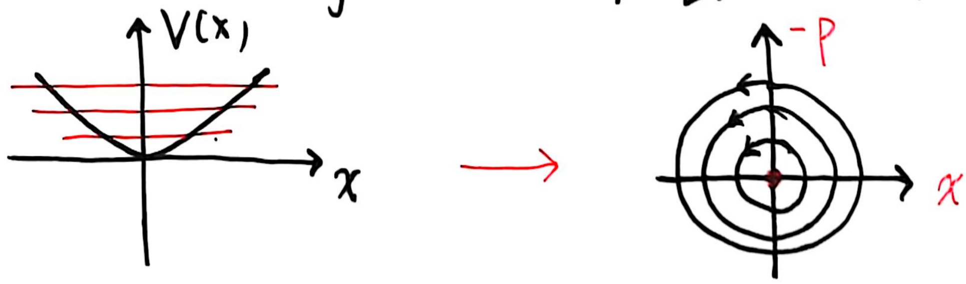
Lecture 1 Review of Classical physics and Old Quantum theory

1° Brief history 1900 — 1925, 1926

2° Hamiltonian Eq from least action principle

Maupertuis principle — $J = \oint \frac{p\,dq}{2\pi}$

canonical transformation $(p, q) \to (J, \theta)$



$\omega = \frac{dE}{dJ}$

3° Classic theory of radiation — quick summary

4° Planck black body radiation — energy quantizat

5° Bohr's old quantum theory

- action quantization
- correspondence theorem

1. History of quantum physics

1900 Black body radiation, Planck's energy quantization

1905 Photoelectric effect — Einstein's hypothesis of photon (quantization of light)

Specific heat of solids — phonon, quantization of lattice vibration

1911 Bohr's model of hydrogen atom

correspondence principle

Bohr - Sommerfeld quantization

$\frac{1}{2\pi}\oint p\,dq = n\hbar$ action quantization

1924 De Broglie matter wave $p = \hbar k = h/\lambda$.

1925-26 Heisenberg's reinterpretation $(x^2)_{ij} = x_{ik}x_{kj}$

Born-Jordan matrix mechanics $[x, p] = i\hbar$

Dirac's mapping to Poisson brackets

1926 Schrödinger equation — wave mechanics

$$i\hbar \frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

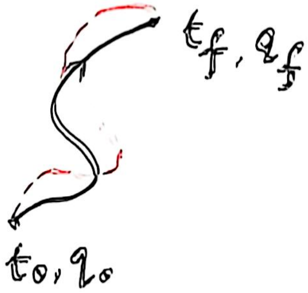
1933, 1948 Dirac, Feynman path integral formulation

$$G(x_b t_b, x_a t_a) = \int Dx(t)\, e^{i\int_{t_a}^{t_b} dt \cdot L(x, \dot{x}, t)}$$

Review of classic mechanics

④ Hamilton Equation from least action principle

$$S[q(t)] = \int_{t_0}^{t_f} dt\, \mathcal{L}(q, \dot{q}, t) = \int (p\dot{q} - H)\, dt$$



$$\begin{cases} \mathcal{L} = p\dot{q} - H(p, q) \\ p = \dfrac{\partial \mathcal{L}}{\partial \dot{q}} \end{cases}$$

$$\delta S = \int_{t_1}^{t_2} \left[\delta p\, \dot{q} + p \frac{d}{dt}(\delta q) - \left(\frac{\partial H}{\partial p} \delta p + \frac{\partial H}{\partial q} \delta q \right) \right] dt$$

$$p \frac{d}{dt}(\delta q) = \frac{d}{dt}(p\,\delta q) - \dot{p}\, \delta q$$

$$= \int_{t_1}^{t_2} dt \left[\delta p \left(\dot{q} - \frac{\partial H}{\partial p} \right) - \delta q \left(\frac{\partial H}{\partial q} + \dot{p} \right) \right] + \underbrace{p\, \delta q \Big|_{t_0}^{t_f}}_{= 0}$$

$$\frac{\delta S}{\delta p} = 0, \quad \frac{\delta S}{\delta q} = 0$$

$$\Rightarrow \begin{cases} \dot{q} = \dfrac{\partial H}{\partial p} \\ \dot{p} = -\dfrac{\partial H}{\partial q} \end{cases}$$

