DMFT, CTQMC, and cRPA methods

DE LA RECHERCHE À L'INDUSTRIE

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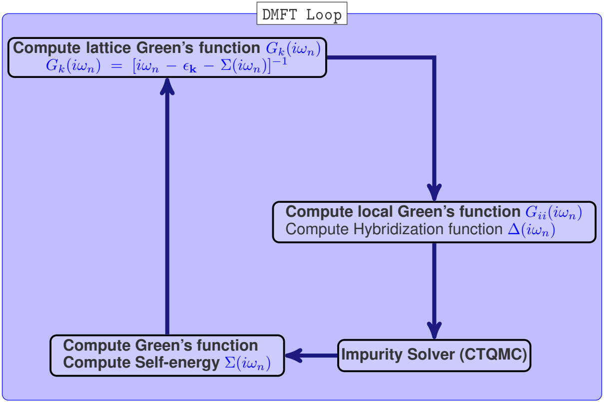
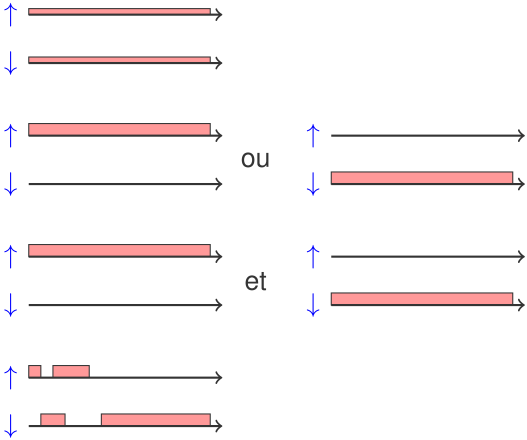
The DMFT Loop

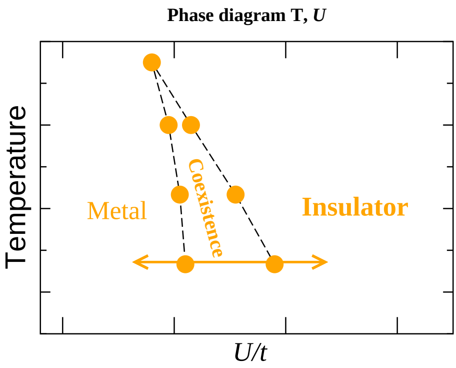


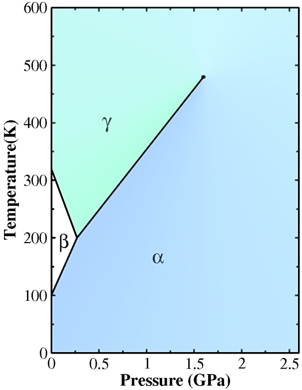
$$\frac{1}{N}\sum_k \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\omega)} = \frac{1}{\omega - \epsilon_0 - \Delta(\omega) - \Sigma(\omega)}$$

Méthode	$E_{\mathrm{Ha+xc}}^{\mathrm{interactions\ e/e}}$
No interaction	$E_{\mathrm{Ha+xc}}^{\mathrm{LDA/GGA}}$
Hartree Fock (Statique)	$U\langle\hat{n}_\uparrow\rangle\langle\hat{n}_\downarrow\rangle$
DMFT (atomic) (Dynamique)	$U\langle\hat{n}_\uparrow\rangle\langle\hat{n}_\downarrow\rangle$
DMFT (CTQMC) (Dynamique)	$U\langle\hat{n}_\uparrow\hat{n}_\downarrow\rangle$



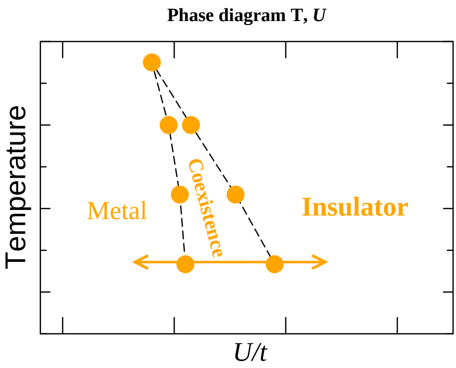
DMFT: Dynamical Mean Field Theory

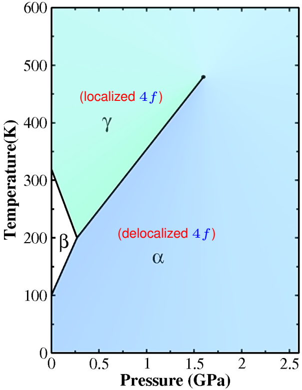




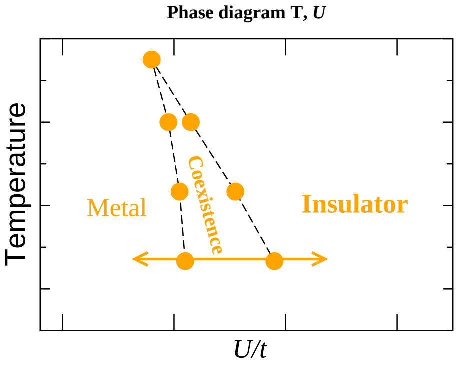
Phase diagram of the Hubbard model in DMFT and experimental phase diagram of cerium.

