Averages

$\frac{1}{c} e^{-\frac{1}{2} \underline{x}^T A \underline{x}}$ is normalised Gaussian

Def: $\langle \ldots \rangle = \frac{1}{c} \int_{\mathbb{R}^n} e^{-\frac{1}{2} \underline{x}^T A \underline{x}} \ldots d^n x$

Example: $\langle 1 \rangle = 1$

Aim: We want $\langle x_{k_1} x_{k_2} \ldots \rangle$

Lemma: $\langle x_{k_1} x_{k_2} \ldots \rangle = 0$ if number of factors is odd

(as contributions to integral from $\underline{x}$ and $-\underline{x}$ cancel)

Generating function

Def: generating function is $\langle \exp(\underbrace{\underline{j}}_{\text{source}}{}^T \underline{x}) \rangle$

This will allow to determine $\langle x_{k_1} x_{k_2} \dots \rangle$ by taking derivs

Lemma: $\langle \exp(\underline{j}^T \underline{x}) \rangle = \exp(\frac{1}{2} \underline{j}^T A^{-1} \underline{j})$

Proof:

$$\langle \exp(\underline{j}^T \underline{x}) \rangle = \frac{1}{C} \int \exp(-\tfrac{1}{2} \underline{x}^T A \underline{x} + \underline{j}^T \underline{x}) \, d^n x$$

$$\underset{\underline{x} = \underline{z} + A^{-1}\underline{j}}{=} \frac{1}{C} \int \exp\left(-\tfrac{1}{2} (\underline{z}^T + \underline{j}^T A^{-1}) A (\underline{z} + A^{-1} \underline{j}) + \underline{j}^T (\underline{z} + A^{-1} \underline{j})\right) d^n z$$

$$= \frac{1}{C} \int \exp\left(-\tfrac{1}{2} \underline{z}^T A \underline{z} - \tfrac{1}{2} \underline{z}^T \underline{j} - \tfrac{1}{2} \underline{j}^T \underline{z} - \tfrac{1}{2} \underline{j}^T A^{-1} \underline{j} + \underline{j}^T \underline{z} + \underline{j}^T A^{-1} \underline{j}\right) d^n z$$

$$= \underbrace{\frac{1}{C} \int \exp(-\tfrac{1}{2} \underline{z}^T A \underline{z}) \, d^n z}_{=1} \; \exp\left(\tfrac{1}{2} \underline{j}^T A^{-1} \underline{j}\right)$$

Two factors

Lemma: $\langle x_k \, x_{k'} \rangle = (A^{-1})_{kk'}$

Proof: $\langle x_k \, x_{k'} \rangle = \langle x_k \, x_{k'} \, e^{\underline{j}^T \underline{x}} \rangle \big|_{\underline{j}=0}$

$$= \frac{\partial}{\partial j_k} \frac{\partial}{\partial j_{k'}} \langle e^{\underline{j}^T \underline{x}} \rangle \big|_{\underline{j}=0}$$

$$= \frac{\partial}{\partial j_k} \frac{\partial}{\partial j_{k'}} \exp\left(\tfrac{1}{2} \underline{j}^T A^{-1} \underline{j}\right)$$

now use $\frac{\partial}{\partial j_k}\left(\tfrac{1}{2} \underline{j}^T A^{-1} \underline{j}\right) = (A^{-1} \underline{j})_k = \sum_n (A^{-1})_{kn} \, j_n$

$$\langle x_k \, x_{k'} \rangle = \frac{\partial}{\partial j_{k'}} \sum_n (A^{-1})_{kn} \, j_n \, \exp\left(\tfrac{1}{2} \underline{j}^T A^{-1} \underline{j}\right) \big|_{\underline{j}=0}$$

must act here!

$$= \sum_n (A^{-1})_{kn} \, \delta_{nk'} = (A^{-1})_{kk'}$$

Wick's theorem

Thm: To obtain $\langle x_{k_1} x_{k_2} \dots \rangle$

- sum over all ways to connect factors pairwise by contraction lines

  e.g. $\langle x_{k_1} x_{k_2} \; x_{k_3} x_{k_4} \rangle$

- in each summand, each contraction line between x_{k_i} and x_{k_e} gives a factor $(A^{-1})_{k_i k_e}$

