Binomial Distributions

- case of large number of trials, with two possible outcomes

N trials, outcomes can be 0 or 1

q - probability that for a particular trial outcome is 0

p - 1

$$q+p=1$$

probability of one particular permutation

$$\boxed{p^{n_1} q^{n_0}}$$

n_1 = number of times outcome was 1

n_0 = ... 0

probability of having n_1 outcomes of 1

$$P(n_1) = \frac{N!}{n_0!\, n_1!} p^{n_1} q^{n_0}$$

$$\sum_{n_1=0}^{N} P(n_1) = \sum_{n_1} \frac{N!}{n_0!\, n_1!} p^{n_1} q^{n_0} = (p+q)^N = 1$$

- can also be written in terms of a continuous variable X;
  - let $P_{X_i}(x)$ denote the probability of outcome for the ith trial

$$P_{X_i}(x) = q\,\delta(x) + p\,\delta(x-1)$$

characteristic function

$$f_{X_i}(k) = \int_{-\infty}^{\infty} e^{ikx} P_{X_i}(x)\,dx = q + p\,e^{ik}$$

let Y_N be stochastic variable such that

$$Y_N = X_1 + \dots + X_N$$

$\Downarrow$

for independent trials

$$P_{Y_N}(y) = \int dx_1 \dots dx_N \, \delta(y - x_1 - \dots - x_N) P_{X_1}(x_1) \dots P_{X_N}(x_N)$$

characteristic function

$$f_{Y_N}(k) = \int dy \, e^{iky} P_{Y_N}(y) = f_{X_1}(k) \dots f_{X_N}(k)$$

$$= (q + p e^{ik})^N$$

expand as $f_{Y_N}(k) = \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} q^{N-n} p^n e^{ikn}$

$$P_{Y_N}(y) = \frac{1}{2\pi} \int e^{-iky} f_{Y_N}(k) \, dk$$

$$= \cancel{\frac{1}{2\pi}} \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} q^{N-n} p^n \delta(y-n)$$

$$= \sum_{n=0}^{N} P_N(n) \delta(y-n)$$

for the moments:

- can be calculated directly
- obtained from characteristic function

1st moment: $\langle n \rangle = -i \partial_k f_{Y_N}(k)$

$$= -i \partial_k [q + p e^{ik}]^N$$

$$= -i \left(N (q + p e^{ik})^{N-1} p e^{ik} i \right)$$

$$= Np$$

2nd moment: $\langle n^2 \rangle = (-i \partial_k)(-i \partial_k) f_{Y_N}(k)$

$$= \dots = (Np)^2 + Npq$$

$\Downarrow$

$$\langle n^2 \rangle - \langle n \rangle^2 = \sqrt{Npq}$$

- to arrive at Gaussian distribution: define

$$P_{Z_N}(z) = \int_{-\infty}^{\infty} dy\, \delta\left(z - \frac{(y-pN)}{\sqrt{pqN}}\right) P_{Y_N}(y)$$

- stochastic variable Z_N is obtained from Y_N

as $$Z_N = \frac{Y_N - \langle Y \rangle}{\sigma_Y}$$

- characteristic function:

$$f_{Z_N}(k) = \int_{-\infty}^{\infty} e^{ikz} P_{Z_N}(z)\, dz$$

$$= \int_{-\infty}^{\infty} dz\, dy\, e^{ikz}\, \delta\left(z - \frac{(y-pN)}{\sqrt{pqN}}\right) P_{Y_N}(y)$$

$$= \int_{-\infty}^{\infty} dy\, e^{ik\frac{(y-pN)}{\sqrt{pqN}}} P_{Y_N}(y)$$

$$= e^{-ikpN/\sqrt{pqN}} \underbrace{\int_{-\infty}^{\infty} dy\, e^{\frac{iky}{\sqrt{pqN}}} P_{Y_N}(y)}_{f_{Y_N}\left(\frac{k}{\sqrt{pqN}}\right)}$$