Example: $\mathcal{L} = \frac{1}{2} m (\dot{q}^2 - \omega^2 q^2)$

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = m\dot{q}$$

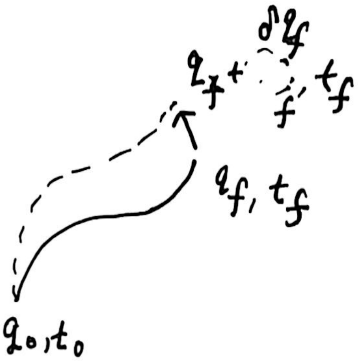
$$H = p\dot{q} - \mathcal{L} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2$$

$$\begin{cases} \dot{q} = \dfrac{\partial H}{\partial p} = \dfrac{p}{m} \\ \dot{p} = -\dfrac{\partial H}{\partial q} = -m\omega^2 q \end{cases}$$

④ Action as function of q, t

Along the physical path, then S is no longer a functional but a function. Let's fix t_0, q_0, then S is a function of t_f, q_f, i.e. $S(q_f, t_f)$.

- Let's calculate $S(q_f + \delta q, t_f)$



Then the physical paths are slightly different.

$$S(q_f + \delta q, t_f) - S(q_f, t_f) = \frac{\partial L}{\partial \dot{q}} \delta q \Big|_{t_0}^{t_f} + \int_{t_0}^{t_f} \underbrace{\left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\right)}_{=0 \text{ along the physical path}} \delta q \, dt$$

t_0, q_0 fixed

$$= p_f \, \delta q_f$$

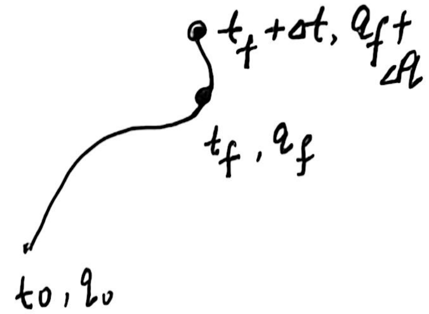
$$\Rightarrow \boxed{\frac{\partial S}{\partial q_f} = p_f}$$

- If we view q_f as a function of t_f, then $S(t_f, q_f(t_f))$ is a function of t_f.

$$S_{(t_f)} = \int_{t_0}^{t_f} dt \; L \quad \Rightarrow \quad \frac{dS}{dt_f} = \int_{t_0}^{t_f + \Delta t} dt \; L - \int_{t_0}^{t_f} dt \; L$$

$$\boxed{\frac{dS}{dt_f} = L.}$$

$$\frac{dS}{dt_f} = \frac{\partial S}{\partial t_f} + \frac{\partial S}{\partial q_f}\dot{q}_f = L$$



$$\boxed{\frac{\partial S}{\partial t_f} = L - p_f\dot{q}_f = -H}$$

If we release both ends $S(t_f q_f, t_0 q_0) \Rightarrow$

$$dS = p_f\, dq_f - H(p_f, q_f)\, dt_f - \left(p_0\, dq_0 - H(p_0, q_0)\, dt_0\right)$$

⊛ Maupertuis principle

The least action principle involves time explicitly. If we are only interested in the shape of path without refering to time, we need to modify the least action principle. We fix t_0 and q_0. The final position q_f is also fixed. But t_f is allowed to vary.

The least action principle does variation: fix t_f, q_f, not E

The Maupertuis principle does variation by fixing q_f, E, but not t_f.

For motions in 2D or even higher dimensions, even E is fixed, the actual shape of the path is still to be determined. In this case, Maupertuis principle is useful.

$$S[q_i(t)] = \int_{t_0}^{t_f} \mathcal{L}\, dt = \int_{t_0}^{t_f} (P_i \dot{q}_i - H)\, dt$$

$$= \int_{\vec{q}_0}^{\vec{q}_f} \vec{p} \cdot d\vec{q} - E(t_f - t_0)$$

Define $S_{abr}[q_i(t)] = S[q_i(t)] + E(t_f - t_0)$

$$= \int_{\vec{q}_0}^{\vec{q}_f} \vec{p} \cdot d\vec{q} \quad \leftarrow \text{abbreviated action}$$

Do variation of S_{abr} around the actual path.

$$\delta S_{abr} = \delta \left[\int_{\vec{q}_0}^{\vec{q}_f} \vec{p} \cdot d\vec{q} \right]$$

To the first order of δq, over the actual path, we only need to find a particular change: Fix $\vec{q}_f$, but vary t_f to $t_f + \Delta t$.

