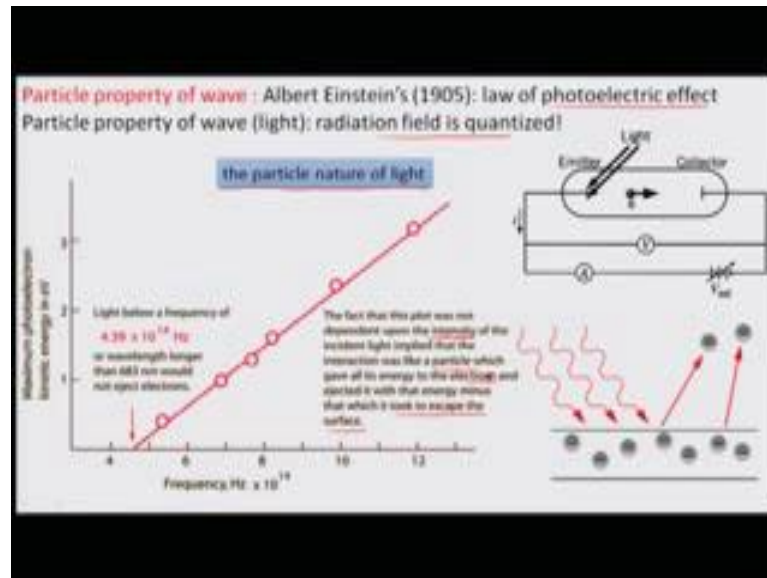
With that let us now look at all the different aspects that we can do for this particular problem. Started with in the first week, where we had these multiple choice questions and their solutions were given. The first one was based on the photoelectric effect which was questioning the concept of photoelectric effect that we discussed. And the question basically was given to find out which of these different choices was important. It sort of was looking for the particle nature of light to be understood.

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In this case, most important parameter or understanding gain from the discretization of the energy that was first proposed by Max Planck, in terms of the Planck's constant h . And this is a visual representation of how the continuous energy picture changed to the discretized energy picture, discrete or quantize energy picture after the principle given by a Max Planck.

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This quanta or the discreteness of the energy in terms of the Planck's constant was the key to bringing the photoelectric effect explanation by Einstein. Where, he was able to show that the radiation field is quantized because no matter how much of a photons you provide beyond a certain energy level, they will be no electron ejection for the photo electric effect; essentially showing that the light below a frequency of say in this particular example of certain hertz or wavelength longer than 683 nanometers would not eject electrons.

The fact that this plot was not dependent on the intensity of the incident light implied that the interaction was like a particle which gave all its energy to the electron and ejected it with that energy minus that which took to escape the surface. This extra energy that was necessary to make this happen is often known as the work function of the surface and so on and so forth. But generally speaking this was the basic concept on the particle nature of light which was been asked in this first question.

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Q 2. The Uncertainty Principle states that if you can measure position and time simultaneously then you cannot measure

- a) Energy
- b) Velocity
- c) Location
- d) a and b


Soln → d) a and b

The second question goes into the uncertainty principle, which states that if you can measure position and time simultaneously then you cannot measure. Here, one of the important things to remember that it actually questions both position and time, and then gives you choices with respect to that; and the correct choices essentially the correlation between these 2 which we now discuss here.

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Heisenberg realized that ...

- In the world of very small particles, one cannot measure any property of a particle without interacting with it in some way
- This introduces an unavoidable uncertainty into the result
- One can never measure all the properties exactly //

