CTQMC

Bernard Amadon
CEA, DAM, DIF
Université Paris-Saclay, CEA, LMCE
Bruyères-le-Châtel, France

Short summary of second quantization (1): the isolated atom

$$H_{\mathrm{atom}} = \sum_{\sigma} \varepsilon_0 d^{\dagger}_{\sigma} d_{\sigma} + U n_{\uparrow} n_{\downarrow} = \varepsilon_0 d^{\dagger}_{\uparrow} d_{\uparrow} + \varepsilon_0 d^{\dagger}_{\downarrow} d_{\downarrow} + U n_{\uparrow} n_{\downarrow}$$

Possible states are:

$$\begin{aligned} |0\rangle &= |00\rangle \\ |\uparrow\rangle &= |10\rangle \\ |\downarrow\rangle &= |01\rangle \\ |\uparrow\downarrow\rangle &= |11\rangle \end{aligned}$$

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$d_\uparrow^\dagger$ creates an electron $\uparrow$, thus

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$n_\uparrow = d^\dagger_\uparrow d_\uparrow$ gives the number of electron $\uparrow$:

$$\begin{aligned} \langle 00|n_\uparrow|00\rangle &= \langle 00|d^\dagger_\uparrow d_\uparrow|00\rangle &&= 0 \\ \langle 10|n_\uparrow|10\rangle &= \langle 10|d^\dagger_\uparrow d_\uparrow|10\rangle &&= \langle 10|d^\dagger_\uparrow|00\rangle &&= \langle 10|10\rangle &&= 1 \\ \langle 01|n_\uparrow|01\rangle &= \langle 01|d^\dagger_\uparrow d_\uparrow|01\rangle &&= 0 \\ \langle 11|n_\uparrow|11\rangle &= \langle 11|d^\dagger_\uparrow d_\uparrow|11\rangle &&= \langle 11|d^\dagger_\uparrow|01\rangle &&= \langle 11|11\rangle &&= 1 \end{aligned}$$

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$n_\downarrow n_\uparrow = 1$ if one electron is present in $\uparrow$ and one in $\downarrow$

$$\begin{aligned} \langle 00|n_\downarrow n_\uparrow|00\rangle &= 0 \\ \langle 10|n_\downarrow n_\uparrow|10\rangle &= \langle 10|n_\downarrow|00\rangle &&= \langle 10|01\rangle &&= 0 \\ \langle 01|n_\downarrow n_\uparrow|01\rangle &= 0 \\ \langle 11|n_\downarrow n_\uparrow|11\rangle &= \langle 11|n_\downarrow|01\rangle &&= \langle 11|11\rangle &&= 1 \end{aligned}$$

Short summary of second quantization (2)

Anticommutation relation, because of the antisymmetry of wavefunction

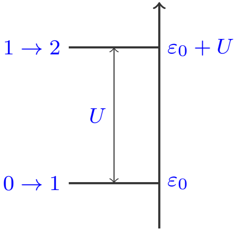
$$|\uparrow\downarrow\rangle \quad = -|\downarrow\uparrow\rangle \quad \Rightarrow \quad d^\dagger_\uparrow d^\dagger_\downarrow|00\rangle \quad = -d^\dagger_\downarrow d^\dagger_\uparrow|00\rangle \quad \Rightarrow \quad d^\dagger_\uparrow d^\dagger_\downarrow \quad = -d^\dagger_\downarrow d^\dagger_\uparrow$$

Isolated atom: exact solution

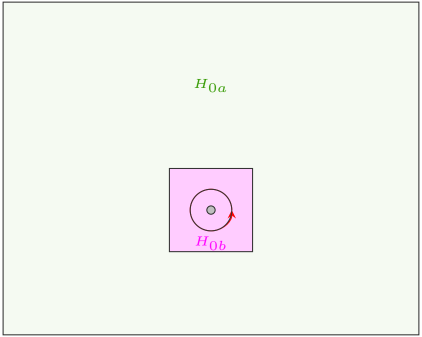
One can compute the energy as a function of the number of electrons:

Configuration	—	$\uparrow$	$\downarrow$	$\downarrow\uparrow$
Energy	0	ε_0	ε_0	$2\varepsilon_0 + U$

One needs an energy ε_0 to go from 0 to 1 electron.
One needs an energy $\varepsilon_0 + U$ to go from 1 to 2 electron.
$\Rightarrow$ Spectral function for the d-electron are formed by Hubbard bands



The Anderson Hamiltonian



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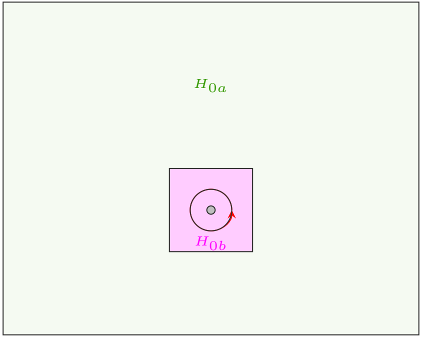

$$H_{\text{Anderson}} = \underbrace{\sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}}_{H_{0a}} + \underbrace{\sum_{\sigma} \varepsilon_0 d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}}_{H_{0b}}$$

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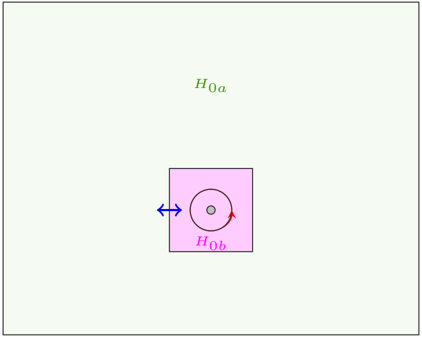

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Anderson model: uncorrelated limit $U = 0$

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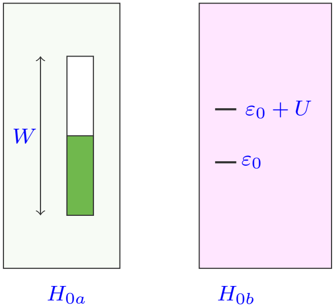
$$\begin{pmatrix} \varepsilon_0 & V_1 & V_2 & \dots & V_k & \dots & V_n \\ V_1 & \varepsilon_1 & 0 & \dots & 0 & \dots & 0 \\ V_2 & 0 & \varepsilon_2 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ V_k & 0 & 0 & \dots & \varepsilon_k & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ V_n & 0 & 0 & \dots & 0 & \dots & \varepsilon_n \end{pmatrix}$$

The Anderson Hamiltonian (solved by CTQMC)



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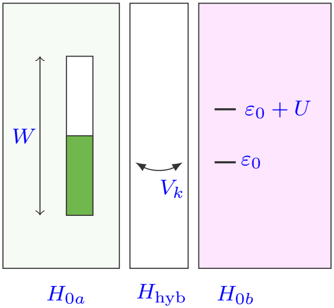

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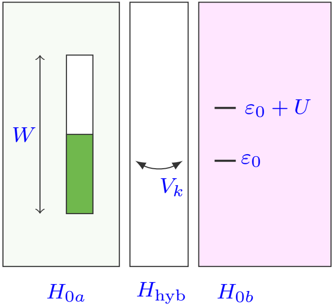

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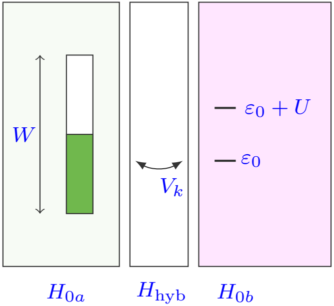

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The main idea is that the atomic problem can be solved exactly and the bath problem can be solved exactly.

Continuous Time Quantum Monte Carlo: Expansion as a function of H_{hyb}

[P. Werner, A. Comanac, L. de medici, M. Troyer and A. J. Millis Phys. Rev. Lett. 97, 076405 (2006)]

The Anderson impurity model.

$$H_{\mathsf{AIM}} = \sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma$$ (Energy of the correlated level)

$$+U n_\uparrow n_\downarrow$$ (Interaction between up and dn orbitals)

$$+\sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$ (levels of the Bath)

$$+\sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} d_\sigma + V_k^* d^\dagger_\sigma c_{k\sigma} \right) (= H_{\mathrm{hyb}})$$ (Hybridization)

$$H_0 = \underbrace{\sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow}_{H_d} + \underbrace{\sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{H_c}$$

$$H_{\mathrm{hyb}} = \sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} d_\sigma + V_k^* d^\dagger_\sigma c_{k\sigma} \right)$$

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&= -\left[e^{+\beta H_0}H_{\text{hyb}}e^{-\beta H_0}\right]A(\beta)
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&= -\left[H_{\mathrm{hyb}}(\beta)\right]A(\beta) \qquad \text{(Heisenberg representation (cf lecture par F. Bruneval) but for imaginary time)}
\end{aligned}$$

This differential equation, where the variable is β, can be solved, taking into account that A and H are operators.