Examples: $\langle x_{k_1} x_{k_2} \rangle = \langle x_{k_1} x_{k_2} \rangle = (A^{-1})_{k_1 k_2}$

$$\langle x_{k_1} x_{k_2} x_{k_3} x_{k_4} \rangle = \langle x_{k_1} x_{k_2} x_{k_3} x_{k_4} \rangle + \langle x_{k_1} x_{k_2} x_{k_3} x_{k_4} \rangle + \langle x_{k_1} x_{k_2} x_{k_3} x_{k_4} \rangle$$

$$= (A^{-1})_{k_1 k_2} (A^{-1})_{k_3 k_4} + (A^{-1})_{k_1 k_3} (A^{-1})_{k_2 k_4} + (A^{-1})_{k_1 k_4} (A^{-1})_{k_2 k_3}.$$

Proof:

- $$\langle x_{k_1} x_{k_2} \dots \rangle = \langle x_{k_1} x_{k_2} \dots \; e^{\underline{j}^T \underline{x}} \rangle \Big|_{\underline{j}=0}$$
$$= \frac{\partial}{\partial j_{k_1}} \frac{\partial}{\partial j_{k_2}} \cdots \langle e^{\underline{j}^T \underline{x}} \rangle \Big|_{\underline{j}=0}$$
$$= \frac{\partial}{\partial j_{k_1}} \frac{\partial}{\partial j_{k_2}} \cdots \exp\left(\tfrac{1}{2} \underline{j}^T A^{-1} \underline{j}\right)$$
- derivative $\frac{\partial}{\partial j_{k_i}}$ gives factor $\sum_n (A^{-1})_{k_i n} \, j_n$
- j_n must be removed by other deriv. $\frac{\partial}{\partial j_{k_l}}$ $(k_l = n)$
  then obtain $(A^{-1})_{j_{k_i} j_{k_l}}$
- Sum over all ways of pairing up derivatives
  pairings visualised by contraction lines

Example: 1 d integrals, $A = 1$

$$\langle \ldots \rangle = \left\langle \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \ldots \right\rangle$$

$$\langle x^2 \rangle = \langle x \quad x \rangle = 1$$

$$\langle x^4 \rangle = \langle x \; x \; x \; x \rangle + \langle x \; x \; x \; x \rangle + \langle x \; x \; x \; x \rangle$$

$$= 3$$

$$\langle x^{2n} \rangle = (2n-1) \cdot (2n-3) \cdot \ldots = (2n-1)!!$$

$\uparrow$ choices for element first factor is contracted with

$\uparrow$ choices for element next remaining factor is contracted with

$$\langle x^6 \rangle = 5!! = 5 \cdot 3 \cdot 1 = 15$$

$$\langle x^8 \rangle = 7!! = 7 \cdot 5 \cdot 3 \cdot 1 = 105$$

Fresnel integrals

$$e^{-\frac{1}{2}\underline{x}^T A \underline{x}} \longrightarrow e^{\frac{i}{2}\underline{x}^T A \underline{x}}$$

A real symmetric, eigenvals $\neq 0$

formally: $A \longrightarrow -iA$

$$(A^{-1})_{kk'} \longrightarrow i\,(A^{-1})_{kk'}$$

derivation:

- $\int e^{\frac{i}{2}ax^2}\,dx = \sqrt{\frac{2\pi}{|a|}}\; e^{i\frac{\pi}{4}\operatorname{sgn} a}$
- $\int e^{\frac{i}{2}\underline{x}^T A \underline{x}}\,d^n x = \frac{(2\pi)^{n/2}}{\sqrt{|\det A|}}\, e^{i\nu\frac{\pi}{4}}$

ν = number of pos. eigenvals.
− number of neg. eigenvals.

absorbed in c

- $\langle e^{-i\underline{j}^T x}\rangle = \exp\left(-\frac{i}{2}\,\underline{j}^T A^{-1}\,\underline{j}\right)$
- $\langle x_k\, x_{k'}\rangle = -\frac{\partial}{\partial j_k}\frac{\partial}{\partial j_{k'}}\exp\left(-\frac{i}{2}\,\underline{j}^T A^{-1}\underline{j}\right)\Big|_{\underline{j}=0} = i\,(A^{-1})_{kk'}$

3.3 Anharmonic oscillator

$$L = T - \mathcal{U} = \underbrace{\frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2}_{\text{quadratic}} - \underbrace{\varepsilon x^4}_{\substack{\text{perturbation} \\ \varepsilon \ll 1}}$$