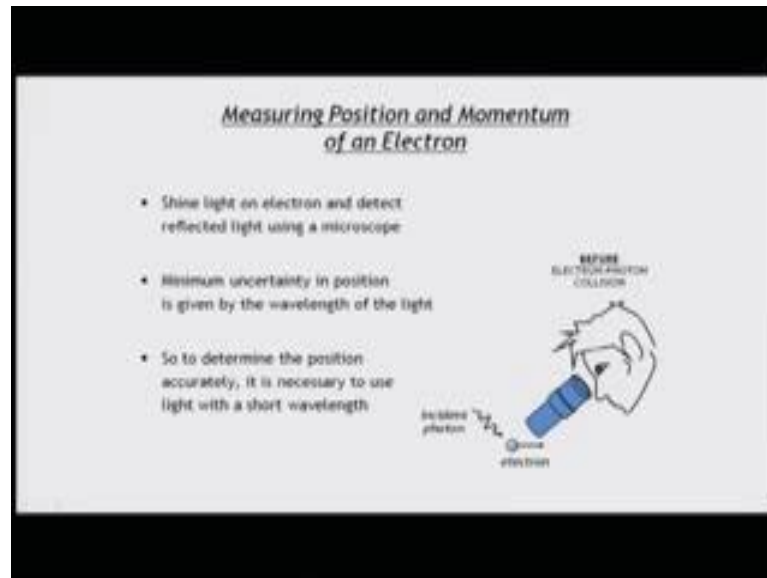


Werner Heisenberg (1901-1976)

This was first realized by Heisenberg, where he was able to understand in the world of very small particles one cannot measure any property of a particle without interacting

with it in some way. This interaction introduces an unavoidable uncertainty into the result and one can never measure all the properties exactly.

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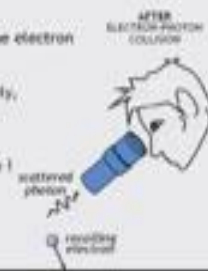


Now, this was the realization of Heisenberg that gave rise to this uncertainty principle. It is illustrated here in some detail. If you shine light on electron and detected reflected light it just using a microscope, then assumes this kind of a way cartoonist picture where the electron photon collision happens before; and minimum uncertainty in position is given by the wavelength of light. To determine the position accurately it is necessary to use light with short wavelength.

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Measuring Position and Momentum of an Electron

- By Planck's law $E = hc/\lambda$, a photon with a short wavelength has a large energy
- Thus, it would impart a large 'kick' to the electron
- But to determine its momentum accurately, electron must only be given a small kick
- This means using light of long wavelength!




However, after the electron photon collision by Planck's law we know that there is a photon with short wavelength has a large energy which would mean, thus it would impart a large kick to the electron, but to determine its momentum accurately electron must only give a small kick.

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Measurement disturbs the system

Before collision


Incident photon



Electron

After collision

Scattered photon



Recoiling electron

The moment you want to actually determine the position very accurately you were almost lost in terms of its momentum and that is the basic idea here because of the re coil of this. This means using light of long wavelength. The measurement disturbs the system

and that is the consequence of this entire problem, because the particles are so small the interaction is large enough to do these issues.

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The Uncertainty Principle

- Classical physics
 - Measurement uncertainty is due to limitations of the measurement apparatus
 - There is no limit in principle to how accurate a measurement can be made
- Quantum Mechanics
 - There is a fundamental limit to the accuracy of a measurement determined by the Heisenberg uncertainty principle
 - If a measurement of position is made with precision Δx and a simultaneous measurement of linear momentum is made with precision Δp , then the product of the two uncertainties can never be less than $\hbar/2\pi$
$$\Delta x \Delta p \geq \hbar$$
 - Heisenberg also recognized the Time Energy Uncertainty relationship:
$$\Delta E \Delta t \geq \hbar$$

How tight? If you can measure position and time simultaneously, then you cannot measure energy.

The uncertainty principle essentially means that there is a fundamental limit to the accuracy of a measurement determined by the Heisenberg's uncertainty principle. And this is different from the classical uncertainty, where the measurement of uncertainty is due to limitations of the measurement apparatus. There is nothing to do with the fundamental limit which is there in terms of quantum mechanics. In this particular case, for example, in classical there is really no limit in principle to how accurately measurement can be made. It all depends on the instrumental apparatus that we are talking about.

