3 Statistical mechanics and path integrals

3.1 Coherent-state path integral

Prototypical example: system of (many!) interacting bosons

Fock basis of many-body Hilbert space:

$$|n_1, n_2, \ldots, n_N\rangle = \prod_{\alpha=1}^{N} \frac{(\hat{a}_\alpha^\dagger)^{n_\alpha}}{\sqrt{n_\alpha!}} |0\rangle$$

where $|0\rangle = |0, \ldots, 0\rangle$ is the (many-body) vacuum state and $\hat{a}_\alpha^\dagger$ ($\hat{a}_\alpha$) creates (annihilates) a boson in the α-th single-particle state.

Commutation relation:

$$[\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger] = \delta_{\alpha,\alpha'} \quad \text{and} \quad [\hat{a}_\alpha, \hat{a}_{\alpha'}] = [\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger] = 0$$

Expansion in basis states:

$$|\Phi\rangle = \sum_{n_1=0}^{\infty} \cdots \sum_{n_N=0}^{\infty} \Phi_{n_1 \ldots n_N} |n_1, \ldots, n_N\rangle$$

Coherent state:

$$\hat{a}_\alpha |\Phi\rangle = \Phi_\alpha |\Phi\rangle \quad \text{for all } \alpha = 1, \ldots, N$$

where $\Phi_\alpha \in \mathbb{C}$.

Expansion coefficients:

$$\Phi_{n_1 \ldots n_N} = \prod_{\alpha=1}^{N} \frac{(\Phi_\alpha)^{n_\alpha}}{\sqrt{n_\alpha!}}$$

Thus:

$$|\Phi\rangle = \sum_{n_1=0}^{\infty} \cdots \sum_{n_N=0}^{\infty} \prod_{\alpha=1}^{N} \frac{(\Phi_\alpha \hat{a}_\alpha^\dagger)^{n_\alpha}}{n_\alpha!} |0\rangle = e^{\sum_\alpha \Phi_\alpha \hat{a}_\alpha^\dagger} |0\rangle$$

Remarks:

- $|\Phi\rangle$ as defined above can easily be shown to satisfy $\hat{a}_\alpha |\Phi\rangle = \Phi_\alpha |\Phi\rangle$ by using $[\hat{a}_\alpha, (\hat{a}_{\alpha'}^\dagger)^n] = n(\hat{a}_\alpha^\dagger)^{n-1} \delta_{\alpha\alpha'}$

- $|\Phi\rangle$ is a superposition of states with arbitrary number of particles

Bra version:

$$\langle\Phi| = \langle 0| e^{\sum_\alpha \Phi_\alpha^* \hat{a}_\alpha} \quad \text{with} \quad \langle\Phi|\hat{a}_\alpha^\dagger = \langle\Phi|\Phi_\alpha^*$$

Particle creation:

$$\hat{a}_\alpha^\dagger |\Phi\rangle = \frac{\partial}{\partial \Phi_\alpha} |\Phi\rangle$$

Overlap of two coherent states:

$$\langle\Phi|\Phi'\rangle = e^{\sum_\alpha \Phi_\alpha^* \Phi_{\alpha'}} \neq 0 \quad \text{(not orthogonal)}$$

Resolution of unity:

$$\mathbb{1} = \int \prod_\alpha \frac{d\Phi_\alpha^* \, d\Phi_\alpha}{2\pi i} e^{-\sum_\alpha \Phi_\alpha^* \Phi_\alpha} |\Phi\rangle\langle\Phi|$$

$\Rightarrow$ Coherent states form an overcomplete "basis"

NB: $\displaystyle\int \frac{d\phi^* d\phi}{2\pi i} e^{-|\phi|^2} |\phi\rangle\langle\phi|$

$\displaystyle = \int_0^\infty \frac{r\,dr}{\pi} \int_0^{2\pi} d\theta\, e^{-r^2} \sum_{m,n=0}^{\infty} \frac{(r e^{i\theta})^m}{\sqrt{m!}} |m\rangle \frac{(r e^{-i\theta})^n}{\sqrt{n!}} \langle n|$

$\displaystyle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\infty dr\, 2r\, e^{-r^2} r^{2n} |n\rangle\langle n| = \sum_n |n\rangle\langle n| = \mathbb{1}$

