Introduction to Many-body Theory

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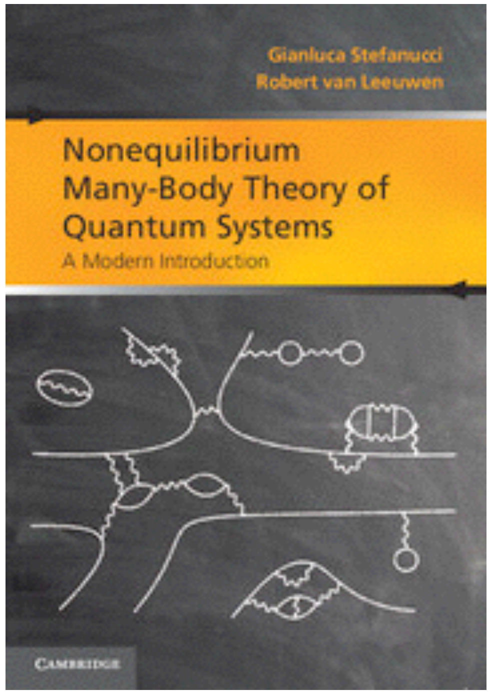
Overview



Part I : Basics

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- Second quantisation
- Time-evolution
- The contour idea

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Introduction to Many-body Theory I

Part I : Basics

- Time-dependent Schrödinger equation
- Second quantisation
- Time-evolution
- The contour idea

Basic quantum mechanics

To describe time-dependent phenomena in nature we have to calculate the time evolution of the relevant quantum states. These states are usually given in a basis representation

$$|\Psi\rangle = \sum_n \Psi_n |n\rangle$$

$$\langle m|n\rangle = \delta_{mn}$$

$\Rightarrow$

$$\langle m|\Psi\rangle = \Psi_m$$

We can therefore write

$$|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle$$

$\Rightarrow$

$$\sum_n |n\rangle\langle n| = 1$$

Resolution of the identity

The time-evolution of a quantum state is given by the Schrödinger equation

$$i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \qquad |\Psi(t_0)\rangle = |\Psi_0\rangle$$

To solve this equation we need to know the representation of the Hamiltonian in a given basis. If we define

$$H_{nm}(t) = \langle n|\hat{H}(t)|m\rangle \qquad c_n(t) = \langle n|\Psi(t)\rangle$$

Then we can write

$$i\partial_t\langle n|\Psi(t)\rangle = \langle n|\hat{H}(t)|\Psi(t)\rangle = \sum_m \langle n|\hat{H}(t)|m\rangle\langle m|\Psi(t)\rangle = \sum_m H_{nm}(t)\langle m|\Psi(t)\rangle$$

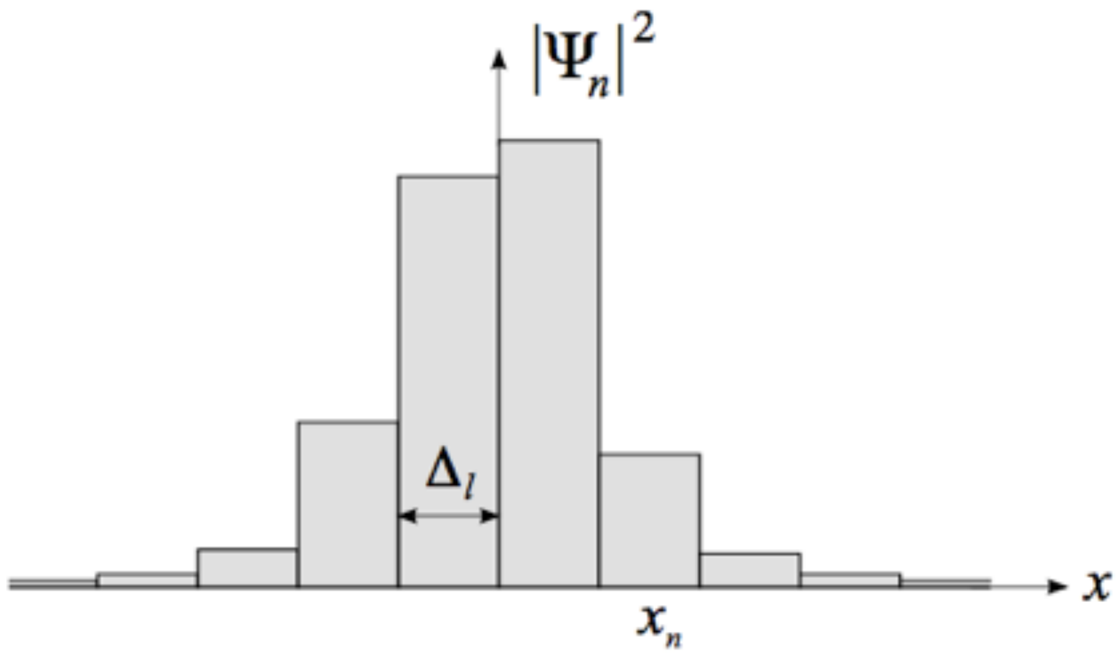
$\Rightarrow$

$$i\partial_t\mathbf{c}(t) = \mathbf{H}(t)\,\mathbf{c}(t)$$

Position basis

We measure a particle to be in interval Δ_n
Its corresponding state is denoted by

$$|x_n\rangle$$



These states have the property

$$\langle x_n | x_m \rangle = \delta_{nm}$$

and form a complete set

$$|\Psi\rangle = \sum_n |x_n\rangle\langle x_n|\Psi\rangle$$

If the system is in state $|\Psi\rangle$ then the probability to measure state $|x_n\rangle$ is

$$P_n = |\langle x_n|\Psi\rangle|^2 = |\Psi(x_n)|^2$$

For one particle in position basis we can, for example, define the Hamiltonian

$$\langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle = (-\frac{1}{2}\nabla^2 + v(\mathbf{x},t))\langle \mathbf{x}|\mathbf{x}'\rangle$$

