2. Functional Field Integrals

Main Goals:
- Develop tools that allow us to obtain an intuitive understanding of quantum many-body problems by keeping the classical limit visible.
- Efficient representation that provides a platform for the non-perturbative solution of quantum-mechanical problems.

Further reading: Altland & Simons chapter 2+3

2.1 Feynman's path integrals in single-particle quantum mechanics

Consider a single-particle Hamiltonian in D=1 of the form

$$\hat{H} = T(\hat{p}) + V(\hat{x}).$$

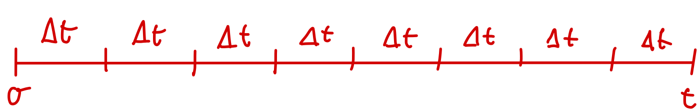
Basic idea of the path integral formalism: Compute the transition amplitude

$$\langle x_f | e^{-\frac{i}{\hbar}\hat{H}t} | x_i \rangle$$

as a sum over all possible trajectories from $|x_i\rangle \to |x_f\rangle$.

The transition amplitude is (generically) difficult to evaluate as the exponential does not factorize.

Feynman's great idea: Divide the total time into N small intervals $\Delta t = \frac{t}{N}$:



The time evolution for the entire interval is $e^{-i\hat{H}t} = \left(e^{-i\hat{H}\Delta t}\right)^N$.

We now insert resolutions of the identity $\mathbb{1} = \int dx\, |x\rangle\langle x|$ after each time step and obtain

$$\langle x_f | e^{-i\hat{H}t} | x_i\rangle = \int \prod_{n=1}^{N-1} dx_n \, \langle x_f | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_{N-1}\rangle \langle x_{N-1} | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_{N-2}\rangle \cdots$$
$$\cdots \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_i\rangle \qquad (2.1)$$

This is just a formal rewriting but represents the basis for useful approximations! Let us consider a single time step Δt:

$$\langle x_{n+1} | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | x_n\rangle = \langle x_{n+1} | e^{-\frac{i}{\hbar}[T(\hat{p}) + V(\hat{x})]\Delta t} | x_n \rangle$$

$e^{\varepsilon\hat{X}} \cdot e^{\varepsilon\hat{Y}} = e^{\varepsilon\hat{X}+\varepsilon\hat{Y}+\underline{\frac{\varepsilon^2}{2}[X,Y]+\cdots}}$ $\longrightarrow$ $\overset{BCH}{=} \langle x_{n+1} | e^{-\frac{i}{\hbar}T(\hat{p})\Delta t} e^{-\frac{i}{\hbar}V(\hat{x})\Delta t} + \mathcal{O}(\Delta t^2) | x_n \rangle$

$\mathbb{1} = \int dp\, |p\rangle\langle p|$ $\curvearrowright$ $= \int dp_{n+1} \underbrace{\langle x_{n+1} | p_{n+1}\rangle}_{\frac{e^{\frac{i}{\hbar}p_{n+1}x_{n+1}}}{\sqrt{2\pi\hbar}}} \underbrace{\langle p_{n+1} | x_n\rangle}_{\frac{e^{-\frac{i}{\hbar}p_{n+1}x_n}}{\sqrt{2\pi\hbar}}} e^{-\frac{i}{\hbar}T(p_{n+1})\Delta t} e^{-\frac{i}{\hbar}V(x_n)\Delta t} + \mathcal{O}(\Delta t^2)$

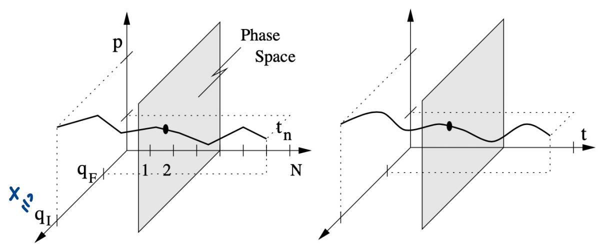
$$= \int \frac{dp_{n+1}}{2\pi\hbar} e^{\frac{i}{\hbar}p_{n+1}(x_{n+1}-x_n)} e^{-\frac{i}{\hbar}T(p_{n+1})\Delta t} e^{-\frac{i}{\hbar}V(x_n)\Delta t} + \mathcal{O}(\Delta t^2).$$

Inserting this into Eq. (2.1) and ignore $\mathcal{O}(\Delta t^2)$, we find

$\langle x_f | e^{-\frac{i}{\hbar}\hat{H}t} | x_i \rangle \simeq$

$$\int\limits_{x_N = x_f,\, x_0 = x_i} \prod_{n=1}^{N-1} dx_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \exp\left\{-\frac{i}{\hbar}\Delta t \sum_n \left[T(p_{n+1}) + V(x_n) - \sum_{n=1}^{N} p_{n+1}(x_{n+1}-x_n)/\Delta t\right]\right\}$$

At each time step, we integrate over the classical coordinates x_n, p_n:



Contributions from trajectories, where $(x_{n+1}-x_n)\cdot p_{n+1} > \hbar$ can be neglected (random phase cancellation) $\rightsquigarrow$ continuum limit

$$\int\limits_{x_N = x_f,\, x_0 = x_i} \prod_{n=1}^{N-1} dx_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \quad \rightsquigarrow \quad \int\limits_{\substack{x(t)=x_f \\ x(0)=x_i}} D(x,p)$$

$$\Delta t \cdot \sum_{n=0}^{N-1} \quad \rightsquigarrow \quad \int_0^t dt'$$

$$p_{n+1}(x_{n+1}-x_n)/\Delta t \quad \rightsquigarrow \quad p\cdot\dot{x}\,\big|_{t'=t_n}$$

$$T(p_{n+1}) + V(x_n) \quad \rightsquigarrow \quad H(x,p)\,\big|_{t'=t_n}$$

Taking the above expressions, we obtain the Hamiltonian formulation of the Feynman path integral:

$$\boxed{\langle x_f | e^{-\frac{i}{\hbar}\hat{H}t} | x_i \rangle = \int_{\substack{x(t)=x_f \\ x(0)=x_i}} D(x,p) \exp\Big\{ \overbrace{\frac{i}{\hbar} \int_0^t dt' \, [\underbrace{p\cdot\dot{x} - H(p,x)}_{\text{Lagrangian}}]}^{\text{Action } S(p,x)} \Big\}}$$

⇝ Quantum transition amplitude as integral over all possible phase space trajectories with given boundary conditions and weighted by the classical action.

For the case of a free particle with $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, we can integrate over p_n explicitly:

$$\langle x_f | e^{-\frac{i}{\hbar}Ht} | x_i \rangle = \int_{\substack{x(t)=x_f \\ x(0)=x_i}} Dx \exp\Big\{ -\frac{i}{\hbar} \int_0^t dt' \, V(x) \Big\} \underbrace{\int Dp \exp\Big\{ -\frac{i}{\hbar} \int dt' \left(\frac{p^2}{2m} - p\cdot\dot{x} \right) \Big\}}_{\text{Gaussian integral over } p}$$

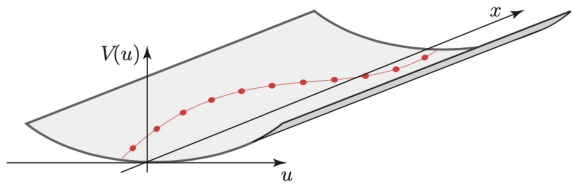
Using $\frac{p^2}{2m} - p\cdot\dot{x} \to \frac{1}{2m}(p - m\dot{x})^2 - \frac{1}{2}m\dot{x}^2$ and $\boxed{\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}}}$, we obtain the Lagrangian formulation:

$$\boxed{\langle x_f | e^{-\frac{i}{\hbar}Ht} | x_i \rangle = \int_{\substack{x(t)=x_f \\ x(0)=x_i}} D(x) \exp\Big\{ \frac{i}{\hbar} \int_0^t dt' \left(\frac{m\dot{x}^2}{2} - V(x) \right) \Big\}}$$

with $D(x) = \lim_{N\to\infty} \left(\frac{N\cdot m}{it2\pi\hbar} \right)^{N/2} \prod_{n=1}^{N-1} dx_n$.

Connection of the path integral to classical mechanics

Consider a flexible string held under constant tension and confined to a "gutter" potential:



Potential energy

Line tension: First consider the segment $x, x+dx$

$$dV_T = \underset{\substack{\uparrow \\ \text{Tension}}}{T}\left[\sqrt{dx^2+du^2}-dx\right] \simeq T\,dx\,(\partial_x u)^2/2$$

du

dx

$$\rightsquigarrow V_T[\partial_x u] = \int dV_T = \frac{1}{2}\int_0^L dx\; T\left[\partial_x u(x)\right]^2$$

External potential: $\rightsquigarrow V_{ext}[u] = \int_0^L dx\; V[u(x)]$

$$\rightsquigarrow H = V_T + V_{ext} = \int_0^L dx \left\{\frac{T}{2}(\partial_x u)^2 + V(x)\right\}$$

The canonical partition function reads

$$Z_{\text{Class. String}} = \operatorname{tr} e^{-\beta H} = \int D u(x)\, \exp\left\{-\beta\int_0^L dx\left[\frac{T}{2}(\partial_x u)^2 + V(x)\right]\right\}$$

Let us now compare this partition function to the Lagrangian formulation of the path integral.

