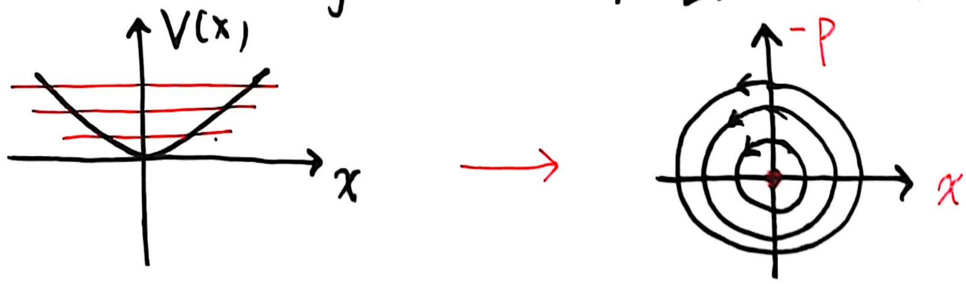
Lecture 1 Review of Classical physics and Old Quantum theory

1° Brief history 1900 — 1925, 1926

2° Hamiltonian Eq from least action principle

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

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



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

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

1913 Bohr's model of hydrogen atom

correspondence principle

1916 Bohr – Sommerfeld quantization

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

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

(*) Hamiltoni Equation from least action principle

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

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

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

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

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

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

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

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

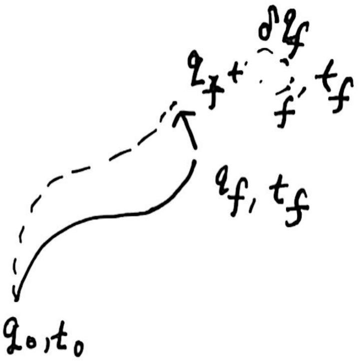
$$H = p\dot{q} - \mathcal{L} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2$$

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

⊛ 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.

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

t_0, q_0 fixed

0 along the physical path

$$= p_f \, \delta q_f$$

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

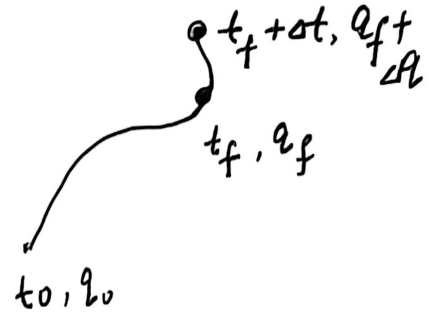
- If we view q_f as a function of t_f, then $S(t_f, q_f(t_f))$ is a function of t_f.

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

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

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

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



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 when E is fixed, the actual path is still to be determined. In this case, the Maupertuis principle is useful.

$$S[q_i(t)] = \int_{t_i}^{t_f} L\, dt = \int_{\vec{q}_0}^{\vec{q}_f} P_i dq_i - E(t_f - t_0)$$

Define S_{abr} $\quad = \int_{\vec{q}_0}^{\vec{q}_f} P_i dq_i = S[q_i(t)] + E(t_f - t_0)$.

we use an arbitary parameter s, such that S_0 and S_f are fixed to characterize a path,

$\gamma(s) = (q(s), p(s))$ and a curve nearby

$\gamma_\epsilon(s) = (q_\epsilon(s), P_\epsilon(s))$ with the boundary condition

$\vec{q}_\epsilon(s_0) = \vec{q}_0, \quad \vec{q}_\epsilon(s_f) = \vec{q}_f$. [fix S_f]

For each s, we require $\boxed{H(q_\epsilon(s), P_\epsilon(s)) = E}$ $\rightarrow$ we do not require $(P_\epsilon(s), q_\epsilon(s))$ is the actual path, but it should on the energy surface $H=E$.

$$\delta H = \frac{\partial H}{\partial q_i}\delta q_i + \frac{\partial H}{\partial p_i}\delta P_i = 0.$$

Now calculate the variation

$$S_{abr}[\gamma] = \int_{s_0}^{s_f} P_i \frac{dq_i}{ds}\, ds$$

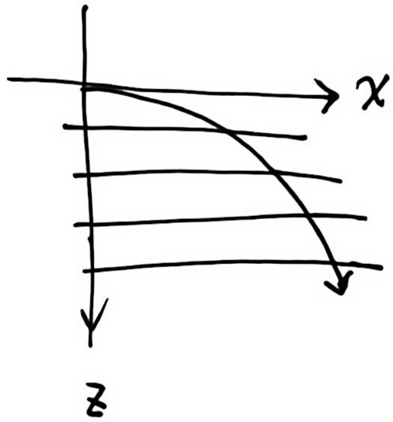
$$\Rightarrow \delta S_{abr}[\gamma] = \int_{s_0}^{s_f} \left(\delta P_i \frac{dq_i}{ds} - \delta q_i \frac{dP_i}{ds}\right) ds + P_i \delta q_i \Big|_{s_0}^{s_f}$$

$$\delta S_{abr}[\gamma] = \int_{s_0}^{s_f} ds \cdot \left(\delta p_i \frac{dq_i}{dt} - \delta q_i \frac{dp_i}{dt} \right) \frac{dt}{ds}$$

$$= \int_{s_0}^{s_f} ds \cdot \frac{dt}{ds} \left[\frac{\partial H}{\partial p_i} \delta p_i + \frac{\partial H}{\partial q_i} \delta q_i \right] = \int_{s_0}^{s_f} ds \frac{dt}{ds} \delta H = 0$$

