I. The contour idea (Stefanucci & van Leeuwen, Chapter 4)

I.1 Time-dependent quantum averages

Goal: Compute a time-dependent quantum average of an operator $\hat{O}(t)$ at time t when the system is initially in the state $|\Psi(t_0)\rangle \equiv |\Psi_0\rangle$

Solution: Propagation of the state via the Schrödinger equation:

$$|\Psi(t)\rangle = \hat{U}(t,t_0)\,|\Psi_0\rangle$$

with, for $t > t_0$, the time evolution operator

$$\hat{U}(t,t_0) \equiv T\left\{e^{-i\int_{t_0}^{t} d\bar{t}\,\hat{H}(\bar{t})}\right\}$$

$T \equiv$ time ordering operator, later times to the left.

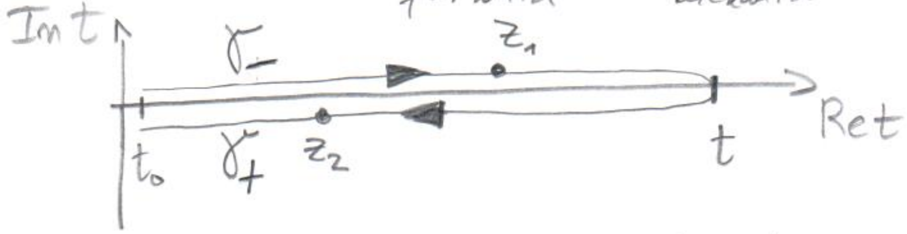
This leads to

$$\boxed{\begin{aligned} O(t) &= \langle\Psi(t)|\,\hat{O}(t)\,|\Psi(t)\rangle \\ &= \langle\Psi_0|\,\bar{T}\left\{e^{-i\int_{t}^{t_0} d\bar{t}\,\hat{H}(\bar{t})}\right\}\hat{O}(t)\,T\left\{e^{-i\int_{t_0}^{t} d\bar{t}\,\hat{H}(\bar{t})}\right\}|\Psi_0\rangle \end{aligned}}$$

→ computing an operator expectation value naturally requires forward + backward propagation in time!

We define the oriented contour γ in the complex time plane — the convenience of the complex time will become clear later — as follows:

$$\gamma \equiv \underbrace{(t_0, t)}_{\substack{\gamma_- \\ \text{forward}}} \oplus \underbrace{(t, t_0)}_{\substack{\gamma_+ \\ \text{backward}}}$$



Note that both γ_+ and γ_- have real time arguments only.

The forward and backward branches are for bookkeeping of time-ordering only — nothing mysterious!

Def.: Operators with contour arguments

$$\hat{A}(z') \equiv \begin{cases} \hat{A}_-(t') & \text{if } z' = t'_- \\ \hat{A}_+(t') & \text{if } z' = t'_+ \end{cases}$$

[$\hat{A}_+$ and $\hat{A}_-$ could be different.]

Def.: Contour time-ordering operator $\mathcal{T}$

$$\mathcal{T}\left\{ \hat{A}_m(z_{P(m)})\, \hat{A}_{m-1}(z_{P(m-1)}) \dots \hat{A}_1(z_{P(1)}) \right\}$$
$$= \hat{A}_m(z_m)\, \hat{A}_{m-1}(z_{m-1}) \dots \hat{A}_1(z_1) \quad \text{with } P \text{ a permutation}$$

and times $z_m \succ z_{m-1} \succ \dots \succ z_1$

"Later on the γ contour"

$\equiv$ further away from the origin at t_{0-}

For two operators $\hat{A}(z_1)$ and $\hat{B}(z_2)$ there are the following possibilities:

$$\mathcal{T}\{\hat{A}(z_1)\,\hat{B}(z_2)\} = \begin{cases} T\{\hat{A}_-(t_1)\,\hat{B}_-(t_2)\} & \text{if } z_1 = t_{1-},\ z_2 = t_{2-} \\ \hat{A}_+(t_1)\,\hat{B}_-(t_2) & \text{if } z_1 = t_{1+},\ z_2 = t_{2-} \\ \hat{B}_+(t_2)\,\hat{A}_-(t_1) & \text{if } z_1 = t_{1-},\ z_2 = t_{2+} \\ \bar{T}\{\hat{A}_+(t_1)\,\hat{B}_+(t_2)\} & \text{if } z_1 = t_{1+},\ z_2 = t_{2+} \end{cases}$$