Let’s first remind the solution for a similar equation for a simple function

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So that:

$$f(x) = f(x_0) + \int_{x_0}^{x} -V(x_1)f(x_0) + (-1)^2\int_{x_0}^{x} V(x_1)\int_{x_0}^{x_1} V(x_2)f(x_2)dx_1dx_2$$

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In this last equation, $x_2 < x_1$. As the integrand of the term is symmetric in x_1 and x_2, it can be rewritten as

$$f(x) = f(x_0) + \int_{x_0}^{x} -V(x_1)f(x_0) + \frac{(-1)^2}{2} \int_{x_0}^{x} \int_{x_0}^{x} V(x_1)V(x_2)f(x_0)dx_1dx_2 + (-1)^3 \int_{x_0}^{x} \int_{x_0}^{x_1} \int_{x_0}^{x_2} \ldots$$

where in this case x_1 and x_2 are not related.

At order three:

$$f(x) = f(x_0) + \int_{x_0}^{x} -V(x_1)f(x_0) + (-1)^2 \int_{x_0}^{x}\int_{x_0}^{x_1} V(x_1)V(x_2)f(x_0)dx_1dx_2 + (-1)^3 \int_{x_0}^{x}\int_{x_0}^{x_1}\int_{x_0}^{x_2} \ldots$$

In this last equation, $x_2 < x_1$. As the integrand of the term is symmetric in x_1 and x_2, it can be rewritten as

$$f(x) = f(x_0) + \int_{x_0}^{x} -V(x_1)f(x_0) + \frac{(-1)^2}{2} \int_{x_0}^{x}\int_{x_0}^{x} V(x_1)V(x_2)f(x_0)dx_1dx_2 + (-1)^3 \int_{x_0}^{x}\int_{x_0}^{x_1}\int_{x_0}^{x_2} \ldots$$

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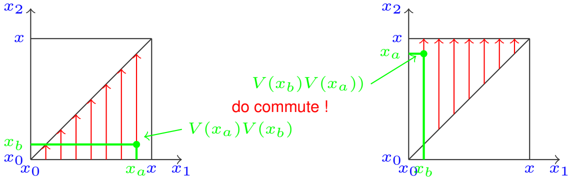

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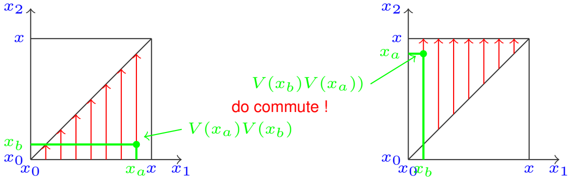

We end with an infinite summation such as:

$$f(x) = f(x_0) + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_{x_0}^{x} dx_1 \ldots \int_{x_0}^{x} dx_k V(x_1)\ldots V(x_k)f(x_0) = f(x_0)\exp\left[\int_{x_0}^{x} -V(x)dx\right]$$

Hybridization expansion

This demonstration can be generalized to the case of matrices

$$\frac{dA(\beta)}{d\beta} = -H_{\mathrm{hyb}}(\beta)A(\beta)$$

We call τ an arbitrary value of β: $A(\tau) = \mathrm{e}^{-\tau H_0}\mathrm{e}^{-\tau H}$

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$$f(x) = f(x_0) + \int_{x_0}^x aV(x_1)f(x_0) + a^2 \int_{x_0}^x \int_{x_0}^{x_1} V(x_1)V(x_2)f(x_0)dx_1 dx_2 + a^3 \dots$$

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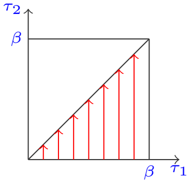

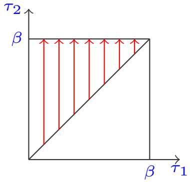

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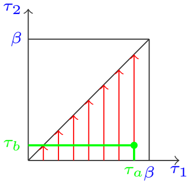

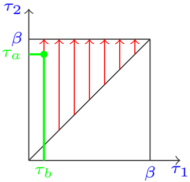

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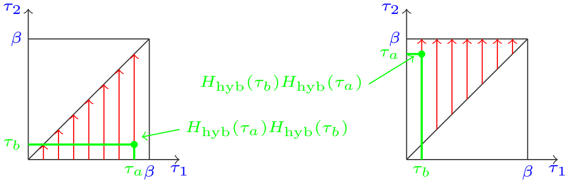

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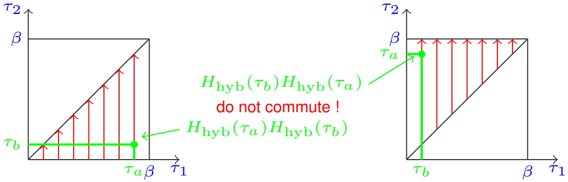

Hybridization expansion and time ordering

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Because

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Let's define the time ordering operator $\mathcal{T}$ such that:

$$\mathcal{T}[H_{\mathrm{hyb}}(\tau_1)H_{\mathrm{hyb}}(\tau_2)] = H_{\mathrm{hyb}}(\tau_1)H_{\mathrm{hyb}}(\tau_2) \quad \tau_2 < \tau_1$$

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It solves the commutation issue and thus:

$$\int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \mathcal{T}[H_{\rm hyb}(\tau_1)H_{\rm hyb}(\tau_2)] = \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \mathcal{T}[H_{\rm hyb}(\tau_1)H_{\rm hyb}(\tau_2)]$$

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One can thus write the whole serie as

$$A(\beta) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \mathcal{T} H_{\mathrm{hyb}}(\tau_1)\ldots H_{\mathrm{hyb}}(\tau_k) = \mathcal{T}\exp\left[-\int_0^\beta H_{\mathrm{hyb}}(\tau)d\tau\right]$$

Hybridization hamiltonian

H_{hyb} is defined by:

$$H_{\text{hyb}} = t \sum_{k\sigma} \left(c^{\dagger}_{k\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{k\sigma} \right)$$

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so

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and we have defined $H_{\mathrm{hyb}}(\tau)$ by:

$$H_{\mathrm{hyb}}(\tau) = \mathrm{e}^{\tau H_0}H_{\mathrm{hyb}}\mathrm{e}^{-\tau H_0}$$

Hence, we can define for all creation and annihilation operators:

$$c_{k\sigma}(\tau) = \mathrm{e}^{\tau H_0}c_{k\sigma}\mathrm{e}^{-\tau H_0}$$

Thus, straighforwardly

$$H_{\mathrm{hyb}}(\tau) = t\sum_{k\sigma}\left(\mathrm{e}^{\tau H_0}c^{\dagger}_{k\sigma}d_{\sigma}\mathrm{e}^{-\tau H_0} + \mathrm{e}^{\tau H_0}d^{\dagger}_{\sigma}c_{k\sigma}\mathrm{e}^{-\tau H_0}\right)$$

so

$$H_{\mathrm{hyb}}(\tau) = t\sum_{k\sigma}\left(\mathrm{e}^{\tau H_0}c^{\dagger}_{k\sigma}\mathrm{e}^{-\tau H_0}\mathrm{e}^{\tau H_0}d_{\sigma}\mathrm{e}^{-\tau H_0} + \mathrm{e}^{\tau H_0}d^{\dagger}_{\sigma}\mathrm{e}^{-\tau H_0}\mathrm{e}^{\tau H_0}c_{k\sigma}\mathrm{e}^{-\tau H_0}\right)$$

thus

$$H_{\mathrm{hyb}}(\tau) = t\sum_{k\sigma}\left(c^{\dagger}_{k\sigma}(\tau)d_{\sigma}(\tau) + d^{\dagger}_{\sigma}(\tau)c_{k\sigma}(\tau)\right)$$

Let's denote the two terms by

$$H_{\mathrm{hyb}}(\tau) = H^{\dagger}_{\mathrm{h}}(\tau) + H_{\mathrm{h}}(\tau)$$

Evolution equation for wave function: $U(t,t')$

Let's define the time evolution operator as the operator $U(t,t')$ such that

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

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$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}|\Psi(t)\rangle$$

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Thus, for a time independant Hamiltonian

$$\hat{U}(t, t_0) = \exp\left[-\frac{i}{\bar{h}}\hat{H}(t - t_0)\right]$$

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Thus, for a time independant Hamiltonian

$$\hat{U}(t,t_0) = \exp\left[-\frac{i}{\bar{h}}\hat{H}(t-t_0)\right]$$

If $\Psi(t_0)$ is an eigenstate of H and that the eigenvalue is E_0, then

$$|\Psi(t)\rangle = \mathrm{e}^{(-iE_0(t-t0)/\bar{h})}|\Psi(t_0)\rangle$$

Thus $\mathrm{e}^{-H\tau}$ can be seen as an evolution operator with an imaginary time.

Hybridization expansion for Z_2

The partition function thus writes:

$$Z = \mathrm{Tr}\left[e^{-\beta H_0} A(\beta)\right] \quad \text{with} \quad A(\beta) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \mathcal{T} H_{\mathrm{hyb}}(\tau_1) \ldots H_{\mathrm{hyb}}(\tau_k)$$

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Let's define $H_{\mathrm{h}}^{\dagger}$ and H_{h}

$$H_{\mathrm{hyb}}(\tau) = t \sum_{k\sigma} \left(c_{k\sigma}^{\dagger}(\tau) d_{\sigma}(\tau) + d_{\sigma}^{\dagger}(\tau) c_{k\sigma}(\tau)\right) = H_{\mathrm{h}}^{\dagger}(\tau) + H_{\mathrm{h}}(\tau)$$

We must have the same number of operator H_{h} and $H_{\mathrm{h}}^{\dagger}$ in order for the trace to be non zero. So that $k = 2n$.