Wick rotation $t \to -i\tau$ — imaginary time evolution

$$\int_0^t i\,dt' \left(\partial_{t'} x\right)^2 \to -\int_0^\tau d\tau' \left(\partial_{\tau'} x\right)^2$$

$$-\int_0^t i\,dt'\, V(x) \to -\int_0^\tau d\tau'\, V(x)$$

This leads to

$$Z_{\text{QM particle}} = \int_{\substack{\text{boundary}\\ \text{conditions}}} Dx\, \exp\left\{ -\frac{1}{\hbar} \int_0^\tau d\tau' \left[\frac{m}{2} \left(\partial_{\tau'} x\right)^2 + V(x) \right] \right\}$$

We can make some useful observations:

(a) Classical partition function of a one-dimensional system coincides with quantum mechanical particle with $t \to -i\tau$, where $\hbar$ plays the role of the temperature.

> More generally: Path integral of a D-dimensional quantum system corresponds to a D+1 dimensional classical system.

(b) Quantum partition function is given by

$$Z_Q = \mathrm{tr}\left(e^{-\beta \hat{H}}\right) = \int dx \, \langle x | e^{-\beta \hat{H}} | x \rangle .$$

$\rightsquigarrow$ Can be interpreted as the dynamical transition amplitude $\langle x | e^{-i\hat{H}t/\hbar} | x \rangle$, evaluated at an imaginary time $t = -i\hbar\beta$.

(c) In the semi-classical limit with $\hbar \to 0$, the path integral is dominated by stationary configurations of the action

$$S = \int dt \; \mathcal{L}(x, \dot{x}, t)$$

$\rightsquigarrow$ Classical equations of motion follow from $\frac{\delta S}{\delta x(t)} = 0 \;\; \forall t$

this approximation is called: saddle point approximation or stationary phase approximation

$$\forall \tilde{t}: \quad 0 = \frac{\delta S}{\delta x(\tilde{t})} = \int dt \; \frac{\partial \mathcal{L}}{\partial x(t)} \underbrace{\frac{\delta x(t)}{\delta x(\tilde{t})}}_{\delta(t-\tilde{t})} + \frac{\partial \mathcal{L}}{\partial \dot{x}(t)} \underbrace{\frac{\delta \dot{x}(t)}{\delta x(\tilde{t})}}_{\partial_t \frac{\delta x(t)}{\delta x(\tilde{t})}} =$$

$$= \int dt \left[\frac{\partial \mathcal{L}}{\partial x(t)} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}(t)} \right) \right] \delta(t - \tilde{t}) = 0$$

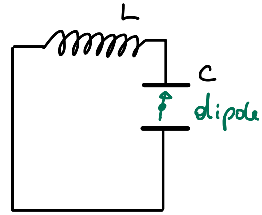
$$\Rightarrow \quad \frac{\partial \mathcal{L}}{\partial x(t)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{x}(t)} = 0 \qquad \text{Euler-Lagrange}$$

Note: Quantum mechanics has not disappeared! It is not just the saddle point that matters but rather the fluctuations around it.

2.2 Effective theories

Goal of quantum many-body physics:
develop effective theories

extremely important concept.



Classical example:
CL circuit with dipole in capacitor

Action for dipole in capacitor

$$S_{dip} = \int dt \left[\frac{m}{2} \dot{x}^2 - \frac{m\omega_0^2}{2} x^2 \right]$$

Action for CL-circuit

$$S_{CL} = \int dt \, \frac{1}{2g} \left(\dot{\mathcal{E}}^2 - \omega_{CL}^2 \, \mathcal{E}^2 \right)$$

$\mathcal{E}$ ... electric field

$\omega_{LC}^2 = \frac{1}{LC}$

inductance, capacitance

Coupling between dipole and field: $\int dt \, e x \mathcal{E}$

The coupled system is described by

$$Z = \int D\mathcal{E} Dx \; e^{i S_{CL} + i S_{dip} + i \int dt \, e x \mathcal{E}}$$

We now assume $\omega_0 \gg \omega_{CL}$ $\rightsquigarrow$ Electric field is perturbed by the presence of the dipole $\rightsquigarrow$ integrate out high frequency motion of dipole.

$$Z = \int D\mathcal{E} \; e^{i S_{CL}[\mathcal{E}] + i S_{int}[\mathcal{E}]}$$

$$e^{iS_{int}(\mathcal{E})} = \int \mathcal{D}x \; e^{i\int dt \left[\frac{m}{2}(\partial_t x)^2 - \frac{m\omega_0^2}{2} x^2 + e x \mathcal{E}\right]}$$

$$\overset{\text{integration by parts}}{=} \int \mathcal{D}x \; e^{-i\int dt \left[\frac{m}{2} x (\partial_t^2 + \omega_0^2) x - e x \mathcal{E}\right]}$$

$$= \mathcal{N} \; e^{i \int dt \frac{e^2}{2m} \mathcal{E} (\partial_t^2 + \omega_0^2)^{-1} \mathcal{E}}$$

↳ Normalization factor (unimportant for now)

Remark: Gaussian integrals with matrices.

In the last step, we have performed the Gaussian integral viewing $\partial_t^2 + \omega_0^2$ as a matrix.

Remember: we took the "artificial" continuum limit when we derived the path integral. In the derivation we rather had terms like: $(x_{n+1} - x_n)/\Delta t \approx \partial_t x$

therefore we can use the formula for Gaussian integrals:

$$\int dx_1 \ldots dx_{N-1} \; e^{-i \sum_{j,k=1}^{N-1} \frac{1}{2} x_j M_{jk} x_k} = \sqrt{\frac{(2\pi)^{N-1}}{\mathrm{Det}(+iM)}}$$

In this formula, we have reintroduced the discrete time $\sim \sum_{jk}$

One can proof this relation by diagonalizing $MU = UD$ and transforming the coordinates $U^\dagger x = y$.

We can also obtain a related formula for shifted integrals

$$\int dx_1 \ldots dx_{N-1} \; e^{-i \sum_{j,k=1}^{N-1} \frac{1}{2} x_j M_{jk} x_k + i \sum_{j=1}^{N-1} a_j x_j} = \sqrt{\frac{(2\pi)^{N-1}}{\mathrm{Det}(iM)}} \cdot e^{\frac{1}{2} i \sum_{j,k=1}^{N-1} a_j (M^{-1})_{jk} a_k}$$

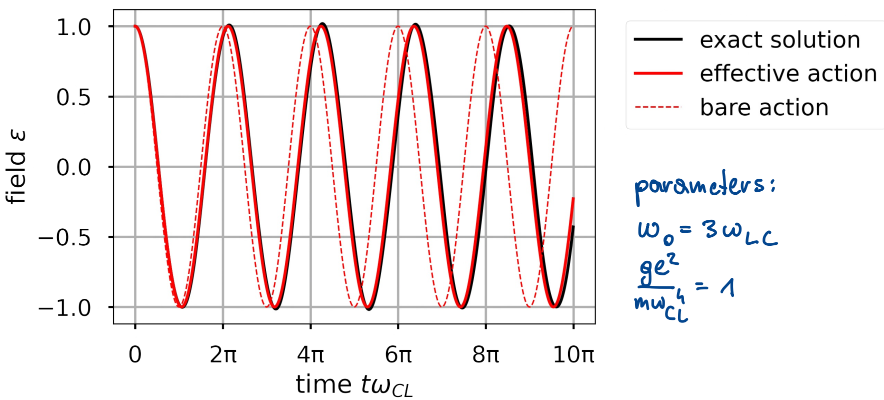
After integrating out the fast dipole motion, we obtain the effective Lagrangian: $S_0(\mathcal{E}) + S_{int}(\mathcal{E}) = \int dt\, \mathcal{L}_{eff}$

$$\mathcal{L}_{eff} = \frac{1}{2g}\left(\dot{\mathcal{E}}^2 - \omega_{CL}^2 \mathcal{E}^2\right) + \frac{e^2}{2m} \mathcal{E} \left(\partial_t^2 + \omega_0^2\right)^{-1} \mathcal{E}$$

Since ω_0 is by assumption the largest scale $(\partial_t^2 + \omega_0^2)^{-1} \approx \frac{1}{\omega_0^2}$

$$\mathcal{L}_{eff} = \frac{1}{2g}\left(\dot{\mathcal{E}}^2 - \omega_{CL}^{*2} \mathcal{E}^2\right) \qquad \omega_{CL}^* = \sqrt{\omega_{CL}^2 + \frac{ge^2}{m\omega_0^2}}$$

After integrating out the high frequency motion of the dipole, the low frequency electric field is described by a simple effective Lagrangian.



parameters:

$\omega_0 = 3\omega_{LC}$

$\frac{ge^2}{m\omega_{CL}^4} = 1$

2.3 Bosonic and Fermionic coherent states

The direct generalization of the Feynman path integral to many-body systems is problematic due to particle indistinguishability and statistics.