$$= e^{-ik\sqrt{\frac{pN}{q}}} f_{Y_N}\left(\frac{k}{\sqrt{pqN}}\right)$$

$$= \left(e^{-ik\sqrt{\frac{p}{qN}}}\right)^N \left(q + p\, e^{i\frac{k}{\sqrt{pqN}}}\right)^N$$

$$= \left(q\, e^{-ik\sqrt{\frac{p}{qN}}} + p\, e^{ik\left(\frac{1}{\sqrt{pqN}} - \sqrt{\frac{p}{qN}}\right)}\right)^N$$

$$\frac{1}{\sqrt{pqN}} - \sqrt{\frac{p}{qN}} = \frac{1}{\sqrt{pqN}} - \frac{p}{\sqrt{pqN}} = \frac{q}{\sqrt{pqN}} = \sqrt{\frac{q}{pN}}$$

$$= \left(q\, e^{-ik\sqrt{\frac{p}{qN}}} + p\, e^{ik\sqrt{\frac{q}{pN}}}\right)^N$$

take the limit $N \to \infty$

$$\left(q e^{-ik\sqrt{\frac{p}{qN}}} + p e^{ik\sqrt{\frac{q}{pN}}}\right)^N$$

$$= \left(q\left(1 - ik\sqrt{\frac{p}{qN}} + \frac{i^2k^2p}{2qN}\right) + p\left(1 + ik\sqrt{\frac{q}{pN}} + \frac{i^2k^2q}{2pN}\right)\right)^N$$

$$= \left(1 - \frac{k^2}{2N}\underbrace{(p+q)}_{1}\right)^N$$

$$= \left(1 - \frac{k^2}{2N}\right)^N = e^{-\frac{k^2}{2}}$$

$\Downarrow$ $\Downarrow$

$$P_Z(z) = \frac{e^{-z^2/2}}{\sqrt{2\pi}}$$

Z has mean 0 and variance 1

Quantum Statistics

- enables consideration of indistinguishability in a quantitative way ⇒ ensemble theory rewritten in terms of operators
  - for now deal with non-interacting systems
  - for high temperatures, low densities ⇒ asymptotically the system tends to the classical limit
  - rigorous evidence is provided for "phase space volume

Quantum-mechanical ensemble theory: the density matrix

- N identical systems $N \gg 1$
  - characterized by Hamiltonian $\hat{H}$
  - physical state of system: $\psi_i(\vec{r},t)$ – wavefunction for kth ensemble member $\psi^k(\vec{r},t)$
    - Schrödinger equation:

$$\hat{H}\psi^k(t) = i\hbar\dot{\psi}^k(t)$$

    - time-independent basis (closed system) $|\varphi_i\rangle$

$$\psi^k(t) = \sum_i a_i^k(t)\,\varphi_i \Rightarrow a_i^k(t) = \int d\vec{r}\,\varphi_i^*(\vec{r})\,\psi^k(\vec{r},t)$$

    - to describe time-evolution of system we can use either $\psi^k(t)$ or coefficients $a_i^k(t)$

$$\hat{H}\psi^k(t) = \sum_i a_i^k(t)\,\hat{H}\varphi_i$$

$$\int d\vec{r}\,\varphi_j^*\hat{H}\psi^k(t) = \sum_i a_i^k(t)\,H_{ji} \qquad H_{ji} = \int d\vec{r}\,\varphi_j^*(\vec{r})\hat{H}\varphi_i(\vec{r})$$

    - time evolution ⇒ matrix equation

meaning of coefficients $a_i^k(t) \Rightarrow$ probability amplitude that system is in state i (ensemble member k)

probability: $|a_i^k(t)|^2 \Rightarrow \sum_i |a_i^k(t)|^2 = 1$

- <u>density operator</u>: $\rho_{mn}(t) = \frac{1}{N} \sum_k a_m^{*k}(t)\, a_n^{k*}(t)$