Aim:

- determine $K(0,0,t)$
- extract ground state energy

  $\left(\frac{i}{\hbar}t \to \beta\right)$

$$K(0,0,t) = \int\limits_{x(0)=x(t)=0} D[x]\ \exp\left(\frac{i}{\hbar}\int_0^t \left(\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2 - \varepsilon x(t')^4\right)dt'\right)$$

Comparison to discrete case

$$\underline{x} = (x_1, x_2, \dots) \quad \longrightarrow \quad x(t')$$

$$\frac{i}{2}\underline{x}^T A\,\underline{x} \quad \longrightarrow \quad \frac{i}{\hbar}S_0 = \frac{i}{\hbar}\int_0^t \left(\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2\right)dt'$$

integrate by parts:

$$\int_0^t \dot{x}(t')^2\,dt' = x(t')\,\dot{x}(t')\Big|_0^t - \int_0^t x(t')\,\ddot{x}(t')\,dt'$$

$$= -\int_0^t x(t')\frac{\partial^2}{\partial t'^2}x(t')\,dt'$$

$$\frac{i}{\hbar}S_0 = \frac{i}{2}\int_0^t x(t')\underbrace{\left(-\frac{m}{\hbar}\right)\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right)}_{\text{corresponds to } A \text{ operator}} x(t')\,dt'$$

Inverse of A

Assume $$(A^{-1}x)(t') = \int_0^t \underbrace{G(t',t'')}_{\text{kernel}} x(t'')\,dt''$$

Then $$x(t') = (AA^{-1}x)(t') = A\int_0^t G(t',t'')\,x(t'')\,dt''$$
$$= \int_0^t \underbrace{AG(t',t'')}_{\overset{!}{=}\,\delta(t'-t'')} x(t'')\,dt''$$

So we need $$\boxed{-\frac{m}{\hbar}\left(\frac{\partial^2}{\partial t'^2}+\omega^2\right)G(t',t'') = \delta(t'-t'')}$$

Also A^{-1} must turn functions with $x(0)=x(t)=0$ into functions satisfying the same requirement.

$$\boxed{G(0,t'')=0, \quad G(t,t'')=0}$$

Prop: $$G(t',t'') = -\frac{\hbar}{m\omega \sin\omega t} \begin{cases} \sin\omega t' \ \sin\omega(t''-t) & t' \leq t'' \\ \sin\omega t'' \ \sin\omega(t'-t) & t' > t'' \end{cases}$$

Proof: boundary cond.

$$G(0,t'') \propto \sin(\omega 0) = 0$$

$$G(t,t'') \propto \sin(\omega(t-t)) = 0$$

for $t' \neq t''$

$$\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right) G(t',t'') = 0$$

Satisfied due to terms $\sin\omega t'$, $\sin\omega(t'-t)$

for $t' = t''$: need to get delta function

$$\frac{\partial}{\partial t'} G(t',t'') = -\frac{\hbar}{m \sin \omega t} \begin{cases} \cos \omega t' \sin \omega(t''-t) & t'<t'' \\ \sin \omega t'' \cos \omega(t'-t) & t'>t'' \end{cases}$$

$$= -\frac{\hbar}{m \sin \omega t} \Big[\cos \omega t' \sin \omega(t''-t)$$

$$+ \Theta(t'-t'') \left(\sin \omega t'' \cos \omega(t'-t) - \cos \omega t' \sin \omega(t''-t) \right) \Big]$$

next $\frac{\partial}{\partial t'}$ can act on

- $\Theta(t'-t'')$: get $\delta(t'-t'')$
- trig. functions : get $-\omega^2 G(t',t'')$

$$\frac{\partial^2}{\partial t'^2} G(t',t'') = -\omega^2 G(t',t'')$$

$$- \frac{\hbar}{m \sin \omega t} \delta(t'-t'') \underbrace{\left(\sin \omega t'' \cos \omega(t'-t) - \cos \omega t' \sin \omega (t''-t) \right)}$$

for $t'' = t'$:

$$\sin(\omega t' - \omega(t'-t)) = \sin \omega t$$

$$= -\omega^2 G(t',t'') - \frac{\hbar}{m} \delta(t'-t'')$$

$$\Rightarrow \; -\frac{m}{\hbar} \left(\frac{\partial^2}{\partial t'^2} + \omega^2 \right) G(t',t'') = \delta(t'-t'') \qquad \square$$