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Let's focus on the term for n=1 to explicit the derivation:

$$Z_1 = \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \mathrm{Tr}\left[\mathcal{T} e^{-\beta H_0} [H_{\mathrm{h}}(\tau_1) + H_{\mathrm{h}}^\dagger(\tau_1)][H_{\mathrm{h}}(\tau_2) + H_{\mathrm{h}}^\dagger(\tau_2)]\right]$$

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$$Z_1 = \frac{2}{2} \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \text{Tr}\left[\mathcal{T} e^{-\beta H_0} [H_\text{h}(\tau_1) H_\text{h}^\dagger(\bar{\tau}_1)]\right]$$

Where we have renamed time for H_h as τ_1 and time for $H_\text{h}^\dagger$ as $\bar{\tau}_1$.

Hybridization expansion for Z_n

$$Z_1 = \frac{2}{2} \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \, \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_0} [H_\mathrm{h}(\tau_1) H_\mathrm{h}^\dagger(\bar{\tau}_1)] \right]$$

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We can generalize this to all case. *Because of the time ordering operator, all the terms with the different ordering of the operator are equivalent, the ordering is fixed by the ordering of time. So we can use only one ordering and we can show that the number of term is* $\frac{(2n)!}{(n!)^2}$

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We can now use $H_\mathrm{h}(\tau) = V_k^\sigma \sum_{k\sigma} \left(c_k^\dagger(\tau) d_\sigma(\tau) \right)$ and $H_\mathrm{h}^\dagger(\bar{\tau}) = V_k^{\sigma *} \sum_{k' \sigma'} \left(d_{\bar{\sigma}}^\dagger(\bar{\tau}) c_k(\bar{\tau}) \right)$ and insert it into e.g. Z_1.

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$$Z_n = \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \int_0^\beta d\bar\tau_1 \ldots \int_0^\beta d\bar\tau_n V_{k_1}^{\sigma_1}V_{\bar k_1}^{\bar\sigma_1 *}\ldots . V_{k_n}^{\sigma_n}V_{\bar k_n}^{\bar\sigma_n *}\mathrm{Tr}\left[\mathcal{T}\mathrm{e}^{-\beta H_0}\right.$$

$$\left.\sum_{k_1..k_n,\bar k_1..\bar k_n}\sum_{\sigma_1..\sigma_n,\bar\sigma_1..\bar\sigma_n} c_{k_n}^\dagger(\tau_n)d_{\sigma_n}(\tau_n)d_{\bar\sigma_n}^\dagger(\bar\tau_n)c_{\bar k_n}(\bar\tau_n)\ldots c_{k_1}^\dagger(\tau_1)d_{\sigma_1}(\tau_1)d_{\bar\sigma_1}^\dagger(\bar\tau_1)c_{\bar k_1}(\bar\tau_1)\right]$$

Separation of Trace over bath and impurity

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \,\mathrm{Tr}\, V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} \left[\mathcal{T} \mathrm{e}^{-\beta H_0} \sum_{k_1, \bar{k}_1} \sum_{\sigma_1, \bar{\sigma}_1} c_{k_1}^{\dagger}(\tau) d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^{\dagger}(\bar{\tau}) c_{\bar{k}_1}(\bar{\tau}) \right]$$

The Trace over quantum states can be done of tensorial product of bath and impurity states so that the trace can be separated in two groups.

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1, \bar{\sigma}_1} \sum_{k_1, \bar{k}_1} \mathrm{Tr}\, V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} \mathrm{Tr}_{\,c} \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^{\dagger}(\tau) c_{\bar{k}_1}(\bar{\tau}) \right] \mathrm{Tr}_{\,d} \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^{\dagger}(\bar{\tau}) \right]$$

Idem for Z_n

Let's now focus on the Bath part:

$$\mathrm{Tr}_{\,c} \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^{\dagger}(\tau) c_{\bar{k}_1}(\bar{\tau}) \right]$$

What is a trace ?

What is a trace

For an hamiltonian in second quantization, the basis is made of state empty or filled.

- For a one particle hamiltonian

  $\mathrm{Tr}\, A = \langle 0|A|0\rangle + \langle 1|A|1\rangle$

- For a two particle hamiltonian

  $\mathrm{Tr}\, A = \langle 00|A|00\rangle + \langle 01|A|01\rangle + \langle 10|A|10\rangle + \langle 11|A|11\rangle$

Separation of Trace over bath and impurity

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \mathrm{Tr}\left[\mathcal{T} e^{-\beta H_0} \sum_{k_1,\bar{k}_1} \sum_{\sigma_1,\bar{\sigma}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} c_{k_1}^\dagger(\tau) d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) c_{\bar{k}_1}(\bar{\tau})\right]$$

The Trace over quantum states can be done of tensorial product of bath and impurity states so that the trace can be separated in two groups (the anticommutation rules give no change).

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} \mathrm{Tr}\, V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} \mathrm{Tr}_c \left[e^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau})\right] \mathrm{Tr}_d \left[e^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau})\right]$$

Idem for Z_n

Let's now focus on the Bath part:

$$\mathrm{Tr}_c \left[e^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau})\right]$$

and we just start with

$$\mathrm{Tr}_c\left[e^{-\beta H_c}\right] = \mathrm{Tr}_c\left[\prod_k e^{-\beta \epsilon_k c_k^\dagger c_k}\right] = \prod_k \mathrm{Tr}_{c_k} e^{-\beta \epsilon_k c_k^\dagger c_k} = \prod_k (\langle 0| e^{-\beta \epsilon_k c_k^\dagger c_k} |0\rangle + \langle 1| e^{-\beta \epsilon_k c_k^\dagger c_k} |1\rangle)$$

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Separation of Trace over bath and impurity

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Let's see how to apply the operator $c_k^\dagger c_k$ on $|0\rangle$ and $|1\rangle$.

$1|0\rangle = |0\rangle$ (n=0)

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Separation of Trace over bath and impurity

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \mathrm{Tr}\left[\mathcal{T} e^{-\beta H_0} \sum_{k_1,\bar{k}_1} \sum_{\sigma_1,\bar{\sigma}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} c_{k_1}^\dagger(\tau) d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) c_{\bar{k}_1}(\bar{\tau})\right]$$

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$\beta^2 \epsilon_k^2 c_k^\dagger c_k c_k^\dagger c_k |1\rangle = \beta^2 \epsilon_k^2 |1\rangle$

$e^{-\beta \epsilon_k c_k^\dagger c_k} |1\rangle = \sum_n \frac{(-\beta)^n \epsilon_k^n}{n!} |1\rangle = e^{-\beta \epsilon_k} |1\rangle$

Separation of Trace over bath and impurity

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \mathrm{Tr}\left[\mathcal{T} e^{-\beta H_0} \sum_{k_1,\bar{k}_1} \sum_{\sigma_1,\bar{\sigma}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} c_{k_1}^\dagger(\tau) d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) c_{\bar{k}_1}(\bar{\tau})\right]$$

The Trace over quantum states can be done of tensorial product of bath and impurity states so that the trace can be separated in two groups (the anticommutation rules give no change).

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} \mathrm{Tr}\, V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} \mathrm{Tr}_c \left[e^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau})\right] \mathrm{Tr}_d \left[e^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau})\right]$$

Idem for Z_n

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$\beta^2 \epsilon_k^2 c_k^\dagger c_k c_k^\dagger c_k |1\rangle = \beta^2 \epsilon_k^2 |1\rangle$

$$e^{-\beta \epsilon_k c_k^\dagger c_k} |1\rangle = \sum_n \frac{(-\beta)^n \epsilon_k^n}{n!} |1\rangle = e^{-\beta \epsilon_k} |1\rangle$$

$$Z_{\mathrm{bath}} = \prod_k (1 + e^{-\beta \epsilon_k})$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

$$\text{Tr}_{\,c}\left[\mathrm{e}^{-\beta H_c}\mathcal{T} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] = \prod_{k\neq k_1} \text{Tr}_{\,c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right] \text{Tr}_{\,c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] =$$

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$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^{\dagger}_{k_1} c_{k_1}} c^{\dagger}_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^{\dagger}_{k_1} c_{k_1}} c^{\dagger}_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

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Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

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$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\ \overbrace{\mathrm{e}^{(\tau H_c)}c^\dagger_{k_1}\mathrm{e}^{(-\tau H_c)}}\ \overbrace{\mathrm{e}^{\bar{\tau}H_c}c_{k_1}(\bar{\tau})\mathrm{e}^{-\bar{\tau}H_c}}\ |0\rangle$$

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$$e^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \overbrace{e^{(\tau H_c)} c^\dagger_{k_1} e^{(-\tau H_c)}}^{c^\dagger_{k_1}(\tau)} \quad \overbrace{e^{\bar{\tau} H_c} c_{k_1}(\bar{\tau}) e^{-\bar{\tau} H_c}\,|0\rangle}^{c_{k_1}(\bar{\tau})|0\rangle}$$

$$e^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \overbrace{e^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} e^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}}^{e^{(\tau H_c)} c^\dagger_{k_1} e^{(-\tau H_c)}} \quad \overbrace{e^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1} e^{(-\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}}^{e^{\bar{\tau} H_c} c_{k_1}(\bar{\tau}) e^{-\bar{\tau} H_c}} \,|0\rangle$$