The Schrödinger equation

$$\hat{h}|\psi(t)\rangle = i\partial_t|\psi(t)\rangle \qquad\qquad \psi(\mathbf{x},t) = \langle \mathbf{x}|\psi(t)\rangle$$

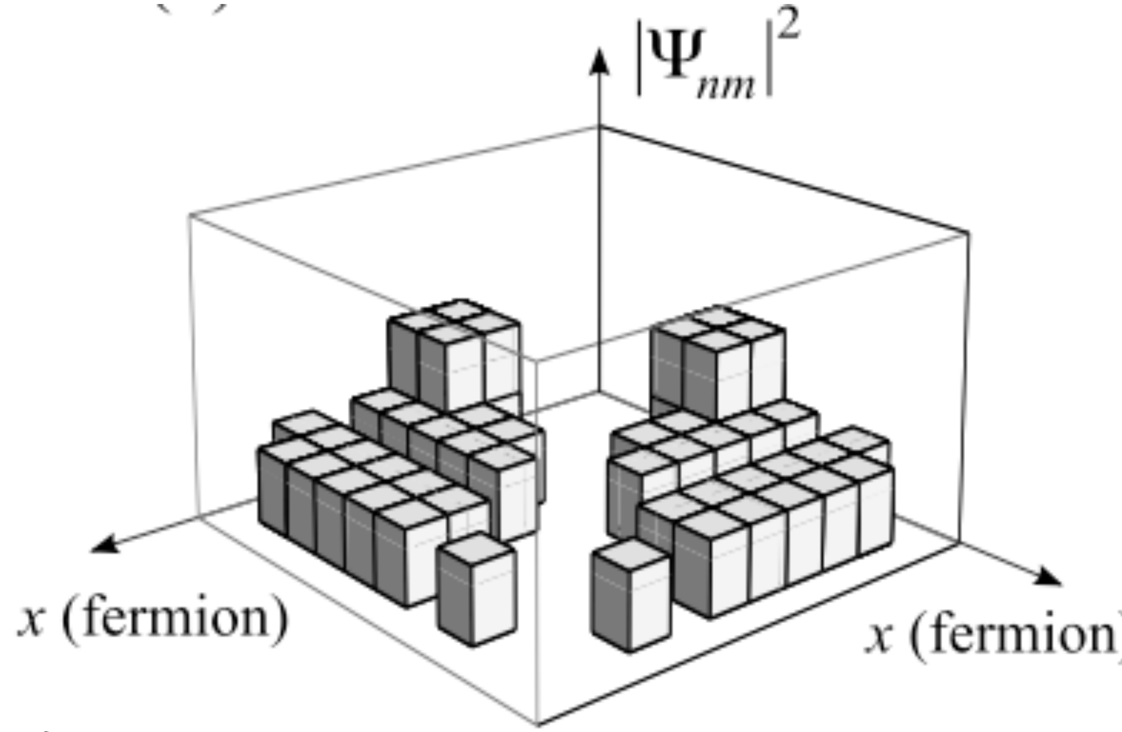
in the position representation then has the form

$$\begin{aligned}
i\partial_t\psi(\mathbf{x},t) &= \langle \mathbf{x}|\hat{h}|\psi(t)\rangle = \int d\mathbf{x}'\, \langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi(t)\rangle \\
&= \int d\mathbf{x}' \left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right) \langle \mathbf{x}|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi(t)\rangle \\
&= \left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right) \psi(\mathbf{x},t)
\end{aligned}$$

Two particles

If we simultaneously measure a particle in intervals Δ_n and Δ_m the state is

$$|x_n\, x_m\rangle$$



The particles are indistinguishable

$$|x_n\, x_m\rangle = \lambda |x_m\, x_n\rangle = \lambda^2 |x_n\, x_m\rangle \rightarrow \lambda = \pm 1$$

The states are normalised

$$\langle x_n x_m | x_{n'} x_{m'}\rangle = \delta_{nn'}\delta_{mm'} \pm \delta_{nm'}\delta_{mn'} = \left| \begin{array}{cc} \delta_{nn'} & \delta_{nm'} \\ \delta_{mn'} & \delta_{mm'} \end{array} \right|_{\pm}$$

Let us consider fermions. Only the states with n > m are linearly independent and we have

$$|\Psi\rangle = \sum_{n>m} |x_n\, x_m\rangle\langle x_n\, x_m|\Psi\rangle$$

$$P_{nm} = |\langle x_n\, x_m|\Psi\rangle|^2 = |\Psi(x_n, x_m)|^2$$

Second quantization

For N fermions we have (with P a permutation)

$$|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = (-1)^P \, |\mathbf{x}_{P(1)} \dots \mathbf{x}_{P(N)}\rangle \qquad \mathbf{x} = \mathbf{r}, \sigma$$

