

# A few words on connected diagrams, size-extensivity, and all that...

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# Structure behind this mess?

$$\mathbf{E}_n^{(1)} = V_{nn}$$

$$\mathbf{E}_n^{(2)} = \frac{|V_{nk_2}|^2}{E_{nk_2}}$$

$$\mathbf{E}_n^{(3)} = \frac{V_{nk_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3}} - V_{nn} \frac{|V_{nk_3}|^2}{E_{nk_3}^2}$$

$$\mathbf{E}_n^{(4)} = \frac{V_{nk_4} V_{k_4 k_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3} E_{nk_4}} - \frac{|V_{nk_4}|^2}{E_{nk_4}^2} \frac{|V_{nk_2}|^2}{E_{nk_2}} - V_{nn} \frac{V_{nk_4} V_{k_4 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_4}} - V_{nn} \frac{V_{nk_4} V_{k_4 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_4}^2} + V_{nn}^2 \frac{|V_{nk_4}|^2}{E_{nk_4}^3}$$

$$= \frac{V_{nk_4} V_{k_4 k_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3} E_{nk_4}} - E_n^{(2)} \frac{|V_{nk_4}|^2}{E_{nk_4}^2} - 2V_{nn} \frac{V_{nk_4} V_{k_4 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_4}} + V_{nn}^2 \frac{|V_{nk_4}|^2}{E_{nk_4}^3}$$

$$\mathbf{E}_n^{(5)} = \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3} E_{nk_4} E_{nk_5}} - \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 n} |V_{nk_2}|^2}{E_{nk_4}^2 E_{nk_5} E_{nk_2}}$$

$$- \frac{V_{nk_5} V_{k_5 k_2} V_{k_2 n} |V_{nk_2}|^2}{E_{nk_2} E_{nk_5}^2 E_{nk_2}} - \frac{|V_{nk_5}|^2}{E_{nk_5}^2} \frac{V_{nk_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3}}$$

$$- V_{nn} \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_4} E_{nk_5}} - V_{nn} \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_4}^2 E_{nk_5}} - V_{nn} \frac{V_{nk_5} V_{k_5 k_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3} E_{nk_5}^2} + V_{nn} \frac{|V_{nk_5}|^2}{E_{nk_5}^2} \frac{|V_{nk_3}|^2}{E_{nk_3}^2} +$$

$$2V_{nn} \frac{|V_{nk_5}|^2}{E_{nk_5}^3} \frac{|V_{nk_2}|^2}{E_{nk_2}} + V_{nn}^2 \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 n}}{E_{nk_4}^3 E_{nk_5}} + V_{nn}^2 \frac{V_{nk_5} V_{k_5 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_5}^2} + V_{nn}^2 \frac{V_{nk_5} V_{k_5 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_5}^3} - V_{nn}^3 \frac{|V_{nk_5}|^2}{E_{nk_5}^4}$$

$$\begin{aligned}
\mathbf{E}_n^{(5)} = & \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3} E_{nk_4} E_{nk_5}} - 2E_n^{(2)} \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 n}}{E_{nk_4}^2 E_{nk_5}} - \frac{|V_{nk_5}|^2}{E_{nk_5}^2} \frac{V_{nk_3} V_{k_3 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_3}} \\
& - 2V_{nn} \left( \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_4} E_{nk_5}} - \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 k_2} V_{k_2 n}}{E_{nk_2} E_{nk_4}^2 E_{nk_5}} + \frac{|V_{nk_5}|^2}{E_{nk_5}^2} \frac{|V_{nk_3}|^2}{E_{nk_3}^2} + 2E_n^{(2)} \frac{|V_{nk_5}|^2}{E_{nk_5}^3} \right) \\
& + V_{nn}^2 \left( 2 \frac{V_{nk_5} V_{k_5 k_4} V_{k_4 n}}{E_{nk_4}^3 E_{nk_5}} + \frac{V_{nk_5} V_{k_5 k_3} V_{k_3 n}}{E_{nk_3}^2 E_{nk_5}^2} \right) - V_{nn}^3 \frac{|V_{nk_5}|^2}{E_{nk_5}^4}
\end{aligned}$$

## Very general and vague statements...

In virtually all fundamental theories of interacting particles and fields, physical properties can be expressed using

- The definition of a configuration space consisting of all possible configurations  $C$  for the system
- The definition of a "probability" for a given state

$$\pi(C) \sim e^{-\int \mathcal{H}/\mathcal{L}} \quad (1)$$

where  $\mathcal{H}$  = Hamiltonian,  $\mathcal{L}$  = Lagrangian.