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$$\mathrm{Tr}_{\,c}\left[\mathrm{e}^{-\beta H_c}\mathcal{T} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] = \prod_{k\neq k_1} \mathrm{Tr}_{\,c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right] \mathrm{Tr}_{\,c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] =$$

$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

$$\frac{Z_{\mathrm{bath}}(=\prod_k(1+\mathrm{e}^{-\beta\epsilon_k}))}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c} c\, \mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad c^\dagger_{k_1}(\tau) \quad c_{k_1}(\bar{\tau})|0\rangle$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \overbrace{\mathrm{e}^{(\tau H_c)} c^\dagger_{k_1} \mathrm{e}^{(-\tau H_c)}} \quad \overbrace{\mathrm{e}^{\bar{\tau} H_c} c_{k_1}(\bar{\tau}) \mathrm{e}^{-\bar{\tau} H_c} |0\rangle}$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \overbrace{\mathrm{e}^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} \mathrm{e}^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}} \quad \overbrace{\mathrm{e}^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1} \mathrm{e}^{(-\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} |0\rangle}$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \mathrm{e}^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} \mathrm{e}^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \quad \mathrm{e}^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1} |0\rangle = 0$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

$$\mathrm{Tr}_{\,c}\left[\mathrm{e}^{-\beta H_c}\mathcal{T} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] = \prod_{k\neq k_1} \mathrm{Tr}_{\,c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right] \mathrm{Tr}_{\,c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] =$$

$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

$$\frac{Z_{\mathrm{bath}}(=\prod_k(1+\mathrm{e}^{-\beta\epsilon_k}))}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c} c \mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1}\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}|1\rangle$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

$$\mathrm{Tr}_c\left[\mathrm{e}^{-\beta H_c}\mathcal{T} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] = \prod_{k\neq k_1} \mathrm{Tr}_{c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right] \mathrm{Tr}_{c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})\right] =$$

$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

$$\frac{Z_{\mathrm{bath}}(=\prod_k(1+\mathrm{e}^{-\beta\epsilon_k}))}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c} c \mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1}\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}|1\rangle$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1}|1\rangle\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1})}$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

$$\mathrm{Tr}_{\,c}\left[\mathrm{e}^{-\beta H_c}\mathcal{T}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})\right] = \prod_{k\neq k_1}\mathrm{Tr}_{\,c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right]\mathrm{Tr}_{\,c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})\right] =$$

$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

$$\frac{Z_{\mathrm{bath}}(=\prod_k(1+\mathrm{e}^{-\beta\epsilon_k}))}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\delta_{k_1\bar{k}_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c}c\mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}|1\rangle$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}|1\rangle\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar{\tau}\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}|0\rangle\mathrm{e}^{(-\bar{\tau}\epsilon_{k_1})}$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar\tau < \tau$ (and $\bar k_1$ and k_1 should be equal)

$$\mathrm{Tr}_c\left[\mathrm{e}^{-\beta H_c}\mathcal{T}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)\right] = \prod_{k\neq k_1}\mathrm{Tr}_{c_k}\left[\mathrm{e}^{-\beta\epsilon_k c^\dagger_k c_k}\right]\mathrm{Tr}_{c_{k_1}}\left[\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)\right] =$$

$$[\prod_{k\neq k_1}(1+\mathrm{e}^{-\beta\epsilon_k})]\delta_{k_1\bar k_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)|1\rangle\right]$$

$$\frac{Z_{\mathrm{bath}}(=\prod_k(1+\mathrm{e}^{-\beta\epsilon_k}))}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\delta_{k_1\bar k_1}\left[\langle 0|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}}c^\dagger_{k_1}(\tau)c_{\bar k_1}(\bar\tau)|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c}c\mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}\mathrm{e}^{(-\bar\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}|1\rangle$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}|1\rangle\mathrm{e}^{(-\bar\tau\epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}\mathrm{e}^{(-\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\bar\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}|0\rangle\mathrm{e}^{(-\bar\tau\epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}\mathrm{e}^{(\tau\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c^\dagger_{k_1}|0\rangle\mathrm{e}^{(-\bar\tau\epsilon_{k_1})}$$

Trace over bath

Now we study the term that appears in Z_1 in the case $\bar{\tau} < \tau$ (and $\bar{k}_1$ and k_1 should be equal)

$$\mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) \right] = \prod_{k \neq k_1} \mathrm{Tr}_{c_k} \left[\mathrm{e}^{-\beta \epsilon_k c^\dagger_k c_k} \right] \mathrm{Tr}_{c_{k_1}} \left[\mathrm{e}^{-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) \right] =$$

$$[\prod_{k \neq k_1} (1 + \mathrm{e}^{-\beta \epsilon_k})] \delta_{k_1 \bar{k}_1} \left[\langle 0 | \mathrm{e}^{-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) | 0 \rangle + \langle 1 | \mathrm{e}^{-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) | 1 \rangle \right]$$

$$\frac{Z_{\mathrm{bath}} (= \prod_k (1 + \mathrm{e}^{-\beta \epsilon_k}))}{(1 + \mathrm{e}^{-\beta \epsilon_{k_1}})} \delta_{k_1 \bar{k}_1} \left[\langle 0 | \mathrm{e}^{-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) | 0 \rangle + \langle 1 | \mathrm{e}^{-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1}} c^\dagger_{k_1}(\tau) c_{\bar{k}_1}(\bar{\tau}) | 1 \rangle \right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c} c \mathrm{e}^{-\tau H_c}$

$$\mathrm{e}^{(-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} \mathrm{e}^{(-\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\bar{\tau} \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1} \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} |1\rangle$$

$$\mathrm{e}^{(-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} \mathrm{e}^{(-\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\bar{\tau} \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c_{k_1} |1\rangle \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} \mathrm{e}^{(-\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\bar{\tau} \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} |0\rangle \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} c^\dagger_{k_1} |0\rangle \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1})}$$

$$\mathrm{e}^{(-\beta \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1} c^\dagger_{k_1} c_{k_1})} |1\rangle \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1})} = |1\rangle \mathrm{e}^{(-\beta \epsilon_{k_1})} \mathrm{e}^{(\tau \epsilon_{k_1})} \mathrm{e}^{(-\bar{\tau} \epsilon_{k_1})} = |1\rangle \mathrm{e}^{(-\epsilon_{k_1})(\beta - (\tau - \bar{\tau}))}$$

Trace over bath $\bar{\tau} < \tau$

Now we study this term for $\bar{\tau} > \tau$:

$$\mathrm{Tr}_{\,c}\left[\mathrm{e}^{-\beta H_c}\mathcal{T}c^\dagger_{k_1}(\tau)c_{\bar{k}_1}(\bar{\tau})\right] = -\prod_{k\neq k_1}\mathrm{Tr}_{\,c_k}\left[\mathrm{e}^{(-\beta\epsilon_k c^\dagger_k c_k)}\right]\mathrm{Tr}_{\,c_{k_1}}\left[\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{\bar{k}_1}(\bar{\tau})c^\dagger_{k_1}(\tau)\right] =$$

$$-\frac{Z_{\mathrm{bath}}}{(1+\mathrm{e}^{-\beta\epsilon_{k_1}})}\left[\langle 0|\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}(\bar{\tau})c^\dagger_{k_1}(\tau)|0\rangle + \langle 1|\mathrm{e}^{(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1})}c_{k_1}(\bar{\tau})c^\dagger_{k_1}(\tau)|1\rangle\right]$$

We remind that $c(\tau) = \mathrm{e}^{\tau H_c}c\mathrm{e}^{-\tau H_c}$. Only the term acting on $|0\rangle$ will be non zero, the same calculation gives

$$\langle 0|\mathrm{e}^{\left(-\beta\epsilon_{k_1}c^\dagger_{k_1}c_{k_1}\right)}c_{k_1}(\bar{\tau})c^\dagger_{k_1}(\tau)|0\rangle = \mathrm{e}^{\epsilon_{k_1}(\tau-\bar{\tau})}$$

Hybridization function F

Let's gather the terms.

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1, \bar{\sigma}_1} \underbrace{\sum_{k_1, \bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right]}_{F_{\sigma_1 \bar{\sigma}_1}(\bar{\tau}_1 - \tau_1)} \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

Hybridization function F

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and

$$F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}-\tau) = Z_{\mathrm{bath}} \sum_{k_1} V_{k_1}^{\sigma_1} V_{k_1}^{\bar{\sigma}_1} \begin{cases} \frac{-e^{-\epsilon_{k_1}(\bar{\tau}-\tau)}}{1+e^{-\beta\epsilon_k}} & \text{if } \bar{\tau}-\tau > 0 \\ \frac{e^{-\epsilon_{k_1}(\beta+(\bar{\tau}-\tau))}}{1+e^{-\beta\epsilon_k}} & \text{if } \bar{\tau}-\tau < 0 \end{cases}$$

This is simply the coupling of non interacting electrons which are evoluting at the frequency of their eigenvalues.

Hybridization function F

Let's gather the terms.

