09/05/25 Lecture — 32 01/12/20

→
- Linear Harmonic Oscillator
- Quantization of EMF
- phonons

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Today we shall see another example of Potential Energy not being Piecewise constant. This example is very important there are many applications of it

It is Linear Harmonic Oscillator

Linear Harmonic Oscillator — I

An important example of one-dimensional motion is that related to the elastic force $F = -cx$, with $c > 0$. As this force can be derived from a potential energy $V = cx^2/2$, the classical Hamiltonian has the form

$$H = \frac{1}{2m}p^2 + \frac{1}{2}cx^2 = E = \text{const.}$$

The equation of motion $\dot{p} = m\ddot{x} = -\partial H/\partial x = -cx$ yields

$$x = x_M \cos(\omega t + \varphi), \qquad \omega = \sqrt{c/m} > 0,$$

where x_M and φ are determined from the initial conditions. This type of motion is called *linear harmonic oscillation*. The Hamiltonian operator is found by replacing p with $-j\hbar\,\mathrm{d}/\mathrm{d}x$, whence Schrödinger's equation reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2 w = Ew.$$

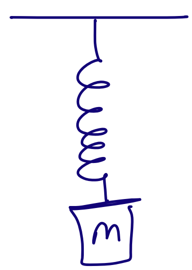
It is worth noting that ω is determined by the parameters of the problem, before quantization. The equation can be recast in normalized form by defining $\epsilon \doteq E/(\hbar\omega)$, $\xi = (m\omega/\hbar)^{1/2}x$:

$$\mathcal{H}'w = \epsilon w, \qquad \mathcal{H}' \doteq \frac{1}{2}\left(\xi^2 - \mathrm{d}^2/\mathrm{d}\xi^2\right).$$

$$\boxed{F = -cx, \quad V = \frac{cx^2}{2}}$$

$$\Rightarrow F = -\frac{d}{dx}V$$ Gradient field

$$F \Rightarrow -cx$$



The above example represents Mass suspended from a spring

Total Energy $\Rightarrow$ $E \Rightarrow H = T + V$

$$H = \frac{p^2}{2m} + \frac{1}{2}cx^2$$

Equation of Motion

$p = m\dot{x} \Rightarrow F = \dot{p} \Rightarrow m\ddot{x}$

& $F = -cx$ given above

oscillatory Behaviour

$$\Rightarrow m\ddot{x} = -cx$$

$$\ddot{x} = -\left(\frac{c}{m}\right)x$$

$$\Rightarrow \boxed{-\ddot{x} = \left(\sqrt{\frac{c}{m}}\right)^2 x}$$

angular frequency

& Sol^n is $x = x_M \cos(\omega t + \phi)$

Maximum displacement.

The equation of motion $\dot{p} = m\ddot{x} = -\partial H/\partial x = -cx$ yields

$$x = x_M \cos(\omega t + \varphi), \qquad \omega = \sqrt{c/m} > 0,$$

where x_M and φ are determined from the initial conditions. This type of motion is called *linear harmonic oscillation*. The Hamiltonian operator is found by replacing p with $-j\hbar\mathrm{d}/\mathrm{d}x$, whence Schrödinger's equation reads

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It is worth noting that ω is determined by the parameters of the problem, before quantization. The equation can be recast in normalized form by defining $\epsilon \doteq E/(\hbar\omega)$, $\xi = (m\omega/\hbar)^{1/2}x$:

$$\mathcal{H}'w = \epsilon w, \qquad \mathcal{H}' \doteq \tfrac{1}{2}\left(\xi^2 - \mathrm{d}^2/\mathrm{d}\xi^2\right).$$

→ Now we have to find Quantum eqⁿ corresponding to these. So we have to go from Classical eqⁿ to Schrodinger eqⁿ Independent of time

✱ (A crystal can be approximated as a superposition of linear oscillators.)

- We already have seen a case about s/s of Atoms bound together that looks complicated but when we expand the P.E of the s/s and truncate it to the 2^{nd} order we find a problem that is eventually seperable.
- We should recall when we introduced the Normal coordinates to the Normal modes of oscillation we split the problem of many particles interacting with each other into a problem in which each degree of freedom is independent from the others.

eqⁿ of individual degree of freedom is the eqⁿ of LH Oscillator.