Utilize the concept of second quantization

⇝ Requires eigenstates of the Fock space operators $\hat{a}_i$ and $\hat{a}_i^\dagger$

⇝ These eigenstates exist: Coherent states!

2.3.1 Bosonic coherent states

What are the eigenstates of Fock space operators $\hat{a}_i$ and $\hat{a}_i^\dagger$?

An eigenstate $|\phi\rangle$ in Fock space can be expanded as

$$|\phi\rangle = \sum_{n_1, n_2, \dots} C_{n_1, n_2, \dots} \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(\hat{a}_2^\dagger)^{n_2}}{\sqrt{n_2!}} \cdots \underbrace{|0\rangle}_{\text{Vacuum}} = \sum_{n_1, n_2 \dots} C_{n_1, n_2 \dots} |n_1, n_2 \dots\rangle$$

An eigenstate of $\hat{a}_j^\dagger$ with $\hat{a}_j^\dagger |\phi\rangle = \phi_j |\phi\rangle$ cannot exist: If the minimum occupation of $|\phi\rangle$ is n_0, then the minimum occupation of $\hat{a}_j^\dagger |\phi\rangle$ is $n_0 + 1$.

However, an eigenstate of $\hat{a}_j$ exists and is given by

$$\boxed{|\phi\rangle = \exp\left(\sum_j \phi_j \hat{a}_j^\dagger\right) |0\rangle} \quad (\phi \mathrel{\hat{=}} \{\phi_j\})$$

coherent state

Proof: Since $\hat{a}_j$ commute with all $\hat{a}_k^+$ for $k \neq j$, we focus on one element j $(\hat{a} = \hat{a}_j)$

$$\hat{a}\,\exp(\phi\,\hat{a}^+)\,|0\rangle = [\hat{a}, \exp(\phi\cdot\hat{a}^+)]\,|0\rangle$$

Expand $\exp(\cdot\cdot)$.

$$= \sum_{n=0}^{\infty} \frac{\phi^n}{n!}\,[\hat{a}, (\hat{a}^+)^n]\,|0\rangle$$

$$\overset{(*)}{=} \sum_{n=1}^{\infty} \frac{n\cdot\phi^n}{n!}\,(\hat{a}^+)^{n-1}\,|0\rangle$$

$$= \phi\cdot\exp(\phi\,\hat{a}^+)\,|0\rangle$$

(*) $\hat{a}(\hat{a}^+)^n = \hat{a}\hat{a}^+(\hat{a}^+)^{n-1} = (1+\hat{a}^+\hat{a})(a^+)^{n-1} = (\hat{a}^+)^{n-1} + \hat{a}^+\hat{a}(\hat{a}^+)^{n-1} \rightsquigarrow [\hat{a}, (\hat{a}^+)^n] = n(a^+)^{n-1}$

Properties of the coherent state: $a_j|\phi\rangle = \phi_j|\phi\rangle$

complex conjugation

(i) Hermitian conjugation: $\forall j$: $\langle\phi|\hat{a}_j^+ = \langle\phi|\bar{\phi}_j$

(ii) The creation operator acts as derivative: $\forall j$: $a_j^+|\phi\rangle = \partial_{\phi_j}|\phi\rangle$

$$\hat{a}^+ e^{\phi\hat{a}^+}|0\rangle = \sum_{n=0}^{\infty}\frac{\phi^n}{n!}(a^+)^{n+1}|0\rangle \overset{n\to m-1}{=} \sum_{m=1}^{\infty}\frac{\phi^{m-1}}{(m-1)!}(a^+)^m|0\rangle = \partial_\phi \sum_{m=0}^{\infty}\frac{\phi^m}{m!}(a^+)^m|0\rangle = \partial_\phi|\phi\rangle$$

(iii) Overlap of coherent states: $\langle\theta| = \langle 0|e^{\sum_j \bar{\theta}_j \hat{a}_j}$

$$\rightsquigarrow \langle\theta|\phi\rangle = \langle 0|e^{\sum_j \bar{\theta}_j\hat{a}_j}|\phi\rangle = e^{\sum_j \bar{\theta}_j\phi_j}\underbrace{\langle 0|\phi\rangle}_{1}$$

$$= e^{\sum_j \bar{\theta}_j\phi_j}$$

Thus the states are not orthogonal!

(iv) Norm of coherent states: $\langle\phi|\phi\rangle = e^{\sum_j \bar{\phi}_j \phi_j}$

(v) Coherent states form an (over) complete set of basis states for the Fock space. Comment: coherent states are not orthogonal
$\rightsquigarrow$ overcounting is compensated by $e^{-\sum_i \bar{\phi}_i \phi_i}$.

$$\boxed{\int \prod_j \frac{d\bar{\phi}_j d\phi_j}{\pi} \cdot e^{-\sum_j \bar{\phi}_j \phi_j} |\phi\rangle\langle\phi| = \mathbb{1}_{\mathcal{F}}}$$

(with $d\bar{\phi}_j d\phi_j = d\,\mathrm{Re}\,\phi_j \, d\,\mathrm{Im}\,\phi_j$)

Unity in Fock space

Proof using Schur's lemma, i.e., show that the expression commutes with all creation and annihilation operators, which implies that it has to be proportional to the identity.

Proof:

$$a_j \int d\bar{\phi}\, d\phi\; e^{-\sum_i \bar{\phi}_i \phi_i} |\phi\rangle\langle\phi|$$

$$= \int d\bar{\phi}\, d\phi\; e^{-\sum_i \bar{\phi}_i \phi_i} \phi_j |\phi\rangle\langle\phi|$$

$$= -\int d\bar{\phi}\, d\phi \left(\partial_{\bar{\phi}_j} e^{-\sum_i \bar{\phi}_i \phi_i} |\phi\rangle\right)\langle\phi|$$

$$\overset{\text{integration by parts}}{=} \int d\bar{\phi}\, d\phi\; e^{-\sum_i \bar{\phi}_i \phi_i} |\phi\rangle \underbrace{\left(\partial_{\bar{\phi}_j} \langle\phi|\right)}_{\langle\phi| a_j}$$

$$\left[\; \partial_{\phi_j} |\phi\rangle = a^\dagger |\phi\rangle \qquad \partial_{\bar{\phi}_j} \langle\phi| = \langle\phi| a \;\right]$$

$$\left[a_j \,,\, \int d(\bar\phi,\phi)\, e^{-\sum_i \bar\phi_i \phi_i} |\phi\rangle\langle\phi| \right] = 0$$

taking the complex conjugate we see that the integral also commutes with $a_j^\dagger$.

$$\rightsquigarrow \quad \int d(\bar\phi,\phi)\, e^{-\sum_i \bar\phi_i \phi_i} |\phi\rangle\langle\phi| \propto \mathbb{1}$$

(vi) Gaussian integrals that will be useful for dealing with coherent states:

$$\boxed{\begin{array}{l}\text{1-Dimensional (complex)} \\ \dfrac{1}{\pi}\displaystyle\int d\bar\phi\, d\phi\; e^{-\bar\phi w \phi + \bar u \phi + \bar\phi v} = \dfrac{1}{w} e^{\bar u v / w}\end{array}}$$

$\bar\phi \to \bar\phi - \bar u/w$

$\phi \to \phi - v/w$

$-(\bar\phi - \frac{\bar u}{w}) w (\phi - \frac{v}{w}) =$

$-\bar\phi w \phi + \bar u \phi + \bar\phi v - \frac{\bar u v}{w}$

$e^{-\bar\phi w \phi + \bar u \phi + \bar\phi v} =$

$e^{-(\bar\phi - \frac{\bar u}{w}) w (\phi - \frac{v}{w}) + \frac{\bar u v}{w}}$

ϕ are vectors

$$\boxed{\begin{array}{l}\text{N-Dimensional (complex)} \\ \displaystyle\int d(\bar\phi,\phi)\, e^{-\bar\phi^T A \cdot \phi + \bar u^T \cdot \phi + \bar\phi^T \cdot v} = \det A^{-1}\, e^{\bar u^T A^{-1} v}\end{array}}$$

with $d(\bar\phi,\phi) = \prod_j \frac{1}{\pi} \underbrace{d\bar\phi_j\, d\phi_j}_{d\,\mathrm{Re}\,\phi_j\; d\,\mathrm{Im}\,\phi_j}$. A is a matrix (A needs to contain a pos. def. hermitian part)

With the above definitions, we can construct the path integral for bosonic systems!