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \underbrace{\sum_{k_1,\bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right]}_{F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1-\tau_1)} \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

and

$$F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}-\tau) = Z_{\mathrm{bath}} \sum_{k_1} V_{k_1}^{\sigma_1} V_{k_1}^{\bar{\sigma}_1} \begin{cases} \frac{-\mathrm{e}^{-\epsilon_{k_1}(\bar{\tau}-\tau)}}{1+\mathrm{e}^{-\beta\epsilon_k}} & \text{if } \bar{\tau}-\tau > 0 \\ \frac{\mathrm{e}^{-\epsilon_{k_1}(\beta+(\bar{\tau}-\tau))}}{1+\mathrm{e}^{-\beta\epsilon_k}} & \text{if } \bar{\tau}-\tau < 0 \end{cases}$$

This is simply the coupling of non interacting electrons which are evoluting at the frequency of their eigenvalues. So that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1-\tau_1) \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

Bath for more operators

We recall that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

Bath for more operators

We recall that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1, \bar{\sigma}_1} \sum_{k_1, \bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

and we have

$$Z_2 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{k_1, k_2, \bar{k}_1, \bar{k}_2} \sum_{\sigma_1, \bar{\sigma}_1, \sigma_2, \bar{\sigma}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2}$$

$$\mathrm{Tr}_c \left[\mathcal{T} \mathrm{e}^{-\beta (H_c)} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau}) c_{k_2}^\dagger(\tau) c_{\bar{k}_2}(\bar{\tau}) \right] \mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-\beta (H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \right]$$

Bath for more operators

We recall that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \text{Tr}_c \left[e^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \text{Tr}_d \left[e^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

and we have

$$Z_2 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} \sum_{\sigma_1,\bar{\sigma}_1,\sigma_2,\bar{\sigma}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2}$$

$$\text{Tr}_c \left[\mathcal{T} e^{-\beta(H_c)} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau}) c_{k_2}^\dagger(\tau) c_{\bar{k}_2}(\bar{\tau}) \right] \text{Tr}_d \left[\mathcal{T} e^{-\beta(H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \right]$$

Let's compute

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2} \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

Bath for more operators

We recall that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} V_{k_1}^{\sigma 1} V_{\bar{k}_1}^{\bar{\sigma}1} \text{Tr}_c \left[e^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \text{Tr}_d \left[e^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

and we have

$$Z_2 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} \sum_{\sigma_1,\bar{\sigma}_1,\sigma_2,\bar{\sigma}_2} V_{k_1}^{\sigma 1} V_{\bar{k}_1}^{\bar{\sigma}1} V_{k_2}^{\sigma 2} V_{\bar{k}_2}^{\bar{\sigma}2}$$

$$\text{Tr}_c \left[\mathcal{T} e^{-\beta(H_c)} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau}) c_{k_2}^\dagger(\tau) c_{\bar{k}_2}(\bar{\tau}) \right] \text{Tr}_d \left[\mathcal{T} e^{-\beta(H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \right]$$

Let's compute

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma 1} V_{\bar{k}_1}^{\bar{\sigma}1} V_{k_2}^{\sigma 2} V_{\bar{k}_2}^{\bar{\sigma}2} \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

We can use anticommutation relation between operator (or use Wick's theorem) to show that:

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma 1} V_{\bar{k}_1}^{\bar{\sigma}1} V_{k_2}^{\sigma 2} V_{\bar{k}_2}^{\bar{\sigma}2} \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

$$- \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_2}(\bar{\tau}_2) \right] \text{Tr} \left[\mathcal{T} e^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_1}(\bar{\tau}_1) \right]$$

Bath for more operators

We recall that

$$Z_1 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \sum_{\sigma_1,\bar{\sigma}_1} \sum_{k_1,\bar{k}_1} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} \mathrm{Tr}_c \left[\mathrm{e}^{-\beta H_c} \mathcal{T} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \mathrm{Tr}_d \left[\mathrm{e}^{-\beta H_d} \mathcal{T} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) \right]$$

and we have

$$Z_2 = \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} \sum_{\sigma_1,\bar{\sigma}_1,\sigma_2,\bar{\sigma}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2}$$

$$\mathrm{Tr}_c \left[\mathcal{T} \mathrm{e}^{-\beta(H_c)} c_{k_1}^\dagger(\tau) c_{\bar{k}_1}(\bar{\tau}) c_{k_2}^\dagger(\tau) c_{\bar{k}_2}(\bar{\tau}) \right] \mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-\beta(H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \right]$$

Let's compute

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2} \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

We can use anticommutation relation between operator (or use Wick's theorem) to show that:

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2} \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

$$- \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_2}(\bar{\tau}_2) \right] \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_1}(\bar{\tau}_1) \right]$$

It comes from the fact that eg. when an electron is annihilated at $\bar{\tau}_1$, it can be the one that was created at τ_1 or τ_2.
Forget the details: it is just a consequence of the antisymmetry of the true wavefunction.

Bath for more operators (2)

From

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2} \Big[\mathrm{Tr}\, \Big[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \Big] \,\mathrm{Tr}\, \Big[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \Big]$$

$$- \mathrm{Tr}\, \Big[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_2}(\bar{\tau}_2) \Big] \,\mathrm{Tr}\, \Big[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_1}(\bar{\tau}_1) \Big] \Big]$$

and using definition of F, we have

$$\big[F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1 - \tau_1) F_{\sigma_2\bar{\sigma}_2}(\bar{\tau}_2 - \tau_2)$$
$$- F_{\sigma_1\bar{\sigma}_2}(\bar{\tau}_2 - \tau_1) F_{\sigma_2\bar{\sigma}_1}(\bar{\tau}_1 - \tau_2)) \big]$$

Bath for more operators (2)

From

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma 1} V_{\bar{k}_1}^{\bar{\sigma}1} V_{k_2}^{\sigma 2} V_{\bar{k}_2}^{\bar{\sigma}2} \Big[\mathrm{Tr} \Big[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \Big] \mathrm{Tr} \Big[\mathcal{T} e^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \Big]$$
$$- \mathrm{Tr} \Big[\mathcal{T} e^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_2}(\bar{\tau}_2) \Big] \mathrm{Tr} \Big[\mathcal{T} e^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_1}(\bar{\tau}_1) \Big] \Big]$$

and using definition of F, we have

$$\big[F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1 - \tau_1) F_{\sigma_2\bar{\sigma}_2}(\bar{\tau}_2 - \tau_2)$$
$$- F_{\sigma_1\bar{\sigma}_2}(\bar{\tau}_2 - \tau_1) F_{\sigma_2\bar{\sigma}_1}(\bar{\tau}_1 - \tau_2)) \big]$$

So that:

$$Z_2 = Z_{\text{bath}} \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{\sigma_1,\bar{\sigma}_1,\sigma_2,\bar{\sigma}_2} \mathrm{Tr}_d \Big[\mathcal{T} e^{-\beta(H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \Big]$$
$$\big[F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1 - \tau_1) F_{\sigma_2\bar{\sigma}_2}(\bar{\tau}_2 - \tau_2) - F_{\sigma_1\bar{\sigma}_2}(\bar{\tau}_2 - \tau_1) F_{\sigma_2\bar{\sigma}_1}(\bar{\tau}_1 - \tau_2)) \big]$$

Bath for more operators (2)

From

$$\sum_{k_1,k_2,\bar{k}_1,\bar{k}_2} V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1} V_{k_2}^{\sigma_2} V_{\bar{k}_2}^{\bar{\sigma}_2} \Big[\mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_1}(\bar{\tau}_1) \right] \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_2}(\bar{\tau}_2) \right]$$

$$- \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_1}^\dagger(\tau_1) c_{\bar{k}_2}(\bar{\tau}_2) \right] \mathrm{Tr} \left[\mathcal{T} \mathrm{e}^{-\beta H_c} c_{k_2}^\dagger(\tau_2) c_{\bar{k}_1}(\bar{\tau}_1) \right] \Big]$$

and using definition of F, we have

$$\big[F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1 - \tau_1) F_{\sigma_2\bar{\sigma}_2}(\bar{\tau}_2 - \tau_2)$$
$$- F_{\sigma_1\bar{\sigma}_2}(\bar{\tau}_2 - \tau_1) F_{\sigma_2\bar{\sigma}_1}(\bar{\tau}_1 - \tau_2))\big]$$

So that:

$$Z_2 = Z_{\text{bath}} \int_0^\beta d\tau_1 \int_0^\beta d\bar{\tau}_1 \int_0^\beta d\tau_2 \int_0^\beta d\bar{\tau}_2 \sum_{\sigma_1,\bar{\sigma}_1,\sigma_2,\bar{\sigma}_2} \mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-\beta(H_d)} d_{\sigma_1}(\tau) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}) d_{\sigma_2}(\tau) d_{\bar{\sigma}_2}^\dagger(\bar{\tau}) \right]$$

$$\big[F_{\sigma_1\bar{\sigma}_1}(\bar{\tau}_1 - \tau_1) F_{\sigma_2\bar{\sigma}_2}(\bar{\tau}_2 - \tau_2) - F_{\sigma_1\bar{\sigma}_2}(\bar{\tau}_2 - \tau_1) F_{\sigma_2\bar{\sigma}_1}(\bar{\tau}_1 - \tau_2))\big]$$

So the full partition functions writes as:

$$Z = Z_{\text{bath}} \sum_n \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 \ldots \int_0^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n,\bar{\sigma}_1..\bar{\sigma}_n}$$

$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d_{\bar{\sigma}_n}^\dagger(\bar{\tau}_n) \ldots d_{\sigma_1}(\tau_1) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

Integration over bath states general case

In the equation:

$$Z = Z_{\text{bath}} \sum_n \frac{1}{n!^2} \int_0^\beta d\tau_1 ... \int_0^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 ... \int_0^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n,\bar{\sigma}_1..\bar{\sigma}_n}$$

$$\text{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\bar{\sigma}_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\bar{\sigma}_1}(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

Integration over bath states general case

In the equation:

$$Z = Z_{\text{bath}} \sum_n \frac{1}{n!^2} \int_0^\beta d\tau_1 ... \int_0^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 ... \int_0^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n,\bar{\sigma}_1..\bar{\sigma}_n}$$

$$\text{Tr}_d \left[\mathcal{T} e^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\bar{\sigma}_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\bar{\sigma}_1}(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

The F are easy to compute because the V are known. Let's rewrite the equation as:

$$Z = Z_{\text{bath}} \sum_n \int_0^\beta d\tau_1 ... \int_{\tau_{n-1}}^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 ... \int_{\tau_{n-1}}^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n,\bar{\sigma}_1..\bar{\sigma}_n}$$

$$\text{Tr}_d \left[\mathcal{T} e^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\bar{\sigma}_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\bar{\sigma}_1}(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

With this formulation we have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$.

