

Introduction to Quantum Mechanics
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Lecture – 07

Heisenberg's formulation of quantum mechanics: Application to harmonic oscillator

So, what we have learnt in the previous 2 lectures is the Heisenberg's formulation of quantum mechanics and 2 things that we have learned so far our number one that quantities like $x(t)$ or $v(t)$ or other derived quantities are to be expressed as a collection of numbers, which we now know are matrices solid as matrices.

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Heisenberg's formulation of
Quantum Mechanics

- Quantities like $x(t)$, or $v(t)$ are to be expressed as matrices

$$x(t) = \begin{bmatrix} x_{11} & x_{12} e^{i\omega_{12}t} & x_{13} e^{i\omega_{13}t} & \dots \\ x_{21} e^{i\omega_{21}t} & x_{22} & x_{23} e^{i\omega_{23}t} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

$$\omega_{12} = -\omega_{21}$$

$$= -\frac{E_2 - E_1}{\hbar}$$

$$\hbar = \frac{h}{2\pi}$$

And I like this for example, if I were to express $x(t)$ I would write this as x_{11} , x_{12} and x_{12} has a time dependence $e^{i\omega_{12}t}$, x_{13} $e^{i\omega_{13}t}$ and so on; x_{21} $e^{i\omega_{21}t}$, x_{22} x_{23} $e^{i\omega_{23}t}$, t here and so on.

Notice that if a quantity is time independent; that means, it does not depend on time all the off diagonal terms anything containing $e^{i\omega_{ij}t}$, ω_{ij} or ω_{ji} would be 0 and the matrix would be diagonal. Let me also point out that ω_{12} is equal to ω_{21} with a minus sign in front which is $-(E_2 - E_1)/\hbar$; \hbar is $h/2\pi$. So, that much is something that we have learned about the kinematic part of the theory, and then we obtain the quantum condition.

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The image shows a whiteboard with the following handwritten text:

Quantum condition

$$2\pi m \sum_{\alpha=-\infty}^{\infty} [\omega_{n+\alpha, n} |C_{n+\alpha, n}|^2 - \omega_{n, n-\alpha} |C_{n, n-\alpha}|^2] = h$$

A bracket on the left side of the equation points to a boxed equation:

$$4\pi m \sum_{\alpha=-\infty}^{\infty} \omega_{n+\alpha, n} |C_{n+\alpha, n}|^2 = h$$

Below this, another equation is written in red:

$$\sum_{-\infty}^{\infty} [\omega_{n+\alpha, n} |C_{n+\alpha, n}|^2 - \omega_{n, n-\alpha} |C_{n, n-\alpha}|^2] = \frac{h}{2}$$

Which said that $2\pi m$ summation of α equals minus infinity to infinity, $\omega_{n+\alpha, n}$ modulus $C_{n+\alpha, n}$ square minus $\omega_{n, n-\alpha}$ modulus $C_{n, n-\alpha}$ square is equal to h and then we also express this as $4\pi m$ summation of α equals minus infinity to infinity, $\omega_{n+\alpha, n}$ modulus $C_{n+\alpha, n}$ square equals h . This can also be written as I will take the first condition, summation minus infinity to infinity $\omega_{n+\alpha, n}$ modulus $C_{n+\alpha, n}$ square minus $\omega_{n, n-\alpha}$ modulus $C_{n, n-\alpha}$ square equals h cross that is also equivalent condition.

So, these are all equivalent, I just wanted to clarify something here before I proceed further and that is along the way while deriving this condition we use the C .

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$$C_{n, n+\alpha} = C_{n+\alpha, n}^*$$

$$C_{n, n-\alpha} = C_{n-\alpha, n}^*$$

$$C_{\tau} = C_{-\tau}^*$$

Question: $C_{\tau} \rightarrow C_{n, n-\tau}$
 $C_{-\tau}$ should it be $C_{n-\tau, n}$ or $C_{n, n+\tau}$??