∴ A crystal can be approximated as a superposition of linear oscillators.

** Another very important problem that can be formally physically different but that can be reduced to set of eq^ns of LHO is that of EMF in vaccum.

EMF in vaccum ⇒ Super position of linear modes of oscillation.

Q) Why is This important to solve LHO ?

Ans If we succeed in solving SE for the LHO Then we can apply sol^ns to many important topics.

Then we can quatize the Motion of the atom of the Crystal using QM by simply replicating the outcome of the calculation that we will see now.

& we also know Quatization of EMF leads to the concept of Photon. it is The interpretation of the Photo Electric experiment.

→ Similarly Quantization of Motion of Atoms in a Crystal will lead to the concept of Phonon. i.e a fictitious particle

Phonons have Energy & Momentum & are the particles that describe oscillation Modes of The Crystal.

- type of motion is called *linear harmonic oscillation*. The Hamiltonian operator is found by replacing p with $-j\hbar\mathrm{d}/\mathrm{d}x$, whence Schrödinger's equation reads

Quantum operator for Momentum

$$\boxed{-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 w}{\mathrm{d}x^2}+\frac{1}{2}m\omega^2x^2w=Ew\,.}$$

- It is worth noting that ω is determined by the parameters of the problem, before quantization. The equation can be recast in normalized form by defining $\epsilon \doteq E/(\hbar\omega)$, $\xi = (m\omega/\hbar)^{1/2}x$:

$$\mathcal{H}'w = \epsilon w\,, \qquad \mathcal{H}' \doteq \tfrac{1}{2}\left(\xi^2 - \mathrm{d}^2/\mathrm{d}\xi^2\right).$$

$\omega = \sqrt{\frac{C}{m}}$

$\Rightarrow C = \omega^2 m$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2W}{dx^2}+\frac{1}{2}m\omega^2x^2W = EW}$$

ω = Angular frequency

W = wave function

- We can notice immediately that the Angular frequency $\omega = \sqrt{c/m}$ is fully determined by the parameters of the Classical case.

we have seen this property in the analysis of the Crystal in that case we had many values of ω^2 which were Eigenvalues of the eqⁿ which we were solving

→ Now we will solve the eqⁿ for P.E not constant but Quadratic w.r.to position.

Renormalising the eqⁿ

It is worth noting that ω is determined by the parameters of the problem, before quantization. The equation can be recast in normalized form by defining $\epsilon \doteq E/(\hbar\omega)$, $\xi = (m\omega/\hbar)^{1/2}x$:

$$\mathcal{H}'w = \epsilon w, \qquad \mathcal{H}' \doteq \tfrac{1}{2}\left(\xi^2 - \mathrm{d}^2/\mathrm{d}\xi^2\right).$$

** Straight forward method to solve the eqⁿ is Brute Force method. i.e we expand solution 'W' formally in a Power series.

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Linear Harmonic Oscillator — II

- The eigenvalues of $\mathcal{H}' \doteq \frac{1}{2}\left(\xi^2 - \mathrm{d}^2/\mathrm{d}\xi^2\right)$ are found by means of auxiliary operators: define

$$\hat{a} \doteq \frac{1}{\sqrt{2}}\left(\xi + \frac{\mathrm{d}}{\mathrm{d}\xi}\right),$$

whence, for all f and g vanishing at infinity,

so They full fill The Normalization Condition.