(vii) Normalization is fixed by taking the vacuum expectation value:

$$\langle 0|\mathbb{1}|0\rangle = \int d(\bar\phi,\phi)\, e^{-\sum_j \bar\phi_j \phi_j} \langle 0|\phi\rangle\langle\phi|0\rangle$$

$$= \int d(\bar\phi,\phi)\, e^{-\sum_j \bar\phi_j \phi_j} = \det \mathbb{1}^{-1} = 1$$

(viii) Expectation value of normal ordered operators $(\hat{a}^+ \dots \hat{a})$

$$\frac{\langle \phi | : \hat{O}(\hat{a}^+, \hat{a}) : | \phi \rangle}{\langle \phi | \phi \rangle} = O(\bar{\phi}, \phi)$$

(ix) Trace of an operator

$$\mathrm{tr}\,\hat{O} = \sum_n \langle n | \hat{O} | n \rangle = \sum_n \int d(\bar{\phi}, \phi) \cdot e^{-\sum \bar{\phi}_j \phi_j} \langle n | \phi \rangle \langle \phi | \hat{O} | n \rangle$$

complete set   insert identity

$$= \int d(\bar{\phi}, \phi)\, e^{-\sum \bar{\phi}_j \phi_j} \langle \phi | \hat{O} | \phi \rangle$$

2.3.2 Fermionic coherent states

In analogy to the bosonic case, we seek a state $|\eta\rangle$ such that $\hat{c}_j |\eta\rangle = \eta_j |\eta\rangle$ for fermionic operators $\hat{c}_j$.

We have to take into account that the fermionic operators anti-commute. For some $j \neq k$, we find

$$\hat{c}_j \hat{c}_k |\eta\rangle = \hat{c}_j \eta_k |\eta\rangle = \eta_j \eta_k |\eta\rangle$$

$$= -\hat{c}_k \hat{c}_j |\eta\rangle = -c_k \eta_j |\eta\rangle = -\eta_k \eta_j |\eta\rangle$$

$\rightsquigarrow$ η cannot be a regular complex number!

$\rightsquigarrow$ η need to anti-commute among each other and with the $\hat{c}$-operators.

Solution: Introduce Grassmann algebra

$$\eta_i \eta_j = -\eta_j \eta_i \qquad \eta_i c_j = -c_j \eta_i$$

$\rightsquigarrow$ anti-commuting numbers (not operators; since they don't act on states)

Besides the anticommutativity, the Grassmann Variables have the following properties:

(i) $\eta_j^2 = 0$ (but note that these are <u>not</u> operators)

(ii) Elements η_j can be added and multiplied by complex numbers:

$$d + d_i \cdot \eta_i + d_j \cdot \eta_j \quad \text{with } d, d_i, d_j \in \mathbb{C}$$

(iii) Differentiation : $\partial_{\eta_i} \eta_j = \delta_{ij}$ (note the ordering $\partial_{\eta_i} \eta_j \eta_i = -\eta_j \partial_{\eta_i} \eta_i = -\eta_j$ for $i \neq j$)

(iv) Integration : $\int d\eta_j = 0$, $\int d\eta_j \, \eta_j = 1$ (i.e., differentiation and integration have the same effect.)

Example : $\int d\eta \, f(\eta) = \int d\eta \left[f_0 + f_1 \eta \right] = f_1 = \partial_\eta f(\eta) \big|_{\eta = 0}$

Taylor expansion ends here since $\eta^2 = 0$.

Reason: Linearity and invariant to shifts of integration variable

- $\int d\eta \, a \, f(\eta) = a \int d\eta \, f(\eta) = a \, f_1$
- $\int d\eta \, f(\eta) = \int d\eta \, f(\eta + \gamma) = \int d\eta \, (f_0 + f_1 \gamma) + f_1 \eta = f_1$

(v) Gaussian integration for Grassmann variables

$$\boxed{\begin{aligned}
&\int d\bar{\eta} \, d\eta \, e^{-\bar{\eta} a \eta} = a \\
&\int d(\bar{\eta}, \eta) \, e^{-\bar{\eta}^T A \eta} = \det A, \text{ with } d(\bar{\eta}, \eta) = \prod_{i=1}^{N} d\bar{\eta}_i \, d\eta_i \\
&\int d(\bar{\eta}, \eta) \, e^{-\bar{\eta}^T A \eta + \bar{\nu}^T \eta + \bar{\eta} \nu} = \det A \, e^{\bar{\nu}^T A^{-1} \nu}
\end{aligned}}$$

With the above preliminaries, we can now introduce the Fermionic coherent states:

$$\boxed{|\eta\rangle = \exp\left(-\sum_j \eta_j \hat{c}_j^\dagger\right)|0\rangle} \qquad (\eta = \{\eta\}) \quad , \text{ Grassmann Variables.}$$

Properties:

(i) These are eigenstates of the fermionic annihilation operators

$$\hat{c}_j|\eta\rangle = c_j(1-\eta_j c_j^\dagger)|0\rangle = \eta_j c_j c_j^\dagger|0\rangle = \eta_j |0\rangle$$

$$= \eta_j (1-\eta_j c_j^\dagger)|0\rangle = \eta_j |\eta\rangle$$

(ii) Adjoint : $\langle\eta| = \langle 0| e^{-\sum_j \hat{c}_j \bar{\eta}_j} = \langle 0| e^{+\sum \bar{\eta}_j \hat{c}_j}$ ($\bar{\eta}_j$ is not complex conj.. ~ different algebra).

(iii) Overlap $\langle\eta|\phi\rangle = \langle 0| e^{-\sum_j \hat{c}_j \bar{\eta}_j}|\phi\rangle = e^{\sum_j \bar{\eta}_j \phi_j}$

(iv) Completeness relation $\int \prod_j d\bar{\eta}_j d\eta_j \, e^{-\sum_j \bar{\eta}_j \eta_j} |\eta\rangle\langle\eta| = \mathbb{1}_{\mathcal{F}}$ (proof like the bosonic case)

(v) $c_i^\dagger|\eta\rangle = -\partial_\eta |\eta\rangle$

Trace formula for an operator $\hat{O}$ with <u>even number</u> of $c, c^\dagger$: ↙ many-body state $c^\dagger c^\dagger c^\dagger|0\rangle$

$$\mathrm{tr}\,\hat{O} = \sum_n \int d(\bar{\eta}\,\eta)\, e^{-\sum_j \bar{\eta}_j \eta_j} \langle n|\hat{O}|\eta\rangle\langle\eta|n\rangle$$

$$= \int d(\bar{\eta}\,\eta)\, e^{-\sum_j \bar{\eta}_j \eta_j} \langle -\eta|\hat{O}|\eta\rangle$$

Note that $\langle -\eta|\hat{O}|\eta\rangle$ is a function of Grassmann variables

Proof of the trace formula for fermions:

$c_1^\dagger c_2^\dagger \cdots c_n^\dagger |0\rangle \qquad \langle 0| c_n c_{n-1} \cdots c_1$

$$\langle \eta | n \rangle = \bar\eta_1 \bar\eta_2 \cdots \bar\eta_n \quad , \quad \langle n | \eta \rangle = \eta_n \eta_{n-1} \cdots \eta_1$$

"move" as pair.

$$\langle n|\eta\rangle\langle\eta|n\rangle = \eta_n \cdots \eta_2 \underbrace{\eta_1 \bar\eta_1} \bar\eta_2 \cdots \bar\eta_n$$

anti-commute

$$= \eta_1\bar\eta_1 \, \eta_2\bar\eta_2 \cdots \eta_n\bar\eta_n$$

$(-\bar\eta_{n-1})(-\bar\eta_n)\eta_n\eta_{n-1}$

$$= (-\bar\eta_1\eta_1)(-\bar\eta_2\eta_2)\cdots(-\bar\eta_{n-1}\eta_{n-1})(-\bar\eta_n\eta_n)$$

$$= (-\bar\eta_1)\cdots(-\bar\eta_{n-1})(-\bar\eta_n)\,\eta_n\eta_{n-1}\cdots\eta_1$$

$$= \langle -\eta|n\rangle\langle n|\eta\rangle$$

Note that fermion coherent states are not contained in the Fock space (η are not complex numbers) $\rightsquigarrow$ They are not observable and there are no classical fields of fermions. Still, fermion coherent states are useful for computations and to formally unify the many-fermion and many-boson problem.

η_i makes only sense under an integral or diff.