- density operator: ensemble average of $a_m^{*k}(t) a_n^k(t)$

diagonal element: $|a_m^k(t)|^2$ - probability

$$\Downarrow$$

$$\sum_n \rho_{nn}(t) = 1$$

equation of motion for the density matrix

$$i\hbar\, \dot{\rho}_{mn}(t) = \frac{1}{N} \sum_{k=1}^{N} \left[i\hbar \left\{ \dot{a}_m^{*k}(t)\, a_n^{*k}(t) + a_m^{*k}(t)\, \dot{a}_n^{*k}(t) \right\} \right]$$

$$= \frac{1}{N} \sum_{k=1}^{N} \left[\left\{ \sum_p H_{mp}\, a_p^k(t)\, a_n^{*k}(t) - \sum_p a_m^k(t)\, a_p^k(t)\, H_{pn} \right\} \right]$$

$$= \sum_p \left\{ H_{mp}\, \rho_{pn}(t) - \rho_{mp}(t)\, H_{pn} \right\}$$

$$\boxed{i\hbar\, \dot{\rho}_{mn}(t) = \hat{H}\hat{\rho} - \hat{\rho}\hat{H}}$$ $\Rightarrow$ quantum Liouville equation

- at equilibrium: $\dot{\rho}_{mn} = 0 \Rightarrow$ must commute with $\hat{H}$

$\Rightarrow \hat{\rho}$ is a function of $\hat{H}$ $\quad \hat{\rho} = \hat{\rho}(\hat{H})$

$\Rightarrow$ must not depend explicitely on time

- represent density matrix in eigenfunctions of $\hat{H}$

$\Rightarrow \hat{\rho}$ diagonal

$H_{mn} = E_n \delta_{mn}$ $\qquad$ $\rho_{mn} = \rho_n \delta_{mn}$

precise dependence of $\hat{\rho}$ on $\hat{H}$ $\Rightarrow$ depends on ensemble

<u>detailed balance</u>: density matrix is symmetric in any representation (not necessarily the energy representation)

$$\rho_{mn} = \rho_{nm}$$

- switch from state $m \to n$ is counterbalanced by a tendency to switch from $n \to m$. (equilibrium)

- expectation value of operator $\hat{G}$

$$\langle \hat{G} \rangle = \frac{Tr\{\hat{\rho}\hat{G}\}}{Tr\,\hat{\rho}}$$ - independent of choice of basis

<u>Various ensembles</u>

<u>Microcanonical Ensemble</u>

- fix N, V, and $E - \frac{\Delta}{2}$, $E + \frac{\Delta}{2}$ $\quad \Delta \ll E$

$\Gamma(N, V, E; \Delta)$ – number of microstates

each microstate is equally likely to occur

$$\rho_{mn} = \rho_n \delta_{mn} \qquad \rho_n = \begin{cases} 1/\Gamma & \text{- for accessible microstate} \\ 0 & \text{- for other states} \end{cases}$$

$$\Downarrow$$

$$S = k \ln \Gamma$$

- no Gibbs paradox: indistinguishability of particles is taken care of by symmetry restriction on the wavefunction rather than as a counting process

- $P=1 \Rightarrow$ pure case $\Rightarrow S=0 \Rightarrow$ third law of thermodynamics

- $P>1$ - mixed case

to construct a diagonal density matrix an additional postulate is needed

$$\rho_{mn} = \frac{1}{N}\sum_{k=1}^{N} a_m^k a_n^{k*} = \frac{1}{N}\sum_{k=1}^{N} |a|^2 e^{i(\theta_m^k - \theta_n^k)}$$

$$= c\langle e^{i(\theta_m^k - \theta_n^k)}\rangle = c\,\delta_{mn}$$

- postulate of equal a priori phases

$\Rightarrow$ incoherent superposition

Canonical Ensemble

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Q} \Rightarrow \rho_{mn} = \rho_n \delta_{mn}$$

$$\langle \hat{G}\rangle = \mathrm{Tr}(\hat{\rho}\hat{G})$$

Grand-canonical ensemble

$$\hat{\rho} = e^{-\beta(\hat{H}^N - \mu\hat{N})}$$

Indistinguishable Particles

- gas of non-interacting particles

  - in this case $H(\vec{p}^N, \vec{q}^N) = \sum_i H_i(\vec{p}_i, \vec{q}_i)$

    $H_i(\vec{p}_i, \vec{q}_i)$ - are the same Hamiltonian, acting on the coordinates/momenta of different particles