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \mathbf{y}_1 \dots \mathbf{y}_N \rangle = \sum_P (-1)^P \prod_{j=1}^{N} \delta(\mathbf{x}_j - \mathbf{y}_{P(j)})$$

Determinant

There is a unique operator $\hat{\psi}^\dagger(\mathbf{x})$ that generates the position basis. It is defined by

$$\begin{aligned}
|\mathbf{x}_1\rangle &= \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\
|\mathbf{x}_1\,\mathbf{x}_2\rangle &= \hat{\psi}^\dagger(\mathbf{x}_2)|\mathbf{x}_1\rangle = \hat{\psi}^\dagger(\mathbf{x}_2)\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\
|\mathbf{x}_1 \dots \mathbf{x}_N\rangle &= \hat{\psi}^\dagger(\mathbf{x}_N)|\mathbf{x}_1 \dots \mathbf{x}_{N-1}\rangle = \hat{\psi}^\dagger(\mathbf{x}_N) \dots \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle
\end{aligned}$$

$\hat{\psi}^\dagger(\mathbf{x})$ is called creation operator

It follows : $\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y}) = -\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})$

Remember that the adjoint of an operator Ô is defined by

$$\langle\Phi|\hat{O}^\dagger|\chi\rangle = \langle\chi|\hat{O}|\Phi\rangle^*$$

The adjoint $\hat{\psi}(\mathbf{x})$ of the creation operator therefore satisfies

$$\begin{aligned}
\langle\mathbf{x}_1\ldots\mathbf{x}_{N-1}|\hat{\psi}(\mathbf{x}_N)|\mathbf{y}_1\ldots\mathbf{y}_N\rangle^* &= \langle\mathbf{y}_1\ldots\mathbf{y}_N|\hat{\psi}^\dagger(\mathbf{x}_N)|\mathbf{x}_1\ldots\mathbf{x}_{N-1}\rangle \\
= \langle\mathbf{y}_1\ldots\mathbf{y}_N|\mathbf{x}_1\ldots\mathbf{x}_N\rangle &= \sum_P(-1)^P\prod_{j=1}^N\delta(\mathbf{y}_j-\mathbf{x}_{P(j)})
\end{aligned}$$

and hence (by expanding the determinant along column N) we have

$$\hat{\psi}(\mathbf{x})|\mathbf{y}_1\ldots\mathbf{y}_N\rangle = \sum_{k=1}^N(-1)^{N-k}\,\delta(\mathbf{x}-\mathbf{y}_k)\,|\mathbf{y}_1\ldots\mathbf{y}_{k-1}\mathbf{y}_{k+1}\ldots\mathbf{y}_N\rangle$$

For example:

$$\begin{aligned}
\hat{\psi}(\mathbf{x})|0\rangle &= 0 \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\rangle &= \delta(\mathbf{x}-\mathbf{y}_1)|0\rangle \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\,\mathbf{y}_2\rangle &= \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\rangle \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\,\mathbf{y}_2\,\mathbf{y}_3\rangle &= \delta(\mathbf{x}-\mathbf{y}_3)|\mathbf{y}_1\,\mathbf{y}_2\rangle - \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\,\mathbf{y}_3\rangle + \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\,\mathbf{y}_3\rangle
\end{aligned}$$

The operator $\hat{\psi}(\mathbf{x})$ is called annihilation operator

It follows (with anti-commutator $[A, B]_+ = AB + BA$):

$$\begin{aligned}
\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})\right]_+ &= \left[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_+ = 0 \\
\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_+ &= \delta(\mathbf{x}-\mathbf{y})
\end{aligned}$$

The density operator is defined by

$$\hat{n}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$$

and has the property

$$\hat{n}(\mathbf{x})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\,|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

For example:

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x})\,\hat{\psi}(\mathbf{x})|\mathbf{y}_1\mathbf{y}_2\rangle &= \hat{\psi}^\dagger(\mathbf{x})\,\left(\delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\rangle\right) \\
&= \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\mathbf{x}\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\mathbf{x}\rangle \\
&= (\delta(\mathbf{x}-\mathbf{y}_1) + \delta(\mathbf{x}-\mathbf{y}_2))|\mathbf{y}_1\mathbf{y}_2\rangle
\end{aligned}$$

The expectation value $n(\mathbf{x}) = \langle\Psi|\hat{n}(\mathbf{x})|\Psi\rangle$

is the particle density of the system in state $|\Psi\rangle$

For N particles we define the Hamiltonian by

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{H} | \mathbf{x}'_1 \dots \mathbf{x}'_N \rangle$$

$$= \left(\sum_j^N -\frac{1}{2}\nabla_j^2 + v(\mathbf{x}_j, t) + \frac{1}{2}\sum_{i \neq j}^N w(\mathbf{x}_i, \mathbf{x}_j) \right) \langle \mathbf{x}_1 \dots \mathbf{x}_N | \mathbf{x}'_1 \dots \mathbf{x}'_N \rangle$$

or equivalently, for any state $|\Psi\rangle$

Many-body wave function

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{H} | \Psi \rangle$$

$$= \left(\sum_j^N -\frac{1}{2}\nabla_j^2 + v(\mathbf{x}_j, t) + \frac{1}{2}\sum_{i \neq j}^N w(\mathbf{x}_i, \mathbf{x}_j) \right) \langle \mathbf{x}_1 \dots \mathbf{x}_N | \Psi \rangle$$

