Path integral

$$K(\underline{r}_f, \underline{r}_0, t) = \langle \underline{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r}_0 \rangle$$

$$= \int \mathcal{D}[\underline{r}]\, e^{iS[\underline{r}]/\hbar}$$

traj. with $\underline{r}(0)=\underline{r}_0, \underline{r}(t)=\underline{r}_f$

classical action

Proof:

- for **small t**

$$\langle \underline{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r}_0 \rangle \simeq \left(\frac{m}{2\pi i\hbar t}\right)^{n/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{\underline{r}_f-\underline{r}_0}{t}\right)^2 - U(\underline{r}_0)t\right)\right]$$

- for **arbitrary t**

split into small intervals & use

$$\mathbb{1} = \int d^n r\, |\underline{r}\rangle\langle\underline{r}|$$

Hamiltonian version:

$$K(\underline{r}_f, \underline{r}_0, t) = \int_{\substack{\underline{r}(0)=\underline{r}_0 \\ \underline{r}(t)=\underline{r}_f}} \mathcal{D}[\underline{r}]\,\mathcal{D}[\underline{p}]\, e^{\frac{i}{\hbar}\int \underline{p}(t')\cdot\dot{\underline{r}}(t') - H(\underline{r}(t'),\underline{p}(t'))\,dt'}$$

Continuum limit

for chain with number of masses $\to \infty$

position ϕ as function of equilibrium pos. x
and time t' : $\phi(x,t')$

$$K(\underbrace{\phi_f, \phi_0}_{\text{functions of } x}, t) = \int \mathcal{D}[\phi]\, e^{\frac{i}{\hbar} \iint \mathcal{L}(\phi(x,t'), \dot{\phi}(x,t'), \phi'(x,t'))\, dx\, dt'}$$

Statistical Mechanics

replace $\frac{i}{\hbar}$ by $\beta = \frac{1}{kT}$

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

$$= \int \mathcal{D}[\underline{r}]\, \exp\Big[\underbrace{- \int_0^\beta \Big(\frac{1}{2} m \Big(\frac{1}{\hbar} \frac{d\underline{r}}{d\beta'} \Big)^2 + U(\underline{r}(\beta')) \Big) d\beta'}_{S_E[\underline{r}]} \Big]$$

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

Perturbation theory

Gaussian averages

$$\langle \ldots \rangle = \frac{1}{c} \int \ldots \exp\left(-\frac{1}{2} \underline{x}^T A \underline{x}\right) d^n x$$

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

$\langle x_{k_1} x_{k_2} \ldots \rangle = 0$ for odd number of factors

for even numbers sum over contractions with

$$\overline{x_{k_i} \ldots\ldots x_{k_j}} = (A^{-1})_{k_i k_j}$$

Anharmonic oscillator

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

$$= \underset{\substack{\uparrow \\ \text{from above}}}{K_{harm}}(0,0,t) \left\langle \exp\left(-\frac{i}{\hbar} \varepsilon \int_0^t x(t')^4 dt'\right) \right\rangle$$

expand in powers of ε

contraction $\overline{x(t') \quad x(t'')}$

gives $i\,G(t',t'')$

where $G(t',t'')$ is integral kernel

$$(A^{-1} x)(t') = \int_0^t G(t',t'')\, x(t'')\, dt''$$

can use <u>Feynman diagrams</u> to keep track of contributions

Second quantisation

- basis of single particle wavefunctions

  $|i\rangle \qquad \varphi_i(\underline{r})$

- two particle wavefunctions must be symmetric/antisymmetric for bosons/fermions

  $|i,j\rangle \qquad \varphi_{i,j}(\underline{r}_1,\underline{r}_2) = C\left(\varphi_i(\underline{r}_1)\varphi_j(\underline{r}_2) \pm \varphi_j(\underline{r}_1)\varphi_i(\underline{r}_2)\right)$

- basis for N particle wavefunctions

  $|i_1, i_2, \dots, i_N\rangle$

  $$\varphi_{i_1 \dots i_N}(\underline{r}_1 \dots \underline{r}_N) = C \sum_{\pi} \varphi_{i_{\pi(1)}}(\underline{r}_1) \dots \varphi_{i_{\pi(N)}}(\underline{r}_N) \begin{cases} 1 \\ \operatorname{sgn}\pi \end{cases}$$

- occupation number representation

  $|n_1, n_2, \dots\rangle$

  particles in state 1   particles in state 2

- **creation & annihilation operators**

for bosons

$$a_i^+ |\ldots n_i \ldots\rangle = \sqrt{n_i+1}\; |\ldots n_i+1 \ldots\rangle$$
$$a_i |\ldots n_i \ldots\rangle = \sqrt{n_i}\; |\ldots n_i-1 \ldots\rangle$$

$$[a_i^+, a_j^+] = [a_i, a_j] = 0 \;, \quad [a_i, a_j^+] = \delta_{ij}$$

for fermions

$$a_i^+ |\ldots n_i=0 \ldots\rangle = (-1)^{\sum_{j=1}^{i-1} n_j} |\ldots n_i=1 \ldots\rangle$$
$$a_i^+ |\ldots n_i=1 \ldots\rangle = 0$$
$$a_i |\ldots n_i=0 \ldots\rangle = 0$$
$$a_i |\ldots n_i=1 \ldots\rangle = (-1)^{\sum_{j=1}^{i-1} n_j} |\ldots n_i=0 \ldots\rangle$$

$$[a_i^+, a_j^+]_+ = [a_i, a_j]_+ = 0, \quad [a_i, a_j^+]_+ = \delta_{ij}$$

- **Hamiltonian** for systems with discrete sites

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$$\hat{H} = \sum_{ij} \underset{\substack{\uparrow \\ \text{single particle} \\ \text{Hamiltonian}}}{H(i,j)}\, a_i^+ a_j + \frac{1}{2} \sum_{ij} \underset{\substack{\uparrow \\ \text{interaction}}}{U_{int}(i,j)}\, a_i^+ a_j^+ a_j a_i$$

Path integral in 2nd quantisation

(for bosons)

$$\mathrm{tr}\, e^{-\frac{i}{\hbar}\hat{H}t}$$

$$= \int\limits_{a_j(t)=a_j(0)} \mathcal{D}[a_1, a_2, \dots] \exp\Big[-\int_0^t dt' \sum_j a_j^*(t')\, \dot{a}_j(t') - \frac{i}{\hbar}\int_0^t dt'\, H(a_1(t'), a_2(t'), \dots, a_1^*(t'), a_2^*(t'), \dots) \Big]$$