$C_{\tau} \rightarrow \tau\omega$ $C_{-\tau} \rightarrow -\tau\omega$

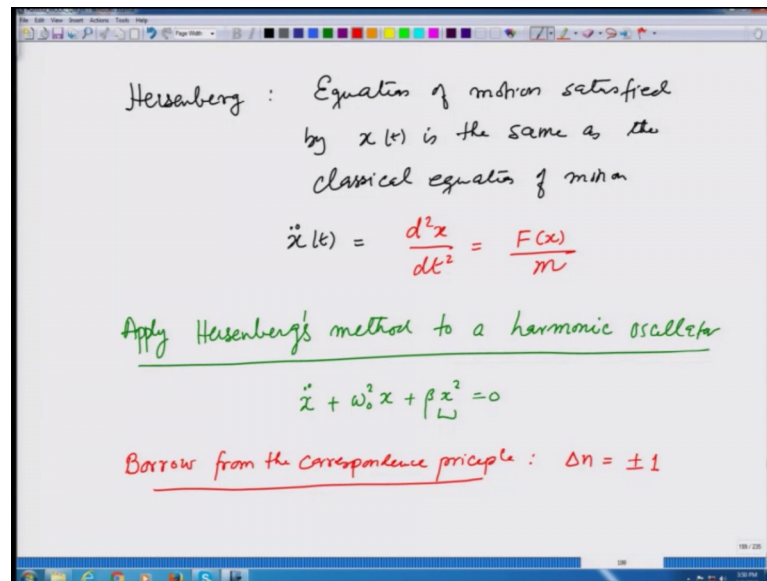
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$\frac{E_n - E_{n-\tau}}{h}$ $\frac{E_{n-\tau} - E_n}{h}$ And not $\frac{E_n - E_{n+\tau}}{h}$

$C_{n, n+\alpha}$ is equal to $C_{n+\alpha, n}^*$ or equivalently $C_{n, n-\alpha}$ is equal to $C_{n-\alpha, n}^*$, and sometimes a question is raised particularly light off that we base all this in correspondence principle, where we have said that C_{τ} was equal to $C_{-\tau}^*$, and the question that arises; question is that C_{τ} suppose it corresponds to in quantum mechanically $C_{n, n-\tau}$, then $C_{-\tau}$ should it be $C_{n-\tau, n}$ or $C_{n, n+\tau}$ that is the question. And what I have claimed is what I have shown in blue on this screen and the reason for this is as follows.

We call that C_{τ} corresponds to the frequency $\tau\omega$, and $C_{-\tau}$ corresponds to the frequency $-\tau\omega$. And $\tau\omega$ quantum mechanically goes to $E_n - E_{n-\tau}$ divided by h cross. Correspondingly $-\tau\omega$ would go to $E_{n-\tau} - E_n$ divided by h cross, and not $E_n - E_{n+\tau}$ divided by h cross it does not go to this and therefore, the correct coefficient for the negative τ quantum mechanically would be $E_{n-\tau} - E_n$, and the corresponding coefficient C would be $C_{n-\tau, n}$ and not $C_{n, n+\tau}$. So, this has been done very carefully and everything is consistent. What we are going to do now is write what the condition on the dynamical condition should be.

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So, what Heisenberg proposed that the equation of motion satisfied by $x(t)$ is the same as the classical equation of motion; that means, $\ddot{x}(t)$ which is same as $\frac{d^2x}{dt^2}$ is going to be equal to $F(x)$ divided by m , except that now each x and each $F(x)$ has to be calculated using these matrices and then you solve the problem. What we are going to do now is apply Heisenberg's method to a harmonic oscillator which also featured in his paper. He took an approach whereby he considered the anharmonic oscillator.

So, the equation for that is $\ddot{x} + \omega_0^2 x + \beta x^2 = 0$. He took an anharmonic oscillator so that he could use his product conditions. We are going to take a slightly different route because I do not want you to get walked down on how to solve for an harmonic oscillator. So, we are going to borrow something from correspondence principle. So, I am going to borrow to solve the problem from the principle, and what I borrow here is that Δn remember we derive can be maximum plus or minus 1. Heisenberg in his paper considered the n harmonic oscillator equation and could obtain $\Delta n = \pm 1$ in the lowest order approximation for ω_0 .