Choose the physical path

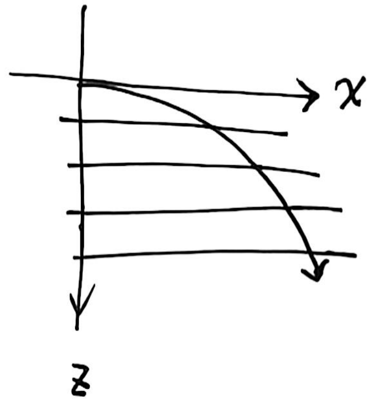
Then $\delta S_{abr} = \left[\dfrac{\partial S(t_f, \vec{q}_f)}{\partial t} + E \right] \Delta t$

$$= [-E + E]\Delta t = 0.$$

$$\Rightarrow \delta\left[\int_{\vec{q}_0}^{\vec{q}_f} \vec{p} \cdot d\vec{q} \right] \Bigg|_{\text{fixed } E} = 0.$$

Excerise:

[illegible]: Consider a projectile motion



$$\int dl \sqrt{2m(E_0 + mgz)}$$

make an analogy to $\int \frac{dl}{v} = \int \frac{n\,dl}{c}$

$n(z) \propto \sqrt{E_0 + mgz}$ increases as z increases, hence the trajactory is like light from the air to the water

Canonical transformation:

The drawback of Newtonian equation of motion is that they explicitly depend on the . coordinates. The Lagrangian formalism improves it, the Lagrangian equation is invariant under coordinate transformation. The Hamiltonian formalism enjoys even larger symmetry. Coordinates and momenta can transform together while maintaining the invariance of the canonical Eq.

We define $\begin{cases} Q = Q(q, p, t) \\ \mathbb{P} = \mathbb{P}(q, p, t) \end{cases}$ such that $\begin{cases} \dot{Q} = \dfrac{\partial H'}{\partial \mathbb{P}} \\ \dot{\mathbb{P}} = -\dfrac{\partial H'}{\partial Q} \end{cases}$

where $H'(\mathbb{P}, Q, t)$ is a new Hamiltonian

Consider $\delta \int (p\,dq - H\,dt) = 0$ (*)

$\delta \int (\mathbb{P}\,dQ - H'\,dt) = 0$ (**)

(*) and (**) are equivalent iff they differ by a total derivative

$p\,dq - H\,dt = \mathbb{P}\,dQ - H'\,dt + dF$ ← generation function

$dF = p\,dq - \mathbb{P}\,dQ + (H - H')\,dt$ $\Rightarrow$ $\boxed{\begin{cases} p = \dfrac{\partial F}{\partial q}, \quad \mathbb{P} = -\dfrac{\partial F}{\partial Q} \\ H' = H + \dfrac{\partial F}{\partial t} \end{cases}}$

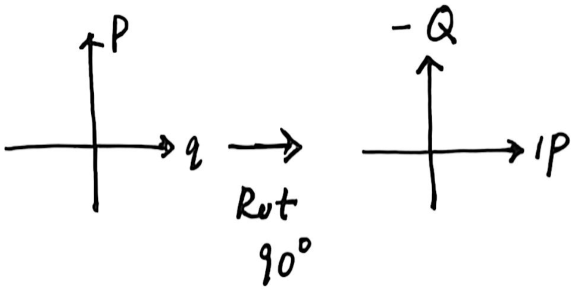
F as function of q, Q, t, $F(q, Q, t)$

For example, let's chouse $F = -qQ$, then $\begin{cases} p = \frac{\partial F}{\partial q} = -Q \\ P = -\frac{\partial F}{\partial Q} = q \end{cases}$

Then $H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2$

$H = \frac{Q^2}{2m} + \frac{1}{2} m \omega^2 P^2$

$H' = H$



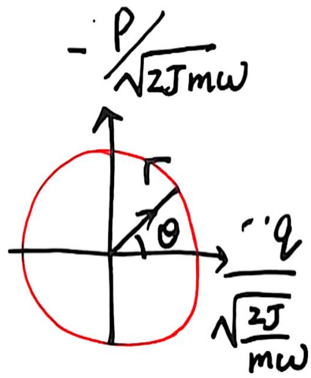
- Solution to harmonic oscillator

$$J = \oint \frac{p\,dq}{2\pi} = \frac{\pi A}{2\pi} m\omega A = \frac{1}{2} m\omega A^2$$

$$= E/\omega$$

action over a period

$$A = \sqrt{\frac{2E}{m\omega^2}} = \sqrt{\frac{2J}{m\omega}} \Rightarrow \begin{cases} q = \sqrt{\frac{2J}{m\omega}} \cos\theta \\ p = -\sqrt{2Jm\omega} \sin\theta \end{cases}$$