Since the one- and two-body potentials are diagonal in the position representation it is easy to express them in second quantisation

For the 2-particle interaction we have

$$\hat{W}|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \frac{1}{2}\sum_{i\neq j}^{N} w(\mathbf{x}_i, \mathbf{x}_j)|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

Since the density operator has the property

$$\hat{n}(\mathbf{x})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\,|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

it follows that

$$\begin{aligned}
\hat{W} &= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\hat{n}(\mathbf{x})\hat{n}(\mathbf{y}) - \frac{1}{2}\int d\mathbf{x}\, w(\mathbf{x},\mathbf{x})\hat{n}(\mathbf{x}) \\
&= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\left(\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y}) - \delta(\mathbf{x}-\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\right) \\
&= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})
\end{aligned}$$

$$\boxed{\hat{W} = \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})}$$

Similarly for the one-body potential

$$\hat{V}(t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \sum_j^N v(\mathbf{x}_j, t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \int d\mathbf{x}\, \hat{n}(\mathbf{x}) v(\mathbf{x}, t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$$

$$\hat{V}(t) = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\, v(\mathbf{x}, t)$$

The kinetic energy operator is only slightly more difficult. Let's illustrate it for 3 particles. Remember that

$$\hat{\psi}(\mathbf{x})|\mathbf{y}_1\, \mathbf{y}_2\, \mathbf{y}_3\rangle \quad = \quad \delta(\mathbf{x} - \mathbf{y}_3)|\mathbf{y}_1\, \mathbf{y}_2\rangle - \delta(\mathbf{x} - \mathbf{y}_2)|\mathbf{y}_1\, \mathbf{y}_3\rangle + \delta(\mathbf{x} - \mathbf{y}_1)|\mathbf{y}_2\, \mathbf{y}_3\rangle$$

$$\hat{\psi}^\dagger(\mathbf{x})\nabla^2\hat{\psi}(\mathbf{x})\,|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle$$

$$= \nabla^2\delta(\mathbf{x} - \mathbf{y}_3)|\mathbf{y}_1\, \mathbf{y}_2\, \mathbf{x}\rangle + \nabla^2\delta(\mathbf{x} - \mathbf{y}_2)|\mathbf{y}_1\mathbf{x}\, \mathbf{y}_3\rangle + \nabla^2\delta(\mathbf{x} - \mathbf{y}_1)|\mathbf{x}\, \mathbf{y}_2\, \mathbf{y}_3\rangle$$

If we therefore define

$$\hat{T} = -\frac{1}{2}\int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x})\nabla^2\hat{\psi}(\mathbf{x})$$

then since T is Hermitian

$$\langle \mathbf{y}_1\mathbf{y}_2\mathbf{y}_3|\hat{T}|\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3\rangle = \langle \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\hat{T}|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle^*$$

$$= -\frac{1}{2}\left(\nabla^2_{\mathbf{y}_1} + \nabla^2_{\mathbf{y}_2} + \nabla^2_{\mathbf{y}_3}\right)\langle \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle^*$$

$$= -\frac{1}{2}\left(\nabla^2_{\mathbf{y}_1} + \nabla^2_{\mathbf{y}_2} + \nabla^2_{\mathbf{y}_3}\right)\langle \mathbf{y}_1\mathbf{y}_2\mathbf{y}_3|\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3\rangle$$

yielding exactly the matrix element of the kinetic energy operator. Hence

$$\hat{H}(t) = \int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x})\left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right)\hat{\psi}(\mathbf{x})$$

$$+\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})$$

We can also rewrite everything in a general basis. If we define

$$\langle \mathbf{x}|n\rangle = \varphi_n(\mathbf{x})$$

then φ_n is an orthonormal set of orbitals

$$\delta_{nm} = \langle n|m\rangle = \int d\mathbf{x}\, \langle n|\mathbf{x}\rangle\langle \mathbf{x}|m\rangle = \int d\mathbf{x}\, \varphi_n^*(\mathbf{x})\varphi_m(\mathbf{x})$$

If we define

$$\hat{a}_n = \int d\mathbf{x}\, \varphi_n^*(\mathbf{x})\hat{\psi}(\mathbf{x}) \qquad \hat{a}_n^\dagger = \int d\mathbf{x}\, \varphi_n(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})$$

then

$$[\hat{a}_n, \hat{a}_m^\dagger]_+ = \delta_{nm} \qquad [\hat{a}_n, \hat{a}_m]_+ = [\hat{a}_n^\dagger, \hat{a}_m^\dagger]_+ = 0$$

$$a_n^\dagger|0\rangle = \int d\mathbf{x}\, \varphi_n(\mathbf{x})\, \underbrace{\hat{\psi}^\dagger(\mathbf{x})|0\rangle}_{|\mathbf{x}\rangle} = \int d\mathbf{x}|\mathbf{x}\rangle\langle\mathbf{x}|n\rangle = |n\rangle$$

In general we can generate N-particle states

$$|n_1 \dots n_N\rangle = \hat{a}^\dagger_{n_N} \dots \hat{a}^\dagger_{n_1} |0\rangle$$