We are going to assume that and our basis of that assumption is going to be borrowing this thing from the correspondence principle right. So, this is what we are going to do. So, let us write it step by step number one.

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(I) $x(t)$ representation

$$\left\{ \begin{array}{l} C_{n, n-1} \quad \omega_{n, n-1} \\ C_{n, n+1} \quad \omega_{n, n+1} \end{array} \right\} \begin{array}{l} C_{n, n-1} e^{i\omega_{n, n-1} t} \\ C_{n, n+1} e^{i\omega_{n, n+1} t} \end{array}$$

(II) Equation of motion:

$$\ddot{x} + \omega_0^2 x = 0$$

$$\left[-\omega_{n, n-1}^2 C_{n, n-1} + \omega_0^2 C_{n, n-1} \right] e^{i\omega_{n, n-1} t} = 0$$

$$\Rightarrow \omega_{n, n-1} = +\omega_0$$

$$\left[-\omega_{n, n+1}^2 C_{n, n+1} + \omega_0^2 C_{n, n+1} \right] = 0 \Rightarrow \omega_{n, n+1} = -\omega_0$$

Xt representation is going to be a collection of numbers of $C_{n, n-1}$ or $C_{n, n+1}$ because maximum n change could be 1 and the corresponding frequency here let it be $\omega_{n, n-1}$ and $\omega_{n, n+1}$. So, that the time dependence can be written as let me write that in a different color $C_{n, n-1} e^{i\omega_{n, n-1} t}$ and the other one as $C_{n, n+1} e^{i\omega_{n, n+1} t}$ that is the time dependence.

Number 2 equation of motion is the same as the classical equation of motion, which says that $x \ddot{\quad} + \omega_0^2 x = 0$. Let us substitute for one of the components. So, I am going to get for example, for the $C_{n, n-1}$ I am going to get $-\omega_{n, n-1}^2 C_{n, n-1} + \omega_0^2 C_{n, n-1} e^{i\omega_{n, n-1} t} = 0$, and this immediately gives me that $\omega_{n, n-1} = \omega_0$. In the same manner I am going to get $-\omega_{n, n+1}^2 C_{n, n+1} + \omega_0^2 C_{n, n+1} = 0$ and this imply $\omega_{n, n+1} = -\omega_0$, but with a minus sign right keep this in mind because one is the frequency when the electron is making a jump from the upper to the lower level and that we have been taking a positive frequency, the other one is going to be a negative frequency.

So, once that is clear from the classical equation of motion we are ready to apply our quantum conditions.

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(3) Quantum condition

$$2\pi m \sum_{\alpha=-\infty}^{\infty} [\omega_{n+\alpha, n} |C_{n+\alpha, n}|^2 - \omega_{n, n-\alpha} |C_{n, n-\alpha}|^2] = h$$

$\alpha = \pm 1$ because $\Delta n = \pm 1$

$$\alpha=1 \quad 2\pi m [\omega_0 |C_{n+1, n}|^2 - \omega_0 |C_{n, n-1}|^2]$$

$$\alpha=-1 \quad + 2\pi m [-\omega_0 |C_{n, n}|^2 + \omega_0 |C_{n, n+1}|^2] = h$$