Excerise:

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 trajacting 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 $\begin{cases} \dot{Q} = \frac{\partial H'}{\partial \mathbb{P}} \\ \dot{\mathbb{P}} = -\frac{\partial H'}{\partial Q} \end{cases}$

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

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

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

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

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

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

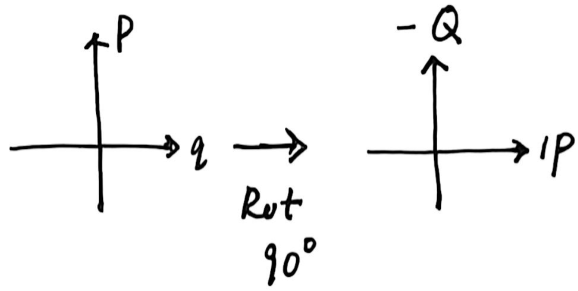
F as function of q, Q, t, $F(q, Q, t)$

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

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

$H' = H$



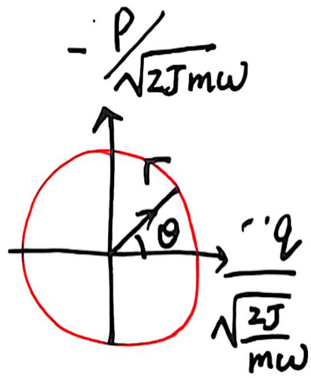
- Solution to harmonic oscillator

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

$= E/\omega$

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

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

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

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

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 $S_{abr}(q,J)$

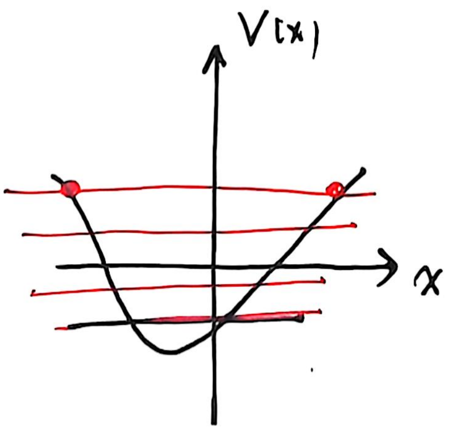
as the generation function

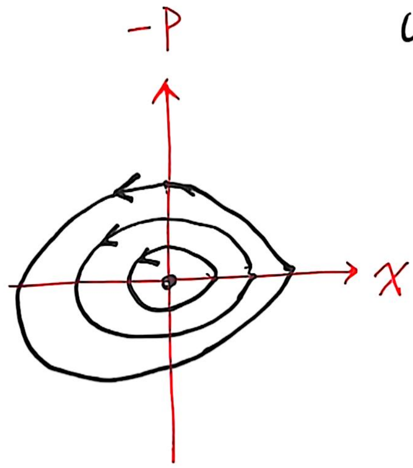
$$P = \left(\frac{\partial S_{abr}}{\partial q}\right)_J \quad \leftrightarrow \quad (P, q) \text{ conjugate}$$

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

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

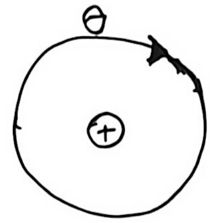
$$\boxed{\theta = \frac{dE}{dJ} \cdot t + \text{const} = \omega(J)\, t + \text{const}}$$





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

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

$$X_n(t) = \sum_{l=-\infty}^{\infty} X_n(l)\, e^{-il\omega_n t},$$

n is a certain mode of osci

l is an integer – order of harmonics

$X_n(l)$ is the harmonic component

$$X_n^2(t) = \sum_{ll'} X_n(l) X_n(l')\, e^{-i(l+l')\omega_n t}$$

$$= \sum_\beta \left(\sum_l X_n(l) X_n(\beta - l) \right) e^{-i\beta\omega_n t}$$

set $\beta = 0$

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

$$\Rightarrow P_l(n) \sim \frac{e^2}{c^3} (l\, \omega_n)^4 \, |X_n(l)|^2$$

$$P = \sum_{l=1}^{\infty} P_l(n)$$

Black-body radiation

Guided by the general principle of thermodynamics and experimental facts

① As $\omega \to 0$, Releigh-Jeans law

$u(\omega)d\omega$: EM energy density $\omega \to \omega + d\omega$

$u(\omega) \sim \omega^2 k_B T$ — equal partition

② Wien's law :