$$\int_{-\infty}^{+\infty} g^* \hat{a} f \,\mathrm{d}\xi = \frac{1}{\sqrt{2}} \int_{-\infty}^{+\infty} \left(g^* \xi f - f \frac{\mathrm{d}g^*}{\mathrm{d}\xi}\right) \mathrm{d}\xi + \frac{1}{\sqrt{2}} \left[g^* f\right]_{-\infty}^{+\infty} =$$

$$= \int_{-\infty}^{+\infty} f \frac{1}{\sqrt{2}} \left(\xi - \frac{\mathrm{d}}{\mathrm{d}\xi}\right) g^* \,\mathrm{d}\xi = \int_{-\infty}^{+\infty} \left(\hat{a}^\dagger g\right)^* f \,\mathrm{d}\xi,$$

with $\hat{a}^\dagger \doteq (\xi - \mathrm{d}/\mathrm{d}\xi)/\sqrt{2}$. As $\hat{a}^\dagger \neq \hat{a}$, $\hat{a}$ is not Hermitian. Also, $\hat{a}$ and $\hat{a}^\dagger$ do not commute; one finds

$$\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \mathcal{I}, \qquad \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 2\mathcal{H}'.$$

- From the above equations, defining a new operator $\mathcal{N} = \hat{a}^\dagger\hat{a}$ one finds $2\mathcal{H}' = (\mathcal{I} + \hat{a}^\dagger\hat{a}) + \hat{a}^\dagger\hat{a} = 2\mathcal{N} + \mathcal{I}$, whence

$$\mathcal{H}'w = \mathcal{N}w + \mathcal{I}w/2 = \epsilon w \quad \Longrightarrow \quad \mathcal{N}w = (\epsilon - 1/2)w \doteq \nu w.$$

One sees that $\mathcal{H}'$ and $\mathcal{N}$ have the same eigenfunctions, while the eigenvalues differ by $1/2$.

Conclusion:

$\mathcal{N}'$ is a product of two first order operators. is Hermetian even though $a, a^\dagger$ are Not Hermetian

$$\int \frac{d}{dx} uv = \int (uv' + vu')$$

$$uv = \int u\,dv + \int v\,du$$

Integration by parts $\Rightarrow$ $\boxed{\int u\,dv = uv - \int v\,du}$

$\rightarrow$

Linear Harmonic Oscillator — III

Operator $\mathcal{N}$ is Hermitian, hence its eigenvalues ν are real; they are also non negative: in fact, scalar multiplication of $\mathcal{N}w = \nu w$ by w yields

$$\boxed{\int_{-\infty}^{+\infty} w^* \hat{a}^\dagger \hat{a} w \, d\xi = \int_{-\infty}^{+\infty} |\hat{a}w|^2 \, d\xi = \nu \int_{-\infty}^{+\infty} |w|^2 \, d\xi \,,}$$

whence $\nu = 0$ iff $\hat{a}w = 0$, otherwise $\nu > 0$. Another relation is found by left multiplying $\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \mathcal{I}$ by $\hat{a}^\dagger$:

$$\mathcal{N}\hat{a}^\dagger - \hat{a}^\dagger\mathcal{N} = \hat{a}^\dagger \implies \mathcal{N}\hat{a}^\dagger = \hat{a}^\dagger(\mathcal{N} + \mathcal{I}) \implies$$

$$\mathcal{N}\hat{a}^\dagger w = \hat{a}^\dagger(\mathcal{N} + \mathcal{I})\,w = \hat{a}^\dagger \nu w + \hat{a}^\dagger w = (\nu + 1)\,\hat{a}^\dagger w \,.$$

In other terms, if ν is an eigenvalue of $\mathcal{N}$ and w is an eigenfunction of ν, then $\nu + 1$ is also an eigenvalue, with eigenfunction $\hat{a}^\dagger w$. This reasoning can be repeated indefinitely: $\mathcal{N}\hat{a}^\dagger\hat{a}^\dagger w = (\nu + 2)\,\hat{a}^\dagger\hat{a}^\dagger w, \ldots$

Similarly, right multiplication of $\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \mathcal{I}$ by $\hat{a}$ yields

$$\hat{a}\mathcal{N} - \mathcal{N}\hat{a} = \hat{a} \implies \hat{a}\,(\mathcal{N} - \mathcal{I}) = \mathcal{N}\hat{a} \implies$$

$$\mathcal{N}\hat{a}w = \hat{a}\,(\mathcal{N} - \mathcal{I})\,w = \hat{a}\nu w - \hat{a}w = (\nu - 1)\,\hat{a}w \,.$$

Scalar product of '$\mathcal{N}$' by 'w'

$\Rightarrow \int_{-\infty}^{\infty} w^* N w \, d\xi$

$\Rightarrow \int_{-\infty}^{\infty} w^* \hat{a}^\dagger \hat{a} w \, d\xi$

$\because$ 'w' is an Eigen function it cannot be equal to zero

$\therefore$ Given an Eigen function 'w' we can calculate full set of eigenfunctions & Eigen values. which are infinite

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Linear Harmonic Oscillator — IV

Assuming Eigenvalues as Integers.

