

# CH1 CANONICAL QUANTIZATION OF FREE FIELDS

## 1.1 Canonical quantization of the free E-M field

→ Using units where  $c=1=\epsilon_0$ , Maxwell's equations reads:

$$\begin{cases} \vec{\nabla} \cdot \vec{E} = \rho & (\text{Gauss}) & \vec{\nabla} \cdot \vec{B} = 0 \\ \vec{\nabla} \times \vec{E} + \partial_0 \vec{B} = 0 & & \vec{\nabla} \times \vec{B} - \partial_0 \vec{E} = \vec{j} \end{cases}$$

with  $\vec{E}(x^\mu)$  the electric field,  $\rho(x^\mu)$  the electric charge density  
 $\vec{B}(x^\mu)$  the magnetic field,  $\vec{j}(x^\mu)$  the electric current density.

PROP The continuity equation reads  $\partial_0 \rho + \vec{\nabla} \cdot \vec{j} = 0$

DEMO Indeed,  $\vec{\nabla} \cdot (\vec{\nabla} \times \vec{B} - \partial_0 \vec{E}) = -\partial_0 \vec{\nabla} \cdot \vec{E} = -\vec{\nabla} \cdot \vec{j}$

$$\Leftrightarrow -\partial_0 \rho = \vec{\nabla} \cdot \vec{j} \text{ where we used } \vec{\nabla} \cdot (\vec{\nabla} \times \vec{B}) = \partial_i \epsilon_{ijk} \partial_j B_k = -\partial_j \epsilon_{jik} \partial_i B_k$$

DEF We introduce the electric 4-vector  $j^\mu$  and the Maxwell tensor  $F^{\mu\nu}$ :

$$j^\mu = \begin{pmatrix} \rho \\ j^1 \\ j^2 \\ j^3 \end{pmatrix} \text{ and } F^{\mu\nu} = \begin{pmatrix} 0 & E^1 & E^2 & E^3 \\ -E^1 & 0 & B^3 & -B^2 \\ -E^2 & -B^3 & 0 & B^1 \\ -E^3 & B^2 & -B^1 & 0 \end{pmatrix}$$

→ Notice  $F^{\mu\nu} = -F^{\nu\mu} \Leftrightarrow F^{\mu\nu} = -F^{\nu\mu}$

PROP The Maxwell eq. are now manifestly Lorentz covariant:

$$\partial_\nu F^{\mu\nu} = j^\mu \quad (1) \text{ and } \epsilon^{\mu\nu\lambda\sigma} \partial_\nu F_{\lambda\sigma} = 0 \Leftrightarrow \partial_{[\nu} F_{\lambda\sigma]} = 0 \quad (2)$$

DEMO Indeed,  $F_{0i} = E^i$ ,  $F_{ij} = \epsilon_{ijk} B^k$

①:  $\partial_i F^{0i} = j^0 \Leftrightarrow \partial_i E^i = \rho$  and with  $\mu=i$ ,  $\nu \neq i$  we get

$$\partial_\nu F^{i\nu} = \partial_0 F^{i0} + \partial_j F^{ij} = -\partial_0 E^i + \partial_j \epsilon^{ijk} B_k = j^i$$

② For  $\mu=0$ ,  $0 = \epsilon^{ijk} \partial_i F_{jk} = \epsilon^{ijk} \partial_i (\epsilon_{jkl} B^l) = 2 \delta_0^i \partial_i B^l = \partial_l B^l$

$$\text{Now, for } \mu=i: 0 = \epsilon^{ijk} \partial_0 F_{jk} + \epsilon^{ij0k} \partial_j F_{0k} + \epsilon^{ij0k} \partial_k F_{j0}$$

$$= \epsilon^{ijk} (-\partial_0 F_{jk} + \partial_j F_{0k} - \partial_k F_{j0}) = \epsilon^{ijk} (-\partial_0 \epsilon_{jkl} B^l - 2 \partial_j E_k)$$

$$= -2(-\partial_0 \delta_0^i B^l - \epsilon^{ijk} \partial_j E_k)$$

PROP The continuity eq. in its invariant form is  $\partial_\mu j^\mu = 0$

## PROP (Helmoltz decomposition)

On  $\mathbb{R}^3$  with suitable fall-off conditions, every vector field  $\vec{v}$  admits a unique decomposition into a longitudinal and a transverse part:  $\vec{v} = \vec{\nabla}\psi + \vec{\nabla} \times \vec{u}$