Grand-canonical partition function:

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

where $\beta = \frac{1}{k_B T}$ the inverse temperature and μ the chemical potential

Hamiltonian (in "second quantization"):

$$\hat{H} = \sum_{\alpha} \underbrace{e_\alpha}_{\substack{\text{energy eigenvalues} \\ \text{for } V=0}} \hat{a}^{+}_{\alpha}\hat{a}_{\alpha} + \sum_{\alpha,\beta,\gamma,\delta} \underbrace{\langle \alpha\beta | V | \gamma\delta\rangle}_{\substack{\text{two-body} \\ \text{interaction}}} \hat{a}^{+}_{\alpha} a^{+}_{\beta} \hat{a}_{\delta}\hat{a}_{\gamma}$$

Particle number operator:

$$\hat{N} = \sum_{\alpha} \hat{a}^{+}_{\alpha}\hat{a}_{\alpha}$$

Partition function:

$$Z = \int \prod_{\alpha} \frac{d\Phi^{*}_{\alpha}\, d\Phi_{\alpha}}{2\pi i}\, e^{-\sum_{\alpha}\Phi^{*}_{\alpha}\Phi_{\alpha}} \langle \Phi | \underbrace{e^{-\beta(\hat{H}-\mu\hat{N})}}_{e^{-\varepsilon(\hat{H}-\mu\hat{N})} \underbrace{\cdot}_{\mathbb{1} = \int \prod \frac{d\Phi^{*} d\Phi}{2\pi i} e^{-\sum\Phi^{*}\Phi} |\Phi\rangle\langle\Phi|} e^{-\varepsilon(\hat{H}-\mu\hat{N})} \underbrace{\cdot}_{\mathbb{1}=\ldots} \cdots \underbrace{\cdot}_{\mathbb{1}=\ldots} e^{-\varepsilon(\hat{H}-\mu\hat{N})}} | \Phi \rangle$$

$\beta \equiv \varepsilon M$

$(M \gg 1)$

$$= \int \prod_{k=0}^{M-1} \prod_{\alpha} \frac{d\Phi^{*}_{\alpha,k}\, d\Phi_{\alpha,k}}{2\pi i}\, e^{-\sum_{k=0}^{M-1}\sum_{\alpha}\Phi^{*}_{\alpha,k}\Phi_{\alpha,k}} \prod_{k=0}^{M-1} \underbrace{\langle \Phi_k | e^{-\varepsilon(\hat{H}-\mu\hat{N})} | \Phi_{k+1}\rangle}_{e^{-\varepsilon\langle\Phi_k|\hat{H}-\mu\hat{N}|\Phi_{k+1}\rangle} + \mathcal{O}(\varepsilon^2)}$$

where $\Phi_0 = \Phi_M = \Phi$.

Normal ordered operators: all $\hat{a}^\dagger_\alpha$ are left of all $\hat{a}_{\alpha'}$

$$\langle \Phi | A(\hat{a}^\dagger_\alpha, \hat{a}_\alpha) | \Phi' \rangle = A(\Phi^*_\alpha, \Phi'_\alpha)\, e^{\sum_\alpha \Phi^*_\alpha \Phi'_\alpha}$$

arbitrary normal-ordered function of $\hat{a}^\dagger_\alpha, \hat{a}_\alpha$

since $a_\alpha |\Phi'\rangle = \Phi'_\alpha |\Phi'\rangle$ and $\langle \Phi | a^\dagger_\alpha = \langle \Phi | \Phi_\alpha$.

NB: $\langle \phi_k | e^{-\varepsilon \tilde{H}} | \phi_{k+1} \rangle$
$= \langle \phi_k | \phi_{k+1} \rangle - \varepsilon \langle \phi_k | \tilde{H} | \phi_{k+1} \rangle$
$= e^{\sum_\alpha \phi^*_k \phi_{k+1}} \underbrace{\left(1 - \varepsilon \tilde{H}(\phi^*_k, \phi_{k+1})\right)}_{e^{-\varepsilon \tilde{H}(\phi^*_k, \phi_{k+1})}}$