We can relate them to position basis states as follows

$$\begin{aligned} |n_1 \dots n_N\rangle &= \int d\mathbf{x}_1 \dots d\mathbf{x}_N \, \varphi_{n_1}(\mathbf{x}_1) \dots \varphi_{n_N}(\mathbf{x}_N) \, \hat{\psi}^\dagger(\mathbf{x}_N) \dots \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\ &= \int d\mathbf{x}_1 \dots d\mathbf{x}_N \, \varphi_{n_1}(\mathbf{x}_1) \dots \varphi_{n_N}(\mathbf{x}_N)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle \end{aligned}$$

and find that their overlaps are given by Slater determinants

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | n_1 \dots n_N \rangle = \sum_P (-1)^P \varphi_{n_1}(\mathbf{x}_{P(1)}) \dots \varphi_{n_N}(\mathbf{x}_{P(N)}) = \begin{vmatrix} \varphi_{n_1}(\mathbf{x}_1) & \dots & \varphi_{n_N}(\mathbf{x}_1) \\ \vdots & & \vdots \\ \varphi_{n_1}(\mathbf{x}_N) & \dots & \varphi_{n_N}(\mathbf{x}_N) \end{vmatrix}$$

The creation and annihilation operators therefore add and remove orbitals from Slater determinants

The Hamiltonian in a general one-particle basis then attains the form

$$\hat{H}(t) = \sum_{ij} h_{ij}(t)\, \hat{a}_i^\dagger\, \hat{a}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl}\, \hat{a}_i^\dagger\, \hat{a}_j^\dagger\, \hat{a}_k\, \hat{a}_l$$

where

$$h_{ij}(t) = \int d\mathbf{x}\, \varphi_i^*(\mathbf{x}) h(\mathbf{x}, t) \varphi_j(\mathbf{x})$$

$$v_{ijkl} = \int d\mathbf{x} d\mathbf{y}\, w(\mathbf{x}, \mathbf{y})\, \varphi_i^*(\mathbf{x}) \varphi_j^*(\mathbf{y}) \varphi_k(\mathbf{y}) \varphi_l(\mathbf{x})$$

The convenient basis states in practice depend on the problem.
Commonly used ones are, for example, Kohn-Sham or Hartree-Fock orbitals

Second quantization: Take home message

- Second quantisation is nothing but a convenient way to generate a many-particle basis that automatically has the correct (anti)symmetry.

  Basis states are created by (anti)-commuting operators with simple (anti)-commutation relations

- As we will see, second quantisation is very convenient in many-body theory as it allows for simple manipulation of perturbative terms without the need to deal with (anti)-symmetrised orbital products

- The derivation of the Hamiltonian in second quantisation is easy in position basis as the Hamiltonian is almost diagonal in this basis

Expectation values

A general expectation value is of the form

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

initial state

where we defined the evolution operator as

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

and the operator Ô(t) in the Heisenberg picture as

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

The Heisenberg operator satisfies an equation of motion

It follows from the Schrödinger equation that

$$i\partial_t \hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t')$$

and therefore that the Heisenberg operator satisfies the equation of motion

$$\partial_t \hat{O}_H(t) = -i\left[\hat{O}_H(t), \hat{H}_H(t)\right] + \left(\partial_t \hat{O}(t)\right)_H$$

For example, you can check that the field operator satisfies

$$[i\partial_t - h(\mathbf{x}t)]\,\hat{\psi}_H(\mathbf{x},t) = \int d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{n}_H(\mathbf{y}t)\hat{\psi}_H(\mathbf{x}t)$$

Let us now derive a more explicit expression for the evolution operator

We start again from the Schrödinger equation $i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle$

If we divide $[t_0, T]$ into small intervals Δ then

$$|\Psi(T)\rangle \approx e^{-i\hat{H}(t_n)\Delta}\dots e^{-i\hat{H}(t_0)\Delta}|\Psi(t_0)\rangle = \mathcal{T}\left\{e^{-i\hat{H}(t_n)\Delta}\dots e^{-i\hat{H}(t_0)\Delta}\right\}|\Psi(t_0)\rangle$$

$$= \mathcal{T}\left\{e^{-i\sum_j^n \hat{H}(t_j)\Delta}\right\}|\Psi(t_0)\rangle$$

where $\mathcal{T}$ denotes time-ordering that orders the latest operator most left.
We used that operators commute under time-ordering

$$\mathcal{T}\left\{\hat{A}(t_1)\hat{B}(t_2)\right\} = \mathcal{T}\left\{\hat{B}(t_2)\hat{A}(t_1)\right\}$$

and hence, in particular

$$\mathcal{T}\left\{e^{\hat{A}(t_1)}e^{\hat{B}(t_2)}\right\} = \mathcal{T}\left\{e^{\hat{A}(t_1)+\hat{B}(t_2)}\right\}$$

In the limit Δ => 0 then

$$|\Psi(T)\rangle = \mathcal{T}\left\{e^{-i\int_{t_0}^{T} dt\,\hat{H}(t)}\right\}|\Psi(t_0)\rangle = \hat{U}(T,t_0)|\Psi(t_0)\rangle$$

Time-evolution operator

By as similar procedure we have

$$U(t_0,T) = e^{i\hat{H}(t_1)\Delta}e^{i\hat{H}(t_2)\Delta}\ldots e^{i\hat{H}(t_n)\Delta} = \bar{\mathcal{T}}\left\{e^{i\sum_j^n \hat{H}(t_j)\Delta}\right\}$$

$$U(t_0,T) = \bar{\mathcal{T}}\left\{e^{i\int_{t_0}^{T}\hat{H}(t)dt}\right\}$$

where $\bar{\mathcal{T}}$ denotes anti-time-ordering that orders the latest operator most right.