- By induction, $\mathcal{N}\hat{a}\hat{a}w = (\nu - 2)\,\hat{a}\hat{a}w$. However, this cannot be repeated indefinitely because the eigenvalue must be non negative. The only acceptable case is $\nu = n$, with $n = 0, 1, 2, \ldots$: it has been shown that $\nu = 0$ iff $\hat{a}w = 0$, hence the induction procedure $\mathcal{N}\hat{a}w = (\nu - 1)\,\hat{a}w = 0$ does not provides any more eigenfunctions as ν reaches zero.
- To determine the eigenfunction(s) w_0 corresponding to $n = 0$ one takes $\hat{a}w = 0$:

$$\boxed{\frac{1}{\sqrt{2}}\left(\xi + \frac{\mathrm{d}}{\mathrm{d}\xi}\right) w_0 = 0\,,} \qquad \frac{\mathrm{d}w_0}{w_0} = -\xi\,\mathrm{d}\xi\,, \qquad \boxed{w_0 = c_0\,\exp(-\xi^2/2)\,,}$$

It is a Gaussian

where $c_0 = \pi^{-1/4}$ is the normalization constant. The eigenfunctions corresponding to $n = 1, 2, \ldots$ are found recursively with $w_1 = \hat{a}^\dagger w_0\,,\ w_2 = \hat{a}^\dagger w_1 = \hat{a}^\dagger\hat{a}^\dagger w_0\,,\ \ldots$ For example,

$$\boxed{w_1 = \frac{1}{\sqrt{2}}\left(\xi w_0 - \frac{\mathrm{d}w_0}{\mathrm{d}\xi}\right) = \frac{1}{\sqrt{2}}\,2\xi\,w_0\,.}$$

Factorization has worked

- It is easily seen that the eigenvalues are not degenerate, and that w_n is even (odd) if n is even (odd).

Linear Harmonic Oscillator — V

- It can be shown that w_n has the form

$$\boxed{w_n(\xi) = \left(n!\, 2^n \sqrt{\pi}\right)^{-1/2} \exp(-\xi^2/2)\, H_n(\xi),}$$

where H_n is the ***Hermite polynomial***

$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{\mathrm{d}^n}{\mathrm{d}\xi^n} \exp(-\xi^2).$$

- The set of the eigenfunctions of the linear harmonic oscillator is a (real) orthonormal set:

$$\int_{-\infty}^{+\infty} w_n w_m \,\mathrm{d}x = \delta_{nm}.$$

By remembering that $\nu = \epsilon - 1/2 = n$ and $\epsilon = E/(\hbar\omega)$, one finds for the energy E the eigenvalues

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \qquad n = 0, 1, 2, \ldots$$

The minimum energy $E_0 = \hbar\omega/2 > 0$ is also called the *zero point energy*.

This is a famous formula which is reminiscent of

Energy of a mode of the Electromagnetic field.

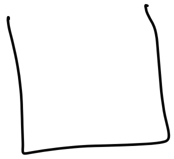
$$E = n\hbar\omega + \frac{1}{2}\hbar\omega \longrightarrow E_0 = \text{zero point Energy}$$

* Quantum Mechanics perspective

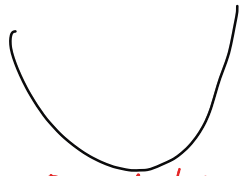
when wavefunction is Normalizable, then the minimum value of Total Energy is strictly larger than the Minimum Potential Energy

This is the case $\because$ the PE is a parabola as This parabola goes upto infinity, LHO is a potential Box but the Box instead of being

piece wise linear



it is



parabola

But The wavefunction is confined inside the limited region of SPACE. So it is Normalizable

Other Properties of the Harmonic Oscillator

Some aspects of the harmonic oscillator are worth mentioning:

- The rest condition of the particle is $x = 0, p = 0$. The quadratic potential $V = cx^2/2$, $c > 0$ corresponds to a linear force $-cx$ which gives rise to an oscillatory motion. The rest condition is thus stable. In turn, the linear force can be thought of as the first-order expansion of a more general force near the equilibrium condition: thus, in many cases the linear oscillator provides the correct perturbation solution.