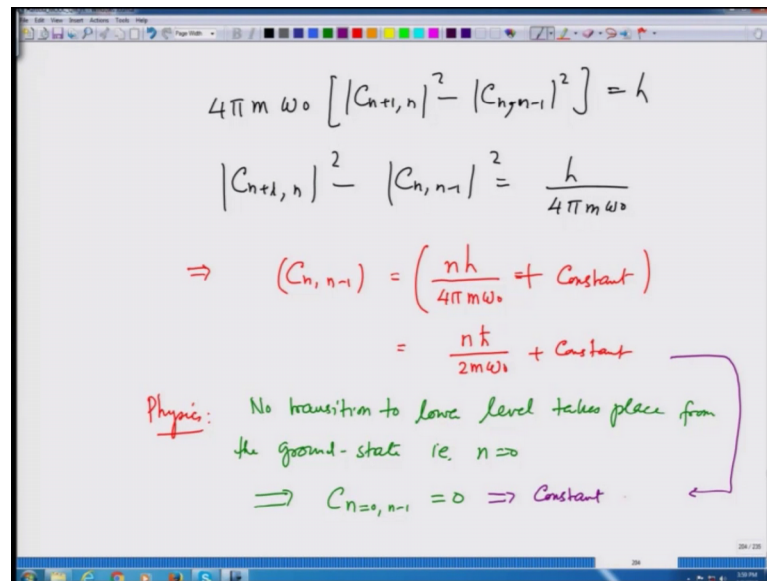
$$4\pi m \omega_0 [|C_{n+1, n}|^2 - |C_{n, n-1}|^2] = h$$

$$|C_{n, n+1}|^2 = |C_{n+1, n}|^2$$

And quantum condition says the $2\pi m$ summation over α $\omega_{n+\alpha, n}$ plus α mod $C_{n+\alpha, n}$ square minus $\omega_{n, n-\alpha}$ mod $C_{n, n-\alpha}$ square is equal to h . Now α in this case is plus or minus 1 because Δn is plus or minus 1. Now α equal to one gives you $2\pi m \omega_0$ that is $n+1$ to mod $C_{n+1, n}$ square minus ω_0 mod $C_{n, n-1}$ square, and α equals minus 1 will give me $2\pi m$ minus ω_0 mod $C_{n, n}$ square minus, minus minus plus ω_0 mod $C_{n, n+1}$ square and some of the 2 would give me h . And you add the 2 terms you are going to get $4\pi m \omega_0$, $C_{n+1, n}$ mod square minus $C_{n, n-1}$ mod squared is equal to h that is what quantum condition gives me, alright.

So, this is the quantum condition and this can help me determine C_n , C_{n+1} and what I have used here I have also used that $C_{n, n+1}$ mod square is same as mod $C_{n+1, n}$ mod square and same thing about $C_{n, n-1}$. So, what quantum condition has given me now is that $4\pi m \omega_0$.

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$$4\pi m \omega_0 \left[|C_{n+1, n}|^2 - |C_{n, n-1}|^2 \right] = \hbar$$
$$|C_{n+1, n}|^2 - |C_{n, n-1}|^2 = \frac{\hbar}{4\pi m \omega_0}$$
$$\Rightarrow C_{n, n-1} = \left(\frac{n\hbar}{4\pi m \omega_0} + \text{Constant} \right)$$
$$= \frac{n\hbar}{2m\omega_0} + \text{Constant}$$

Physics: No transition to lower level takes place from the ground-state i.e. $n=0$

$$\Rightarrow C_{n=0, n-1} = 0 \Rightarrow \text{Constant}$$

$|C_{n+1, n}|^2 - |C_{n, n-1}|^2$ is equal to \hbar or $|C_{n+1, n}|^2 - |C_{n, n-1}|^2 = \frac{\hbar}{4\pi m \omega_0}$ and this immediately implies the solution is very straightforward that $|C_{n, n-1}|^2$ is equal to $\frac{n\hbar}{4\pi m \omega_0}$ which I can also write as $\frac{n\hbar}{2m\omega_0}$ plus some constant. Heisenberg had said that that constant should be determined from quantum conditions. This I can also write as $\frac{n\hbar}{2m\omega_0} + \text{Constant}$.

Now, we are going to use some physics. Physics is no transition to lower level takes place from the ground state that is $n=0$ and this implies that $|C_{n=0, n-1}|^2$ should be equal to 0, which immediately tells you from this equation that constant is equal to 0.