Maxwell: isotropic massless radiation $p = \frac{1}{3}u$

Stefan-Boltzmann: Start from $dU = TdS - pdV$

$$U = uV \Rightarrow \quad Tds = (u+p)dV + Vdu$$

$$ds = \frac{4u}{3T}dV + \frac{Vdu}{T} = \frac{4u}{3T}dV + \frac{V}{T}\frac{du}{dT}dT$$

$$\frac{\partial^2 S}{\partial V \partial T} = \frac{\partial^2 S}{\partial T \partial V} \Rightarrow \frac{\partial}{\partial V}\left(\frac{\partial S}{\partial T}\right)_V = \frac{\partial}{\partial V}\left(\frac{V}{T}\frac{du}{dT}\right) = \frac{1}{T}\frac{du}{dT}$$

$$\frac{\partial}{\partial T}\left(\frac{\partial S}{\partial V}\right)_T = \frac{\partial}{\partial T}\left(\frac{4u}{3T}\right) = \frac{4}{3}\left[\frac{1}{T}\frac{du}{dT} - \frac{u}{T^2}\right]$$

$$\Rightarrow \frac{du}{dT} = \frac{4u}{T} \Rightarrow \ln u = 4\ln T + \text{const} \Rightarrow \boxed{u = aT^4}$$

For adiabatic process

$$0 = Tds = d(uV) + pdV \Rightarrow du \cdot V + u\,dV + \frac{u}{3}\,dV = 0$$

$$\left.\begin{array}{l} \dfrac{du}{u} + \dfrac{4}{3}\dfrac{dV}{V} = 0 \\ u = aT^4 \end{array}\right\} \Rightarrow \frac{dT}{T} = -\frac{1}{3}\frac{dV}{V} \Rightarrow T \sim V^{-1/3}$$

$$\omega \sim L^{-1} \sim V^{-1/3}$$

$$\Rightarrow u(\omega) \sim V^{-1} f\left(\frac{\omega}{T}\right) \sim \left(\frac{\omega}{c}\right)^3 f\left(\frac{\omega}{T}\right)$$

If $f(\frac{\omega}{T}) = T/\omega$ → Releigh-Jeans law $\quad u(\omega) \propto k_B T$

" radiation gas" → $f(\frac{\omega}{T}) \sim e^{-\hbar\omega/k_BT}$ $\quad u(\omega) \propto e^{-\hbar\omega/k_BT}$

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

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

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

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

$$\Rightarrow \frac{\partial(\frac{1}{T})}{\partial u} = -\frac{k_B}{u^2}$$

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

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

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

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

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

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

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

$$1 + \frac{\hbar\omega}{u} = \text{const}\cdot e^{\hbar\omega/k_B T}$$

check $\hbar\omega \to 0 \Rightarrow$ const $= 1$, 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

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

$$\frac{\partial E}{\partial J} = \omega = \dot{\theta}$$

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

Einstein — Bohr

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

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

$$\boxed{\omega_{l\leftarrow n} = \omega_{m\leftarrow n} + \omega_{l\leftarrow m}}$$

③ Intensity correspondence (Bohr).

The radiation power $P_{n-l\leftarrow n} \longrightarrow P_l(n)$ in the limit $n \gg l$.

transition from $n \to n - l$

the l-th harmonics of the classic motion in the state n.

② Correspondence theorems

1. Correspondence between spectral and mechanical frequencies.

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

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

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

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

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

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

$$\hbar\,\omega_{m\leftarrow n} = E_n - E_m = E(n\hbar) - E(m\hbar) = \frac{\partial E}{\partial J}\Big|_{J=n\hbar} (n-m)\hbar$$

$$\boxed{\hbar\omega_{n-l\leftarrow n} = l\,\hbar \frac{\partial E}{\partial J}\Big|_{J=n\hbar} \to \boxed{}\; l\,\hbar\,\omega_n \qquad \text{define } \omega_n = \frac{\partial E}{\partial J}\Big|_{J=n\hbar}.}$$

2. Correspondence between transition probability and vibration amplitude

The transition rate $n \to n-l$ in the limit $n \to \infty$, it behaves

$$A_{n-l \leftarrow n} = \frac{e^2 (l\omega(n))^3}{3\hbar c^3} |X_n(l)|^2$$

$$\uparrow \quad X_n(t) = \sum_{l=-\infty}^{+\infty} X_n(l)\, e^{-il\omega_n t}$$

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

$$\ddot{x}_n(t) = \sum_l X_n(l)\,(-)(l\omega_n)^2\, e^{-il\omega_n t}$$

$$\overline{|\ddot{x}_n(t)|^2} = \sum_l |X_n(l)|^2 (l\omega_n)^4$$

$$\overline{P(t)} = \frac{4}{3}\frac{e^2}{c^3}\omega_n^4 \sum_{l=1}^{\infty} l^4 |X_n(l)|^2 = P(n)$$

$$P_l(n) = \frac{4}{3}\frac{e^2}{c^3}\omega_n^4\, l^4\, |X_n(l)|^2 \leftarrow (l\omega_n)^4 = \omega_{n-l,n}^4$$

$$\to \hbar\omega_{n-l\leftarrow n} A_{n-l\leftarrow n}$$

$$\Rightarrow \boxed{A_{n-l,n} = \frac{4}{3}\frac{e^2}{\hbar c^3}\omega_{n-l,n}^3 |X_n(l)|^2}$$