Properties expressed as

$$\bar{Q} = \langle Q \rangle_{\pi}$$

- Classical statistical physics:  $\mathcal{C} = (x, v) \quad \pi(\mathcal{C}) \sim e^{-\beta E(\mathcal{C})}$
- Quantum statistical physics:  $\mathcal{C} = \text{path} = x(t) \quad \pi(\mathcal{C}) \sim e^{-\int_0^\beta dt \mathcal{H}(x(t))}$
- Quantum mechanics in real time:  $\mathcal{C} = \text{path} = x(t) \quad \pi(\mathcal{C}) \sim e^{-\int_0^\beta dt \mathcal{L}(x(t))}$
- Quantum mechanics in imaginary time ( $t \rightarrow it$ , QMC):  
 $\mathcal{C} = \text{path} = x(t) \quad \pi(\mathcal{C}) \sim e^{-\int_0^\beta dt \mathcal{H}(x(t))}$
- Quantum Field Theory:  $\mathcal{C} = \text{field} = \phi(x, t) \quad \pi(\mathcal{C}) \sim e^{-\int dx dt \mathcal{H} / \mathcal{L}(\phi)}$

Let us call  $Z$  the normalization of the probability

$$\pi(\mathcal{C}) = \frac{e^{-\int \mathcal{H}/\mathcal{L}}}{Z}$$

$$Z = \int_{\text{all } \mathcal{C}} e^{-\int \mathcal{H}/\mathcal{L}}$$

In all these theories the ground-state energy can be written as the logarithm of the normalization

$$E_0 \sim \ln Z = \ln \langle e^{-\int \mathcal{H}/\mathcal{L}} \rangle \quad (2)$$

that **the logarithm of an average of an exponential function**

This is this property which is **at the root of the "connected structure" of all these theories**

# Let us see how it works in quantum mechanics

Let us define some reference Hamiltonian  $H_0$  so that

$$H_0 \Phi_i^{(0)} = E_i^{(0)} \Phi_i^{(0)}$$

and

$$H = H_0 + \lambda V$$

with

$$H \Phi_i = E_i \Phi_i$$

All exact eigenstates are taken normalized here. The ground-state energy can be written as

$$E_0 = \lim_{t \rightarrow +\infty} -\frac{1}{t} \ln \langle \Phi_0^{(0)} | e^{-tH} | \Phi_0^{(0)} \rangle$$



This property results from

$$e^{-tH}|\Phi_0^{(0)}\rangle = \sum_i e^{-tE_i} \langle \Phi_i | \Phi_0^{(0)} \rangle |\Phi_i\rangle$$

with  $E_0 \leq E_1 \leq E_2 \leq \dots$  and then

$$\langle \Phi_0^{(0)} | e^{-tH} | \Phi_0^{(0)} \rangle \sim_{t \rightarrow +\infty} e^{-tE_0} \langle \Phi_0 | \Phi_0^{(0)} \rangle^2 + O(e^{-t(E_1-E_0)})$$

## Path integral formalism of quantum mechanics

$$\langle \Phi_0^{(0)} | e^{-tH} \Phi_0^{(0)} \rangle = \langle \Phi_0^{(0)} | e^{-\tau(H_0 + \lambda V)} e^{-\tau(H_0 + \lambda V)} \dots e^{-\tau(H_0 + \lambda V)} | \Phi_0^{(0)} \rangle$$

where  $\tau = t/N$ . Now, we use the following decomposition

$$\langle x | e^{-\tau(H_0 + \lambda V)} | x' \rangle = \langle x | e^{-\tau H_0} | x' \rangle e^{-\tau \lambda V(x)} \delta(x - x')$$

which is **exact** in the  $\tau = 0$ -limit. So that

$$\langle \Phi_0^{(0)} | e^{-tH} | \Phi_0^{(0)} \rangle = \lim_{N \rightarrow +\infty} \int dx_0 \dots dx_{N-1} \langle \Phi_0^{(0)} | e^{-\tau H_0} | x_1 \rangle \langle x_1 | e^{-\tau H_0} | x_2 \rangle \dots \langle x_{N-1} | e^{-\tau H_0} | \Phi_0^{(0)} \rangle e^{-\lambda \tau \sum_{i=1}^N V(x_i)}$$