- The normalized form is $-\mathrm{d}^2 w_n/\mathrm{d}\xi^2 + \xi^2 w_n = 2\epsilon_n w_n$. Let

$$u_n(\eta) \doteq \mathcal{F} w_n = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} w_n(\xi) \exp(-j\eta\xi)\, \mathrm{d}\xi\,.$$

Due to the properties of the Fourier transform it is $\mathcal{F}\mathrm{d}^2 w_n/\mathrm{d}\xi^2 = -\eta^2 u_n$, $\mathcal{F}\xi^2 w_n = -\mathrm{d}^2\eta_n/\mathrm{d}\eta^2$. Fourier transforming the equation thus yields $\eta^2 u_n - \mathrm{d}^2 u_n/\mathrm{d}\eta^2 = 2\epsilon_n u_n$, namely, the same equation written in terms of u_n and with the same eigenvalue. As the ϵ_n are not degenerate, it follows $u_n \propto w_n$, namely, the eigenfunctions of the harmonic oscillator are Fourier self-transforms.

→ * Quantization of EMF

Quantization of the E.M. Field — I

* We want to calculate the TE inside the Box!

(Q) Why do you want to calculate the TE?

Ans when we want to operate the Quantization of EMF and we want to write down the Schrodinger Equation!

The energy of the e.m. field in a volume $V = d_1 d_2 d_3$ can be expressed in terms of modes as

$$\boxed{W_{em} = \sum_{k\sigma} W_{k\sigma}}, \qquad \boxed{W_{k\sigma} = 2\varepsilon_0 V\, \omega^2\, s_{k\sigma} s^*_{k\sigma}},$$

→ energy associated individual Monochromatic wave

where $\sigma = 1, 2$, $\boldsymbol{k} = \Sigma_{i=1}^{3} 2\pi n_i \boldsymbol{i}_i / d_i$, $n_i = 0, \pm 1, \pm 2, \ldots$, and $\omega = ck$. The relation between each $s_{k\sigma}$ and the corresponding canonical variables $q_{k\sigma}, p_{k\sigma}$ is

→ position

→ Momentum operator

polarisation which is indication of Spin of Photon

$$2\sqrt{\varepsilon_0 V}\, \omega\, s_{k\sigma} = \omega q_{k\sigma} + j p_{k\sigma}\,.$$

Replacing the above in $W_{k\sigma}$ yields the three equivalent forms

This is similar to the eq^n of Linear Harmonic oscillator.

$$W_{k\sigma} = \begin{cases} (1/2)\,(p^2_{k\sigma} + \omega^2 q^2_{k\sigma}) \\ (1/2)\,(p^2_{k\sigma} + \omega^2 q^2_{k\sigma}) + (j\omega/2)\,(q_{k\sigma} p_{k\sigma} - p_{k\sigma} q_{k\sigma}) \\ (1/2)\,(p^2_{k\sigma} + \omega^2 q^2_{k\sigma}) - (j\omega/2)\,(q_{k\sigma} p_{k\sigma} - p_{k\sigma} q_{k\sigma}) \end{cases}$$

- However, the quantum Hamiltonians corresponding to the different forms of $W_{k\sigma}$ are not equivalent, as $p_{k\sigma}$ does not commute with $q_{k\sigma}$. In fact, the replacements

$$q_{k\sigma} \leftarrow \hat{q}_{k\sigma} = q_{k\sigma}\,, \qquad p_{k\sigma} \leftarrow \hat{p}_{k\sigma} = -j\hbar\, \partial/\partial q_{k\sigma}$$

yield $q_{k\sigma} p_{k\sigma} - p_{k\sigma} q_{k\sigma} \leftarrow \hat{q}_{k\sigma} \hat{p}_{k\sigma} - \hat{p}_{k\sigma} \hat{q}_{k\sigma} = j\hbar\,.$

→ Remember, The SE provides us with The Eigenvalues of The Energy. So, we must start from classical formula of Energy for EMF and Then we must introduce the Quantization.