**DEMO** We consider a field  $\vec{v}$  such that  $v \sim 1/r$  when  $r \rightarrow \infty$ . Then the Laplacian  $\Delta$  is invertible.

$$\rightarrow (\vec{\nabla} \times (\vec{\nabla} \times \vec{v}))_i = \epsilon_{ijk} \partial_j \epsilon_{klm} \partial_l v_m = (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \partial_j \partial_l v_m \\ = \partial_m \partial_i v_m - \partial_l \partial_l v_i = \vec{\nabla}(\vec{\nabla} \cdot \vec{v}) - \Delta \vec{v}$$

$$\rightarrow \Delta \vec{v} = \vec{\nabla}(\vec{\nabla} \cdot \vec{v}) - \vec{\nabla} \times (\vec{\nabla} \times \vec{v}) \Leftrightarrow \vec{v} = \vec{\nabla} \Delta^{-1}(\vec{\nabla} \cdot \vec{v}) - \vec{\nabla} \times \Delta^{-1}(\vec{\nabla} \times \vec{v}) \quad \square$$

$\hookrightarrow$  Explicitly,  $\psi = \Delta^{-1}(\vec{\nabla} \cdot \vec{v})$  and  $\vec{u} = -\Delta^{-1}(\vec{\nabla} \times \vec{v})$

$\rightarrow$  For  $\vec{v}$  such that  $\vec{\nabla} \cdot \vec{v} = 0$ , we have  $\vec{v} = \vec{\nabla} \times \vec{u}$   
For  $\vec{v}$  such that  $\vec{\nabla} \times \vec{v} = 0$ , we have  $\vec{v} = \vec{\nabla} \psi$

$\rightarrow$  We can build  $\Delta^{-1}$  explicitly using Green function, namely solving  $\Delta \phi(\vec{x}) = -\delta^{(3)}(\vec{x} - \vec{y}) \Leftrightarrow \phi(\vec{x}) = \frac{1}{4\pi} \frac{1}{|\vec{x} - \vec{y}|}$  so that if

$$\Delta \phi(x) = j(x), \quad \phi(\vec{x}) = \frac{-1}{4\pi} \int d^3y \frac{j(y)}{|\vec{x} - \vec{y}|} \sim \Delta^{-1} j(\vec{x})$$

$\rightarrow$  Since  $\vec{\nabla} \cdot \vec{B} = 0$ , we can write  $\vec{B} = \vec{\nabla} \times \vec{A}$  with  $\vec{A}$  a vector potential. Using  $\vec{\nabla} \times \vec{E} + \partial_0 \vec{B} = 0$ :  $\vec{\nabla} \times (\vec{E} + \partial_0 \vec{A}) = 0 \Leftrightarrow \vec{E} = -\partial_0 \vec{A} - \vec{\nabla} \phi$  for some  $\phi$ , a scalar potential.

$\hookrightarrow \phi$  and  $\vec{A}$  are not uniquely defined. Let's consider  $\phi', \vec{A}'$  such that  $\vec{B} = \vec{\nabla} \times \vec{A}'$  and  $\vec{E} = -\partial_0 \vec{A}' - \vec{\nabla} \phi' \Rightarrow \vec{\nabla} \times (\vec{A}' - \vec{A}) = 0$

$\Rightarrow \vec{A}' = \vec{A} + \vec{\nabla} \chi$  and from  $0 = \vec{\nabla}(\partial_0 \chi + \phi' - \phi)$ , we see that  $\phi' = \phi - \partial_0 \chi + f(t)$  such that  $\lim_{r \rightarrow \infty} f(t) = 0 \Leftrightarrow f(t) = 0 \forall r$

**DEF** Defining  $A_\mu = (-\phi, A_1, A_2, A_3)$ , we get  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ , and the gauge transformations of  $A_\mu$  read:  
 $A'_\mu = A_\mu + \partial_\mu \chi$

$\rightarrow$  The 2 quantization methods (canonical and path integral) require an action or a hamiltonian. We rewrite Maxwell eq. such that it comes from a variational principle.

