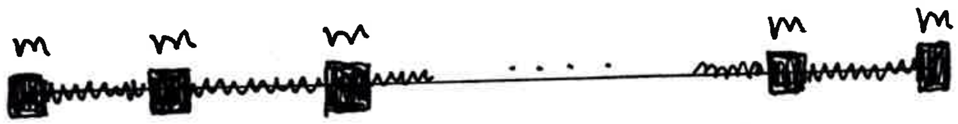
2.4 Elastic chain

N+1 masses connected by springs:



$\phi_0 = 0 \quad \phi_1 \quad \phi_2 \quad \ldots \quad \phi_{N-1} \quad \phi_N = C$

spring const: k
natural length: 0

$$\underline{\phi} = (\phi_1, \phi_2, \ldots, \phi_{N-1})$$

Lagrangian:

$$L(\underline{\phi}, \underline{\dot{\phi}}) = \sum_{i=1}^{N-1} \frac{1}{2} m \dot{\phi}_i^2 - \sum_{i=0}^{N-1} \frac{1}{2} k (\phi_{i+1} - \phi_i)^2$$

Path integral:

$$K(\underline{\phi}_f, \underline{\phi}_0, t) = \langle \underline{\phi}_f | e^{-\frac{i}{\hbar} \hat{H} t} | \underline{\phi}_0 \rangle = \int\limits_{\substack{\underline{\phi}(t') \text{ with} \\ \underline{\phi}(0) = \underline{\phi}_0,\, \underline{\phi}(t) = \underline{\phi}_f}} D[\underline{\phi}]\, e^{\frac{i}{\hbar} S[\underline{\phi}]}$$

$$S[\underline{\phi}] = \int_0^t dt' \, L(\underline{\phi}(t'), \underline{\dot{\phi}}(t'))\, dt'$$

Continuum limit $N \to \infty$

regard ϕ as function of t' and equilibrium position

$$x = i \underbrace{\frac{c}{N}}_{=a} \in \mathbb{R}$$

$$\phi_i(t') = \phi(\underbrace{ia}_{=x}, t')$$

i.e. a field, assume ϕ is smooth

summand in Lagrangian:

$$\frac{1}{2} m \dot{\phi}_i^2 \qquad - \frac{1}{2} k (\phi_{i+1} - \phi_i)^2$$

$$= \frac{1}{2} m \dot{\phi}(ia, t')^2 \quad - \frac{1}{2} k \underbrace{(\phi((i+1)a, t') - \phi(ia, t'))}_{\approx \phi'(ia, t')\, a}{}^2$$

$(\phi' = \text{deriv. w.r.t. } x)$

$$\simeq \frac{1}{2} \frac{m}{a} \int_{ia}^{(i+1)a} \dot{\phi}(x, t')^2 dx \; - \frac{1}{2} k a \int_{ia}^{(i+1)a} \phi'(x, t')^2 \, dx$$

Lagrangian:

$$L(\underline{\Phi}, \dot{\underline{\Phi}}) \simeq \int_0^{\ell} dx \left(\frac{1}{2} \frac{m}{a} \dot{\phi}(x,t')^2 - \frac{1}{2} k a \phi'(x,t')^2 \right)$$

approx. becomes better and better as $N \to \infty$

Path integral in continuum limit:

$$K(\phi_f, \phi_0, t) = \int D[\phi] \; e^{\frac{i}{\hbar} S[\phi]}$$

functions of x

$\phi(x,t')$
with $\phi(x,0) = \phi_0(x)$
$\phi(x,t) = \phi_f(x)$

$$S[\phi] = \int_0^t dt' \int_0^{\ell} dx \underbrace{\left(\frac{1}{2} \frac{m}{a} \dot{\phi}(x,t')^2 - \frac{1}{2} k a \phi'(x,t')^2 \right)}_{\text{Lagrangian density } \mathcal{L}(\phi, \dot{\phi}, \phi')}$$

Boundary conditions

due to $\phi_0(t') = 0$: $\phi(0, t') = 0$

due to $\phi_N(t') = C$: $\phi(C, t') = C$

Convergence:

$a \propto \frac{1}{N}$

need $m \propto \frac{1}{N}$

$k \propto N$

2.5 Path integrals in Statistical Mechanics

consider a system that can exchange energy with environment

probability for a state with energy E_j

$$\propto e^{-\frac{E_j}{kT}} = e^{-\beta E_j}$$

Boltzmann const. temperature $\beta = \frac{1}{kT}$

for normalisation one needs the partition function

$$Z = \sum_j e^{-\beta E_j} = \mathrm{tr}\, e^{-\beta \hat{H}}$$

can also consider matrix elements

$$\langle \underline{r}_f | e^{-\beta \hat{H}} | \underline{r}_0 \rangle$$

might contain positions of many particles

Path integral

recall

$$\langle \underline{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r}_0 \rangle = \int \mathcal{D}[\underline{r}] \exp\left(\frac{i}{\hbar}\int_0^t \left[\frac{1}{2} m \dot{\underline{r}}(t')^2 - \mathcal{U}(\underline{r}(t'))\right] dt'\right)$$

heuristically, replace

$$e^{-\frac{i}{\hbar}\hat{H}t} \longrightarrow e^{-\beta\hat{H}} \qquad \frac{i}{\hbar}t \longrightarrow \beta$$

$$\frac{i}{\hbar}t' \longrightarrow \beta' \qquad t' \longrightarrow \frac{\hbar}{i}\beta' \qquad \frac{d}{dt'} \longrightarrow \frac{i}{\hbar}\frac{d}{d\beta'}$$

this gives

$$\langle \underline{r}_f | e^{-\beta\hat{H}} | \underline{r}_0 \rangle = \int\limits_{\underline{r}(0)=\underline{r}_0,\, \underline{r}(\beta)=\underline{r}_f} \mathcal{D}[\underline{r}] \exp\left(\int_0^\beta \left[\frac{1}{2} m \left(\frac{i}{\hbar}\frac{d}{d\beta'}\underline{r}\right)^2 - \mathcal{U}(\underline{r}(\beta'))\right] d\beta'\right)$$

$$= \int\limits_{\underline{r}(0)=\underline{r}_0,\, \underline{r}(\beta)=\underline{r}_f} \mathcal{D}[\underline{r}] \exp\Bigg(\underbrace{-\int_0^\beta \left[\frac{1}{2}\frac{m}{\hbar^2}\left(\frac{d\underline{r}}{d\beta'}\right)^2 + \mathcal{U}(\underline{r}(\beta'))\right] d\beta'}_{\text{Euclidian action } S_E[\underline{r}]}\Bigg)$$

Extract ground state energy

$$\langle \underline{r}_f | \underbrace{e^{-\beta \hat{H}}}_{} | \underline{r}_0 \rangle$$

$$= \sum_j |\psi_j\rangle e^{-\beta E_j} \langle \psi_j |$$

$$= \sum_j \langle \underline{r}_f | \psi_j \rangle \, e^{-\beta E_j} \langle \psi_j | \underline{r}_0 \rangle$$

for $\beta \to \infty$ dominating term is proportional to $e^{-\beta E_0}$

can use this to determine E_0

e.g. harmonic oscillator

$$K(x_f, x_0, t) = \sqrt{\frac{m\omega}{2\pi\hbar \sin\omega t}} \exp\left(\frac{i}{\hbar} \frac{m\omega}{2\sin\omega t}\left((x_0^2 + x_f^2)\cos\omega t - 2x_0 x_f\right) - i\frac{\pi}{4}\right)$$

$$K(0,0,t) = \sqrt{\frac{m\omega}{2\pi\hbar \sin\omega t}}\, e^{-i\frac{\pi}{4}}$$

$$t \to \frac{\hbar}{i}\beta$$

$$\langle 0| e^{-\beta\hat{H}} |0\rangle = \sqrt{\frac{m\omega}{2\pi\hbar \sin\omega\frac{\hbar}{i}\beta}}\; e^{-i\frac{\pi}{4}}$$

$$\propto \left(\sin \omega\frac{\hbar}{i}\beta\right)^{-1/2}$$

$$= \left(\frac{1}{2i}\left(e^{i\omega\frac{\hbar}{i}\beta} - e^{-i\omega\frac{\hbar}{i}\beta}\right)\right)^{-\frac{1}{2}}$$