If the bath does not mix spins ...

$$Z = Z_{\text{bath}} \sum_n \int_0^\beta d\tau_1 ... \int_{\tau_{n-1}}^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 ... \int_{\tau_{n-1}}^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n, \bar{\sigma}_1..\bar{\sigma}_n}$$

$$\text{Tr}_d \left[\mathcal{T} \text{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\bar{\sigma}_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\bar{\sigma}_1}(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

If the bath does not mix spins ...

$$Z = Z_{\text{bath}} \sum_n \int_0^\beta d\tau_1 ... \int_{\tau_{n-1}}^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 ... \int_{\tau_{n-1}}^\beta d\bar{\tau}_n \sum_{\sigma_1..\sigma_n,\bar{\sigma}_1..\bar{\sigma}_n}$$
$$\text{Tr}_d \left[\mathcal{T} e^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\bar{\sigma}_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\bar{\sigma}_1}(\bar{\tau}_1) \right] \det[F(\bar{\tau} - \tau)]$$

We can separate spins and have spin dependant indices if F is a matrix that does not couple spins.

$$Z = Z_{\text{bath}} \left[\prod_\sigma \left(\sum_{n_\sigma} \int_0^\beta d\tau_1^\sigma ... \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \int_0^\beta d\bar{\tau}_1^\sigma ... \int_{\bar{\tau}_{n-1}^\sigma}^\beta d\bar{\tau}_n^\sigma \right) \right] \times$$
$$\text{Tr}_d \left[\mathcal{T} e^{-(\beta H_d)} \prod_\sigma d_\sigma(\tau_n^\sigma) d^\dagger_\sigma(\bar{\tau}_n^\sigma) ... d_\sigma(\tau_1^\sigma) d^\dagger_\sigma(\bar{\tau}_1^\sigma) \right] \left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)] \right)$$

everything depends on spin, but spin are separated

Let's forget spin and try to understand the Tr $_d$

We have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$. Let's now focus on

$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) \right]$$

Let's forget spin and try to understand the Tr_d

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Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

Let's forget spin and try to understand the Tr_d

We have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$. Let's now focus on

$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^{\dagger}_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1) \right]$$

Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

$$\mathrm{Tr}_d \left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1) \right]$$

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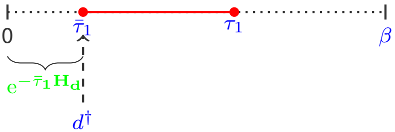
$$\mathrm{Tr}_d\left[\mathcal{T}\mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right]$$

Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

$$\mathrm{Tr}_d\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right]$$

So only non zero term in the Tr is:

$$\begin{aligned}\mathrm{Tr}_d\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right] &= \langle 0|\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)|0\rangle \\ &= \langle 0|\mathrm{e}^{-(\beta H_d)} \mathrm{e}^{\tau_1 H_d} d_{\sigma_1} \mathrm{e}^{-\tau_1 H_d} \mathrm{e}^{\bar{\tau}_1 H_d} d^\dagger_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 \mathbf{H_d}}|0\rangle\end{aligned}$$



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$$\text{Tr}_d\left[\mathcal{T}\mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right]$$

Let’s start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

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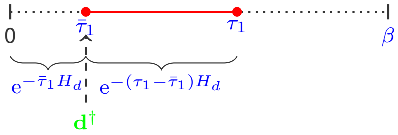


Let's forget spin and try to understand the Tr $_d$

We have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$. Let's now focus on

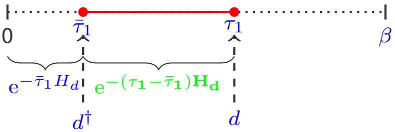
$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) \right]$$

Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

$$\mathrm{Tr}_d \left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) \right]$$

So only non zero term in the Tr is:

$$\begin{aligned} \mathrm{Tr}_d \left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) \right] &= \langle 0 | \mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) | 0 \rangle \\ &= \langle 0 | \mathrm{e}^{-(\beta H_d)} \mathrm{e}^{\tau_1 H_d} d_{\sigma_1} \mathrm{e}^{-\tau_1 \mathbf{H_d}} \mathrm{e}^{\bar{\tau}_1 \mathbf{H_d}} d^\dagger_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 H_d} | 0 \rangle \end{aligned}$$



Let's forget spin and try to understand the $\mathrm{Tr}_{\,d}$

We have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$. Let's now focus on

$$\mathrm{Tr}_{\,d}\left[\mathcal{T}\mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right]$$

Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

$$\mathrm{Tr}_{\,d}\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1)\right]$$

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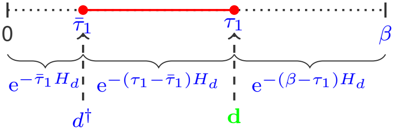

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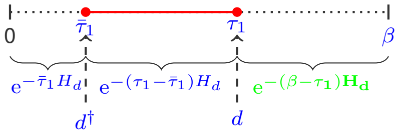

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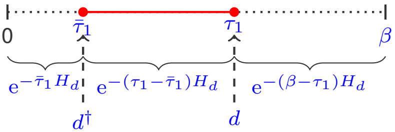

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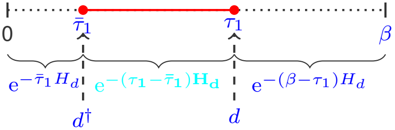


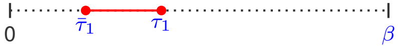
Role of τ versus $\bar{\tau}$?

$$\bar{\tau}_1 < \tau_1 \qquad \text{Tr}_{\,d}\mathcal{T}\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)\right] = <0|\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)|0>$$

cea

Role of τ versus $\bar{\tau}$?

$$\bar{\tau}_1 < \tau_1 \qquad \mathrm{Tr}\,_d\mathcal{T}\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)\right] = < 0|\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)|0 >$$

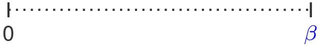


$$\bar{\tau}_1 > \tau_1 \qquad \mathrm{Tr}\,_d\mathcal{T}\left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)\right] = < 1|\mathrm{e}^{-(\beta H_d)} d^{\dagger}_{\sigma_1}(\bar{\tau}_1) d_{\sigma_1}(\tau_1)|1 >$$

More operators

$$\mathrm{Tr}_{\,d}\left[\mathcal{T}\mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^{\dagger}_{\sigma_n}(\bar{\tau}_n) \ldots d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)\right]$$

n=0



More operators

$$\text{Tr}_{\,d}\left[\mathcal{T}\mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^{\dagger}_{\sigma_n}(\bar{\tau}_n) \ldots d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1)\right]$$

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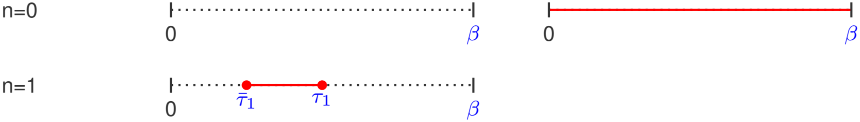

More operators

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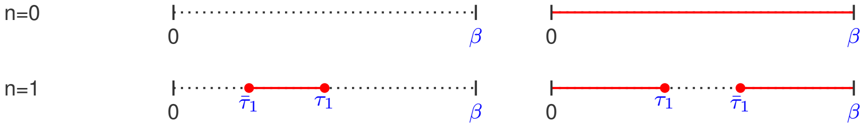

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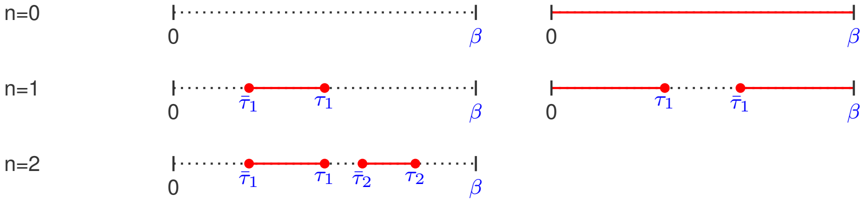

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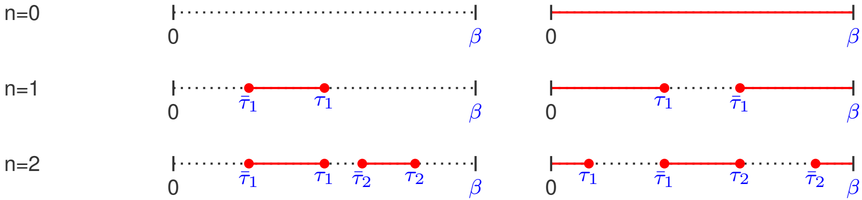