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$$\ddot{x} + \omega_0^2 x = 0$$

(1) $\omega_{n, n-1} = \omega_0$ for all n 's
 $\omega_{n, n+1} = -\omega_0$ for all n 's

(2) $|C_{n, n-1}|^2 = \left(\frac{n\hbar}{2m\omega_0}\right)$

Energy: Since energy is conserved, only diagonal elements of Energy matrix $\neq 0$

$$E_n = \frac{1}{2} m v_n^2 + \frac{1}{2} k x_n^2$$

$$E_n = \frac{1}{2} m v_{n,n}^2 + \frac{1}{2} m \omega_0^2 x_{nn}^2$$

So, taking the harmonic oscillator equation the first step the classical equation gave me that $\omega_{n, n-1}$ is equal to ω_0 for all n 's and $\omega_{n, n+1}$ is minus ω_0 for all n 's.

Number 2 we applied the quantum condition that is what we did we applied the quantum condition and got that $|C_{n, n-1}|^2$ is equal to $\frac{n\hbar}{2m\omega_0}$ what about the energy of the system. So, we have got on these transition matrix element now energy. Since energy is conserved only diagonal elements of energy matrix are not equal to 0, because if there were diagonal elements they will necessarily involve $e^{i\omega t}$ and that would make a time dependent.

So, if I want to calculate the energy for the n th level, this would be equal to one half $m v_n^2$ for the n th level plus one half $k x_n^2$ for the n th level, and this is one half m in quantum mechanical notation it will be $\frac{1}{2} m v_{n,n}^2$ because that is the diagonal term plus one half k is $\frac{1}{2} m \omega_0^2 x_{nn}^2$, and that will be the energy for the n th level. This is what we need to calculate now for the system to get the n th level energy and let us do that next.

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$$\begin{aligned}
 \chi^2(t)_{nn} &= \sum C_{n,n'} C_{n',n} \\
 &= \sum |C_{nn'}|^2 \\
 (n' = n \pm 1) &= |C_{n,n+1}|^2 + |C_{n,n-1}|^2 \\
 &= \frac{(n+1)\hbar}{2m\omega_0} + \frac{n\hbar}{2m\omega_0} \\
 &= \left(n + \frac{1}{2}\right) \frac{\hbar}{m\omega_0} \\
 \langle \hat{H} \rangle_{nn} &= \sum (i\omega_{nn'} C_{nn'}) (i\omega_{n'n} C_{n'n}) \\
 &= -\sum \omega_{nn'} \omega_{n'n} |C_{nn'}|^2 \\
 \text{Since } \omega_{nn'} &= -\omega_{n'n} \\
 &= \sum \omega_{nn'}^2 |C_{nn'}|^2 \\
 \text{Taking } n' &= n \pm 1 \\
 &= \omega_0^2 |C_{n,n+1}|^2 + \omega_0^2 |C_{n,n-1}|^2
 \end{aligned}$$

What is x this is represented by the C_n numbers? So, x^2 would be nothing but summation according to overrule $C_{n,n'} C_{n',n}$ right that is what it is and this is nothing but summation mod $C_{n,n'}^2$.

Now, we have seen that n' could be $n \pm 1$ and therefore, because of this I am going to have $C_{n,n+1}^2$ plus $C_{n,n-1}^2$ and these have been calculated this is nothing but $(n+1)\hbar / 2m\omega_0$ plus $n\hbar / 2m\omega_0$ which comes out to be therefore, $(n + \frac{1}{2})\hbar / m\omega_0$ what about $\langle \hat{H} \rangle_{nn}$? $\langle \hat{H} \rangle_{nn}$ is going to be nothing but summation $i\omega_{nn'} C_{nn'}$ times $i\omega_{n'n} C_{n'n}$ this is $-\sum \omega_{nn'} \omega_{n'n} |C_{nn'}|^2$ which is nothing but minus $\omega_{nn'} \omega_{n'n} |C_{nn'}|^2$

Since $\omega_{nn'} = -\omega_{n'n}$, we get this equal to summation $\omega_{nn'}^2 |C_{nn'}|^2$ and therefore, taking $n' = n \pm 1$ and all $\omega_{nn'} = \omega_0$, we get this whole thing to be equal to $\omega_0^2 (|C_{n,n+1}|^2 + |C_{n,n-1}|^2)$ which is the same as for x^2 and therefore, this value is also going to be equal to $(n + \frac{1}{2})\hbar / m\omega_0$.