$H(\theta, J) = J\omega \quad (J>0)$

we view the motion as around a circle in phase space

$$\theta = \cos^{-1}\frac{x}{\sqrt{2J/m\omega}} = \omega(t-t_0)$$

$$\begin{cases} \dot{\theta} = \frac{\partial H}{\partial J} = \omega \\ \dot{J} = -\frac{\partial H}{\partial \theta} = 0 \end{cases}$$

$$J = \left(\frac{p}{\sqrt{m\omega 2}}\right)^2 + \left(\sqrt{\frac{m\omega}{2}}\, q\right)^2$$

General case, J is a single variable function of E, hence

$$S_{abr}(q,E) = \int_{q_0}^{q} dq\; p(q,E)$$ can be expressed as

$$S_{abr}(q,J) = \int_{q_0}^{q} dq\; p(q,J),$$ then treat $S_{abr}(q,J)$

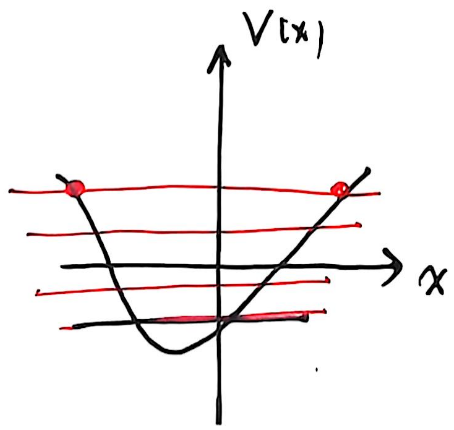
as the generation function

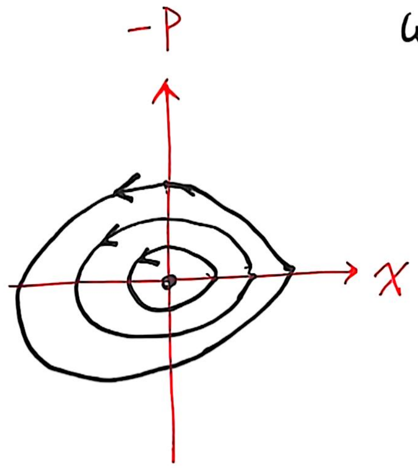
$$p = \left(\frac{\partial S_{abr}}{\partial q}\right)_J \qquad \leftrightarrow \quad (p, q) \text{ conjugate}$$

$$\theta' = -\left(\frac{\partial S_{abr}}{\partial J}\right)_q \qquad \leftrightarrow \quad (\theta', J) \text{ conjugate} \rightarrow (J, \theta = -\theta')$$

$H' = H = E(J)$ since $S_{abr}(q,J)$ is independent on time

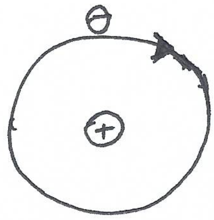
$$\boxed{\theta = \frac{dE}{dJ} \cdot t + \text{const} = \omega(J)\, t + \text{const}}$$





$$\omega = \left.\frac{dE}{dJ}\right|_J$$

Classic theory of radiations



1. dipole radiation power

$$P \sim \frac{e^2 a^2}{c^3} \qquad a: \text{acceleration}$$

dimensional analysis $\quad \frac{e^2}{} \frac{L^2}{T^4} \cdot \frac{T^3}{L^3} = \frac{e^2}{L \cdot T} = \frac{E}{T} = \text{power}$

$$a \sim \omega^2 x \Rightarrow \boxed{P \sim \frac{e^2}{c^3} x^2 \omega^4}$$

more precisely

$$P = \frac{2e^2}{3c^3} \ddot{x}^2$$

2. Fourier expansion — harmonics

$$X_n(t) = \sum_{\alpha=-\infty}^{\infty} a_\alpha e^{i \alpha \omega_n t}$$

, where Here a_α is the harmonic component, α is an integer order of harmonics.