DEF

The Maxwell action reads

$$S[A_\mu; j^\mu] \equiv \int d^4x \left\{ \frac{-1}{4} F_{\mu\nu} F^{\mu\nu} + j^\mu A_\mu \right\}$$

→ Its variation reads

$$\delta S \sim \frac{-1}{2} (\delta F_{\mu\nu}) F^{\mu\nu} + \delta A_\mu \cdot j^\mu$$

$$\sim \partial_\nu \delta A_\mu F^{\mu\nu} + \delta A_\mu \cdot j^\mu \sim (-\partial_\nu F^{\mu\nu} + j^\mu) \delta A_\mu \stackrel{!}{=} 0 \Leftrightarrow \partial_\nu F^{\mu\nu} = j^\mu$$

### ⊙ Hamiltonian formulation of EM

→ To go to the hamiltonian formalism, we need to compute the conjugate momenta  $p_i \equiv \frac{\partial L}{\partial \dot{q}^i} \Leftrightarrow \pi_\mu \equiv \frac{\partial L}{\partial \dot{A}_\mu}$

$$\text{We write } S = \int dt \int d^3x \left\{ \frac{-1}{2} F_{0i} F^{0i} - \frac{1}{4} F_{ij} F^{ij} + A_\mu j^\mu \right\} \quad \epsilon_{ijk} \epsilon^{ijl} = 2\delta_k^l$$

$$= \int dt \int d^3x \left\{ \frac{1}{2} \partial_0 A_i \partial_0 A^i - \frac{1}{2} B_i B^i + A_i j^i + A_0 j^0 + A_0 \partial_0 \partial_i A^i - \frac{1}{2} A_0 \Delta A_0 \right\}$$

↳ The conjugate momentum  $\frac{\partial L}{\partial [\partial_0 A_0]} = 0$  doesn't appear in the action!

We cannot perform a Legendre transform. But since

$$S \sim \int A_0 (\partial_0 \partial_i A^i + j^0 - \frac{1}{2} \Delta A_0), \text{ imposing } \delta_0 S \stackrel{!}{=} 0 \Rightarrow A_0 = \frac{1}{\Delta} (\partial_0 \partial_i A^i + j^0)$$

↳ The EOM for  $A_0$  can be solved algebraically for  $A_0$  without invoking initial conditions  $\Rightarrow$  we can inject the solution in the action.

This gives to a reduced action principle. The reduced action reads:

$$S = \int d^4x \left\{ \frac{1}{2} \partial_0 A^i \partial_0 A_i + \frac{1}{2} \frac{1}{\Delta} (\partial_0 \partial_i A^i + j^0) (\partial_0 \partial_k A^k + j^0) - \frac{1}{2} B_i B^i + A_i j^i \right\} \\ = S[A^i; j^\mu]$$

→ Using Helmholtz decomposition, we write for  $A_i$ :

$$\vec{A} = \vec{\nabla} \varphi + \vec{\nabla} \times \vec{\omega} \equiv \vec{\nabla} \varphi + \vec{\nabla} \perp \vec{\omega} \text{ with } \vec{\nabla} \cdot \vec{\omega} \perp = 0 \text{ and } \varphi \equiv \Delta^{-1} (\vec{\nabla} \cdot \vec{A})$$

$$A_i = \partial_i (\Delta^{-1} \partial_j A^j) + A_i^\perp \text{ such that } \vec{\nabla} \cdot \vec{A}^\perp = 0$$

→ We also have that  $\vec{B} = \vec{\nabla} \times \vec{A} = \vec{\nabla} \times \vec{A}^\perp$