* Energy of EMF inside The Box = Sum of Individual

energies associated to the Monochromatic components of the EMF

- All three eqn of $W_{k\sigma}$ are valid.

Quantization of the E.M. Field — II

Single Mode of oscillation

- The Hamiltonians corresponding to the different forms of $W_{k\sigma}$ read

$$\mathcal{H}_{k\sigma} = \begin{cases} \mathcal{H}^0_{k\sigma} \doteq (1/2)\left(-\hbar^2\partial^2/\partial q^2_{k\sigma} + \omega^2 q^2_{k\sigma}\right) \\ \mathcal{H}^-_{k\sigma} \doteq (1/2)\left(-\hbar^2\partial^2/\partial q^2_{k\sigma} + \omega^2 q^2_{k\sigma}\right) - \hbar\omega/2 \\ \mathcal{H}^+_{k\sigma} \doteq (1/2)\left(-\hbar^2\partial^2/\partial q^2_{k\sigma} + \omega^2 q^2_{k\sigma}\right) + \hbar\omega/2 \end{cases}$$

- The corresponding Schrödinger equations are

$$\begin{cases} \mathcal{H}^0_{k\sigma} w^0_{k\sigma} = E^0_{k\sigma} w^0_{k\sigma} \\ \left(\mathcal{H}^0_{k\sigma} - \hbar\omega/2\right) w^-_{k\sigma} = E^-_{k\sigma} w^-_{k\sigma} \\ \left(\mathcal{H}^0_{k\sigma} + \hbar\omega/2\right) w^+_{k\sigma} = E^+_{k\sigma} w^+_{k\sigma} \end{cases}$$

- The eigenvalues of $\mathcal{H}^0_{k\sigma}$ are $(n_{k\sigma} + 1/2)\,\hbar\omega$ and are non degenerate. Writing the second equation as

$$\mathcal{H}^0_{k\sigma}\, w^-_{k\sigma} = \left(E^-_{k\sigma} + \hbar\omega/2\right)\, w^-_{k\sigma}$$

shows that $w^-_{k\sigma} = w^0_{k\sigma}$ and $E^-_{k\sigma} + \hbar\omega/2 = E^0_{k\sigma}$, whence $E^-_{k\sigma} = n_{k\sigma}\,\hbar\omega$. Similarly, $w^+_{k\sigma} = w^0_{k\sigma}$ and $E^+_{k\sigma} - \hbar\omega/2 = E^0_{k\sigma}$, whence $E^+_{k\sigma} = (n_{k\sigma} + 1)\,\hbar\omega$.

* apparently all the three eqns provide us with the same Eigen values.

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Quantization of the E.M. Field — III

As the energy of the e.m. field is the sum of the energy of the single modes, the three cases considered above yield:

$$\begin{cases} \Sigma_{k\sigma}(n_{k\sigma}+1/2)\,\hbar\omega \\ \Sigma_{k\sigma}\,n_{k\sigma}\,\hbar\omega \\ \Sigma_{k\sigma}(n_{k\sigma}+1)\,\hbar\omega \end{cases}$$

with $\omega = ck$. In the first and third case the sum over k diverges due to the terms $\hbar\omega/2$ and $\hbar\omega$, respectively. This cannot be accepted as the total energy must be finite. On the contrary, for the sum of the second case to converge it is sufficient that $n_{k\sigma}$ vanishes from some k on. The correct Hamiltonian is thus $\mathcal{H}^{-}_{k\sigma}$. Letting $n_k = n_{k1} + n_{k2}$, the energy of the e.m. field reads

$$\boxed{W_{\text{em}} = \sum_k n_k\,\hbar\omega\,,}$$

namely, it is the sum of the energies of each mode of oscillation. The latter, in turn, is an integer multiple of the elementary energy $\hbar\omega(\boldsymbol{k})$. This result provides the justification of the concept of photon. The integer $n_{k\sigma}$ is the *occupation number* of the pair $\boldsymbol{k}, \sigma$, whereas n_k is the number of photons of the mode corresponding to $\boldsymbol{k}$.