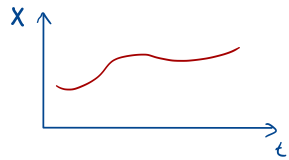
2.4 Functional field integral for the partition function

Concept of the functional field integral:

Degrees of freedom | Path integral

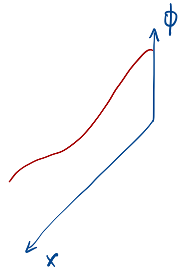
QM: $x \to x(t)$

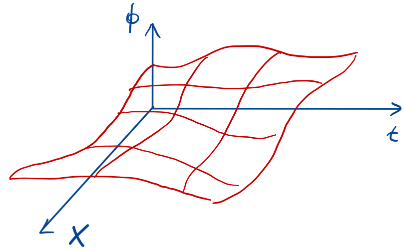
$\bullet x$



e.g. matter, spin, ...

Field theory: $\phi(x) \to \phi(x,t)$





$\rightsquigarrow$ integration is over a d+1 dimensional manifold.

Goal: Express the grand canonical partition function

$$Z = \operatorname{tr} e^{-\beta(\hat{H} - \mu \cdot \hat{N})} \qquad \hat{N} = \sum_j \hat{n}_j$$

chemical potential

for a generic interacting many-body system (bosons or fermions) as a path integral in imaginary time τ with $\tau \in [0, \beta]$.

Why do we focus on the partition function?

(i) Calculation of correlation functions will be straight forward once we know how to compute Z.

(ii) Extract thermodynamic properties.

2.4.1 Quantum partition function

We first apply the trace formula for bosons ($\zeta = +1$) or fermions ($\zeta = -1$):

$$Z = \int d(\bar{\psi}, \psi)\, e^{-\sum_j \bar{\psi}_j \psi_j} \langle \zeta \psi | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi \rangle$$

Let us assume that the Hamiltonian is normal ordered $\hat{H}(\hat{a}^\dagger, \hat{a}) = :H(\hat{a}^\dagger, \hat{a}):$.
(for example $\hat{H} = \sum_{i,j} h_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l} V_{ijkl}\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$).

$e^{a^\dagger a} = 1 + a^\dagger a + \frac{1}{2} a^\dagger a a^\dagger a + \dots$

Note that the exponential $e^{-\beta(\hat{H} - \mu \hat{N})}$ is not normal ordered and thus we cannot simply replace $a^\dagger \to \bar{\psi}$ and $a \to \psi$!

To resolve this, we follow Feynman's idea and decompose Z into infinitely small imaginary time steps $\Delta\tau = \beta/N$ with $N \to \infty$ and only keep the leading order in $\Delta\tau$:

$$e^{-\hat{H}\Delta\tau} = 1 - \hat{H}(\hat{a}^\dagger, a)\,\Delta\tau + \mathcal{O}(\Delta\tau^2)$$

$\rightsquigarrow$ This expression is normal ordered!

Consider now

$$\langle \zeta \psi | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi \rangle = \langle \zeta \psi | e^{-\Delta\tau(\hat{H} - \mu \hat{N})}\, \underset{\mathbb{1}_{\mathcal{F}}}{\uparrow}\, e^{-\Delta\tau(\hat{H} - \mu \hat{N})} \cdots\cdots \underset{\mathbb{1}_{\mathcal{F}}}{\uparrow} \cdots \underset{\mathbb{1}_{\mathcal{F}}}{\uparrow}\, e^{-\Delta\tau(\hat{H} - \mu \hat{N})} | \psi \rangle.$$

and insert a resolution of the identity

$$\underset{\text{Fock space}}{\mathbb{1}_{\mathcal{F}}} = \int d(\bar{\psi}_n, \psi_n)\, e^{-\bar{\psi}_n \cdot \psi_n} | \psi_n \rangle \langle \psi_n |$$

with ψ_n being vectors with elements $\{\psi_j\}_n$.

For each term we find

$$\langle \psi^{n+1} | e^{-\Delta\tau(\hat{H}-\mu\hat{N})} | \psi^n \rangle = \langle \psi^{n+1} | 1 - \Delta\tau (\hat{H}-\mu\hat{N}) | \psi^n \rangle + \mathcal{O}(\Delta\tau^2)$$

$$= \langle \psi^{n+1} | \psi^n \rangle - \Delta\tau \langle \psi^{n+1} | \hat{H}-\mu\hat{N}) | \psi^n \rangle + \mathcal{O}(\Delta\tau^2)$$

$$\langle \phi | \phi \rangle = e^{\sum_j \bar{\phi}_j \phi_j} \qquad = \langle \psi^{n+1} | \psi^n \rangle \left[1 - \Delta\tau \left(H(\bar{\psi}^{n+1}, \psi^n) - \mu N(\bar{\psi}^{n+1}, \psi) \right] + \mathcal{O}(\Delta\tau^2) \right.$$

$$\simeq e^{\sum_j \bar{\psi}_j^{n+1} \psi_j^n} \, e^{-\Delta\tau \left(H(\bar{\psi}^{n+1}, \psi^n) - \mu N(\bar{\psi}^{n+1}, \psi^n) \right)}.$$

Note that $\langle \psi^{n+1} | \psi^n \rangle$ is bilinear in ψ and commutes with everything

Collecting all the terms, we obtain

$$Z = \int d(\bar{\psi}, \psi) \, e^{-\sum_j \bar{\psi}^n \psi^n} \langle \zeta \psi | e^{-\beta(\hat{H}-\mu\hat{N})} | \psi \rangle$$

$$= \int \prod_{n=0}^{N} d(\bar{\psi}^n, \psi^n) \, e^{-\sum_{n=0}^{N-1} \left\{ \bar{\psi}^n \cdot \psi^n - \bar{\psi}^{n+1} \cdot \psi^n + \Delta\tau \left(H(\bar{\psi}^{n+1}, \psi^n) - \mu N(\bar{\psi}^{n+1}, \psi^n) \right) \right\}}$$

$$\bar{\psi}^0 = \zeta \bar{\psi}^N$$
$$\psi^0 = \zeta \psi^N$$

Boundary conditions reflect the trace in Z

Next we take the continuum limit with $\sum_n \Delta\tau \to \int_0^\beta d\tau$ and $\psi_j^n \to \psi_j(\tau)$:

$$\boxed{\begin{aligned} Z &= \int D(\bar{\psi}, \psi) \, e^{-S(\bar{\psi}, \psi)} \\ S(\bar{\psi}, \psi) &= \int_0^\beta d\tau \left[\bar{\psi}(\tau) \, \partial_\tau \psi(\tau) + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi) \right] \\ D(\bar{\psi}, \psi) &= \lim_{N\to\infty} \prod_{n=0}^{N} d(\bar{\psi}^n, \psi^n) \\ &\text{Boundary conditions: } \psi(\tau=0) = \zeta \psi(\tau=\beta) \text{ and } \bar{\psi}(\tau=0) = \zeta \bar{\psi}(\tau=\beta) \end{aligned}}$$

⇝ Partition function Z expressed as a functional integral over the fields $\bar{\psi}$ and ψ with weights $e^{-S(\bar{\psi},\psi)}$.

⇝ For the example Hamiltonian shown above, we find

$$S(\bar{\psi},\psi) = \int_0^\beta d\tau \left\{ \sum_{ij} \bar{\psi}_i(\tau) \left[(\partial_\tau - \mu)\delta_{ij} + h_{ij} \right] \psi_j(\tau) + \sum_{ijkl} V_{ijkl}\, \bar{\psi}_i(\tau) \bar{\psi}_j(\tau) \psi_k(\tau) \psi_l(\tau) \right\}$$

(Quantum partition function expressed as integral over fields $\psi_j(\tau)$).

Often it is convenient to work with a frequency representation instead of imaginary time: Matsubara frequency representation

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \psi_n \cdot e^{-i\omega_n \tau}, \quad \psi_n = \frac{1}{\sqrt{\beta}} \cdot \int_0^\beta d\tau\, \psi(\tau)\, e^{i\omega_n \tau}$$

$$\bar{\psi}(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \bar{\psi}_n\, e^{i\omega_n \tau}, \quad \bar{\psi}_n = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, \bar{\psi}(\tau)\, e^{-i\omega_n \tau}$$

with $n \in \mathbb{Z}$ and Matsubara frequencies $\omega_n = \begin{cases} \pi 2n/\beta & \text{for bosons.} \\ \pi(2n+1)/\beta & \text{for fermions.} \end{cases}$

Difference between bosons and fermions: Boundary conditions $\psi(0) = \zeta \psi(\beta)$ leading to $\zeta \cdot e^{-i\omega_n \beta} = 1$.