→ We also have that  $\int d^3x \, q^i \omega_i = \int d^3x \, (q^{i\perp} \omega_i^\perp + q^{i\parallel} \omega_i^\parallel)$

$$\text{with } q^{i\parallel} \equiv q^{i\perp} + q^{i\perp}$$



→ The reduced action becomes

$$S = \int d^4x \left\{ \frac{1}{2} \partial_0 A_i^\perp \partial_0 A_i^\perp - \frac{1}{2} B^i B_i + \frac{1}{2} f^0 \Delta f^0 + A_i^\perp f_i^\perp \right\} \quad \text{with } B^i = B^i(A_i^\perp)$$

→ Computing  $\frac{\delta L}{\delta A_i^\perp} = 0$ , we get  $\partial_0^2 \vec{A}_\perp = -\vec{\nabla} \times (\vec{\nabla} \times \vec{A}_\perp) + \vec{f}_\perp$   
 $\partial_0^2 \vec{A}_\perp = \Delta \vec{A}_\perp + \vec{f}_\perp$

↳ We can now write the conjugate momenta to  $A_i^\perp$ :

$$\pi_i^\perp(\vec{x}, t) = \frac{\delta L}{\delta \partial_0 A_i^\perp(\vec{x}, t)} = \partial_0 A_i^\perp(t, \vec{x})$$

→ The above formulation doesn't depend on  $A_0 = -\phi$  nor  $\vec{A}_\parallel$ , we are in the Coulomb gauge. We're left with the physical dof only.

DEF | Eliminate the non physical dof from a system before quantifying it is called reduction before quantization.

→ The hamiltonian now reads:

$$H = \int d^3x \left\{ \frac{1}{2} \pi_i^\perp \pi_i^\perp + \frac{1}{2} B^i B_i - \frac{1}{2} f^0 \Delta f^0 - A_i^\perp f_i^\perp \right\}$$

Since  $\vec{E} = -\partial_0 \vec{A} + \vec{\nabla} A_0$ ,  $\vec{E}_\parallel = -\vec{\nabla}_\parallel A_0$  and  $\vec{E}_\perp = \vec{\nabla} \times \vec{A}_\perp$ , we can rewrite

$$H = \int d^3x \left\{ \frac{1}{2} (\vec{E}^\perp \vec{E}_\perp + B^i B_i) - A_i^\perp f_i^\perp \right\}$$

## ② Electromagnetic radiation in a box:

→ We obtained wave equations:  $\begin{cases} \dot{A}_i^\perp = \pi_i^\perp \\ \dot{\pi}_i^\perp = \Delta A_i^\perp \end{cases}$

Indeed, if  $f^\mu = 0$ , the E-M theory reduces on the classical level to the free wave eq. for  $\vec{A}_\perp$ . To see it, we compute

$$\delta H = \int d^3x \left\{ \delta \pi_i^\perp \cdot \pi_i^\perp - \delta A_i^\perp (\Delta A_i^\perp - \partial_0^2 (\vec{\nabla} \cdot \vec{A}_\perp)) \right\}$$

so that the Hamiltonian BOM are

$$\dot{A}_i^\perp = \{A_i^\perp, H\} = \frac{\delta H}{\delta \pi_i^\perp} = \pi_i^\perp \quad \text{and} \quad \dot{\pi}_i^\perp = \{\pi_i^\perp, H\} = -\frac{\delta H}{\delta A_i^\perp} = \Delta A_i^\perp$$

Then,  $\ddot{\pi}_i^\perp = \ddot{A}_i^\perp = \Delta A_i^\perp \Leftrightarrow \partial_\mu \partial^\mu A_i^\perp = 0$

→ In a box of size of length  $L$  with periodic boundary conditions, we can write  $A_i(x)$  in a Fourier space:

$$A_i(x) = \bar{A}_i(t) + \sum_{\vec{k} \neq 0} \sqrt{\frac{\hbar}{2\omega L^3}} \tilde{A}_i(\vec{k}, t) e^{i\vec{k} \cdot \vec{x}}$$

with  $k^i = \frac{2\pi n^i}{L}$ ,  $n^i \in \mathbb{Z}$ ,  $\omega(k) = \sqrt{k^2} = |k|$  and the factor  $\sqrt{\hbar/2\omega L^3}$  is chosen for convenience.