<u>Note:</u> backward, $+$ is always later than forward, $-$

Now we can rewrite the operator expectation value in a more compact way:

$$O(t) = \langle \Psi_0 | \mathcal{T}\left\{ e^{-i\int_{\gamma_+} d\bar{z}\,\hat{H}(\bar{z})}\,\hat{O}(t_\pm)\,e^{-i\int_{\gamma_-} d\bar{z}\,\hat{H}(\bar{z})} \right\} | \Psi_0 \rangle$$

Inside the $\mathcal{T}$ sign all operators can be treated as if they commute — remember that $\mathcal{T}$ will order them contour-chronologically anyway — and therefore we have the shorthand notation

$$O(t) = \langle \Psi_0 | \mathcal{T}\left\{ e^{-i\int_{\gamma} d\bar{z}\,\hat{H}(\bar{z})}\,\hat{O}(t_\pm)\right\} | \Psi_0 \rangle$$

with $\int_\gamma \equiv \int_{\gamma_-} + \int_{\gamma_+}$

Note that all physical observables including the Hamiltonian $\hat{H}$ have $\hat{O}(t_\pm) \equiv \hat{O}(t)$, they are the same on both γ_+ and γ_-.

Here $\hat{O}(t)$ is <u>not</u> $\hat{O}_H(t) \equiv$ operator in Heisenberg picture.

The time argument is meant as a reminder <u>where</u> to insert the operator along the contour!

Now we can extend the contour up to $+\infty$:

$$\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\, \hat{O}(t_-)\right\} = \hat{U}(t_0,\infty)\,\hat{U}(\infty,t)\,\hat{O}(t)\,\hat{U}(t,t_0)$$

$$= \hat{U}(t_0,t)\,\hat{O}(t)\,\hat{U}(t,t_0)$$

and

$$\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\, \hat{O}(t_+)\right\} = \hat{U}(t_0,t)\,\hat{O}(t)\,\hat{U}(t,\infty)\,\hat{U}(\infty,t_0)$$

$$= \hat{U}(t_0,t)\,\hat{O}(t)\,\hat{U}(t,t_0)$$

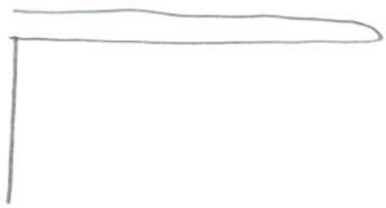
which shows that $\hat{O}(t)$ <u>does not change</u> if we extend the contour: $\boxed{O(z) = \langle \Psi_0 | \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\, \hat{O}(z)\right\} | \Psi_0 \rangle}$

$\gamma \equiv$ "Keldysh contour", dating back to Keldysh's classic paper on nonequilibrium Green's functions (1964)

But: Schwinger used the contour already in 1961.
It is sometimes called "Schwinger-Keldysh contour".

1st lecture (1 hour)

We will call it "the contour" only. It will be extended to include imaginary times — (Wick rotation) then it looks like an "L" and we also call it the L-shaped contour.



Slide: show some simple movies computed on Keldysh contour

I.2 Time-dependent ensemble averages

Now: pure state ⟶ mixed state (e.g., thermal ensemble)

$|\Psi_0\rangle$ ⟶ probability distribution $\{w_n\}$ with $w_n \in [0,1]$ and $\sum_n w_n = 1$ of finding the system in state $|\chi_n\rangle$ with $\langle \chi_n | \chi_n \rangle = 1$ (normalized) but $\langle \chi_n | \chi_m \rangle \neq 0$ for $n \neq m$ in general (no orthogonality required)

Expectation value: $\quad O(t_0) = \sum_n w_n \langle \chi_n | \hat{O}(t_0) | \chi_n \rangle$

Def.: density matrix operator

$$\hat{\rho} = \sum_n w_n |\chi_n\rangle\langle\chi_n|$$

$\hat{\rho} = \hat{\rho}^+$ (self-adjoint)

$\langle \Psi | \hat{\rho} | \Psi \rangle = \sum_n w_n |\langle \Psi | \chi_n \rangle|^2 \geq 0$ (positive-semidefinite)

Let $\{|\psi_k\rangle\}$ be a generic orthonormal basis set.