In quantum mechanics, we have these 2 very important aspects; one related to the position which is the position accuracy and the simultaneous measurement of the linear momentum with precision Δp . Then the product of the 2 can never be less than this. This is one part of the uncertainty. Heisenberg also recognized the time energy uncertainty relationship which is related to the energy of the system as well as the time, that is been used and there are 2 different uncertainties and the problem probe both of them that is why the answer was for both the cases, when position and velocity are the ones which cannot be measured simultaneously. And similarly time and energy cannot

be mentions simultaneously when all these four parameters are there. That is the reason why the answer was given in that particular way.

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Q 3. The wave function is

- a) a measure of light
- b) used to determine the exact position of a particle
- c) a mathematical description of a quantum entity
- d) all of the above

Soln → c) a mathematical description of a quantum entity

This particular problem is perhaps easier which basically introduces and looks at the concept of the wave function, which is just a mathematical description of a quantum entity.

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Wave function in Quantum Mechanics

- In 1925, Austrian physicist Erwin Schrodinger proposed an equation (the celebrated Schrodinger wave equation) that accurately described the motion of the wave that accompanies the electron. This wave, represented by the Greek letter ψ , gave precise predictions for the behavior of atoms
- The wave function is a complex function (a function containing quantities that are complex numbers) and is constructed in such a way that performing an operation to take the modulus of the complex function for a given state results in a real value that represents the probability density of a result that corresponds to that state. This is how the wave function is transformed into a meaningful physical prediction

This wave function, represented by the Greek letter ψ , is a mathematical description of a quantum entity

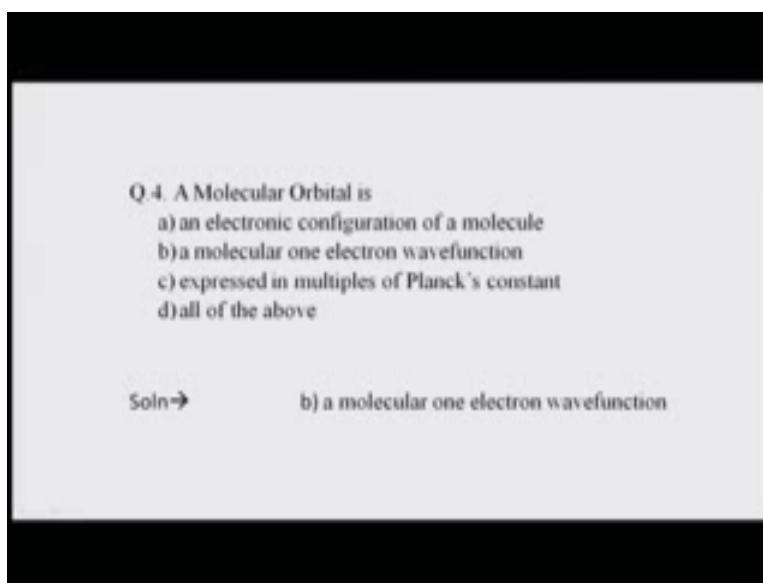
And in a little bit more detail manner here is the description which we have already looked at before. But in a very précised sense, this is the Schrodinger's proposed

equation that accurately describes the motion of wave that accompanies the electron. This wave represented by the Greek letter psi gave precise predictions for the behavior of atoms.

The wave function is a complex function, a function containing quantities that are complex numbers and is constructed in such a way that performing an operation to take the modulus of the complex function for a given state results in a real value that represents the probability density of a result that corresponds to that state. This is how wave function is transformed into a meaningful physical prediction. That is the importance of the wave function that it actually embeds all the physical important information that is necessary.

The wave function represented by Greek letter psi is a mathematical description of a quantum entity and that is what the choice answer would have appeared.