Calculation of trace: need spins

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar{\tau}_1^\downarrow) d_\uparrow^\dagger(\bar{\tau}_1^\uparrow)|00 >$$

$\sigma = \uparrow$

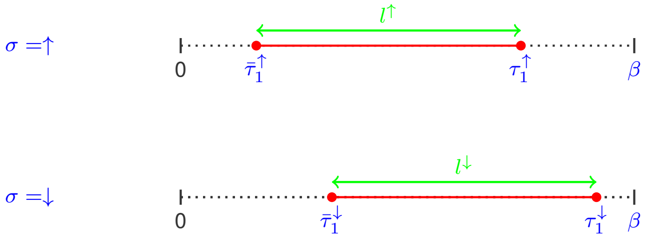
$\sigma = \downarrow$

$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar{\tau}_1^\downarrow) d_\uparrow^\dagger(\bar{\tau}_1^\uparrow)|00 >=$$

Calculation of trace: need spins

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar{\tau}_1^\downarrow) d_\uparrow^\dagger(\bar{\tau}_1^\uparrow)|00 >$$

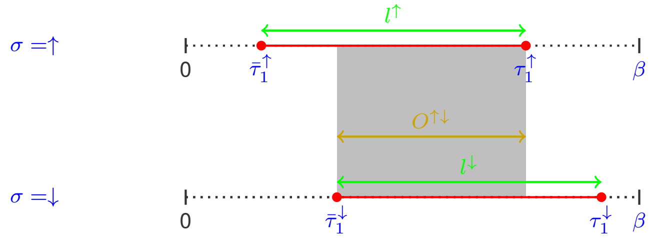


$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar{\tau}_1^\downarrow) d_\uparrow^\dagger(\bar{\tau}_1^\uparrow)|00 >= \exp\left[-\varepsilon_0(l^\uparrow + l^\downarrow)\right]$$

Calculation of trace: need spins

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar\tau_1^\downarrow) d_\uparrow^\dagger(\bar\tau_1^\uparrow)|00 >$$



$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

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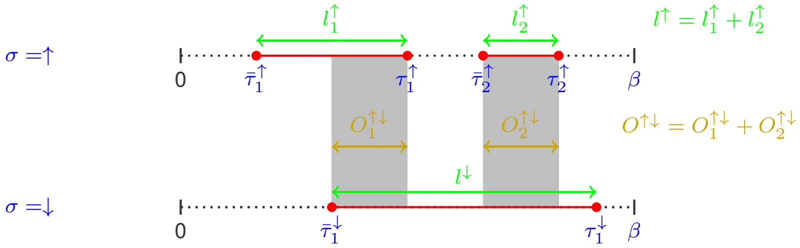
Calculation of trace: need spins

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_2^\uparrow) d_\uparrow^\dagger(\bar\tau_2^\uparrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar\tau_1^\downarrow) d_\uparrow^\dagger(\bar\tau_1^\uparrow)|00 >$$



$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

$$< 00|\mathrm{e}^{-(\beta H_d)} d_\downarrow(\tau_1^\downarrow) d_\uparrow(\tau_2^\uparrow) d_\uparrow^\dagger(\bar\tau_2^\uparrow) d_\uparrow(\tau_1^\uparrow) d_\downarrow^\dagger(\bar\tau_1^\downarrow) d_\uparrow^\dagger(\bar\tau_1^\uparrow)|00 > = \exp\left[-\varepsilon_0(l^\uparrow + l^\downarrow) - U O^{\uparrow\downarrow}\right]$$

Expression of the partition function

We add:

$$Z = Z_{\mathrm{bath}} \left[\prod_{\sigma} \left(\sum_{n_\sigma} \int_0^\beta d\tau_1^\sigma \ldots \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \int_0^\beta d\bar{\tau}_1^\sigma \ldots \int_{\bar{\tau}_{n-1}^\sigma}^\beta d\bar{\tau}_n^\sigma \right) \right] \times$$

$$\mathrm{Tr}_d \left[\mathcal{T} e^{-(\beta H_d)} \prod_\sigma d_\sigma(\tau_n^\sigma) d_\sigma^\dagger(\bar{\tau}_n^\sigma) \ldots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\bar{\tau}_1^\sigma) \right] \left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)] \right)$$

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$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} \prod_\sigma d_\sigma(\tau_n^\sigma) d_\sigma^\dagger(\bar{\tau}_n^\sigma) \ldots d_\sigma(\tau_1^\sigma) d_\sigma^\dagger(\bar{\tau}_1^\sigma) \right] \left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)] \right)$$

We now have

$$Z = Z_{\mathrm{bath}} \left[\prod_\sigma \left(\sum_{n_\sigma} \int_0^\beta d\tau_1^\sigma \ldots \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \int_0^\beta d\bar{\tau}_1^\sigma \ldots \int_{\bar{\tau}_{n-1}^\sigma}^\beta d\bar{\tau}_n^\sigma \right) \right] \times$$

$$\exp\left[-\varepsilon_0 (l_\tau^\uparrow + l_\tau^\downarrow) + U O_\tau^{\uparrow\downarrow} \right] \left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)] \right)$$

- Where $l^\uparrow$, $l^\downarrow$ and $O^{\uparrow\downarrow}$ are functions of all the $\tau_1^\sigma \ldots \tau_n^\sigma$.
- $F(\tau - \bar{\tau})$ is also a function of all the $\tau_1^\sigma \ldots \tau_n^\sigma$.
- This integration can be sampled by Monte Carlo.

Monte carlo

We have

$$Z = Z_{\text{bath}} \left[\prod_\sigma \left(\sum_{n_\sigma} \int_0^\beta d\tau_1^\sigma \ldots \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \int_0^\beta d\bar{\tau}_1^\sigma \ldots \int_{\bar{\tau}_{n-1}^\sigma}^\beta d\bar{\tau}_n^\sigma \right) \right] \times$$

$$\exp\left[-\varepsilon_0 (l_\tau^\uparrow + l_\tau^\downarrow) + U O_\tau^{\uparrow\downarrow} \right] \left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)] \right)$$

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The partition function can be rewritten as

$$Z = \sum_x f(x)$$

Monte carlo

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$$Z = Z_{\rm bath}\left[\prod_\sigma\left(\sum_{n_\sigma}\int_0^\beta d\tau_1^\sigma \ldots \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \int_0^\beta d\bar\tau_1^\sigma \ldots \int_{\bar\tau_{n-1}^\sigma}^\beta d\bar\tau_n^\sigma\right)\right]\times$$

$$\exp\left[-\varepsilon_0(l_\tau^\uparrow + l_\tau^\downarrow) + UO_\tau^{\uparrow\downarrow}\right]\left(\prod_\sigma \det[F_\sigma(\bar\tau - \tau)]\right)$$

The partition function can be rewritten as

$$Z = \sum_x f(x)$$

Where for each x, we have to specify an expansion order for each spin n_σ

$$f(x) = Z_{\rm bath}(d\tau)^{2(n_\uparrow + n_\downarrow)}\exp\left[-\varepsilon_0(l_\tau^\uparrow + l_\tau^\downarrow) + UO_\tau^{\uparrow\downarrow}\right]\left(\prod_\sigma \det[F_\sigma(\bar\tau - \tau)]\right)$$

- Metropolis algorithm is used to sample the configurations according to the distribution function

Reminder: Monte Carlo, detailled balance and Metropolis algorithm

- The goal is to compute $\langle A \rangle = \frac{1}{Z} \int dx f(x) A(x)$ with $Z = \int f(x) dx$

Reminder: Monte Carlo, detailled balance and Metropolis algorithm

- The goal is to compute $\langle A \rangle = \frac{1}{Z} \int dx f(x) A(x)$ with $Z = \int f(x) dx$
- a Markov chain is a sequence of configuration x such that $\langle A \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_i A(x_i)$
    - Starting from a configuration x, the probability to generate x' is such that $\sum_{x'} p(x \to x') = 1$

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$$\sum_{x'} p(x)p(x \to x') = \sum_{x'} p(x')p(x' \to x)$$

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- Metropolis algorithm

$$p(x \to x') = \min \left(\frac{p(x')}{p(x)}, 1 \right)$$

Reminder: Monte Carlo, detailled balance and Metropolis algorithm

Metropolis algorithm:

$$p(x \to x') = \min\left(\frac{p(x')}{p(x)}, 1\right)$$

Corresponding transition probability

	$p(x) > p(x')$	$p(x') > p(x)$
$p(x \to x')$	$p(x')/p(x)$	1
$p(x)p(x \to x')$	$p(x')$	$p(x)$
$p(x' \to x)$	1	$p(x)/p(x')$
$p(x')p(x' \to x)$	$p(x')$	$p(x)$