⇝ For the example Hamiltonian above, the action in frequency representation reads:

$$S[\bar{\psi},\psi] = \sum_{ijn} \bar{\psi}_{in} \left[(-i\omega_n - \mu)\delta_{ij} + h_{ij} \right] \psi_{jn} + \frac{1}{\beta} \sum_{ijkl, n_i} V_{ijkl}\, \bar{\psi}_{in_1} \bar{\psi}_{jn_2} \psi_{kn_3} \psi_{ln_4} \cdot \delta_{n_1+n_2,\, n_3+n_4}$$

(using the identity $\int_0^\beta d\tau\, e^{-i\omega_n \tau} = \beta\, \delta_{\omega_n, 0}$)

The expression further simplifies when expressing h_{ij} in k-space (i.e. when diagonalizing h_{ij}) $\rightsquigarrow$ $h_{ij} u_{jk} = u_{ik} \varepsilon_k$

For a free particle $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ The action then reads:

$$S = \sum_{nk} \bar{\psi}_{kn} (-i\omega_n + \varepsilon_k - \mu) \psi_{kn} + \frac{1}{\beta V} \sum_{\substack{kk'q \\ nn'm}} V(q) \bar{\psi}_{k+q,n+m} \bar{\psi}_{k'-q,n'-m} \psi_{k',n'} \psi_{k,n}$$

2.4.2 Coherent state path integral for the transition amplitude

For the transition amplitude (real time) we find

$$\langle \phi_1 | \underbrace{\hat{U}(t,0)}_{\text{time evolution operator}} | \phi_0 \rangle = \langle \phi_1 | \underset{\mathbb{1}_\varepsilon}{\uparrow} e^{-i/\hbar \int_0^t dt' H} \underset{\mathbb{1}_\varepsilon}{\uparrow} | \phi_0 \rangle$$

arbitrary states

coherent states

$$= \int d(\bar{\psi}_t \psi_t)\, d(\bar{\psi}_0 \psi_0)\, e^{-\bar{\psi}_t \psi_t - \bar{\psi}_0 \psi_0}\, \bar{\phi}_1(\psi_t)\, \phi_0(\psi_0) \langle \psi_t | \hat{U} | \psi_0 \rangle$$

Here $|\phi_i\rangle$ are arbitrary states and $|\psi_i\rangle$ are coherent states.

We can now use the previous results to express $\langle \psi_t | U(t,0) | \psi_0 \rangle$ as a path integral:

$$\boxed{\begin{aligned} \langle \psi_t | U(t,0) | \psi_0 \rangle &= \int D(\bar{\psi}, \psi)\, e^{\frac{i}{\hbar} S[\bar{\psi}, \psi]} \\ S(\bar{\psi}, \psi) &= \int_0^t dt' \left\{ i \bar{\psi} \partial_t \psi - H[\bar{\psi}, \psi] \right\} \end{aligned}}$$

assuming normal order of $\hat{H}$.

Same expression as obtained from Wick rotation.

2.4.3 Partition function of the non-interacting gas

We now consider the Hamiltonian of free quantum particles

$$\hat{H} = \sum_\alpha \underbrace{\varepsilon_\alpha}_{\text{single particle eigenvalues.}} \overbrace{\hat{a}^\dagger_\alpha \hat{a}_\alpha}^{\hat{=}\ \hat{n}_\alpha \text{ counting \# of particles in state } \alpha.},$$

where $\hat{a}^\dagger_\alpha$ $\hat{a}_\alpha$ can be bosonic or fermionic operators.

Let us first consider the quantum partition function

$$Z = \mathrm{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n | e^{-\beta(\hat{H}-\mu\hat{N})} | n \rangle .$$

The action assumes the form

$$\left(\text{Recall}: S[\bar{\psi},\psi] = \sum_{ijn} \bar{\psi}_{in} \left[(-i\omega_n - \mu)\delta_{ij} + h_{ij} \right] \psi_{jn} \right)$$

$$S(\bar{\phi},\phi) = \sum_\alpha \sum_{\omega_n} \bar{\phi}_{\alpha n} (-i\omega_n + \xi_\alpha) \phi_{\alpha n}, \quad \text{with } \xi_\alpha = \varepsilon_\alpha - \mu \text{ and Matsubara freq. } \omega_n.$$

Since the particles are independent, we find that the partition function decouples $Z = \prod_\alpha Z_\alpha$ with (i.e. it is a product of Gaussian states)

$$Z_\alpha = \int D(\bar{\phi}_\alpha, \phi_\alpha) \cdot e^{-\sum_{\omega_n} \bar{\phi}_{\alpha n}(-i\omega_n + \xi_\alpha)\phi_{\alpha n}}$$

$$= \prod_n \left\{ \beta(-i\omega_n + \xi_\alpha) \right\}^{-\zeta}$$

For the last equality, we evaluated the complex (Bosons) and Grassmann (Fermions) Gaussian integral. The factor β needs to be there for dimensional reasons and results from the Jacobian in the measure $D(\bar{\phi},\phi)$.
We now have to compute an infinite product over factors $i\omega_n - \xi_\alpha$.

For convenience, we take the logarithm of the partition function and consider the free energy

$$F_\alpha = -T \ln Z_\alpha = \frac{1}{\beta} \cdot \sum_n \ln\left[\beta(-i\omega_n + \xi_\alpha)\right]$$

How to perform the frequency summation?

Let us introduce a general framework to perform such summations.

Matsubara summations

Evaluate sums of the form

$$\frac{1}{\beta} \cdot \sum_n f(i\omega_n) \quad \text{with} \quad \omega_n = \begin{cases} 2\pi n/\beta & \text{bosons} \\ (2n+1)\pi/\beta & \text{fermions} \end{cases}$$

Basic idea:

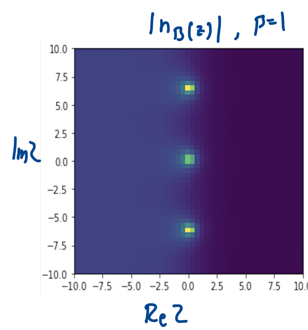
(i) Rewrite the sum as a contour integral in the complex plane using auxiliary functions with simple poles at the Matsubara frequencies.

We choose the following auxiliary functions (multiple choices are possible):

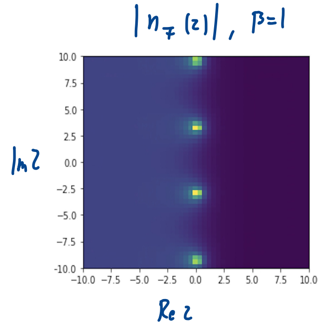
Bosons:

Bose-Einstein distribution $n_B(z) = \frac{1}{e^{\beta z} - 1}$ has poles at $z_n = i\omega_n = i\frac{2\pi \cdot n}{\beta}$ with residues $\mathrm{Res}\left[n_B(z), z = z_n\right] = \beta^{-1}$

$$\left[\lim_{z \to z_n} (z - z_n) \frac{1}{e^{\beta z} - 1} \overset{\text{del Hospital}}{=} \lim_{z \to z_n} \frac{1}{\beta e^{\beta z}} = \beta^{-1}\right]$$



Fermions:



Fermi-Dirac distribution $n_F(z) = \frac{1}{e^{\beta z}+1}$ has poles at $z_n = i\omega_n = \frac{i\pi(2n+1)}{\beta}$ with residues $\mathrm{Res}\left[n_F(z), z=z_n\right] = -\beta^{-1}$

(ii) Choose a contour such that all poles of the auxiliary function are enclosed:
Contour integral = sum of residues

(iii) Residue theorem then allows us to perform the summation by integrating over the proper contour.

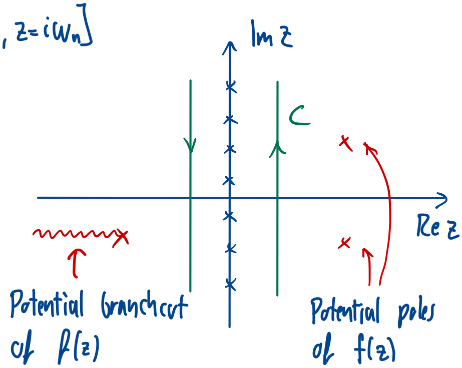
$$\boxed{\frac{1}{\beta}\sum_n f(i\omega_n) = \zeta \cdot \oint_C \frac{dz}{2\pi i}\, n_{\beta,F}(z) \cdot f(z)} \quad (*)$$

Proof: $\zeta \oint_C \frac{dz}{2\pi i}\, n_{\beta,F}(z) \cdot f(z) =$

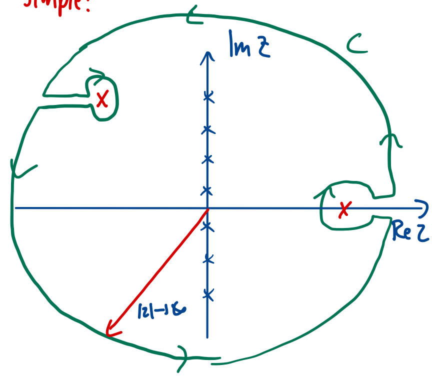
$$= \zeta \cdot \sum_n \mathrm{Res}\left[n_{\beta,F}(z) \cdot f(z), z = i\omega_n\right]$$

$$= \frac{1}{\beta} \cdot \sum_n f(i\omega_n)$$

Residues of $n_{\beta,F}(z)$ are $\frac{\zeta}{\beta}$.