→ by going in Fourier space, resolving the wave equation becomes simple.

→ The general solution follows from  $(\partial_t^2 + \omega^2) \tilde{A}_i(\vec{k}, t) = 0$

$\Rightarrow \tilde{A}_i(\vec{k}, t) = c_i(\vec{k}) e^{-i\omega t} + c_i^*(\vec{k}) e^{i\omega t}$ ,  $c_i(\vec{k}) \in \mathbb{C}$  and  $\bar{A}_i(t) = \bar{A}_i + \bar{\pi}_i t$  with  $\bar{A}_i, \bar{\pi}_i \in \mathbb{R}$ . In what follow, we discard the 0-mode:  $\bar{A}_i = \bar{\pi}_i = 0$

→ Since  $A_i^T$  must be transverse,  $\vec{\nabla} \cdot \vec{A}_\perp = 0 \Rightarrow k_i \tilde{A}_i(\vec{k}, t) = 0$

DEF We introduce polarization vectors  $\vec{e}^m(k)$  such that  $e_i^3 = \frac{|k|}{|k|}$  and  $k_i e_i^{1,2} = 0$ . They furnish an orthonormal frame:  $\sum_m e_i^m e_j^m = \delta_{ij}$

→ We can then write  $c_i(\vec{k}) = a_1(\vec{k}) e_i^1(\vec{k}) + a_2(\vec{k}) e_i^2(\vec{k}) = a_s(\vec{k}) e_i^s(\vec{k})$   
 $\hookrightarrow$  2 dof corresponding to the 2 Fourier coeff.

→ Explicitly, we could pick:

$$\vec{e}^1 = \frac{1}{k_\perp} (k_2, -k_1, 0); \vec{e}^2 = \frac{1}{k k_\perp} (k_1, k_2, k k_3, -k_\perp^2) \text{ with } k_\perp = \sqrt{k_1^2 + k_2^2}$$

→ Discarding the 0-mode (subdominant in the calculation of the partition function), the general solution (with transverse condition) becomes:

$$A_i(x) = \sum_{\vec{k} \neq 0} \sqrt{\frac{\hbar}{2\omega(k)V}} \left( a_s(\vec{k}) e_i^s(\vec{k}) e^{ikx} + a_s^*(\vec{k}) e_i^s(\vec{k}) e^{-ikx} \right)$$

$$\text{with } kx = k_\mu x^\mu = -\omega t + \vec{k} \cdot \vec{x}$$

→ In the box, the hamiltonian reduces to:

$$H(t) = \frac{1}{2} \int_{\text{box}} d^3x \left( E_i^\perp(\vec{x}) E_i^\perp(\vec{x}) + B_i(\vec{x}) B_i(\vec{x}) \right)$$

$\hookrightarrow$  We need to compute  $E_i^\perp = -\partial_0 A_i^\perp$  and  $\vec{B} = \vec{\nabla} \times \vec{A}$

$$\rightarrow E_i^{\perp} = -\partial_0 A_i^{\perp} = i \sum_{\mathbf{k} \neq 0} \sqrt{\frac{\hbar}{2\omega V}} \left( \omega(\mathbf{k}) a_s(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} e^{i\mathbf{k} \cdot \mathbf{x}} - \omega a_s^* e^{i\mathbf{k} \cdot \mathbf{x}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

$$\rightarrow B^i(\mathbf{x}) = i \sum_{\mathbf{k} \neq 0} \sqrt{\frac{\hbar}{2\omega V}} \left( \epsilon^{ijk} k_j a_s(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} e^{i\mathbf{k} \cdot \mathbf{x}} - \epsilon^{ijk} k_j a_s^* e^{i\mathbf{k} \cdot \mathbf{x}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

Prop Using  $\int_{\text{box}} d^3x \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{x}] = V \delta^3(\mathbf{k}-\mathbf{k}')$ , one gets

$$H = \sum_{\mathbf{k} \neq 0} \hbar \omega a_s^*(\mathbf{k}) a_s(\mathbf{k})$$

→ The hamiltonian becomes a superposition of harmonic oscillators, degenerated in  $s=1,2$ , the transverse polarisations.