Then

$$O(t_0) = \sum_k \sum_n w_n \langle \chi_n | \psi_k \rangle \langle \psi_k | \hat{O}(t_0) | \chi_n \rangle$$

$$= \sum_k \langle \psi_k | \hat{O}(t_0)\, \hat{\rho} \,| \psi_k \rangle$$

$$\equiv \mathrm{Tr}\left[\hat{O}(t_0)\,\hat{\rho}\right] = \mathrm{Tr}\left[\hat{\rho}\,\hat{O}(t_0)\right]$$

trace in the Fock space $\mathcal{F}$

= trace over a complete set of many-body states

In particular, since $\hat{O}(t_0) = \mathbb{1} \Rightarrow O(t_0) = 1$ due to $|\chi_n\rangle$s being normalized, one has

$$\mathrm{Tr}[\hat{\rho}] = 1. \quad (*)$$

We choose kets $|\psi_k\rangle$ as eigenkets of $\hat{\rho}$:

$$\hat{\rho}\,|\psi_k\rangle = \rho_k\,|\psi_k\rangle$$

$$\Rightarrow \hat{\rho} = \sum_k \rho_k |\psi_k\rangle\langle\psi_k| \quad \text{with } \rho_k \in [0,1],\ \sum_k \rho_k = 1$$

$$\Rightarrow \mathrm{Tr}[\hat{\rho}^2] \leq 1 \quad (**)$$

Most general expression fulfilling these constraints $(*), (**)$:

$$\rho_k = \frac{e^{-x_k}}{\sum_p e^{-x_p}}$$

with $x_k \in \mathbb{R}$.

We can write $x_k = \beta E_k^M$ with $\beta > 0$

and define

$$\hat{H}^M = \sum_k E_k^M |\Psi_k\rangle\langle\Psi_k|$$

$$\Rightarrow \boxed{\hat{\rho} = \sum_k \frac{e^{-\beta E_k^M}}{Z} |\Psi_k\rangle\langle\Psi_k| = \frac{e^{-\beta \hat{H}^M}}{Z}}$$

with the partition function

$$\boxed{Z \equiv \sum_k e^{-\beta E_k^M} = \mathrm{Tr}\left[e^{-\beta \hat{H}^M}\right]}$$

M: "Matsubara"

For example, in a grand-canonical ensemble we choose

$$\hat{H}^M = \hat{H} - \mu \hat{N} \quad \text{and} \quad \beta = \frac{1}{k_B T}$$

$k_B \equiv$ Boltzmann constant

$T \equiv$ temperature

$\mu =$ chemical potential

$\hat{N} =$ total particle number operator

Next: time evolution of ensemble averages.

Ensemble time evolution:

Evolve each subsystem of the ensemble, then perform the weighted average. Same $\hat{H}(z)$ for all of them!

$$O(z) = \sum_n w_n \langle \chi_n | \hat{U}(t_0, z) \hat{O}(z) \hat{U}(z, t_0) | \chi_n \rangle$$

$$= \mathrm{Tr}\left[\hat{\rho}\, \hat{U}(t_0, z)\, \hat{O}(z)\, \hat{U}(z, t_0) \right]$$

$$= \mathrm{Tr}\left[\hat{\rho}\, \mathcal{T}\left\{ e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{O}(z) \right\} \right]$$

$$= \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}^M} \mathcal{T}\left\{ e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \hat{O}(z) \right\} \right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}^M} \right]} \quad (*)$$

We observe the following:

(1) $\mathcal{T}\left\{ e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})} \right\} = \hat{U}(t_0, \infty)\, \hat{U}(\infty, t_0) = \hat{\mathbb{1}}$