The detailed balance is fullfilled with the Metropolis algorithm

$$p(x)p(x \to x') = p(x')p(x' \to x)$$

Reminder: Monte Carlo, detailled balance and Metropolis algorithm

- proposal probability and acceptance probability

$$p(x \to x') = p_{\text{prop}}(x \to x') p_{\text{acc}}(x \to x')$$

- Detailed balance

$$p(x)p(x \to x') = p(x')p(x' \to x)$$

becomes

$$p(x)p_{\text{prop}}(x \to x')p_{\text{acc}}(x \to x') = p(x')p_{\text{prop}}(x' \to x)p_{\text{acc}}(x' \to x)$$

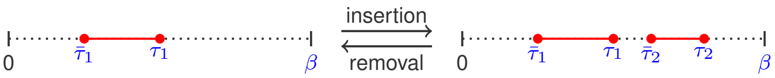
- Metropolis algorithm

$$p_{\text{acc}}(x \to x') = \min\left(\frac{p(x')}{p(x)} \frac{p_{\text{prop}}(x' \to x)}{p_{\text{prop}}(x \to x')}, 1\right)$$

Monte Carlo moves

Basic moves

- insertion/removal of a segment



Monte Carlo moves

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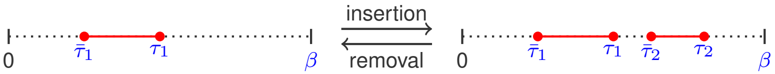
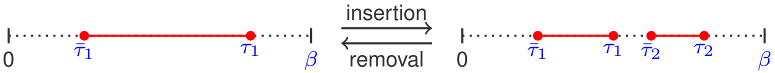
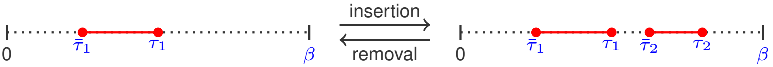


- insertion/removal of a anti-segment



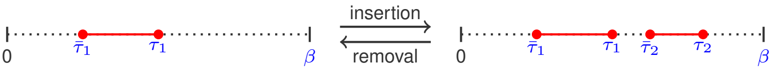
Description of the insertion/removal of a segment

- For a segment insertion:



(a)

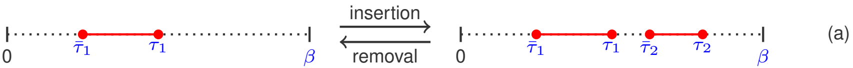
Description of the insertion/removal of a segment



(a)

- For a segment insertion:
- Choose insertion or removal with the probability 1/2

Description of the insertion/removal of a segment



- For a segment insertion:
- Choose insertion or removal with the probability 1/2
- Choose a time $\bar{\tau}_2$ within $d\tau$ ($\beta/d\tau$ times are available).

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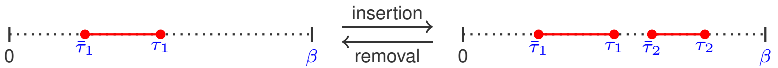

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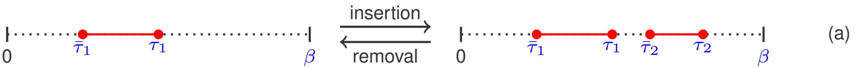

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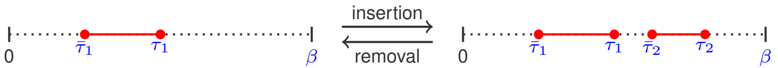

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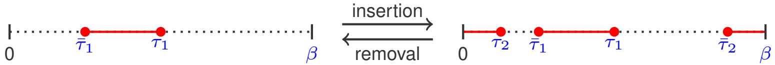
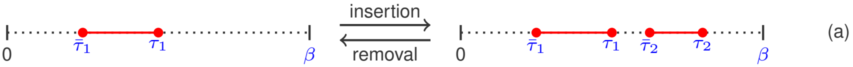


(b)

Description of the insertion/removal of a segment



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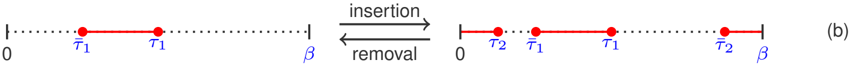

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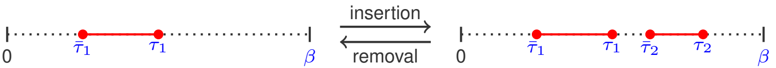

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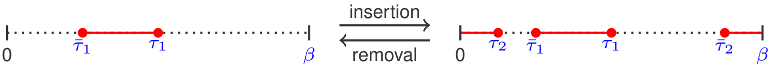

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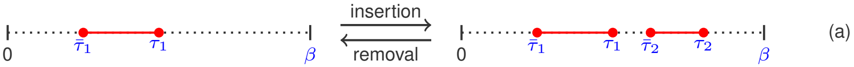

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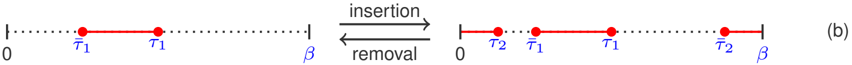

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- Then we use the Metropolis expression for the acceptance probability:

$$p_{\text{acc}}(x \to x') = \min\left(\frac{p(x')}{p(x)}\frac{p_{\text{prop}}(x' \to x)}{p_{\text{prop}}(x \to x')}, 1\right)$$

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- Using the probability $p(x)$ from the partition function

$$p(x) = Z_{\mathrm{bath}}(d\tau)^{2(n_\uparrow + n_\downarrow)} \exp\left[-\varepsilon_0(l_\tau^\uparrow + l_\tau^\downarrow) + U O_\tau^{\uparrow\downarrow}\right]\left(\prod_\sigma \det[F_\sigma(\bar{\tau} - \tau)]\right)$$

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- For an insertion of a segment $p(x)$ and $p(x')$

$$p_{\mathrm{acc}}(x \to x') = \min\left(\frac{\beta l_{\mathrm{max}}}{n+1}\frac{\det[F']}{\det[F]}\frac{\exp\left[-\varepsilon_0(l_\tau^{\uparrow\prime} + l_\tau^{\downarrow\prime}) + UO_\tau^{\uparrow\downarrow\prime}\right]}{\exp\left[-\varepsilon_0(l_\tau^\uparrow + l_\tau^\downarrow) + UO_\tau^{\uparrow\downarrow}\right]}, 1\right)$$

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- similar expression can be obtained for other moves.

Measurements

- Occupations

$$\langle n_\sigma \rangle = \frac{1}{Z} \mathsf{Tr}\left[\mathrm{e}^{(-\beta H)} \hat{n}_\sigma \right] = \frac{1}{\beta} \frac{1}{Z} \sum_x f(x) l^\sigma$$

- Double occupation (and interaction energy)

$$\langle n_\downarrow n_\uparrow \rangle = \frac{1}{\beta} \frac{1}{Z} \sum_x f(x) O^{\uparrow\downarrow}$$

Negative sign problem

$$Z = \int f(x) dx$$

$$\langle \hat{A} \rangle = \frac{1}{Z} \mathrm{Tr} \left(\mathrm{e}^{-\beta \hat{H}} \hat{A} \right)$$

On quantum systems, it can happen that $f(x) < 0$ for some x. How to randomly choose a configuration with a negative (or even complex) probability ?

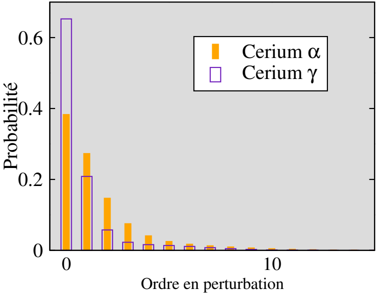
$$\langle A \rangle_{f(x)} = \frac{\int dx f(x) A(x)}{\int dx f(x)} = \frac{\int dx f(x) A(x)}{\int dx f(x)} = \frac{\int dx |f(x)| \mathrm{sgn}(f(x)) A(x)}{\int dx |f(x)| \mathrm{sgn}(f(x))}$$

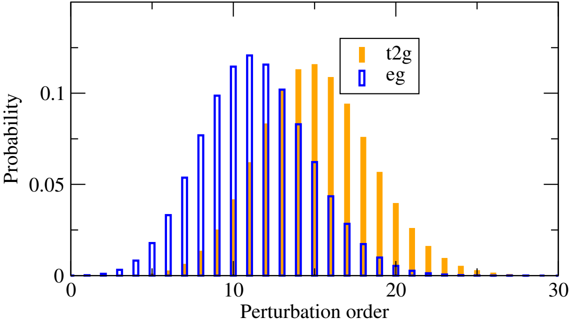
$$\langle A \rangle_{f(x)} = \frac{\langle \mathrm{sgn}(f(x)) A(x) \rangle_{|f(x)|}}{\langle \mathrm{sgn}(f(x)) \rangle_{|f(x)|}}$$

We can thus sample $\mathrm{sgn}(f(x))A(x)$ with the probability $|f(x)|$.
Similarly, for complex $f(x) = |f(x)|\mathrm{e}^{i\theta(x)}$, We can sample $\mathrm{e}^{i\theta(x)} A(x)$ with the probability $|f(x)|$.

Comparison between Iron and Cerium

- d orbitals in iron are much diffuse than f orbitals in cerium.
- V_k is thus much larger
- The expansion as a function in V_k needs more term in iron in comparison to cerium.





Conclusion

- For more general interaction for multiorbital case (d or f), the algorithm is more complex.
- Calculation of Green's function can be done using Legendre coefficients.
- Interaction expansion is also possible.
- Global moves can be necessary for multi-orbital systems.

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