So, you have gotten $\langle \hat{H} \rangle_{nn}$, we have gotten ω_0 energy e .

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$$E_{nn} = \frac{1}{2} m v^2 + \frac{1}{2} m \omega_0^2 x^2$$

$$= \frac{1}{2} m \omega_0^2 (n + \frac{1}{2}) \frac{\hbar}{m \omega_0} + \frac{1}{2} m \omega_0^2 (n + \frac{1}{2}) \frac{\hbar}{m \omega_0}$$

$$= (n + \frac{1}{2}) \hbar \omega_0$$

$$E_n = (n + \frac{1}{2}) \hbar \omega_0$$

Notice $n=0$ gives $E_0 = \frac{\hbar \omega_0}{2}$ Zero point energy

$$\Delta E = \hbar \omega_0 = h \nu_0$$

Rate of Energy coming out $\left(\frac{dE}{dt}\right)_{n, n-1}$
 \rightarrow Einstein A coeff

E_n is one half mv^2 plus one half $m\omega_0^2 x^2$ which then comes out to be one half mv^2 we have just calculated is nothing but ω_0^2 , n plus a half \hbar cross over $m\omega_0$, and the second term is one half $m\omega_0^2 x^2$ this is also n plus a half \hbar cross over $m\omega_0$.

So, this comes out to be m cancels. So, does one of the ω_0 zeros same thing here and you get n plus a half \hbar cross ω_0 that is the energy.

So, according to Heisenberg's quantum mechanics then we get e for the n th level to be equal to n plus a half \hbar cross ω_0 notice n equal to 0 gives e_0 to the \hbar cross ω_0 $\times 2$ it is not 0 energy as in the classical sense or even in Wilson's Sommerfeld field quantum conditions the lowest energy the ground state energy is \hbar cross ω_0 by 2 . This is known as 0 point energy, and ΔE is still \hbar cross ω_0 or $h\nu_0$ which it should be if we were to reduce the blackbody radiation formula. So, that comes out correctly and the energy has 0 point energy what Heisenberg has been able to do in all this is calculate the energy purely from quantum mechanical considerations, where the quantum mechanical quantities are expressed as matrices quantum conditions and equation of motion help you determine these coefficients that he proposed.

What about the rate of energy coming out or dE/dt when transition is made from n to n minus 1 and that gives you Einstein's a coefficient also, remember we had earlier calculated it using correspondence principle. So, let us do that.

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$$\begin{aligned} \left(\frac{dE}{dt}\right)_{n,n-1} &= \left[\frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{a^2}{c^3} \right]_{avg} \\ &= \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{\omega_{n,n-1}^4 (A_{n,n-1})^2}{c^3} \\ &= \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{\omega_0^4 (A_{n,n-1})^2}{c^3} \\ x(t) &= \sum C_n e^{i\tau\omega_n t} \\ &= 2C_n \cos(\tau\omega_0 t) \\ A_{n,n-1} &= 2C_{n,n-1} \Rightarrow A_{n,n-1}^2 = 4|C_{n,n-1}|^2 \\ &= \frac{4\hbar}{2m\omega_0} \\ &= \left(\frac{2\hbar}{m\omega_0}\right) \end{aligned}$$

dE/dt n to n minus 1 by dt , I am going to use the classical formula is going to be given as time averaged of 2 thirds e square over $4\pi\epsilon_0$, acceleration raise 2 acceleration square divided by C cube this is the formula we had used and when I take the average I take the average of this, this comes out to be one third e square over $4\pi\epsilon_0$ ω alpha right n to n minus 1 raise to 4 amplitude square divided by C cube.