- $\psi_E(\vec{p}^N, \vec{q}^N)$: $H(\vec{p}^N, \vec{q}^N)\psi_E(\vec{p}^N, \vec{q}^N) = E\psi_E(\vec{p}^N, \vec{q}^N)$

  since Hamiltonian is a sum of one-particle Hamiltonians

$$\Rightarrow \psi_E(\vec{p}^N, \vec{q}^N) = \prod_{i=1}^{N} \varphi_{\varepsilon_i}(\vec{p}_i, \vec{q}_i)$$

$$E = \sum_i \varepsilon_i$$

$$H_i(\vec{p}_i, \vec{q}_i)\varphi_{\varepsilon_i}(\vec{p}_i, \vec{q}_i) = \varepsilon_i \varphi_{\varepsilon_i}(\vec{p}_i, \vec{q}_i)$$

$$\Downarrow$$

$$H_i(\vec{q}_i)\varphi_{\varepsilon_i}(\vec{q}_i) = \varepsilon_i \varphi_{\varepsilon_i}(\vec{q}_i)$$

since in quantum mechanics there is no phase space $\Rightarrow$ momenta and position are representations, not distinct variables as in classical mechanics

- for each $\varepsilon_i \Rightarrow$ can have a number of particles in energy state $\varepsilon_i \Rightarrow n_i$

$$\sum_i n_i = N$$

$$\sum_i n_i \varepsilon_i = E$$

$$\Psi_E(\vec{q}^N) = \prod_{m=1}^{n_1} \varphi_1(m) \prod_{p=n_1+1}^{n_1+n_2} \varphi_2(p) \dots$$

- one can permute coordinates

$$P\Psi_E(\vec{q}^N) = \prod_{m=1}^{n_1} u_1(P_m) \prod_{p=n_1+1}^{n_1+n_2} u_2(P_p) \dots$$

permutation: coordinates $1, 2, \dots, N$
are replaced as $P1, P2, \dots, PN$

- in classical physics $\Rightarrow$ permutations lead to physically distinct states

$\Rightarrow$ the number of distinct states $W = \dfrac{N!}{n_1! \, n_2! \dots}$

$\Rightarrow$ Gibbs correction: $W = \dfrac{1}{n_1! \, n_2! \dots}$ (divide by $N!$)

BUT!!! quantum mechanically a permutation does not lead to a physically distinct state

- interchange of particles, when it in ~~the sa~~ different states $\Rightarrow$ does not change state of the system

quantum ~~mechanically~~ mechanically the question "which particle is in which state?" does not make sense

$\Rightarrow$ number of microstates $W = 1$, provided that the set of occupations n_i are not disallowed on physical grounds

- simple product wavefunction $\prod_{m=1}^{n_1} \psi_{\xi_1}(m) \prod_{p=n_1+1}^{n_2+n_1} \psi_{\xi_2}(p) \ldots$

  not appropriate to describe a system of indistinguishable particles: permutations lead to inequivalent states

- to construct an appropriate wavefunction notice that

$$\psi \to P\psi : \quad |\psi|^2 = |P\psi|^2 \quad \text{since } P^2 = I$$

two possibilities: $P\psi = \psi$ symmetric
$P\psi = -\psi$ antisymmetric

- for anti-symmetric case

$$\psi_A(\vec{q}) = \begin{vmatrix} u_1(1) & \cdots & u_1(N) \\ \vdots & & \\ u_N(1) & \cdots & u_N(N) \end{vmatrix}$$