$\rightsquigarrow$ As long as we are careful to not cross any singularities, we are free to distort the contour such that the integral can be done. This is not always simple!



If the product $n_{\beta,\mp} \cdot f(z)$ decays faster than z^{-1} for $|z| \to \infty$, we can inflate the original contour to an infinite circle. Since the outer contour at the outer perimeter does not contribute, we are then left with integrals around the singularities of $f(z)$.

In the simple case of isolated singularities at $\{z_n\}$, the infinite sum can be reduced to the evaluation of a finite number of residues!

Let us now return to the partition function of the non-interacting quantum gas and evaluate the Matsubara sum

$$F = \frac{\zeta}{\beta} \sum_{\alpha} \sum_{i\omega_n} \ln(\xi_\alpha - i\omega_n) \quad \text{with } \xi_\alpha = \varepsilon_\alpha - \mu .$$

Problem: The sum formally diverges!

We need to recall how the functional integral was constructed $\rightsquigarrow$ Convergence generating factor appears because of the normal ordering in the Hamiltonian!

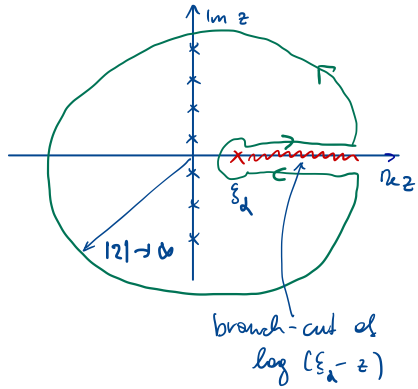
The fields $\bar{\psi}(\tau)$ in the Hamiltonian are evaluated at infinitesimally later than $\psi(\tau)$, i.e. $H[\bar{\psi}(\tau+\Delta\tau), \psi(\tau)]$ with $\Delta\tau \to 0^+$.

Now keep track of $\Delta\tau$:

$$F = \frac{\zeta}{\beta} \sum_\alpha \sum_{i\omega_n} \ln\left(\xi_\alpha - i\omega_n \cdot e^{-i\omega_n \cdot 0^+}\right)$$

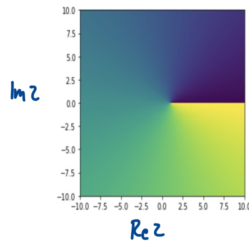
with (*)

$$= \sum_\alpha \oint_C \frac{dz}{2\pi i}\, n_{B/F}(z) \ln\left(\xi_\alpha - z \cdot e^{-z\cdot 0^+}\right).$$



To simplify the integral, we use

$$n_{B/F} = \frac{\zeta}{\beta} \partial_z \ln\left(1 - \zeta e^{-\beta z}\right) \quad \left(= \frac{1}{e^{-\beta z} - \zeta}\right)$$



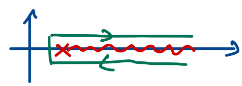
$$F = \sum_\alpha \oint_C \frac{dz}{2\pi i} \left[\frac{\zeta}{\beta} \partial_z \ln\left(1 - \zeta e^{-\beta z}\right)\right] \ln\left(\xi_\alpha - z \cdot e^{-z \cdot 0^+}\right).$$

Integration by parts

$$= -\frac{\zeta}{\beta} \cdot \sum_\alpha \oint_C \frac{dz}{2\pi i} \ln\left(1 - \zeta e^{-\beta z}\right) \frac{1}{z e^{-z 0^+} - \xi_\alpha}$$

The factor e^{-z0^+} ensures that the integral vanishes along the outer perimeter!

$$F = -\frac{\zeta}{\beta} \sum_\alpha \int_{\xi_\alpha - 0^+}^{\infty} \frac{d\varepsilon}{2\pi i} \ln\left(1 - \zeta \cdot e^{-\beta\varepsilon}\right) \left[\frac{1}{\varepsilon + i0^+ - \xi_\alpha} - \frac{1}{\varepsilon - i0^+ - \xi_\alpha}\right]$$



$$= -\frac{\zeta}{\beta} \sum_\alpha \int_{\xi_\alpha - 0^+}^{\infty} \frac{d\varepsilon}{\cancel{2\pi i}} \ln\left(1 - \zeta e^{-\beta\varepsilon}\right) (-\cancel{2\pi i})\, \delta(\varepsilon - \xi_\alpha)$$

$$= \boxed{\frac{\zeta}{\beta} \cdot \sum_\alpha \ln\left(1 - \zeta \cdot e^{-\beta\xi_\alpha}\right)}$$

$\rightsquigarrow$ As expected for non-interacting Fermions/Bosons!

2.4.4 Matsubara Green's functions and correlation functions

A useful way to compare theoretical result to experiments is to calculate correlation functions of some operators $\hat{A}$ and $\hat{B}$:

$$C_{A,B} = \langle T_\tau \hat{A}(\tau) \hat{B}(\tau') \rangle$$

with τ being the imaginary time and time-dependent operators in the Heisenberg picture.

T_τ indicates the time ordering such that

$$\langle T_\tau \hat{A}(\tau) \hat{B}(\tau') \rangle = \begin{cases} \langle \hat{A}(\tau) \hat{B}(\tau') \rangle & \tau > \tau' \\ \underbrace{\zeta}_{-1 \text{ if } \hat{A},\hat{B} \text{ anti commute.}} \langle \hat{B}(\tau') \hat{A}(\tau) \rangle & \tau < \tau' \end{cases}.$$

The expectation value of an operator $\hat{O}$ at inverse temperature β is

$$\langle \hat{O} \rangle = \frac{1}{Z} \mathrm{Tr}[e^{-\beta \hat{\mathcal{H}}} \hat{O}] \qquad \text{with } \hat{\mathcal{H}} = \hat{H} - \mu \hat{N}.$$

This we know how to express in terms of a functional integral

$$\boxed{C_{A,B}(\tau-\tau') = \frac{1}{Z} \int D(\bar{\psi},\psi)\, A[\bar{\psi}(\tau)\psi(\tau)]\, B[\bar{\psi}(\tau')\psi(\tau')]\, e^{-S[\bar{\psi},\psi]}.}$$

Note that the functional integral computes time ordered correlations!

Let us check this for $\tau > \tau'$:

$$\langle \hat{A}(\tau) \hat{B}(\tau') \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta\hat{\mathcal{H}}} e^{\tau \hat{\mathcal{H}}} \hat{A} e^{-\tau\hat{\mathcal{H}}} e^{\tau'\hat{\mathcal{H}}} \hat{B} e^{-\tau'\hat{\mathcal{H}}} \right]$$

$$= \frac{1}{Z} \mathrm{Tr}\left[\underbrace{e^{-(\beta-\tau)\hat{\mathcal{H}}}}_{\tau\to\beta} \underset{\uparrow}{\hat{A}}\ \underbrace{e^{-(\tau-\tau')\hat{\mathcal{H}}}}_{\tau'\to\tau} \underset{\uparrow}{\hat{B}}\ \underbrace{e^{-\tau'\hat{\mathcal{H}}}}_{0\to\tau'} \right]$$

We now perform the same steps as in the construction of the field integral in 2.4.1 (i.e., breaking the time evolution into small time steps and insert resolutions of the identity after each step):

$$\langle \hat{A}(\tau)\hat{B}(\tau')\rangle = \frac{1}{Z}\int \prod_n d(\bar{\psi}^n \psi^n)\, \langle \zeta\psi | e^{-\Delta\tau \mathcal{H}} | \psi^N\rangle\langle\psi^N| e^{-\Delta\tau\mathcal{H}}|\psi^{N-1}\rangle \cdots$$

$$\cdots \langle \psi^{i+1}| e^{-\Delta\tau\mathcal{H}}|\psi^i\rangle\langle\psi^i|\hat{A}|\psi^{i-1}\rangle\langle\psi^{i-1}|e^{\Delta\tau\mathcal{H}}|\psi^{i-2}\rangle\cdots$$

$$\cdots \langle \psi^{j+1}| e^{-\Delta\tau\mathcal{H}}|\psi^j\rangle\langle\psi^j|\hat{B}|\psi^{j-1}\rangle\langle\psi^{j-1}|e^{-\Delta\tau\mathcal{H}}|\psi^{j-2}\rangle\cdots$$

$$\cdots \langle\psi^1|e^{-\Delta\tau\mathcal{H}}|\psi\rangle,$$

where $i\Delta\tau > \tau > (i-1)\delta\tau$ and $j\Delta\tau > \tau' > (j-1)\Delta\tau$.