Then:

$$Z = \lim_{M \to \infty} \int \prod_{k=0}^{M-1} \prod_\alpha \frac{d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}}{2\pi i}\, e^{-\sum_{k=0}^{M-1} \sum_\alpha \Phi^*_{\alpha,k} (\Phi_{\alpha,k} - \Phi_{\alpha,k+1})}$$
$$\times\, e^{-\sum_{k=0}^{M-1} \varepsilon \left[H(\Phi^*_{\alpha,k}, \Phi_{\alpha,k+1}) - \mu \sum_\alpha \Phi^*_{\alpha,k} \Phi_{\alpha,k+1} \right]}$$

$$=: \int_{\Phi_\alpha(0) = \Phi_\alpha(\beta)} \mathcal{D}\Phi^*_\alpha(\tau)\, \mathcal{D}\Phi_\alpha(\tau)\, e^{-S[\Phi^*_\alpha(\tau), \Phi_\alpha(\tau)]}$$

"functional integral"

with the "imaginary time" $\tau = \frac{k}{M} \beta$ and the <u>action</u>:

$$S = \int_0^\beta d\tau \left\{ \sum_\alpha \Phi^*_\alpha(\tau) (-\partial_\tau - \mu) \Phi_\alpha(\tau) + H[\Phi^*_\alpha(\tau), \Phi_\alpha(\tau)] \right\}$$

Remarks:

- $D\Phi^*_\alpha$ and $D\Phi_\alpha$ should be understood as the "sum" over all complex functions $\Phi_\alpha(\tau)$ that satisfy $\Phi_\alpha(0) = \Phi_\alpha(\beta)$
- Quantum number α labels states in the single-particle basis, e.g., momentum $\vec{q}$, position $\vec{x}$, lattice site i

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Example (nonrel. bosons of mass m interacting via $V(\vec{x}-\vec{y})$):

$$S = \int_0^\beta d\tau \int d^d\vec{x} \left[\Phi^*(\vec{x},\tau)\left(-\partial_\tau - \mu - \frac{\hbar^2 \vec{\nabla}^2}{2m}\right)\Phi(\vec{x},\tau) + \int d^d\vec{y}\, |\Phi(\vec{x},\tau)|^2 \, V(\vec{x}-\vec{y})\, |\Phi(\vec{y},\tau)|^2 \right]$$

Example ("Higgs" bosons interacting via $V(\vec{x}-\vec{y}) = \lambda\, \delta(\vec{x}-\vec{y})$):

$$S = \int_0^\beta d\tau \int d^d\vec{x} \left[\frac{1}{2}\Phi(\vec{x},\tau)(-\partial_\mu^2 + \underbrace{m^2}_{\text{"Higgs" mass}})\Phi(\vec{x},\tau) + \lambda\, \Phi(\vec{x},\tau)^4 \right],$$

where $(\partial_\mu) = \left(\frac{1}{c}\frac{\partial}{\partial\tau}, \vec{\nabla}\right)$, $\mu = 0, \dots, d$.

Example (Dirac fermion coupled to order-parameter field):

e.g., quarks — e.g., mesons

$$S = \int_0^\beta d\tau \int d^d\vec{x} \left[\bar{\Psi}(\vec{x},\tau)\gamma^\mu \partial_\mu \Psi(\vec{x},\tau) + \frac{1}{2}\Phi(\vec{x},\tau)(-\partial_\mu^2 + m^2)\Phi(\vec{x},\tau) + g\, \Phi(\vec{x},\tau)\bar{\Psi}(x,\tau)\Psi(\vec{x},\tau) \right]$$

g: Yukawa coupling

where $\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}\mathbb{1}$ Dirac matrices

Fourier transform:

$$\Phi(\vec{r},\tau) = \frac{1}{\beta} \int \frac{d\vec{k}}{(2\pi)^d} \sum_{\omega_n = \frac{2\pi n}{\beta}} \Phi(\vec{k},\omega_n)\, e^{i\vec{k}\cdot\vec{r} + i\omega_n \tau} \quad , n = 0, \pm 1, \pm 2, \dots$$