$\Rightarrow$ no two particles can be in the same state
(determinant gives ~~the same~~ zero)

$$\Rightarrow \quad W(\{n_i\}) = \begin{cases} 1 & \text{if } \sum_i n_i = N \\ 0 & \text{if } \sum_i n_i \neq N \end{cases}$$

- for bosons: no restriction on number of states
  - appropriate wavefunction $\Rightarrow$ permanent

Density matrix of a system of free particles

position representation / canonical ensemble

N-particle system (N, T, V)

$$\langle \vec{r}_1, \dots, \vec{r}_N | \frac{e^{-\beta \hat{H}}}{Q_N(\beta)} | \vec{r}_1', \dots, \vec{r}_N' \rangle$$ = density matrix

$$Q_N(\beta) = \int d\vec{r}_1 \dots d\vec{r}_N \langle \vec{r}_1, \dots \vec{r}_N | e^{-\beta H} | \vec{r}_1, \dots, \vec{r}_N \rangle$$

- using energy identity: $\sum_E |\psi_E\rangle\langle\psi_E| = 1$

$$\int \sum_E \langle r_1, \dots, r_N | \psi_E \rangle e^{-\beta E} \langle \psi_E | \vec{r}_1', \dots, \vec{r}_N' \rangle$$

- assume system is non-interacting

$$\Rightarrow E = \frac{\hbar^2}{2m}(k_1^2 + \dots + k_N^2)$$

$$u_{\vec{k}}(\vec{r}) = V^{-1/2} \exp[i(\vec{k} \cdot \vec{r})]$$

$$\vec{k} = 2\pi V^{-1/3} \vec{n}$$

- wavefunction is given by Slater determinant

$$\psi_E = \frac{1}{\sqrt{N!}} \sum_P \delta_P P[u_{\vec{k}_1}(\vec{r}_1) \dots u_{\vec{k}_N}(\vec{r}_N)]$$

$P \rightarrow$ permutation operator

$$\delta_P = \begin{cases} [+1]^P & \text{for even permutation} \rightarrow \text{bosons} \\ [-1]^P & \text{for odd permutation} \rightarrow \text{fermions} \end{cases}$$

P - order of permutation

- note about permutation operator
  - One can permute either coordinates or momenta

$$P u_{n_1}(\vec{r}_1) \cdots u_{n_N}(\vec{r}_N) = u_{n_1}(P\vec{r}_1) \cdots u_{n_N}(P\vec{r}_N)$$

$$P u_{n_1}(\vec{r}_1) \cdots u_{n_N}(\vec{r}_N) = u_{Pn_1}(\vec{r}_1) \cdots u_{Pn_N}(\vec{r}_N)$$

- for the partition function $\Rightarrow$ we sum over all permutations
  $\Rightarrow$ we can sum over either all momentum permutations or over all coordinate permutations

$\psi_E(1, \dots, N) \Rightarrow$ use momentum representation

$$\psi_{\vec{k}}(1, \dots, N) = \frac{1}{\sqrt{N!}} \sum_P \delta_P \, \cancel{\psi_{n_1}} \, [u_{n_1}(P1) \cdots u_{n_N}(PN)]$$

- question is, what does the density matrix look like in this case?
- simplest thing to do is to consider two particles

$$\psi_{n_1 n_2}(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} u_{n_1}(1) & u_{n_1}(2) \\ u_{n_2}(1) & u_{n_2}(2) \end{vmatrix}$$

$$\langle \vec{r}_1 \vec{r}_2 | e^{-\beta \hat{H}} | \vec{r}_1' \vec{r}_2' \rangle$$

$$= \frac{1}{4} \sum_{n_1 n_2} \begin{bmatrix} u^*_{n_1}(1) & u^*_{n_1}(2) \\ u_{n_2}(1) & u_{n_2}(2) \end{bmatrix} e^{-\beta\left(\frac{k_1^2}{2} + \frac{k_2^2}{2}\right)} \begin{vmatrix} u^*_{n_1}(1') & u^*_{n_1}(2') \\ u^*_{n_2}(1') & u^*_{n_2}(2') \end{vmatrix} e^{-\frac{\beta}{2}(k_1^2 + k_2^2)}$$