$$\rightsquigarrow \langle \hat{A}(\tau)\hat{B}(\tau')\rangle = \frac{1}{Z}\int D(\bar{\psi},\psi)\, A[\bar{\psi}(\tau),\psi(\tau)]\, B[\bar{\psi}(\tau'),\psi(\tau')]\cdot e^{-S[\bar{\psi},\psi]}$$

For $\tau < \tau'$ the construction proceeds analogously $\square$

<u>Example</u>: One of the most relevant time-ordered correlation functions is the single particle Green function (GF).

position x

$$\boxed{G(x',\tau',x,\tau) = -\langle T_\tau\, \hat{a}(x',\tau')\, \hat{a}^\dagger(x,\tau)\rangle.}$$

For space- and time-translational systems, the GF only depends on relative coordinates $\rightsquigarrow$ consider $G(x'-x,\tau'-\tau)$ and take the Fourier transform

$$G(x-x', \tau-\tau') = -\langle T_\tau \sum_{k,k'} e^{-i(k'x'-kx)} \hat{a}_{k'}(\tau') \hat{a}^\dagger_k(\tau) \rangle$$

$R = \frac{x+x'}{2}$

$r = x'-x$

$$\downarrow = -\langle T_\tau \sum_{k,k'} e^{-i(k'-k)\cdot R} \cdot e^{-\frac{k+k'}{2} r} \hat{a}_{k'}(\tau') \hat{a}^\dagger_k(\tau) \rangle$$

$\frac{1}{V}\int d^D R$

$$\downarrow = -\langle T_\tau \sum_k e^{-ikr} \hat{a}_k(\tau') \hat{a}^\dagger_k(\tau) \rangle$$

$$= \sum_k e^{-ikr} G(k, \tau'-\tau)$$

Thus we define

$$\boxed{G(k,\tau) = -\langle T_\tau \hat{a}_k(\tau) \hat{a}^\dagger_k(0) \rangle}$$

Let us consider the case of non-interacting particles:

$$\hat{\mathcal{H}} = \hat{H} - \mu \hat{N} = \sum_k (\varepsilon_k - \mu) \hat{a}^\dagger_k \hat{a}_k$$

$$\rightsquigarrow \hat{a}_k(\tau) = e^{\tau(\hat{H}-\mu\hat{N})} \cdot \hat{a}_k e^{-\tau(\hat{H}-\mu\hat{N})} = e^{-(\varepsilon_k-\mu)\tau} \hat{a}_k$$

$$\rightsquigarrow G_0(k,\tau) = -\Theta(\tau) \langle \hat{a}_k(\tau) \hat{a}^\dagger_k(0) \rangle - \zeta \Theta(-\tau) \langle \hat{a}^\dagger_k(0) \hat{a}_k(\tau) \rangle$$

$$= -\Theta(\tau) e^{-(\varepsilon_k-\mu)\tau} \underbrace{\langle \hat{a}_k \hat{a}^\dagger_k \rangle}_{1+\zeta n_k} - e^{-(\varepsilon_k-\mu)\tau} \zeta \cdot \Theta(-\tau) \underbrace{\langle \hat{a}^\dagger_k \hat{a}_k \rangle}_{= n_k}$$

$$= -\Theta(\tau) e^{-(\varepsilon_k-\mu)\cdot\tau} - \zeta \cdot e^{-(\varepsilon_k-\mu)\tau} n_k$$

$n_k = (e^{-\beta(\varepsilon-\mu)} - \zeta)^{-1}$

$$\downarrow = -e^{-(\varepsilon_k-\mu)\tau} \left[\Theta(\tau) + \frac{\zeta}{e^{\beta(\varepsilon_k-\mu)} - \zeta} \right].$$

2.4.5 Generating Functionals

Define the generating functional by coupling the fields $\bar{\psi}, \psi$ to external source fields J and $\bar{J}$.

$$Z[\bar{J}, J] = \int D(\bar{\psi}, \psi) \exp\left[-S(\bar{\psi}, \psi) + \sum_{k,n} \left(\bar{J}(k, i\omega_n)\psi(k, i\omega_n) + \bar{\psi}(k, i\omega_n) J(k, i\omega_n)\right)\right]$$

Arbitrary correlation functions of the fields $\bar{\psi}, \psi$ can now be obtained by taking functional derivatives of $Z[\bar{J}, J]$ with respect to the external source fields:

± 1 for bosons / fermions.

$$\boxed{\langle \psi(k, i\omega_n)\bar{\psi}(k, i\omega_n)\rangle = \frac{1}{Z[0,0]} \zeta \cdot \frac{\delta^2 Z[J, \bar{J}]}{\delta \bar{J}(k, i\omega_n)\delta J(k, i\omega_n)}\Big|_{\bar{J}=J=0}}$$

For non-interacting particles, we can compute $Z[\bar{J}, J]$ exactly [use a short hand notation $k = (i\omega_n, k)$]:

$$Z_0[\bar{J}, J] = \int D(\bar{\psi}, \psi)\, e^{-\sum_k \bar{\psi}(k)[-G_0^{-1}(k)]\psi(k) + \sum_k [\bar{J}(k)\psi(k) + \bar{\psi}(k) J(k)]}$$

combine sum over all $(k, i\omega_n)$.

Gaussian integration

$$= Z_0[0,0] \cdot \exp\left[-\sum_k \bar{J}(k) G_0(k) J(k)\right]$$

$$\rightsquigarrow \langle \psi_{k_0}\bar{\psi}_{k_0}\rangle_0 = \zeta \frac{\delta^2}{\delta\bar{J}(k_0)\delta J(k_0)} \exp\left[-\sum_k \bar{J}(k) G_0(k) J(k)\right]\Big|_{\bar{J}=J=0} = -G_0(k_0)$$

Higher order correlation functions: n-particle Green function

$$\boxed{\langle \psi(q_1)\cdots\psi(q_n)\bar{\psi}(k_n)\cdots\bar{\psi}(k_1)\rangle = \frac{1}{Z[0,0]} \frac{\zeta^n \delta^{2n} Z[\bar{J}, J]}{\delta\bar{J}(q_1)\cdots\delta\bar{J}(q_n)\delta J(k_n)\cdots\delta J(k_1)}\Big|_{\bar{J}=J=0}}$$

For non-interacting particles, these correlation functions can be evaluated easily using properties of Gaussian integrals : Wicks theorem

$$\langle \psi(q_1)\cdots\psi(q_n)\,\bar\psi(k_n)\cdots\bar\psi(k_1)\rangle_0 = \left.\frac{\zeta^n\,\delta^{2n}\exp\left[-\sum_k \bar J(k)\,G_0(k)\,J(k)\right]}{\delta\bar J(q_1)\cdots\delta\bar J(q_n)\,\delta J(k_n)\cdots\delta J(k_1)}\right|_{\bar J = J = 0}$$

e.g. $\langle \hat a_i \hat a_j \hat a_k^\dagger \hat a_l^\dagger\rangle$

$$= \frac{\delta}{\delta\bar J(q_1)}\cdots\frac{\delta}{\delta\bar J(q_n)}\left[\bar J(k_n)\,G_0(k_n)\cdots\bar J(k_1)\,G_0(k_1)\right](-1)^n$$

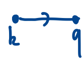
$$= G_0(k_n)\cdots G_0(k_1)\cdot\sum_{\text{perm }P}\zeta^{\sigma(P)}\,\delta_{q_n,k_{P(n)}}\cdots\delta_{q_1,k_{P(1)}}\,(-1)^n$$

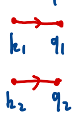
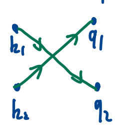
with $\sigma(P) = \begin{cases} 0 & \text{even permutation} \\ 1 & \text{odd permutation}\end{cases}$

$\rightsquigarrow$ For free particles, the n-particle Green function can be reduced to a product of single-particle Green functions!

Graphical representation:

Momentum conservation

$n=1$ $\langle \psi_q \bar\psi_k\rangle =$  $= -G_0(k)\cdot\delta_{k,q}$

$n=2$ $\langle \psi_{q_1}\psi_{q_2}\bar\psi_{k_2}\bar\psi_{k_1}\rangle =$  $+\ \zeta$ 

$$= G_0(k_1)\,G_0(k_2)\left[\delta_{k_1,q_1}\delta_{k_2,q_2} + \zeta\,\delta_{k_1,q_2}\delta_{k_2,q_1}\right]$$