The evolution operator can then be written as

$$\hat{U}(t_1, t_2) = \begin{cases} \mathcal{T} e^{-i \int_{t_1}^{t_2} dt\, \hat{H}(t) dt} & t_1 < t_2 \\ \bar{\mathcal{T}} e^{+i \int_{t_2}^{t_1} dt\, \hat{H}(t) dt} & t_2 < t_1 \end{cases}$$

and the expectation value

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

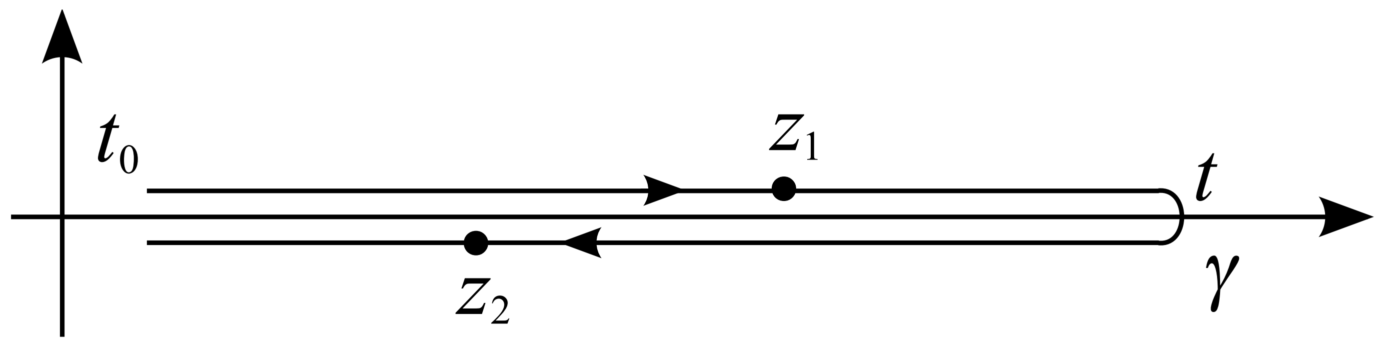
can therefore be written as

$$\langle \hat{O}(t) \rangle = \langle \Psi_0 | \, \bar{\mathcal{T}} e^{i \int_{t_0}^{t} dt\, \hat{H}(t) dt} \, \hat{O}(t) \, \mathcal{T} e^{-i \int_{t_0}^{t} dt\, \hat{H}(t) dt} \, | \Psi_0 \rangle$$

If we expand in powers of the Hamiltonian then a typical term is

$$\bar{\mathcal{T}} \left\{ \hat{H}(t_1) \ldots \hat{H}(t_n) \right\} \hat{O}(t) \, \mathcal{T} \left\{ \hat{H}(t_1') \ldots \hat{H}(t_n') \right\}$$

early ← late   late ← early



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

We define a contour γ consisting of two copies of the interval $[t_0 , t]$ .A generic element z of γ can lie on the forward branch γ_- or the backward branch γ_+

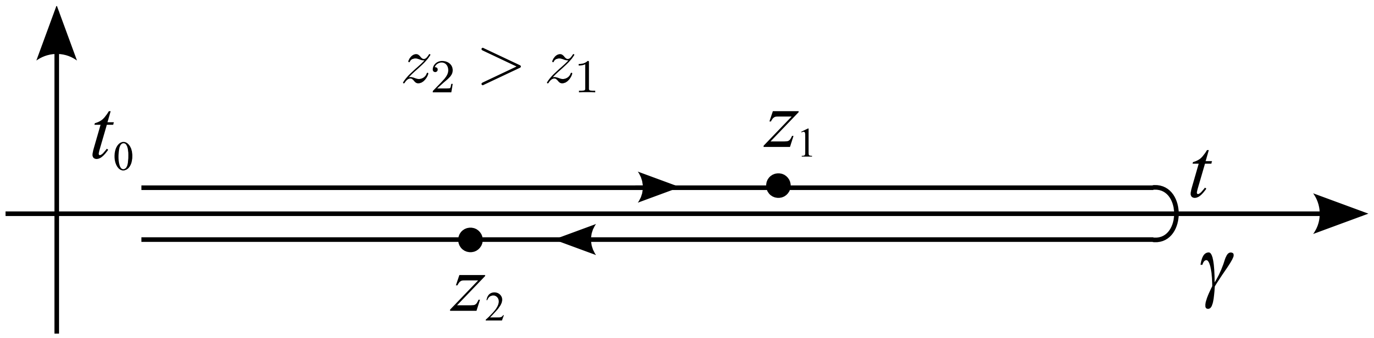
Notation

$z = t'_-$ when $z \in \gamma_-$ and its real value is t'

$z = t'_+$ when $z \in \gamma_+$ and its real value is t'