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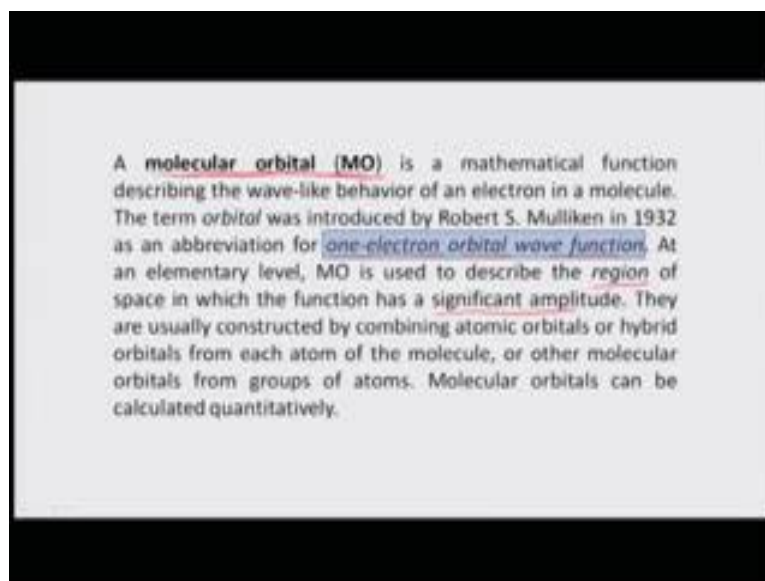
Q.4. A Molecular Orbital is

- a) an electronic configuration of a molecule
- b) a molecular one electron wavefunction
- c) expressed in multiples of Planck's constant
- d) all of the above

Soln → b) a molecular one electron wavefunction

Similarly, the next question is on the combined condition of atomic orbital's which is a molecular orbital. And this is defined in many different ways, but this is a particular definition which is been looked at here.

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And there is a little right up on it that I have put up for you now so that it becomes clear. A molecular orbital is a mathematical function that describes the wave like behavior of an electron in a molecule. The term orbital was introduced by Mulliken in 1932, as an abbreviation for one electron orbital wave function. And that is the reason why the most appropriate connection between the molecular orbital is to the one electron orbital wave function.

At an elementary level molecular orbital is used to describe the region of space in which the function has significant amplitude. They are usually constructed by combining atomic orbital's or hybrid orbital's from each atom of the molecule or other molecular orbitals from groups of atoms. Molecular orbital's can be calculated quantitatively. That is why molecular orbitals have a lot of important positions and interactions to take care and I thought a little bit more detail on what we have done before is necessary. And here the most important part to keep in mind is that the is a mathematical entity which has to do with one electron orbital wave function and it sort of like connecting to the molecular orbital in that sense.

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Q 5. The concept that all moving particles have wave characteristics is attributed to _____

a) Bohr
b) de Broglie
c) Heisenberg
d) Einstein

Soln → b) de Broglie

de Broglie, in his 1924 PhD thesis, proposed that just as light has both wave-like and particle-like properties, electrons with momentum p also have wave-like properties with wavelength (λ):

$$\lambda = \frac{h}{p}$$

This relationship is now known to hold for all types of matter

There are 2 questions on de Broglie. The first one is just trying to see that you connect the de Broglie to the concept that he essentially introduced; this is a matter wave characteristic. And anything related to the wave like nature of matter is now considered to be related to de Broglie, so that was the point of this particular question. And this is the concept that he introduced through his thesis, PhD thesis in 1924 where he proposed that just like light both wave like and particle like properties electrons with momentum P , also have wave like properties like sorry with wavelength λ ; such that λ is related to the Planck's constant over the momentum.

Now, this relationship is now known to hold for all types of matter and not just for electrons. Although it was initially proposed by him in his thesis for the electrons, but it was for everything.

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Q.6. Ratio of de Broglie wavelengths for a cricket ball of mass 0.4 kg to that of a ${}^4\text{He}$ atom, both of which are travelling at 1 km/s:

a) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1.67\times 10^{-26}:1$

b) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1:1.67\times 10^{-26}$

c) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1:1.67\times 10^{26}$

d) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1:1$

Soln \rightarrow a) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1.67\times 10^{-26}:1$

Now in the next question taking on to the fact that this matter wave is universal fact, the question is raised on how the ratio of that goes between them. And so the ratio of de Broglie wavelength for a cricket ball of a given mass to that of helium atom, both of which are traveling at the same speed just for argument sake is being looked at.