We define the density of probability

$$\pi(x_1, \dots, x_{N-1}) = \langle \Phi_0^{(0)} | e^{-\tau(H_0 - E_0^{(0)})} | x_1 \rangle \prod_{i=1}^{N-2} \langle x_i | e^{-\tau(H_0 - E_0^{(0)})} | x_{i+1} \rangle \langle x_{N-1} | e^{-\tau(H_0 - E_0^{(0)})} | \Phi_0^{(0)} \rangle$$

We have

$$\pi \geq 0$$

and

$$\int dx_1 \dots dx_{N-1} \pi(x_1, \dots, x_{N-1}) = \langle \Phi_0^{(0)} | e^{-t(H_0 - E_0^{(0)})} | \Phi_0^{(0)} \rangle = 1$$

So

$$E_0 = \lim_{t \rightarrow +\infty} -\frac{1}{t} \ln \left[ e^{-tE_0^{(0)}} \langle e^{-\lambda \int_0^t V[x(t)]} \rangle_{\pi} \right]$$

and we have the **exact equality** expressing the energy as the log of the average of an exponential

$$E_0 = E_0^{(0)} - \lim_{t \rightarrow +\infty} -\frac{1}{t} \ln \langle e^{-\lambda \int_0^t V[x(t)]} \rangle_{\pi} \quad (3)$$

Let us decompose the exponential

$$\begin{aligned}
 E_0 &\sim \ln \left\langle \sum_{n=0}^{\infty} \frac{(-\lambda)^n}{n!} \int_0^t dt_1 \dots \int_0^t dt_n V[x(t_1)] \dots V[x(t_n)] \right\rangle_{\pi} \\
 &\sim \ln \left[ 1 - \frac{\lambda}{1!} \int_0^t d1 \langle V_1 \rangle + \frac{\lambda^2}{2!} \int_0^t \int_0^t d1 d2 \langle V_1 V_2 \rangle + \dots \right] \\
 &\sim \ln \left[ 1 - \lambda \int_0^t d1 \langle V_1 \rangle + \lambda^2 \int_0^t \int_{t_1}^t d1 d2 \langle V_1 V_2 \rangle + \lambda^3 \int_0^t \int_{t_1}^t \int_{t_2}^t d1 d2 d3 \langle V_1 V_2 V_3 \rangle \dots \right]
 \end{aligned}$$

Denoting

$$R(t) = e^{-t(H_0 - E_0^{(0)})}$$

$$\int_0^t d1 \langle V_1 \rangle = \int_0^t d1 \langle \Phi_0^{(0)} | R(t_1) V R(t - t_1) | \Phi_0^{(0)} \rangle = t \langle \Phi_0^{(0)} | V | \Phi_0^{(0)} \rangle$$

$$\begin{aligned} \int_0^t \int_{t_1}^t d1 d2 \langle V_1 V_2 \rangle &= \int_0^t \int_{t_1}^t d1 d2 \langle \Phi_0^{(0)} | R(t_1) V R(t_2 - t_1) V R(t - t_2) | \Phi_0^{(0)} \rangle \\ &= t \int_0^t du_1 \langle \Phi_0^{(0)} | V R(u_1) V | \Phi_0^{(0)} \rangle \end{aligned}$$

$$\int_0^t \int_{t_1}^t \int_{t_2}^t du_1 du_2 \langle V_1 V_2 V_3 \rangle = t \int_0^t \int_{u_2}^t \langle \Phi_0^{(0)} | V R(u_1) V R(u_2) V | \Phi_0^{(0)} \rangle$$

etc.

We have

$$\ln(1+x) = 1 - x + x^2/2 + \dots$$

Then

$$E_0 = E_0^{(0)} + \lambda \langle V_1 \rangle - \lambda^2 \int_0^\infty \langle (V_1 - \langle V \rangle)(V_2 - \langle V \rangle) \rangle + \dots$$