n is a certain mode of oscillation

$$X_n^2(t) = \sum_{\alpha \alpha'} a_\alpha a_{\alpha'} e^{i(\alpha+\alpha')\omega_n t}$$

$$= \sum_\beta \left(\sum_\alpha a_{\beta-\alpha} a_\alpha \right) e^{i \beta \omega_n t}$$

$$\Rightarrow y_\beta = \sum_\alpha a_{\beta-\alpha} a_\alpha$$

$\omega_n, 2\omega_n, 3\omega_n, \cdots\cdots$

3 $\quad P_\alpha(n) \sim \frac{e^2}{c^3} (\alpha \omega_n)^4 |a|_\alpha^2 \qquad P = \sum_{\alpha=1}^{\infty} P_\alpha(n)$

How Planck derived his formula?

Actually Planck was guided by the general principle of thermodynamics and experiment fact. 1 The radiative power at $\omega \to 0$ obeys the Releigh-Jeans law, i.e

$$k_B T \propto u(\omega),$$

u is the ave~~r~~erge energy for a E&M mode at the fregnency ω.

2 At $\omega \to \infty$, the experiment curve shows

$$u_{(\omega)} \propto e^{-\hbar\omega/k_B T}.$$

The question is that the two forms of $u(\omega) = \begin{cases} k_B T & \omega \to 0 \\ \# e^{-\hbar\omega/k_B T} & \omega \to +\infty \end{cases}$ are two different. How to find an unified formula to controll is an interesting question.

Planck considered to view the low ω and high ω as two subsystems. They reach thermal equilibrium via the same ~~temperature~~. At low ω frequency regin

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_V \Rightarrow \frac{\partial}{\partial u}\left(\frac{1}{T}\right) = \left(\frac{\partial^2 S}{\partial u^2}\right)_V$$

since $u \propto T \Rightarrow \frac{1}{T} = \frac{k_B}{u}$

$$\Rightarrow \frac{\partial(\frac{1}{T})}{\partial u} = -\frac{k_B}{u^2} \text{ ~~where } \cancel{C_1 \text{ is a constant}}~~ .$$

· At high freguesy. $\ln u = -\frac{\hbar\omega}{k_B T} + \text{cnst}$

$$\frac{\partial \ln u}{\partial(\frac{1}{T})} = -\frac{\hbar\omega}{k_B} \Rightarrow \frac{1}{u}\frac{\partial u}{\partial \frac{1}{T}} = -\frac{\hbar\omega}{k_B}$$

$$\partial(\tfrac{1}{T})/\partial u = -\frac{k_B/\hbar\omega}{u}$$

Then $\partial(\frac{1}{T})/\partial u$ can be unified as

$$\partial(\tfrac{1}{T})/\partial u(\omega) = -\frac{k_B}{u(u+\hbar\omega)} \rightarrow \begin{cases} -\frac{k_B}{u^2} & \omega \to 0 \\ -\frac{k_B}{u\hbar\omega} & \omega \to \infty \end{cases}$$

$$\Rightarrow \frac{\partial(\frac{1}{k_B T})}{\partial u} = \left[\frac{1}{u+\hbar\omega} - \frac{1}{u}\right]\frac{1}{\hbar\omega}$$

$$\frac{\hbar\omega}{k_B T} = \ln\frac{u+\hbar\omega}{u} + \text{Const} \Rightarrow$$

$$1 + \frac{\hbar\omega}{u} = \text{cnst.}\, e^{\hbar\omega/k_B T}$$

check $\hbar\omega \to 0 \Rightarrow$ cnst $= 1$, with $u = k_B T$

$$\Rightarrow \frac{\hbar\omega}{u} = e^{\hbar\omega/k_B T} - 1$$

$$\Rightarrow \boxed{U(\omega) = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}}$$

old quantum theory — Bohr theory

① Quantization condition – Bohr - Sommerfeld

$$\boxed{\oint \frac{p\,dx}{2\pi} = n\hbar \,, \quad n = 0, 1, 2, \cdots}$$

② Frequency ω_{nm} and the power of light associated with the transition

Einstein – Bohr

$$\boxed{\left.\begin{aligned} \omega_{nm} &= \frac{1}{\hbar}(E_n - E_m) \\ P_{nm} &= A_{nm}(E_n - E_m) \end{aligned}\right\}}$$

A_{nm} is the transition rate, i.e. the probability from $n \to m$ in unit time.