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de Broglie equation relating matter with momentum p to its wavelength (λ) is given by:

$$\lambda = \frac{h}{p} \quad \text{where } h \text{ is the Planck Constant.}$$
$$\frac{\lambda_{\text{cricket ball}}}{\lambda_{\text{He-atom}}} = \frac{h/p_{\text{cricket ball}}}{h/p_{\text{He-atom}}} = \frac{p_{\text{He-atom}}}{p_{\text{cricket ball}}} = \frac{m_{\text{He-atom}} \cdot \text{velocity}}{m_{\text{cricket ball}} \cdot \text{velocity}}$$

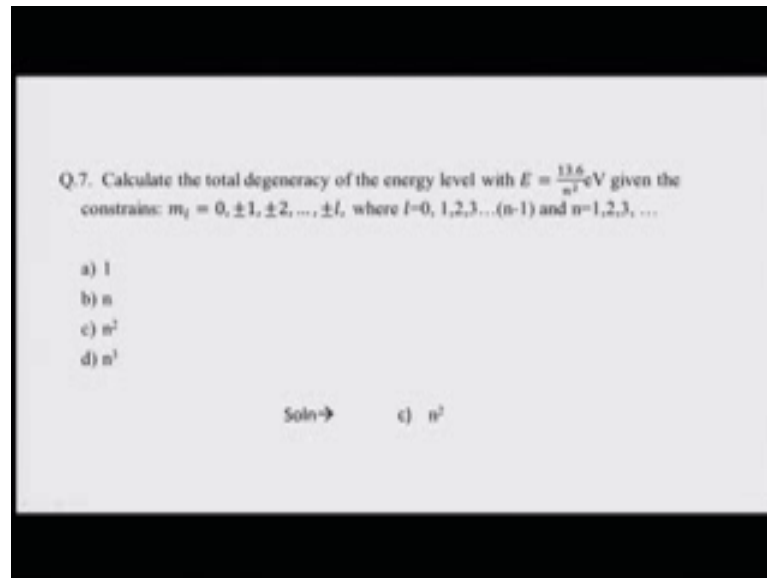
Since velocity of both the cricket ball (mass = 0.4 kg) and He-atom (mass = $4 \times 1.67 \times 10^{-27}$ kg) is 1 km/s, we get:

a) $\lambda_{\text{cricket ball}}:\lambda_{\text{He-atom}}::1.67\times 10^{-26}:1$

To do this problem, it is important that you use the de Broglie relation with that relates matter with momentum and its wavelength. And take a ratio of the 2 cases and realize that the wavelength is inversely proportional to mass and the velocity.

Now, since velocity has been kept same so it essentially means that you have to only consider the mass of the system for both of them and once you do that you just get a ratio of the 2 masses; in this particular case 0.4 and 4 coming from the helium is cancelled and you are left with a order of magnitude value which is simply relating the conversion between the 2.

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Q.7. Calculate the total degeneracy of the energy level with $E = \frac{13.6}{n^2} \text{eV}$ given the constraints: $m_l = 0, \pm 1, \pm 2, \dots, \pm l$, where $l = 0, 1, 2, 3, \dots, (n-1)$ and $n = 1, 2, 3, \dots$

a) 1
b) n
c) n^2
d) n^3

Soln → c) n^2

The next question looks at a degeneracy of a particular state. For example, this is a 13.6 over N square electron volt, is the energy, is the as you know for the hydrogen atom, and it is under the constraints that the state has all these other characteristics; and you are suppose to find the solution.

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For each quantum level n , there are $l = 0, 1, 2, \dots, (n-1)$ angular momentum states, each of which would have a degeneracy of $m_l = 0, \pm 1, \pm 2, \dots, \pm l$. This means that each l state is $2l + 1$ degenerate.