→ By defining  $a_s(\mathbf{k}, t) = a_s(\mathbf{k}) e^{-i\omega t}$ , we get  $\dot{a}_s(\mathbf{k}, t) = -i\omega a_s(\mathbf{k}, t)$  and  $\frac{d}{dt} a_s(\mathbf{k}, t) = \{a_s(\mathbf{k}, t), H\}$  only if we have the

following Poisson brackets:

$$\{a_s(\mathbf{k}), a_{s'}^*(\mathbf{k}')\} = -\frac{i}{\hbar} \delta_{\mathbf{k}, \mathbf{k}'} \delta_{s, s'} \text{ and } \{a_s(\mathbf{k}), a_{s'}(\mathbf{k}')\} = 0$$

$$\{a_s^*(\mathbf{k}), a_{s'}^*(\mathbf{k}')\} = 0$$

↳ This is equivalent to  $\{A_i^{\perp}(\mathbf{x}), \pi_j^{\perp}(\mathbf{y})\} = \delta_{ij}^{\perp} \delta_{\mathbf{x}, \mathbf{y}}$

## ⊙ A digression on the harmonic oscillator:

→ Consider a collection of  $n$  decoupled harmonic oscillators with frequencies  $\omega_a$ ,  $a=1, \dots, n$ .

→ The associated lagrangian is  $L = \frac{1}{2} \dot{q}^a \dot{q}_a - \frac{1}{2} \omega_{ab}^2 q^a q^b$  with  $\omega_{ab}^2 \equiv \omega_{(a)}^2 \delta_{ab}$

→ Canonical momenta are  $\partial L / \partial \dot{q}^a = \dot{q}_a \equiv p_a$  and the hamiltonian is  $H = \frac{1}{2} p_a p^a + \frac{1}{2} \omega_{ab}^2 q^a q^b$

→ The Poisson brackets are canonical:  $\{q^a, p_b\} = \delta^a_b$ ,  $\{q^a, q^b\} = 0 = \{p_a, p_b\}$

→ We perform a change of variables:

$$\hat{a}_a \equiv \frac{\sqrt{\omega_a}}{\sqrt{2\hbar}} \hat{q}^a + i \frac{\hat{p}_a}{\sqrt{2\hbar \omega_a}} ; \hat{a}_a^* = \frac{\sqrt{\omega_a}}{\sqrt{2\hbar}} \hat{q}_a - i \frac{\hat{p}_a}{\sqrt{2\hbar \omega_a}}$$

Inverting, we get:

$$\hat{q}^a = \sqrt{\frac{\hbar}{2\omega_a}} (\hat{a}_a + \hat{a}_a^*) \text{ and } \hat{p}_a = -i \sqrt{\frac{\hbar \omega_a}{2}} (\hat{a}_a - \hat{a}_a^*)$$



→ The canonical commutation relations become:  
 $[\hat{a}^a, \hat{a}^{+b}] = \delta^{ab}$  and  $[\hat{a}^a, \hat{a}^b] = 0 = [\hat{a}^{+a}, \hat{a}^{+b}]$   
 and the hamiltonian is given by:  
 $H = \hbar \omega_{ab} (\hat{a}^{+a} \hat{a}^b + \frac{1}{2} \delta^{ab})$

→ We used the quantization rule: for  $A(q, p), B(q, p)$  two function on the phase space with Poisson bracket  $\{A, B\}$ , their equivalent quantum operator follows the following commutation relation:  
 $[A, B] = i\hbar \{A, B\} + \mathcal{O}(\hbar^2)$

↳ The time evolution is given by  $\dot{f} = \{f, H\}$  for any  $f = f(q, p)$ .