This is consistent with the Rydberg – Ritz combination law

$$\boxed{\omega_{nl} = \omega_{nm} + \omega_{ml}}$$

③ Intensity correspondence (Bohr).

The radiation power $P_{n,n-\alpha} \longrightarrow P_\alpha(n)$ in the limit $n \gg \alpha$.

$P_{n,n-\alpha}$: transition from $n \to n-\alpha$

$P_\alpha(n)$: the α-th harmonics of the classic motion in the state n.

2 Correspondence theorems

1. Correspondence between spectral and mechanical frequencies.

The spectra frequency $\omega_{n,n-\alpha}$ from the quantum state $n \to n-\alpha$, corresponds to the α-harmonics of mechanical frequency $\alpha\omega(n)$.

i.e. $\boxed{\omega_{n,n-\alpha} = \alpha\,\omega_n}$

Proof: In classic physics, the abberivated action $\boxed{J(E) = \oint \frac{p\,dx}{2\pi}}$,

$$2\pi \frac{\partial J}{\partial E} = \oint \left.\frac{\partial p}{\partial E}\right|_q dq = \oint dq\Big/\frac{\partial H}{\partial p} = \oint dq/\dot{q} = \oint dt = T$$

$$\Rightarrow \quad \boxed{\partial E/\partial J = \omega}$$

assume $E_n = E(J = n\hbar)$, $E_m = E(J = m\hbar)$

$$\hbar\,\omega_{nm} = E_n - E_m = E(n\hbar) - E(m\hbar) = \left.\frac{\partial E}{\partial J}\right|_{J=n\hbar} (n-m)\hbar$$

$$\boxed{\hbar\,\omega_{n,n-\alpha} = \alpha\,\hbar \left.\frac{\partial E}{\partial J}\right|_{J=n\hbar} \to \alpha\,\hbar\,\omega_n}$$

$$\boxed{\text{define } \omega_n = \left.\frac{\partial E}{\partial J}\right|_{J=n\hbar}.}$$

2. Correspondence between transition probability and viabration amplitude: —

The transition rate $n \to n-\tau$ in the limit of $n \to \infty$, it behaves.

$$A_{n,n-\alpha} = \frac{e^2 (\alpha\omega(n))^3}{3\hbar c^3} |a_\alpha(n)|^2$$

the α-th harmonics of $X_n(t) = \sum_{\alpha=-\infty}^{+\infty} a_\alpha(n) e^{i\omega_n \alpha t}$.

Proof: $$p(t) = \frac{2e^2}{3c^3} \ddot{x}_n^2$$

$$x_n(t) = \sum_\alpha a_\alpha(n) e^{i\alpha\omega_n t}, \quad \ddot{x}_n(t) = \sum_\alpha a_\alpha(n)(-)(\alpha\omega_n)^2 e^{i\alpha\omega_n t}$$

$$|\ddot{x}_n(t)|^2 = \sum_{\alpha\alpha'} a_\alpha(n) a^*_{\alpha'}(n) (\alpha\omega_n)^2 (\alpha'\omega_n)^2 e^{i(\alpha-\alpha')\omega_n t}$$

$$= \sum_\alpha |a_\alpha(n)|^2 \alpha^4 \omega_n^4 + \sum_{\alpha\neq\alpha'} a_\alpha(n) a^*_{\alpha'}(n) (\alpha\alpha')^2 \omega_n^4 e^{i(\alpha-\alpha')\omega_n t}$$

$$\Rightarrow \overline{p(t)} = \frac{4}{3}\frac{e^2}{c^3}\omega_n^4 \sum_{\alpha=1}^{\infty} \alpha^4 |a_\alpha(n)|^2 = P(n)$$

$$P_\alpha(n) = \frac{4}{3}\frac{e^2}{c^3}\omega_n^4 \alpha^4 |a_\alpha(n)|^2$$

$$P_\alpha(n) \longrightarrow \hbar\omega_{n,n-\alpha} A_{n,n-\alpha} \to \frac{4}{3}\frac{e^2}{c^3} \omega^4_{n,n-\alpha} |X_{n,n-\alpha}|^2$$

$$\parallel \; \alpha\omega_n$$

$$A_{n,n-\alpha} = \frac{4}{3}\frac{e^2}{\hbar c^3}\omega^3_{n,n-\alpha} |X_{n-\alpha,n}|^2$$