Thus, the total degeneracy for level n is:

$$\sum_{l=0}^{n-1} (2l + 1) = 2 \times \sum_{l=0}^{n-1} l + \sum_{l=0}^{n-1} 1 = \frac{2n(n-1)}{2} + n = n^2$$

And this involves realizing that each quantum level N for an atom; that is the principle quantum number there are 0 to N minus 1 angular momentum states each of which have a degeneracy of again 0 plus minus 1, all the way to plus minus L which means that each L state will have $2L + 1$ degeneracy.

The total degeneracy given that each N state can have any volume from 0 to N minus 1 would then mean a summation of this entire $2L + 1$ over 0 to N plus 1. Once you do the summation, you will find that it is a series where the answer comes out to be N squared. That is how this little math's is suppose to take you there.

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Q8. Considering a harmonic oscillator model for H_2 and HD , and assuming the same force constants for both the molecules, the lowest energy state for H_2 is (tick the correct choice)

- a) Higher than that of HD
- b) Lower than that of HD
- c) Equal to that of HD
- d) Not related to that of HD

Soln → a) Higher than that of HD

The next couple of questions on this is are essentially looking at the properties of these molecules to some level, but based on very simplistic arguments considering a harmonic oscillator model for hydrogen molecule and an H D molecule and assuming that the same force constants exist for both molecules. The lowest energy state for H_2 is you have to find out that to. Basically you would need to know the how many oscillator model form of energy.

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For a Harmonic Oscillator: $E_n = \left(n + \frac{1}{2}\right) h\nu$, $n = 0, 1, 2, \dots$ $k = \frac{1}{2k}$

where the frequency of vibration is: $\omega = \sqrt{\frac{k}{m}}$

Assuming the same force constants (k) for both the molecules, the lowest energy state for both would have an inverse relation to their respective mass:

$$E_0 = h \sqrt{\frac{k}{m}}$$

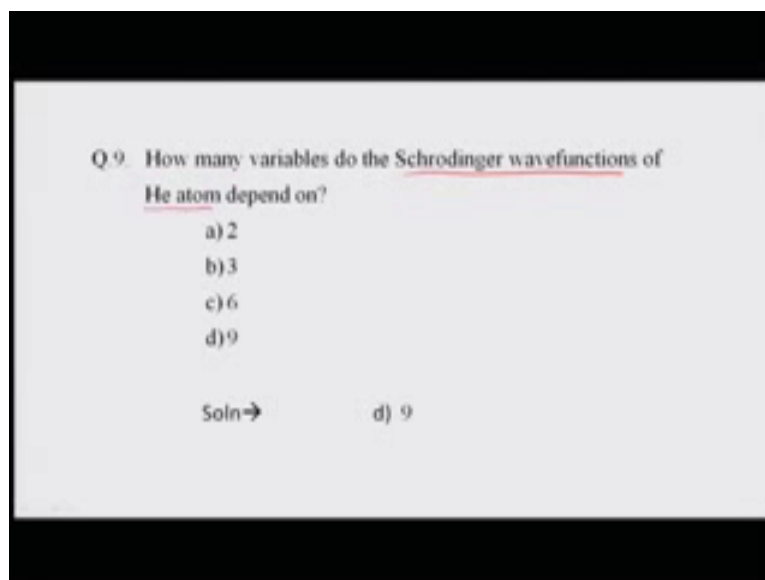
Since Hydrogen molecule has lower mass as compared to HD molecule, the lowest energy state for H_2 is higher than that of HD .

And the harmonic for a harmonic oscillator, energy states are given by this where V is the quantum number, where V can go from anywhere from 0 to whatever number; and then here the way the energy essentially exist makes sure that there is a 0 point energy and a because at V equal to 0 the energy exists, it is half h cross ω . h cross by the way as we all know is h over to 2π .

Now the frequency of vibration is given by the spring constant over or the force constant over the mass or reduce mass as the system maybe, and assuming that this has been given in the problem that the same force constant exists for the both the molecules. The lowest energy state for both will have an inverse relationship with respect to their masses, with respect to their respective mass which means that you will have the E_0 being proportional to 1 over root M .