Now, we have already seen that $\omega_{n,n-1}$ and all these things are the same as ω_0 . So, this is going to be one third e square over $4\pi\epsilon_0$ ω_0 raise to 4 amplitude square n to n minus 1 transition amplitude divided by C cube. What about this amplitude? Again go back to the classical $C_{n,n}$ and I will say that the $x(t)$ was written as summation, $C_n e^{i\tau\omega_n t}$ for the n th level t , which could be written as taking C to be real as $2C_n \cos(\tau\omega_0 t)$. In the quantum mechanical sense then I am going to write that the amplitude n to n minus 1 is going to be $2C_{n,n-1}$ making that correspondence and this implies that $A_{n,n-1}^2$ is going to be 4 times $C_{n,n-1}^2$ which we have already calculated to be $4\hbar$ cross over $2m\omega_0$.

So, this comes out to be $2 \hbar$ cross over $m \omega_0$, I will substitute this in the formula here and get dE by dt n to n minus 1 to be equal to one third e^2 over four pi epsilon 0 ω_0 raise to 4 over C cubed and $4 a$ n square I get $2 \hbar$ cross over $m \omega_0$. Let us cancel a few terms this ω_0 gives me ω_0 cubed and therefore, I get this 2 I can bring in front and therefore, I can write dE dt transition from n to n minus 1 is equal to 2 thirds, e^2 over $4 \pi \epsilon_0 \omega_0$ cubed at \hbar over $m c$ cubed.

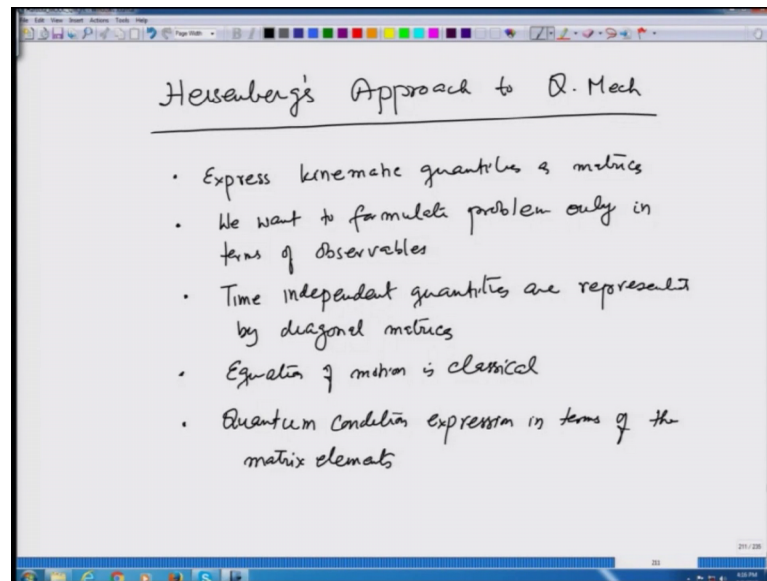
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$$\begin{aligned} \left(\frac{dE}{dt}\right)_{n, n-1} &= \frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{\omega_0^3 \hbar}{m c^3} n \\ &= \hbar \omega_0 A_{n, n-1} \\ \Rightarrow A_{n, n-1} &= \frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{\omega_0^2}{m c^3} n \end{aligned}$$

I recall that this is also equal to \hbar cross ω_0 times the Einstein coefficient for a to n , n minus 1 and this immediately gives me the answer that the Einstein coefficient n minus 1 is going to be 2 thirds e^2 over $4 \pi \epsilon_0 \omega_0$ square over $m c$ cubed. There is an n also because the C_n factor has n and this is precisely the answer we had obtained earlier. So, quantum mechanically we have also calculated this through a purely quantum mechanical calculation.

So, let me now conclude this lecture on Heisenberg's application of his equation to harmonic oscillator and write.

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So, this is basically Heisenberg's approach to quantum mechanics is conclude number one express kinematic quantities as matrices. And that is done because we want to formulate problem only in terms of observables time independent quantities are represented by diagonal matrices, then equation of motion is classical and quantum condition expressed in terms of the matrix elements.

So, this is the conclusion of Heisenberg's approach, this was made more general and put on a stronger footing and something called the matrix mechanics, to which I will just give you a brief introduction in the next lecture.