We can define operators on the contour

$$\hat{O}(z') = \begin{cases} \hat{O}_-(t') & z' = t'_- \\ \hat{O}_+(t') & z' = t'_+ \end{cases}$$



$$\mathcal{T}_\gamma \left\{ \hat{A}_{P(1)}(z_{P(1)}) \dots \hat{A}_{P(1)}(z_{P(1)}) \right\} = \hat{A}_1(z_1) \dots \hat{A}_n(z_n) \quad z_1 > \dots > z_n$$

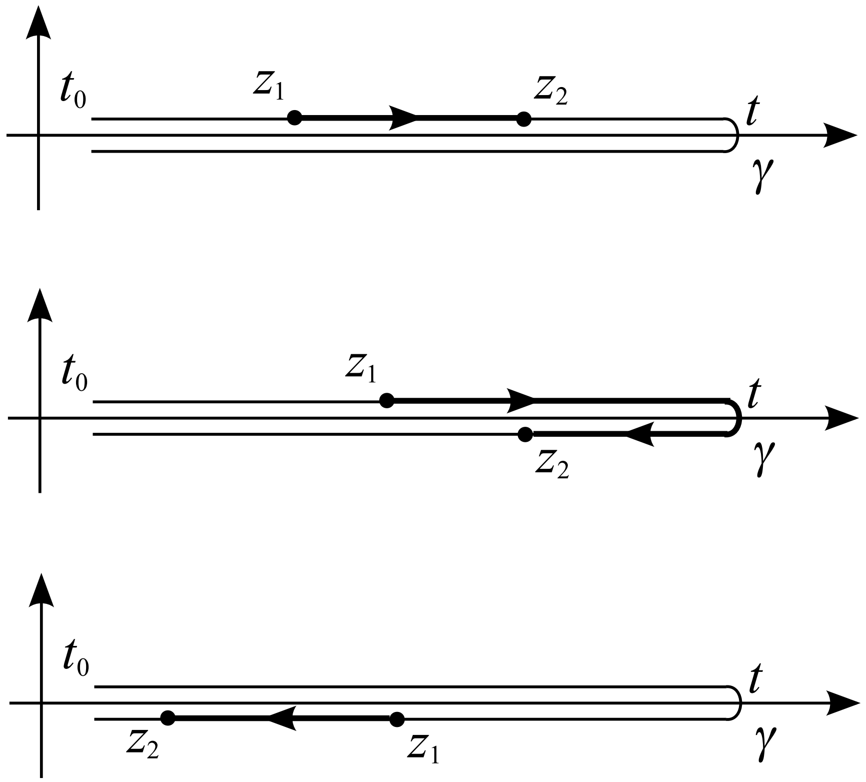
With this definition we can write

$$\bar{\mathcal{T}} \left\{ \hat{H}(t_1) \dots \hat{H}(t_n) \right\} \hat{O}(t) \, \mathcal{T} \left\{ \hat{H}(t'_1) \dots \hat{H}(t'_n) \right\}$$
$$= \mathcal{T}_\gamma \left\{ \hat{H}(t_{1+}) \dots \hat{H}(t_{n+}) \hat{O}(t) \hat{H}(t'_{1-}) \dots \hat{H}(t'_{n-}) \right\}$$

where

$$\hat{H}(z = t'_\pm) = \hat{H}(t')$$

With this trick we can write the expectation value in a compact way



$$\int_{z_1}^{z_2} d\bar{z}\,\hat{A}(\bar{z}) = \begin{cases} \int_{t_1}^{t_2} d\bar{t}\,\hat{A}_-(\bar{t}) & \text{if } z_1 = t_{1-} \text{ and } z_2 = t_{2-} \\ \int_{t_1}^{t} d\bar{t}\,\hat{A}_-(\bar{t}) + \int_{t}^{t_2} d\bar{t}\,\hat{A}_+(\bar{t}) & \text{if } z_1 = t_{1-} \text{ and } z_2 = t_{2+} \\ \int_{t_1}^{t_2} d\bar{t}\,\hat{A}_+(\bar{t}) & \text{if } z_1 = t_{1+} \text{ and } z_2 = t_{2+} \end{cases}$$

The expectation value can then be written as

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

and since the operators commute under the time-ordering

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

It will be useful to extend the concept of expectation value to ensembles

$$\langle \hat{O}_H(t) \rangle = \sum_n w_n \langle \Psi_n | \hat{O}_H(t) | \Psi_n \rangle = \mathrm{Tr} \left\{ \hat{\rho}\, \hat{O}_H(t) \right\}$$

$$\hat{\rho} = \sum_n w_n |\Psi_n\rangle\langle\Psi_n| \qquad \sum_n w_n = 1 \qquad w_m \geq 0$$

where we defined $\mathrm{Tr}\ \hat{A} = \sum_m \langle \Phi_m | \hat{A} | \Phi_m \rangle$ with $|\Phi_m\rangle$ any complete orthonormal set

An important special case is

$$w_n = \frac{e^{-\beta E_n}}{\sum_m e^{-\beta E_m}} \qquad \hat{H}^M |\Psi_n\rangle = E_n |\Psi_n\rangle \qquad \hat{H}^M = \hat{H}(t_0) - \mu \hat{N}$$

$$\hat{\rho} = \sum_n w_n |\Psi_n\rangle\langle\Psi_n| = \frac{e^{-\beta \hat{H}^M}}{\mathrm{Tr}\ \left\{ e^{-\beta \hat{H}^M} \right\}}$$