And since hydrogen mass is a lower mass as compare to the H_2 molecule, the lowest energy for H_2 will then therefore be higher than that of H , because a its inversely proportional so you will be slightly lower in energy then an H_2 . That is the level of identification that we are suppose to make for these kinds of the problems.

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Now, similarly the other simple question was based on the ideas to how to look for wave functions and realize how many variables are necessary for describing a wave function. For a Schrodinger wave function of helium atom, he was asked how many coordinates or how many variables this depend on.

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For He atom:

Potential energy part is:

$$\frac{-Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 R}$$

Wavefunction depends on $\psi(r_1, r_2, R)$

With these parameters, when we consider all possibilities, we find this to be a 9-dimensional problem.

electron position Nuclear position

Essentially, the wavefunction depends on 3 variables, each of which depend on 3 variables, implying its wavefunction would depend on 9 variables.

In order to do that, the best thing is to draw a simplistic picture of say the helium atom which has 1 nucleus and 2 electrons. Now the potential part of this will have the electron electron repulsion part, where there is R^{-1} which is the relative distance between the 2 electrons. And the 2 coulombic attractions would be between the nuclei and the nucleus.

The potential energy part will have a 3 components, one of them is repulsive and the other 2 being attractive.


And therefore the wave function will depend on each of these 3 parameters. And each of these parameters is dependent on entire set of 3 possibilities. So, what we are essentially saying is, if we consider all possibilities we get a 9 dimensional problem. More clearly helium atom has 1 nucleus as we mentioned and 2 electrons each of which would depend on 3 variables implying that it is a wave function would therefore depend on all possible 9 variables.

This is how this problem has been looked at, and this is the sort of the way these problems have been designed and done in this kind of problem set.

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Q.10 The lowest rotational energy gap for the linear carbon-dioxide ($^{12}\text{C}^{16}\text{O}_2$) molecule under the assumption that it is a 3D rigid rotor with the carbon at the center of the rotating axis and the two ^{16}O atoms are exactly at Bohr radius (53×10^{-12} m) from the central ^{12}C atom can be calculated to be

- a) 16.6 cm^{-1}
- b) 166 cm^{-1}
- c) 1.66 cm^{-1}
- d) 53 cm^{-1}



There is a one issue in the last problem of this week 1 which while I was going through a solving it, I realize that this question were the lowest rotational energy gap of the linear carbon dioxide molecule is being questioned under the assumption that it is a 3 D rigid rotor. This is a completely thought problem because it is thought of as a linear molecule and assume to be a 3 D rigid rotor, where the carbon is set to be at the center of the rotating axis and 2 oxygen atoms exactly at Bohr radius, so it is taken as 53 picometer on both sides, from the central carbon atoms. The carbon is consider to be the center and this has been asked with the idea that whether you can calculate this to be a number which comes out to be a exactly one of these.

Unfortunately, perhaps I did not do it very with a lot of effort but have when I was doing it quickly I could not get exact match to one of these problems and one of these answers which I given here and that is actually little bit a way a difficulties. So, what have decided is that I will open the problem for you and then we will look in to this problem further into the next lecture because I do not think will have much time in this lecture to finish the problem. But what we will do is will open up this problem for this now, and if we are not able to get any answer, then we will have to see why there must have been and printing typing error on my side on while making the question; and let us see.

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For a 3D rigid rotor, the energy of the l^{th} state is: $E_l = \frac{h^2 l(l+1)}{8\pi^2 I}$ that results in

an energy gap: $\Delta E = \frac{h^2((l+1)(l+2) - l(l+1))}{8\pi^2 I hc} = \frac{h(l+1)}{4\pi^2 I c} \text{ cm}^{-1}$

The lowest rotational energy gap in cm^{-1} (i.e., when $l=0$) = $\frac{h}{4\pi^2 \mu c R^2}$

The reduced mass (μ) for the defined system is $\frac{16 \times 12}{12+16} \times 1.67 \times 10^{-27} \text{ kg} = 11.45 \times 10^{-27} \text{ kg}$
and $R = 53 \times 10^{-12} \text{ m}$.