$$= \left(\frac{1}{2i}\left(e^{\omega\hbar\beta} - e^{-\omega\hbar\beta}\right)\right)^{-\frac{1}{2}}$$

$$\underset{\beta\to\infty}{\simeq} \left(\frac{1}{2i}\right)^{-1/2} e^{-\beta\left(\frac{1}{2}\hbar\omega\right)}$$

ground state energy

3 Perturbation theory

3.1 Motivation

$$K(\underline{r}_f, \underline{r}_0, t) = \int D[\underline{r}]\, e^{\frac{i}{\hbar}\int L\, dt'}$$

can be evaluated exactly if L is quadratic in $\underline{r}, \dot{\underline{r}}$

otherwise try to expand

$$L(\underline{r}, \dot{\underline{r}}) = \underbrace{L_0(\underline{r}, \dot{\underline{r}})}_{\text{quadratic}} + \underbrace{\varepsilon}_{\varepsilon \ll 1}\, \underbrace{L_1(\underline{r}, \dot{\underline{r}})}_{\text{perturbation, e.g. } \underline{r}^4}$$

$$K(\underline{r}_f, \underline{r}_0, t) = \int D[\underline{r}]\, e^{\frac{i}{\hbar}\int L_0\, dt'}\, \underbrace{e^{\frac{i\varepsilon}{\hbar}\int L_1\, dt'}}_{\simeq 1 + \frac{i\varepsilon}{\hbar}\int L_1\, dt'}$$

change approx. by $\frac{i\varepsilon}{\hbar}\int D[\underline{r}]\left(\int L_1\, dt'\right) e^{\frac{i\varepsilon}{\hbar}\int L_0\, dt'}$

need Fresnel integrals with prefactors

Similar problems

- $\boxed{\begin{array}{l}\text{discrete Gaussian / Fresnel with prefactors e.g.} \\ \displaystyle\int x_{k_1} x_{k_2} \cdots e^{-\frac{1}{2}\underline{x}^T A \underline{x}} \, d^n x\end{array}}$
- partition function for perturbed L $\left(\frac{i}{\hbar} t \to \beta\right)$
- statistical averages
- correlation functions

$$\int D[x] \; x(t_1)\, x(t_2)\, e^{\frac{i}{\hbar}\int_0^t L(x(t'),\dot{x}(t'))\,dt'}$$

3.2 Wick's theorem

aim: evaluate integrals

$$\int x_{k_1} x_{k_2} \cdots \; e^{-\frac{1}{2}\underline{x}^T A \underline{x}} \, d^n x$$

$\underline{x} = (x_1, x_2, \dots)$

A real symmetric, positive definite ($\underline{x}^T A \underline{x} > 0$ for $\underline{x} \neq 0$)

Prop:

$$\int e^{-\frac{1}{2}\underline{x}^T A \underline{x}} \, d^n x = \frac{(2\pi)^{n/2}}{\sqrt{\det A}} =: c$$

(generalises $\int e^{-\frac{1}{2}ax^2} dx = \sqrt{\frac{2\pi}{a}}$)

Proof:

- for diagonal matrix $A = \begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}$

$$\int \exp\left(-\frac{1}{2}\underline{x}^T A \underline{x}\right) d^n x = \int \exp\left(-\frac{1}{2}\sum_k a_k x_k^2\right) d^n x = \prod_k \sqrt{\frac{2\pi}{a_k}} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$

- for general $A = O^T \underbrace{\begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}}_{=D} O$ ← orth. matrix $O^T = O^{-1}$

$$\int \exp\left(-\frac{1}{2}\underline{x}^T O^T D O \underline{x}\right) d^n x$$

$$= \int \exp\left(-\frac{1}{2}\underline{y}^T D \underline{y}\right) d^n y = \frac{(2\pi)^{n/2}}{\sqrt{\det D}} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$

$\underline{y} = O\underline{x}$, $\underline{y}^T = \underline{x}^T O^T$

$|\det O| = 1$

$\boxed{\text{Averages}}$

$\frac{1}{c} e^{-\frac{1}{2}\underline{x}^T A \underline{x}}$ 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 $\langle \exp(\underset{\uparrow\,\text{source}}{\underline{j}^T} \underline{x}) \rangle$

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:

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

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

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

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