Matsubara frequencies

Action (nonrel. bosons with $V=0$):

$$S = \frac{1}{\beta} \int \frac{d^d\vec{k}}{(2\pi)^d} \sum_{\omega_n} \left(-i\omega_n + \frac{\hbar^2 k^2}{2m} - \mu\right) |\Phi(\vec{k},\omega_n)|^2$$

Propagator:

$$G(\omega_n, k) = \frac{\beta}{-i\omega_n + \frac{\hbar^2 k^2}{2m} - \mu} = \beta \, \frac{+i\omega_n + \frac{\hbar^2 k^2}{2m} - \mu}{\omega_n^2 + \left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2}$$

Remarks:

- For $T>0$ all modes with $\omega_n \neq 0$ ($|n| \geq 1$) have a finite gap $\propto T$
  $\Rightarrow$ cannot contribute to a nonanalyticity in $Z = \int \mathcal{D}\Phi \mathcal{D}\Phi^* e^{-S}$
  $\Rightarrow$ "non-critical modes"
- For $T>0$ system can be understood as having finite extent β in imaginary time $\tau \in [0,\beta)$
  $\Rightarrow$ correlation time τ_c at criticality : $\tau_c \gg \beta$
  $\Rightarrow$ critical configurations $\Phi(\tau) \approx \Phi(0)$ for all $\tau \in [0,\beta)$.
  $\Rightarrow$ only $\omega_{n=0} = 0$ mode contributes to critical properties at finite T
- Statics and dynamics decouple at $T>0$

- For $T=0$ we have $\tau \in [0,\infty)$ and ω becomes continuous:
$$\frac{1}{\beta}\sum_{\omega_n} \rightarrow \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}$$

$\Rightarrow$ continuum of small-ω modes contribute at a quantum critical point

$\Rightarrow$ quantum critical behavior in d dimensions (often) resembles classical critical behavior in $d+z$ dimensions
("quantum-to-classical mapping", see Chapter 6)

3.2 Mean-field approximation: Landau theory

Assume critical point at $T>0$: retain only critical ($\omega_0=0$) modes
Effective action (bosons with $V(\vec{x}-\vec{y}) = \lambda\,\delta(\vec{x}-\vec{y})$):

$$S[\Phi] = \beta \int d^d\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\nabla}\Phi(\vec{r})|^2 - \mu |\Phi(\vec{r})|^2 + \lambda |\Phi(\vec{r})|^4 \right]$$

Remark:
Using $\Phi = \phi_1 + i\phi_2$ with , $a=1,2$ real scalar field, the action reads
$$S[\vec{\phi}] = \beta \int d^d\vec{r} \left[\sum_{a=1}^{N} \frac{\hbar^2}{2m} (\vec{\nabla}\phi^a)^2 - \sum_{a=1}^{N} \mu\, \phi^a\phi^a + \lambda \left(\sum_{a=1}^{N} \phi^a\phi^a\right)^2 \right]$$
for $N=2$.

"Ginzburg-Landau-Wilson theory"
"O(N) model"
"ϕ^4 theory"

Partition function:

$$Z = \int \mathcal{D}\vec{\phi}\; e^{-S[\vec{\phi}]}$$

will be dominated by configurations that minimize $S[\vec{\phi}]$

Saddle-point approximation (= mean-field approximation)

$$Z \approx e^{-S[\vec{\phi}_0]} \quad \text{with} \quad \left.\frac{\delta S}{\delta \vec{\phi}}\right|_{\vec{\phi}_0} = 0 \quad \text{and} \quad \left.\frac{\delta^2 S}{\delta\vec{\phi}\,\delta\vec{\phi}^T}\right|_{\vec{\phi}_0} \text{ pos. definite}$$

where we have neglected fluctuations $S[\phi] - S[\phi_0] = \frac{1}{2}\,\delta\vec{\phi}^T \cdot \frac{\delta^2 S}{\delta\phi\,\delta\vec{\phi}^T}\,\delta\vec{\phi} + \mathcal{O}(\delta\phi^3)$

Free energy:

$$F = -k_B T \ln Z$$

$$= k_B T\, S[\vec{\phi}_0]$$

$\Rightarrow$ recover Landau-Ginzburg theory with parameters

$$(a, b, \xi_0^2) \propto \left(-2\mu, 4\lambda, \frac{\hbar^2}{2m}\right)$$

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