So, the lowest rotational energy gap in cm^{-1} =

$$\frac{h}{4\pi^2 \mu c R^2} = \frac{6.6 \times 10^{-34}}{4 \times 11.45 \times 10^{-27} \times (3.14 \times 53 \times 10^{-12})^2 \times 3 \times 10^{10}} \text{ cm}^{-1}$$

The question is based on the idea that we know how the energy of a 3 D rigid rotor looks like and that is sort of given in terms of a this expression where the energy of the Lth state can be written in this term. Very often you are used to the H cross terms, however in this particular case since we are going to write in terms wave numbers I have taken out the H cross and therefore we have gotten these a pi sitting in there. If you write in terms of H cross, these pi square terms vanish and it is perhaps sometimes easier to remember them a in that forms. So we often write them in the H cross terms with 2 I.

That is roughly what we do because 4 pi squared gets absorbed as soon as we say H cross in there. By irrespective whatever we remember your energy is going to look like this and this results in an energy gap in terms of L to L plus 1 let us say you will get something of this form. And if you write it in terms of in wave numbers then you are going to divide the answer by H C; that is the idea. And in this particular case when you divide by H C you have to remember to use your value of C in terms of centimeters per second.

Generally, in these cases what is done is it is taken as 3 times roughly 3 times 10 to the power 10 centimeters per second; this is the velocity of light which is taken instead of 10 to the power 8, 3 times 10 to the power 8 meters per second. This is just to make sure that we can get the wave number unit at the end. So, we have here the quantum number L rotation constant I. Now I is related to the reduced mass in this case, so I is mu R

squared; R is the distance. In our particular model when we have the carbon sitting in the center and the oxygen sitting linearly on the other side, the R is basically this distance that we are looking at, which has been given to us. The μ is the reduce mass.

Now, the reduce mass can be taken in many different ways. In this particular case, the simplest 1 is to consider only the carbon and the oxygen because those are the only 2 points that we are looking at the rest of the same. However, in reality by just considering it to be a 3 body system, you can always utilize the harmonic mean for this system also. In spectroscopy however, there is a little bit more involved manner of doing this, that is why the problem was simply simplified by providing the assumption that it is a linear level by this particular case.

In the simplest way of looking at 3 body kind of a situation like this reduce mass will just be the three masses; in this case oxygen, carbon and oxygen. This could also be used, but to make it even simpler we just kept between the 2 to get rough estimate and we have to always use the unit for conversion into the kilogram that was it goes. And the R has been given as we mentioned in the question. The moment of inertia I can then be calculated, although this particular way of calculating the moment of inertia has a lot of assumption in it. And any way by going by this root we can get some form from where we can get the lowest rotational energy gap, which we have described here by just plugging in the values.

It so turns out that once we plug in these values in order to get the number in terms of wave numbers and at least I did not find it to come close enough to the values that we are used to. The best became to us I think not what we have given as choice. So as we had been talking to you about this problem it does not give any of the results that we have been talking, that we have provided in this problem. So this last problem in that week's problem set had the difficulty that the printed solutions that were provided as options did not actually come as any of the answers that we are looking at here, either when you do it in the approximate sense that we present here or any of the other sense that we do here. And therefore, I do not think you will find any solution which will be in connection correct to the options that are given.

In that way what I am going to do is we are not going to have that as a grade numbering for you, we will take that part of, but the solution part was important to show you as how

to do this problem because there is more important to realize how to do a problem rather than to just be able to get some marks for it.

So, what I have done here is that I have given you an idea as to how to do this problem in case, something of similar nature comes out. It can be very many very much more complicated as I have been mentioning here, but many times we will be essentially looking at the problem in a much more simpler way to make sure that we are getting the main aspects of the problem.

In the next week, we will be looking at the other problems such that we have been giving you. And with this I would like to close today's lecture. See you next time.

Thank you.