$$= \frac{1}{4} \sum_{n_1 n_2} \left(u_{n_1}(1) u_{n_2}(2) - u_{n_1}(2) u_{n_2}(1) \right) \left(u^*_{n_1}(1') u^*_{n_2}(2') - u_{n_1}(2') u_{n_2}(1') \right)$$

$$\frac{1}{2}\Big[\frac{1}{2}\sum_{n_1 n_2}\Big[u_{n_1}(1)\,e^{-\frac{\beta}{2}k_1^2}\,u_{n_1}(1')\Big]\Big[u_{n_2}(2)\,e^{-\frac{\beta}{2}k_2^2}\,u_{n_2}(2')\Big]$$

$$+\frac{1}{2}\sum_{n_1 n_2}\Big[u_{n_1}(2)\,e^{-\frac{\beta}{2}k_2^2}\,u_{n_1}(2')\Big]\Big[u_{n_2}(1)\,e^{-\frac{\beta}{2}k_1^2}\,u_{n_2}(1')\Big]$$

$$-\frac{1}{2}\sum_{n_1 n_2}\Big[u_{n_1}(1)\,e^{-\frac{\beta}{2}k_1^2}\,u_{n_1}(2')\Big]\Big[u_{n_2}(2)\,e^{-\frac{\beta}{2}k_2^2}\,u_{n_2}(1')\Big]$$

$$-\frac{1}{2}\sum_{n_1 n_2}\Big[u_{n_1}(2)\,e^{-\frac{\beta}{2}k_1^2}\,u_{n_1}(1')\Big]\Big[u_{n_2}(1)\,e^{-\frac{\beta}{2}k_2^2}\,u_{n_2}(2')\Big]\Big]$$

consider the particular term: $\sum_{n_1} u(1)\,e^{-\frac{\beta}{2}k_1^2}\,u(1')$

$$= \sum_{n_1} u_{n_1}(\vec{r}_1)\,e^{-\beta\epsilon_{n_1}}\,u(\vec{r}_1') = \langle \vec{r}_1|\,\hat{\rho}^{(1)}\,|\vec{r}_1'\rangle$$

- this is the one-body density matrix in the coordinate representation

$$= \frac{1}{2}\begin{bmatrix} \langle 1|\hat{\rho}^{(1)}|1'\rangle & \langle 1|\hat{\rho}^{(1)}|2'\rangle \\ \langle 2|\hat{\rho}^{(1)}|1'\rangle & \langle 2|\hat{\rho}^{(1)}|2'\rangle \end{bmatrix} \Rightarrow \text{determinant}$$

- we have evaluated the one-body density matrix for a free particle

$$\langle \vec{r}|\,\hat{\rho}\,|\vec{r}'\rangle = \langle \vec{r}|\,e^{-\beta\frac{\hat{p}^2}{2m}}\,|\vec{r}'\rangle$$

$$= \left(\frac{m}{2\pi\beta}\right)^{3/2}\exp\left(-\frac{m}{2\beta}(\vec{r}-\vec{r}')^2\right)$$

$\lambda = \frac{2\pi\beta}{m} \Rightarrow$ de Broglie wavelength

- density matrix will look like

$$\left(\frac{m}{2\pi\beta}\right)^3\Big[\exp\left(-\frac{m}{2\beta}(\vec{r}_1-\vec{r}_1')^2-\frac{m}{2\beta}(\vec{r}_2-\vec{r}_2')^2\right)$$

$$-\exp\left(-\frac{m}{2\beta}(\vec{r}_1-\vec{r}_2')^2-\frac{m}{2\beta}(\vec{r}_2-\vec{r}_1')^2\right)\Big]$$

consider the density matrix for two particle system in the path integral representation