• First order

$$E_1 = \langle V_1 \rangle = \langle \Phi_0^{(0)} | V | \Phi_0^{(0)} \rangle$$

• Second-order

$$\begin{aligned} E_2 &= - \int_0^\infty \langle (V_1 - \langle V \rangle)(V_2 - \langle V \rangle) \rangle = - \int_0^\infty du \langle \Phi_0^{(0)} | (V - \langle V \rangle) e^{-u(H_0 - E_0^{(0)})} (V - \langle V \rangle) | \Phi_0^{(0)} \rangle \\ &= - \sum_{i=0} \langle \Phi_0^{(0)} | (V - \langle V \rangle) | \Phi_i^{(0)} \rangle^2 \int_0^\infty du e^{-u(E_i^{(0)} - E_0^{(0)})} = - \sum_{\mathbf{i} \neq \mathbf{0}} \langle \Phi_0^{(0)} | V | \Phi_i^{(0)} \rangle^2 \int_0^\infty du e^{-u(E_i^{(0)} - E_0^{(0)})} \\ &= - \sum_{i \neq 0} \frac{\langle \Phi_0^{(0)} | V | \Phi_i^{(0)} \rangle^2}{E_i^{(0)} - E_0^{(0)}} \end{aligned}$$

Let  $X$  be random variable with probability  $\pi(x)$ . The moments are defined as

$$M_n = \int \pi(x) x^n = \langle x^n \rangle$$

Generating function for the moments

$$G(\lambda) = \langle e^{\lambda x} \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n \langle e^{\lambda x} \rangle}{\partial \lambda^n} (0) \lambda^n = \sum_{n=0}^{\infty} \frac{M_n}{n!} \lambda^n$$



Here

$$E_0(\lambda) \sim \ln \langle e^{\lambda X} \rangle_\pi$$

where the random variable  $X$  is

$$X = - \int_0^t V[x(t)]$$

Because of the logarithm **the moments are not the appropriate quantities**. Indeed, we would like instead

$$\ln \langle e^{\lambda x} \rangle_\pi = \sum_{n=0}^{\infty} \frac{C_n}{n!} \lambda^n$$

that is

$$\langle e^{\lambda x} \rangle = \sum_{n=0}^{\infty} \frac{M_n}{n!} \lambda^n = \exp \left\{ \sum_{n=0}^{\infty} \frac{C_n}{n!} \lambda^n \right\}$$

The  $C_n$  are the **cumulants**.

Easy to calculate by expanding the exponential

$$C_1 = M_1$$

$$C_2 = M_2 - M_1^2$$

$$C_3 = M_3 - 3M_2M_1 + 2M_1^3$$

$$C_4 = M_4 - 4M_3M_1 - 3M_2^2 + 12M_2M_1^2 - 6M_1^4$$

$$C_5 = M_5 - 5M_4M_1 - 10M_3M_2 + 20M_3M_1^2 + 30M_2^2M_1 - 60M_2M_1^3 + 24M_1^5$$

$$C_6 = M_6 - 6M_5M_1 - 15M_4M_2 + 30M_4M_1^2 - 10M_3^2 + 120M_3M_2M_1 \\ - 120M_3M_1^3 + 30M_2^3 - 270M_2^2M_1^2 + 360M_2M_1^4 - 120M_1^6$$

$$E_0 = E_0^{(0)} - \lim_{t \rightarrow +\infty} \frac{1}{t} \ln \langle e^{-\lambda \int_0^t V[x(t)]} \rangle_{\pi} \quad (4)$$

If the system decomposes into two independent parts

$$V = V_A + V_B$$

$$\pi = \pi_A \pi_B$$

$$E_0 = E_0^{(0)} - \lim_{t \rightarrow +\infty} \frac{1}{t} \ln \left[ \langle e^{-\lambda \int_0^t V_A[x_A(t)]} \rangle_{\pi_A} \langle e^{-\lambda \int_0^t V_B[x_B(t)]} \rangle_{\pi_B} \right]$$

$$E_0 = E_0^A + E_0^B$$

But we have also

$$\begin{aligned} E_n &= - \lim_{t \rightarrow \infty} \frac{1}{t} \frac{\partial^n \ln \langle e^{-\lambda \int V} \rangle}{\partial \lambda^n} (0) \\ &= - \lim_{t \rightarrow \infty} \frac{1}{t} \left[ \frac{\partial^n \ln \langle e^{-\lambda \int V_A} \rangle}{\partial \lambda^n} (0) + \frac{\partial^n \ln \langle e^{-\lambda \int V_B} \rangle}{\partial \lambda^n} (0) \right] \end{aligned}$$

which gives

$$E_n = E_n^A + E_n^B$$

The energy is size-extensive **order by order** in perturbation



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