### ③ Hilbert space:

→ For 1 HO, a complete set of orthonormal states is given by  
 $|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle$ , with  $\langle m | n \rangle = \delta_{mn}$

→ For  $n$  HO, the Hilbert space  $\mathcal{H}$  is the Fock space generated by the creation operators  $\hat{a}_s^+(k)$  for each mode  $k, s$ :

$$\mathcal{H} = \bigotimes_{k,s} \mathcal{H}_{k,s} \text{ with } |n_{k,s}\rangle \equiv \frac{(\hat{a}_s^+(k))^{n_{k,s}}}{\sqrt{n_{k,s}}} |0\rangle \in \mathcal{H}_{k,s}$$

↳ The hamiltonian operator in the normal ordered form is given by  
 $\hat{H} = \sum_{k,s} \hbar \omega(k) \hat{a}_{(s)}^+(k) \hat{a}_{(s)}(k)$  (dropped the 1/2)

# 1.2 Partition function and Thermodynamics

DEF] The partition function  $Z$  is defined as  
 $Z \equiv \text{Tr} \{ \exp \{ -\beta \hat{H} \} \}$  where  $\beta = (k_B T)^{-1}$

→ For a sum of non interacting HO, the partition function factorizes:

$$Z = \text{Tr} e^{-\beta \hat{H}} = \prod_{\mathbf{k}, s} \sum_{n_{\mathbf{k}, s}} \langle n_{\mathbf{k}, s} | e^{-\beta \hat{H}_{\mathbf{k}, s}} | n_{\mathbf{k}, s} \rangle$$

$$= \prod_{\mathbf{k}, s} \sum_{n_{\mathbf{k}, s}} \exp \{ -\beta \hbar \omega_{\mathbf{k}, s} n_{\mathbf{k}, s} \}$$

$$\sum_{n=0}^{\infty} c^n = (1-c)^{-1}$$

$$= \prod_{\mathbf{k}, s} (1 - e^{-\beta \hbar \omega_{\mathbf{k}, s}})^{-1}$$

$$\rightarrow \text{We get } \ln Z = - \sum_{\mathbf{k}, s} \ln(1 - e^{-\beta \hbar \omega_{\mathbf{k}, s}}) = -2 \sum_{\mathbf{k}} \ln(1 - e^{-\beta \hbar \omega_{\mathbf{k}}})$$

→ Using the Euler-Maclaurin formula:  $\sum_{n \in \mathbb{Z}} \rightarrow \int_{-\infty}^{\infty} dn = \frac{L}{2\pi} \int_{-\infty}^{\infty} dk$  with  $k = \frac{2\pi n}{L}$   
 and taking  $V \rightarrow \infty$ , we get:

$$\ln Z = -2 \cdot \left( \frac{L}{2\pi} \right)^3 \int d^3 k \ln(1 - e^{-\beta \hbar k})$$

$$= -2 \cdot \frac{V}{(2\pi)^3} \cdot 4\pi \int_0^{\infty} dk \cdot k^2 \cdot \ln(1 - e^{-\beta \hbar k})$$

$$k \mapsto x/\beta \hbar$$

$$e^{-\beta \hbar k} \mapsto e^{-x}$$

$$= -\frac{V}{\pi^2} \cdot \frac{1}{\beta \hbar} \cdot \frac{1}{(\beta \hbar)^2} \int_0^{\infty} dx \cdot x^2 \cdot \ln(1 - e^{-x})$$

$$x^2 = f'; \ln(1 - e^{-x}) = g$$

$$\text{and } \int f'g = [fg] - \int fg'$$

$$= -\frac{\beta^{-3} V}{\hbar^3 \pi^2} \cdot (-1) \cdot \int_0^{\infty} dx \cdot \frac{x^3}{3} \cdot \frac{1}{1 - e^{-x}}$$

$$= \frac{\beta^{-3} V}{3 \hbar^3 \pi^2} \int_0^{\infty} \frac{x^3}{e^x - 1} = \frac{\beta^{-3} V}{3 \hbar^3 \pi^2} \cdot \Gamma(4) \cdot \zeta(4)$$

$$\Gamma(4) = 3!; \zeta(4) = \pi^4/90$$

We get:

$$\ln Z = \frac{\beta^{-3} V \pi^2}{45 \hbar^3} = \frac{b}{3} \cdot V \cdot \beta^{-3}$$

$$\rightarrow U = \langle H \rangle = -\partial_{\beta} \ln Z = b V \beta^{-4} \Leftrightarrow \beta = (U/bV)^{-1/4}$$