$$\langle \vec r_1 \vec r_2 | \hat\rho^{(2)} | \vec r_1' \vec r_2' \rangle = [\langle \vec r_1 | \hat\rho^{(1)} | \vec r_1' \rangle \langle \vec r_2 | \hat\rho^{(1)} | \vec r_2' \rangle - \langle \vec r_1 | \hat\rho^{(1)} | \vec r_2' \rangle \langle \vec r_2 | \rho^{(1)} | \vec r_1' \rangle]$$

$$\langle \vec r_1 | \hat\rho^{(1)} | \vec r_1' \rangle = \cancel{\int D[\vec r(\tau)]} \langle \vec r_1 | e^{-\beta \hat H^{(1)}} | \vec r_1' \rangle \qquad (\hat H^{(1)} = \frac{\hat p^2}{2m}$$

$$= \langle \vec r_1 | \left[e^{-\frac{\beta \hat H^{(1)}}{P}} \right]^P | \vec r_1' \rangle = \prod_{i=0}^{P} \langle \vec s_i | e^{-\beta \frac{H}{P}} | \vec s_{i+1} \rangle$$

$$\vec s_0 = \vec r_1 \qquad \vec s_{P+1} = \vec r_1'$$

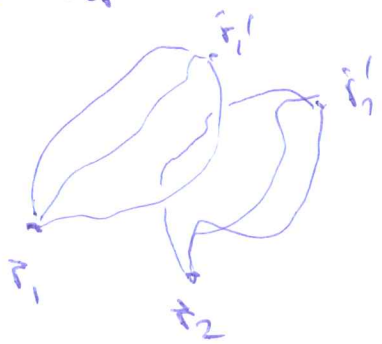
$$= \int_{\vec s(0) = \vec r_1}^{\vec s(\beta) = \vec r_1'} D[\vec s(\tau)] \, e^{-\int_0^\beta d\tau \, \frac{m \dot{\vec r}^2(\tau)}{2}}$$

- integral over all paths in which particle 1 travels from position $\vec r_1$ at imaginary time $\tau = 0$ to position $\vec r_1'$ at imaginary time $\tau = \beta$

$$\langle \vec r_1 | \hat\rho^{(1)} | \vec r_1' \rangle \langle \vec r_2 | \hat\rho^{(1)} | \vec r_2' \rangle = \int_{\vec s_1(0) = \vec r_1}^{\vec s_1(\beta) = \vec r_1'} D[\vec s_1(\tau)] \int_{\vec s_2(0) = \vec r_2}^{\vec s_2(\beta) = \vec r_2'} D[\vec s_2(\tau)] \, e^{-\int_0^\beta d\tau [H_1^{(1)}(\tau) + H_2^{(1)}(\tau)]}$$

- integral over paths in which particle 1 travels from $\vec r_1$ to $\vec r_1'$ in imaginary time $(0 \to \beta)$ and particle 2 travels from $\vec r_2$ to $\vec r_2'$ in imaginary time $(0 \to \beta)$

pictorial representation of paths



consider second term

$$\langle \vec r_1 | \hat\rho^{(1)} | \vec r_2{}' \rangle \langle \vec r_2 | \hat\rho^{(1)} | \vec r_1{}' \rangle$$

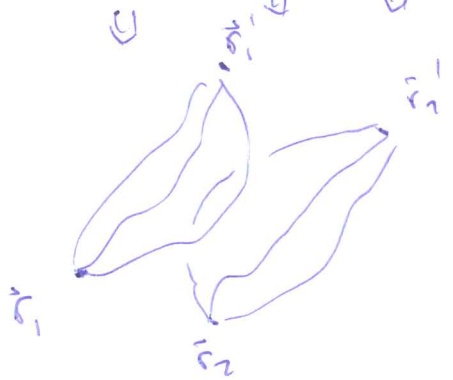
in this case path-integral representation corresponds to