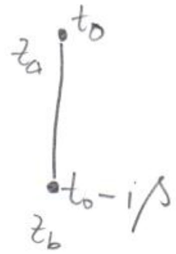
$\Rightarrow$ can be inserted into the trace in the denominator of $(*)$

(2) The exponential can be written as

$$e^{-\beta \hat{H}^M} = e^{-i\int_{\gamma^M} d\bar{z}\, \hat{H}^M(\bar{z})}$$

where γ^M is a contour $z_a \longrightarrow z_b$ with

$$z_b - z_a = -i\beta$$

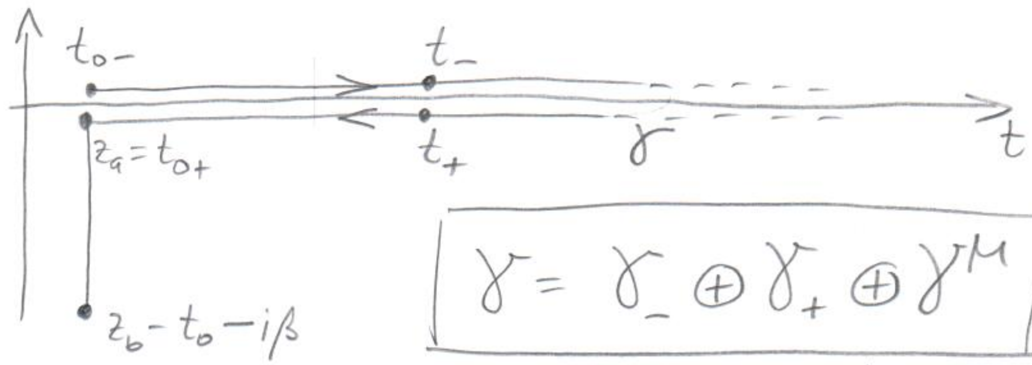


(1), (2) $\to$ (*) gives

$$O(z) = \frac{\mathrm{Tr}\left[e^{-i\int_{\gamma^M} d\bar{z}\, \hat{H}^M(\bar{z})}\, \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\, \hat{O}(z)\right\}\right]}{\mathrm{Tr}\left[e^{-i\int_{\gamma^M} d\bar{z}\, \hat{H}^M(\bar{z})}\, \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\right\}\right]}$$

Note: statistical averaging = time propagation along imaginary time axis γ^M.

We can add γ^M to the two-branch contour!



$$\boxed{\gamma = \gamma_- \oplus \gamma_+ \oplus \gamma^M}$$

"the contour"

<u>Note:</u> In practice the contour has a finite length corresponding to the maximal time at which we can compute observables.

("probe the system")

We finally have

$$O(z) = \frac{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\, \hat{O}(z)\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\, \hat{H}(\bar{z})}\right\}\right]}$$

II. Path integrals

(Altland & Simons, Chapter 3+4)

In particular: The Feynman path integral

II.1. General path integral formalism

Path integral in quantum mechanics: alternative description to the operator/canonical quantization approach. Equivalent!

Advantages of the path integral:

- classical limit of QM always visible
- efficient formulation of non-perturbative approaches, e.g., instanton solution to quantum tunneling; the proof of renormalizability of the electroweak theory by t'Hooft in 1971 was performed in the path integral formalism and has to this date not been achieved in the canonical approach (see F. Close, "The Infinity Puzzle")
- path integrals are easily generalized to higher-dimensional field integrals, see later.

Basic idea: expansion around the classical path of a quantum particle given by the principle of least action.

II.2 Construction of the path integral

Starting point: time-dependent Schrödinger equation (time-independent $\hat{H}$ for simplicity)

$$i\hbar \partial_t |\psi\rangle = \hat{H} |\psi\rangle$$

$\Rightarrow$ formal integration yields the time evolution operator

$$\hat{U}(t',t) = e^{-i\hat{H}(t'-t)/\hbar}$$

$$|\psi(t')\rangle = \hat{U}(t',t)\,|\psi(t)\rangle$$

In real space (q) we can write

$$\psi(q',t') = \langle q'|\psi(t')\rangle = \langle q'|\hat{U}(t',t)|\psi(t)\rangle$$