PHOTON

$$\boxed{W_{em} = \sum_k n_k \hbar\omega}$$

integer number

individual Quantum energy associated to the Angular Frequency 'ω' i.e 'k'

→ we can also find an expression for the Momentum of the EMF in classical terms

• we use Pointing Theorem which is a Theorem of the conservation of the Energy.

This explains the interaction of particles in space with EMF of the interaction 4w there will result in Energy exchange!

Quantization of the E.M. Field — IV

The momentum of the e.m. field in a volume V expressed in terms of modes reads

wave vector of individual component

$$\mathbf{\Pi}_{\rm em} = \sum_{k\sigma} \mathbf{\Pi}_{k\sigma}\,, \qquad \mathbf{\Pi}_{k\sigma} = 2\varepsilon_0 V \omega\, \boldsymbol{k}\, s_{k\sigma} s^*_{k\sigma}\,.$$

The same quantization procedure used for the energy can be applied here to yield

$$\mathbf{\Pi}_{k\sigma} = \frac{1}{c} 2\varepsilon_0 V \omega^2 s_{k\sigma} s^*_{k\sigma} \frac{\boldsymbol{k}}{k} \quad \leftarrow \quad \hat{\mathbf{\Pi}}_{k\sigma} = \frac{1}{c} \mathcal{H}^-_{k\sigma} \frac{\boldsymbol{k}}{k}\,.$$

The eigenvalues of the ith component of $\hat{\mathbf{\Pi}}_{k\sigma}$ are thus

$$\frac{1}{c} n_{k\sigma} \hbar\omega \frac{k_i}{k} = n_{k\sigma} \hbar k_i\,.$$

As a consequence, the eigenvalues of $\hat{\mathbf{\Pi}}_{k\sigma}$ are $n_{k\sigma}\,\hbar\boldsymbol{k}$. Letting $n_k = n_{k1} + n_{k2}$, the momentum of the e.m. field reads

$$\mathbf{\Pi}_{\rm em} = \sum_k n_k \hbar\boldsymbol{k}\,,$$

namely, it is the sum of the momenta of each mode of oscillation. The latter, in turn, is an integer multiple of the elementary momentum $\hbar\boldsymbol{k}$. This result provides the justification of taking $\hbar\boldsymbol{k}$ as momentum of the photon.

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Phonons — I

The Schrödinger equation for a system of K electrons and N nuclei is split into a system of two equations,

$$(\mathcal{T}_e + U_e + U_{ea} + U_{\text{ext}})\, u = E_e u\,,$$

$$(\mathcal{T}_a + U_a + E_e + U_u)\, v = E v\,.$$

It is assumed that the first equation has been solved for $\boldsymbol{R} = \boldsymbol{R}_0$, so that $E_e(\boldsymbol{R}_0)$ and $U_u(\boldsymbol{R}_0)$ are known. Letting

$$V_a(\boldsymbol{R}) \doteq U_a(\boldsymbol{R}) + E_e(\boldsymbol{R}_0) + U_u(\boldsymbol{R}_0)\,,$$

the operator $\mathcal{T}_a + V_a$ is the quantum equivalent of a classical Hamiltonian function $T_a + V_a$. If the displacements $|\boldsymbol{R} - \boldsymbol{R}_0|$ of the nuclei with respect to the equilibrium position are small, V_a can be expanded to second order around $\boldsymbol{R}_0$. Then, separating the second-order term into normal coordinates b_σ, whose conjugate moments are $\dot{b}_\sigma$, provides

Equillibrium PE

$$\boxed{\underbrace{T_a}_{\text{K.E}} + \underbrace{V_a}_{\text{PE}} = \sum_{\sigma=1}^{3N} H_\sigma + V_{a0}}\,, \qquad \boxed{H_\sigma \doteq \frac{1}{2}\dot{b}_\sigma^2 + \frac{1}{2}\omega_\sigma^2 b_\sigma^2}\,.$$

Normal co-ordinate depends on time

Total energy of Set of Atoms

Hamiltonian in clanical term

At some point we discussed about Crystal or Set of Atoms and we considered that the forces among these items are very strong so the displacements of the Atoms w.r.to the Equillibrium positions is very small.