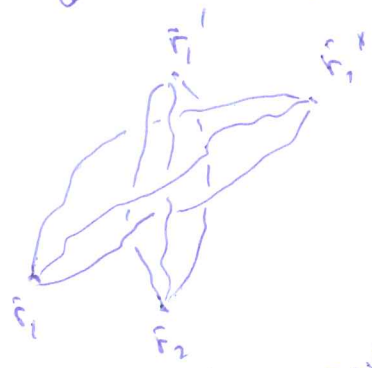
$$\int_{\vec s_1(0)=\vec r_1}^{\vec s_1(\beta)=\vec r_2{}'} \int_{\vec s_2(0)=\vec r_2}^{\vec s_2(\beta)=\vec r_1{}'} \mathcal{D}[\vec s_1(\tau)]\mathcal{D}[\vec s_2(\tau)]\, e^{-\int_0^\beta d\tau \left[\frac{\dot{\vec s}_1^{\,2}(\tau)}{2m} + \frac{\dot{\vec s}_2^{\,2}(\tau)}{2m}\right]}$$

- here particle 1 starts at $\vec r_1$ but ends up at $\vec r_2{}'$ and vice versa

$$\langle 1 2 | \hat\rho^{(2)} | 1' 2' \rangle = \cancel{\langle 1 | \hat\rho^{(1)} | 1' \rangle \langle 2 | \hat\rho^{(1)} | 2' \rangle}$$

$$= \langle 1 | \hat\rho^{(1)} | 1' \rangle \langle 2 | \hat\rho^{(1)} | 2' \rangle - \langle 1 | \hat\rho^{(1)} | 2' \rangle \langle 2 | \hat\rho^{(1)} | 1' \rangle$$





exchanging paths

for the partition function of two particles we can write first the diagonal elements of $\hat\rho$

$$\langle 1 2 | \hat\rho^{(2)} | 1 2 \rangle = \frac{1}{2\lambda^6} \left[1 - \exp\left[-\frac{\pi(\vec r_1 - \vec r_2)^2}{\lambda^2}\right] \exp\left[-\frac{\pi(\vec r_2 - \vec r_1)^2}{\lambda^2}\right] \right]$$

partition function $\int d\vec r_1 d\vec r_2 \langle 1 2 | \hat\rho^{(2)} | 1 2 \rangle$

many-bodies generalization:

$$\langle 1,\dots,N|\hat{\rho}^{(N)}|1',\dots,N'\rangle = \frac{1}{N!}\begin{vmatrix} \langle 1|\hat{\rho}^{(1)}|1'\rangle & \cdots & \langle 1|\hat{\rho}^{(1)}|N'\rangle \\ \vdots & & \\ \langle N|\hat{\rho}^{(1)}|1'\rangle & \cdots & \langle N|\hat{\rho}^{(1)}|N'\rangle \end{vmatrix}$$

write $\langle \vec{r}_i|\hat{\rho}^{(1)}|\vec{r}_j\rangle = \frac{1}{\lambda^3}\exp\left(-\frac{m}{2\beta}(\vec{r}_i-\vec{r}_j)^2\right) = \frac{1}{\lambda^3} f_{ij}$

diagonal element:

$$\langle 1,\dots,N|\hat{\rho}^{(N)}|1,\dots,N\rangle = \frac{1}{N!\,\lambda^{3N}}\begin{vmatrix} 1 & f_{12} & \cdots & f_{1N} \\ f_{21} & 1 & & \vdots \\ \vdots & & 1 & \vdots \\ f_{N1} & \cdots & & 1 \end{vmatrix}$$

$$Q = \frac{1}{N!}\frac{1}{\lambda^{3N}}\int d\vec{r}_1\dots d\vec{r}_N\left[1 - \sum_{i<j} f_{ij}f_{ji} + \sum_{i<j<k} f_{ij}f_{jk}f_{ki} + \dots\right]$$

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two particle case:

$$V_s(r) = -kT\ln\left[1 \pm \exp\left(-\frac{2\pi r^2}{\lambda^2}\right)\right]$$

effective exchange potential