This corresponds to an initial system at inverse temperature β and chemical potential μ

$$e^{-\beta \hat{H}^M} = e^{-i[(t_0 - i\beta) - t_0]\hat{H}^M} = \hat{U}(t_0 - i\beta, t_0)$$

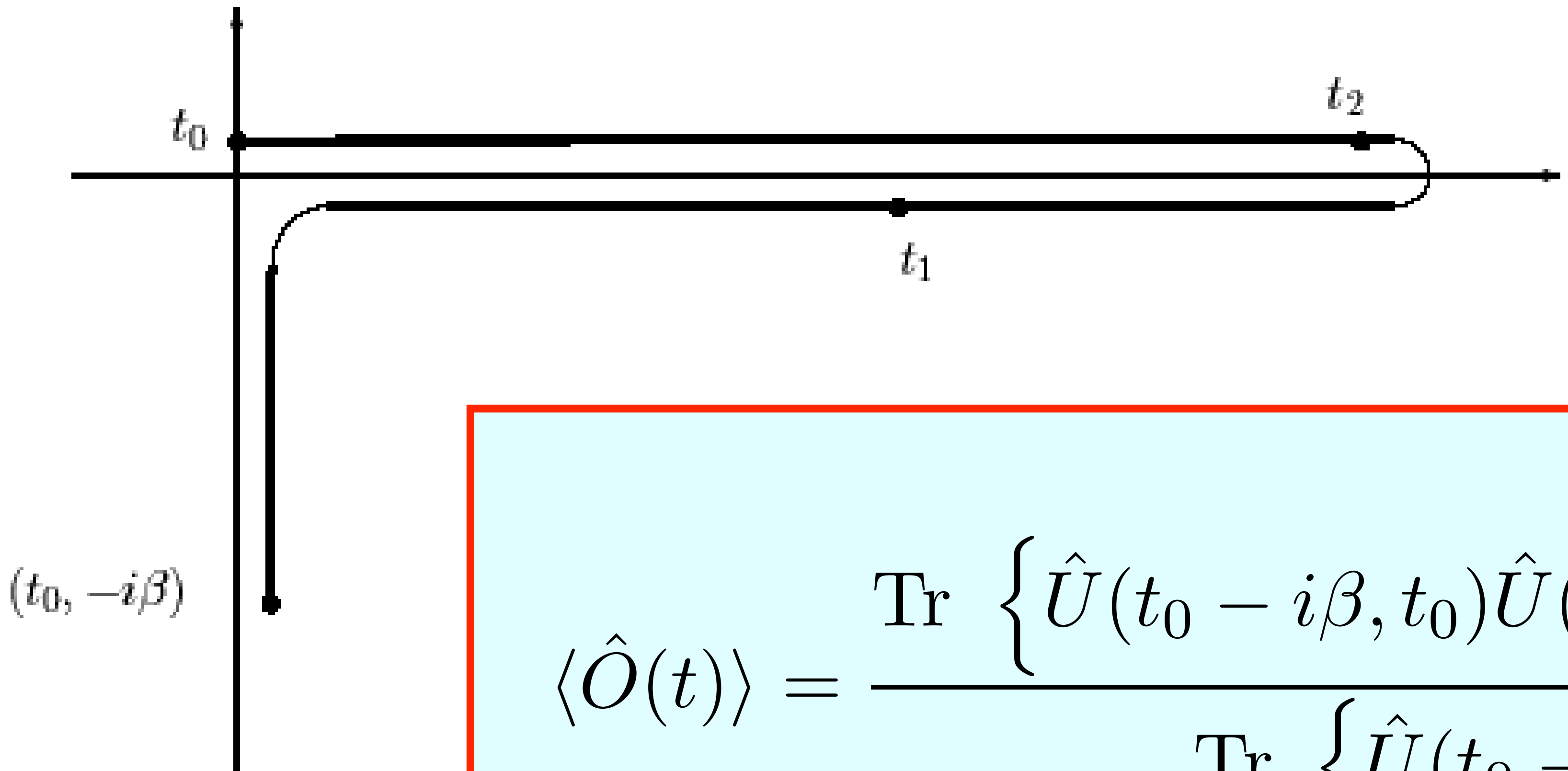
If we therefore define

$$\hat{H}(z) = \begin{cases} \hat{H}(t) & z \in [t_0, \infty[\\ \hat{H}^M & z \in [t_0, t_0 - i\beta] \end{cases}$$

then we can write

$$\langle \hat{O}(t) \rangle = \frac{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0) \right\}}{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}$$

(L.V.Keldysh, Sov.Phys.JETP20, 1018 (1965),
Konstantinov, Perel', JETP12,142 (1961))



$$\langle \hat{O}(t) \rangle = \frac{\text{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0) \right\}}{\text{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}$$

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}(z)} \hat{O}(t) \right\}}{\text{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}(z)} \right\}}$$

Time ordering is now defined along the extended contour

Time-ordering: Take home message

- Time-ordering is a direct consequence of the structure of time-dependent Schrödinger equation.

- Expectation values consist of a time-ordered evolution operator for the ket state and an anti-time-ordering for the bra state

- The expectation of any operator value can be rewritten in terms of a single time-ordered exponential by introducing contour ordering

- In case of systems prepared in an initial ensemble the expectation value can be rewritten as a time-ordering on a contour with an additional vertical track