Then at this point we have potential Energy to the second order, Then we found the Quadratic form of the Potential Energy.

Due to some properties the Tn QF is PD & Symmetric and it can be Diagonalised

After this process of Diagonalising TE of Material in classical terms we have found the Normal co-ordinates and the Normal Modes of oscillations.

$$\boxed{\text{Total Energy} = T_a + V_a = \sum_{r=1}^{3N} H_r + V_{a0}}$$

$$\boxed{H_r = \frac{1}{2}\dot{b}_r^2 + \frac{1}{2}\omega_r^2 b_r^2}$$

Hamiltonian in classical situation

This angular frequency is given by the classical formula, There is no Quantisation

→ Now offcourse, Quantization consists of Transforming Kinetic Energy into Kinetic operator

Phonons — II

- As a consequence, the quantum operator takes the form

$$\mathcal{T}_a + V_a = \sum_{\sigma=1}^{3N} \mathcal{H}_\sigma + V_{a0}\,, \qquad \mathcal{H}_\sigma \doteq -\frac{\hbar^2}{2}\frac{\partial^2}{\partial b_\sigma^2} + \frac{1}{2}\omega_\sigma^2 b_\sigma^2\,.$$

This is the corresponding Schrodinger eqn.

- Introducing the above into $(\mathcal{T}_a + V_a)v = Ev$ yields

$$\left(\sum_{\sigma=1}^{3N} \mathcal{H}_\sigma\right) v = E' v\,, \qquad E' \doteq E - V_{a0}\,.$$

As the operator is the sum of operators acting on individual degrees of freedom, the above can be split into $3N$ equations

$$\mathcal{H}_\sigma v_{\sigma\zeta_\sigma} = E_{\sigma\zeta_\sigma} v_{\sigma\zeta_\sigma}\,, \qquad E' = \sum_{\sigma=1}^{3N} E_{\sigma\zeta_\sigma}\,,$$

where index $\sigma = 1, 2, \ldots, 3N$ refers to the degrees of freedom, whereas $\zeta_\sigma = 0, 1, 2, \ldots$ is the set of eigenvalue indices corresponding to a given σ. The Schrödinger equation for the individual degree of freedom is of the linear harmonic-oscillator type, whence

$$E_{\sigma\zeta_\sigma} = \left(\zeta_\sigma + \frac{1}{2}\right)\hbar\omega_\sigma\,, \qquad \zeta_\sigma = 0, 1, 2, \ldots\,.$$

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Phonons — III

- The eigenvalues of $(\mathcal{T}_a + V_a)v = Ev$ are then

$$E = V_{a0} + \sum_{\sigma=1}^{3N} \left(\zeta_\sigma + \frac{1}{2}\right) \hbar\omega_\sigma .$$

- The oscillation of the normal coordinate of index σ is also called a *mode* of the system of nuclei.
  The energy associated to each mode has the same form as that of a mode of the e.m. field. By analogy with the e.m. case, a particle of energy $\hbar\omega_\sigma$ is introduced, called *phonon*, and the energy of the mode is ascribed to the set of phonons belonging to the mode.
  The integers ζ_σ are the *occupation numbers* of the normal modes of oscillation. As the phonons are bosons, the equilibrium distribution of the ζ_σ is given by the Bose-Einstein statistics.
- The simplest way to describe the interaction of an electron with the nuclei is using the quantum-mechanical, first-order perturbation theory applied to the two-particle collision of an electron and a phonon.

** we continue in the next class by considering another Problem "Electron inside a Crystal"

we will use the conclusion drawn from the Piecewise constant Potentials to describe the Eigenvalues of the e^-s in the Crystal.