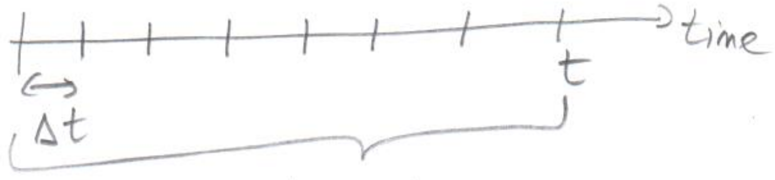
$$= \int dq \; U(q',t';q,t)\,\psi(q,t)$$

$$U(q',t';q,t) \equiv \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle$$

(q',q)-component of the time evolution operator

= "propagator"

Feynman's idea: infinitesimal time evolutions



$$t = N \cdot \Delta t$$

$$e^{-i\hat{H}t/\hbar} = \left[e^{-i\hat{H}\Delta t/\hbar}\right]^N$$

formal rewriting, but: for Δt much smaller than the relevant excitation energies of $\hat{H}$, the terms $\hat{H}\Delta t/\hbar$ can be treated perturbatively.

If $\hat{H} = \hat{T} + \hat{V}$ = kinetic + potential energy,

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{T}\Delta t/\hbar} e^{-i\hat{V}\Delta t/\hbar} + \mathcal{O}(\Delta t^2).$$

Advantage: eigenstates of $\hat{T}$ and $\hat{V}$ are known independently:

$$(*) \quad \langle q_f | \left[e^{-i\hat{H}\Delta t/\hbar}\right]^N | q_i \rangle \simeq \langle q_f | \wedge e^{-i\hat{T}\Delta t/\hbar} e^{-i\hat{V}\Delta t/\hbar} \wedge \cdots \wedge$$
$$\times e^{-i\hat{T}\Delta t/\hbar} e^{-i\hat{V}\Delta t/\hbar} | q_i \rangle$$

Now we insert at "$\wedge$" positions the identity

$$(**) \quad id = \int dq_n \int dp_n \, |q_n\rangle\langle q_n | p_n\rangle\langle p_n|$$

$\{|q_n\rangle\}, \{|p_n\rangle\}$: complete sets of position-/momentum eigenstates

(**) into (*) and use $\langle q|p\rangle = \langle p|q\rangle^*$

$$= e^{iqp/\hbar}/(2\pi\hbar)^{1/2} \; ;$$

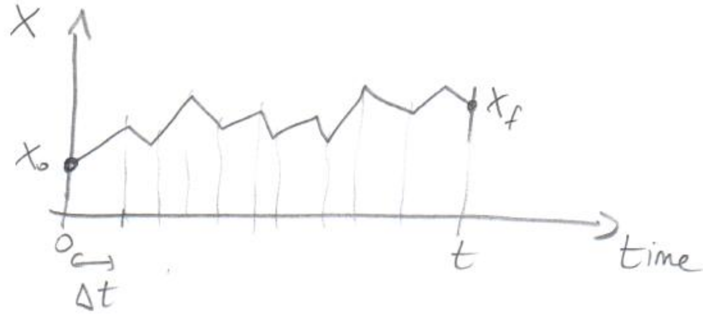
$$\langle q_f|e^{-iHt/\hbar}|q_i\rangle \simeq \int_{\substack{q_N = q_f \\ q_0 = q_i}} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \quad \times$$

(***)

$$\times\, e^{-i\frac{\Delta t}{\hbar}\sum_{n=0}^{N-1}\left(V(q_n)+T(p_{n+1})-p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}\right)}$$

=> $(2N-1)$-dimensional integral over eigenvalues.

=> at each time step $t_n = n\Delta t$, $n=1,\dots,N$ we integrate over a pair of coordinates $x_n = (q_n, p_n)$ parametrizing classical phase space



– if $p_{n+1}(q_{n+1}-q_n) > \hbar$ the phase of the exponential exceeds 2π. Paths with this behavior will destructively interfere leading to cancellation.

=> smooth variation of important paths

=> motivates continuum limit

end lecture 2 (1.5 hrs)