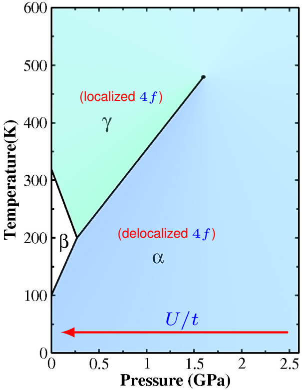
Dynamical Mean Field Theory: the Hubbard model





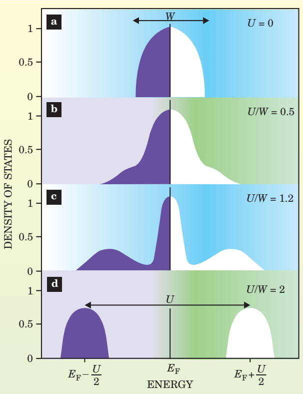
Phase diagram of the Hubbard model in DMFT and experimental phase diagram of cerium.



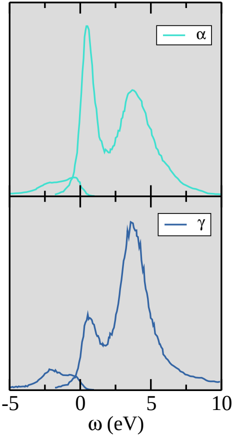


Phase diagram of the Hubbard model in DMFT and experimental phase diagram of cerium.

Hubbard bands: high energy is required to add or remove an electron



[G.Kotliar *et al* Phys. Today, AIP, 57, 53-59 (2004)]



[E. Weschke, *et al* Phys. Rev. B 44, 8304 (1991)
M. Grioni, *et al* Phys. Rev. B 55, 2056 (1997)]

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

Possible states are:

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

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

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$d_{\uparrow}$ suppress an electron $\uparrow$, thus

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

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$d^\dagger_\uparrow$ creates an electron $\uparrow$, thus

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

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

Possible states are:

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

$d_\uparrow$ suppress an electron $\uparrow$, thus

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

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

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

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

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

$$H_{\text{atom}} = \sum_\sigma \varepsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow = \varepsilon_0 d^\dagger_\uparrow d_\uparrow + \varepsilon_0 d^\dagger_\downarrow d_\downarrow + U n_\uparrow n_\downarrow$$

Possible states are:

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

$d_\uparrow$ suppress an electron $\uparrow$, thus

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

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

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

(cf Lecture by Emmanuel Fromager on second quantization)

Short summary of second quantization (2)

Anticommutation relation, because of the antisymmetry of wavefunction

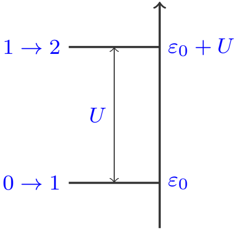
$$|\uparrow\downarrow\rangle \quad = -|\downarrow\uparrow\rangle \quad \Rightarrow \quad d^\dagger_\uparrow d^\dagger_\downarrow |00\rangle \quad = -d^\dagger_\downarrow d^\dagger_\uparrow |00\rangle \quad \Rightarrow \quad d^\dagger_\uparrow d^\dagger_\downarrow \quad = -d^\dagger_\downarrow d^\dagger_\uparrow$$

Isolated atom: exact solution

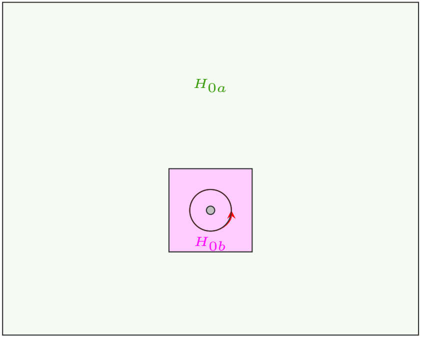
One can compute the energy as a function of the number of electrons:

Configuration	—	↑	↓	↓↑
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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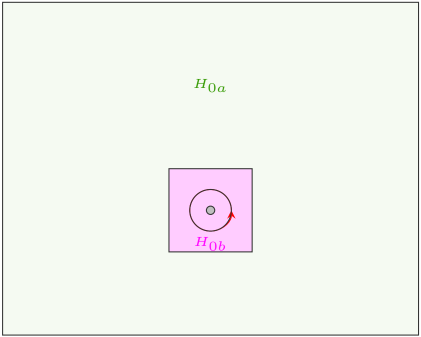

$$H_{\text{Anderson}} = \underbrace{\sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{H_{0a}} + \underbrace{\sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow}_{H_{0b}}$$

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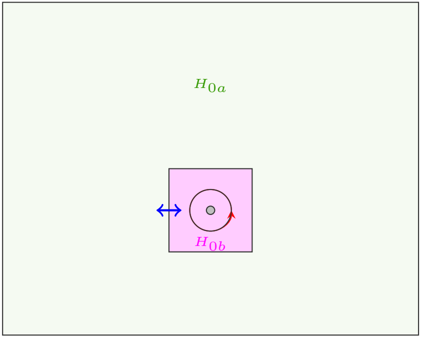

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Anderson model: uncorrelated limit $U = 0$

$$H_{\text{Anderson}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow + \sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma} \right)$$

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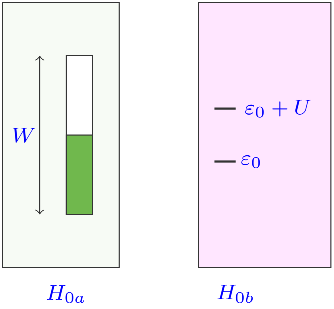
$$\begin{pmatrix} \varepsilon_0 & V_1 & V_2 & \dots & V_k & \dots & V_n \\ V_1 & \varepsilon_1 & 0 & \dots & 0 & \dots & 0 \\ V_2 & 0 & \varepsilon_2 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ V_k & 0 & 0 & \dots & \varepsilon_k & \dots & 0 \\ \dots & \dots & \dots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

The Anderson Hamiltonian (solved by CTQMC)



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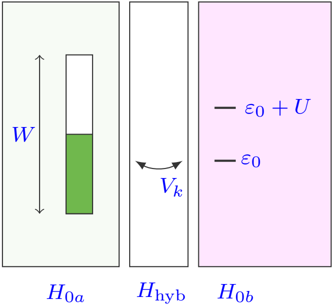

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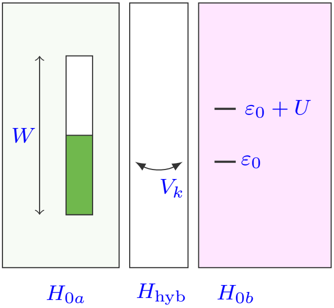

$$H_{\rm Anderson} = \underbrace{\sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{H_{0a}} + \underbrace{\sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow}_{H_{0b}} + \underbrace{\sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma} \right)}_{H_{\rm hyb}}$$

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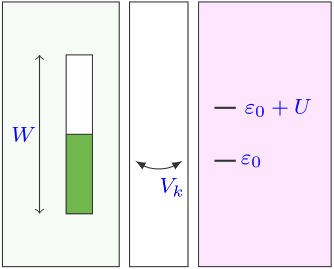

H_{0a} $H_{\rm hyb}$ H_{0b}

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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 $H_{\rm hyb}$

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

The Anderson impurity model.

$$H_{\mathrm{AIM}} = \sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma$$ (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)

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

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

The partition function can be written as

$$Z = \text{Tr}\left[\mathrm{e}^{-\beta H}\right]$$

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$$\frac{dA(\beta)}{d\beta} = H_0\mathrm{e}^{\beta H_0}\mathrm{e}^{-\beta H} - \mathrm{e}^{\beta H_0}H\mathrm{e}^{-\beta H}$$

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\frac{dA(\beta)}{d\beta} &= H_0 e^{\beta H_0} e^{-\beta H} - e^{\beta H_0} H e^{-\beta H} \\
&= -e^{\beta H_0} (H - H_0) e^{-\beta H} \\
&= -e^{\beta H_0} (H_{\text{hyb}}) e^{-\beta H}
\end{aligned}$$

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&= -e^{\beta H_0}(H - H_0) e^{-\beta H} \\
&= -e^{\beta H_0}(H_{\text{hyb}}) e^{-\beta H} \\
&= -e^{\beta H_0}(H_{\text{hyb}}) e^{-\beta H_0} \times e^{\beta H_0} e^{-\beta H}
\end{aligned}$$

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&= -e^{\beta H_0}(H_{\text{hyb}}) e^{-\beta H} \\
&= -e^{\beta H_0}(H_{\text{hyb}}) e^{-\beta H_0} \times e^{\beta H_0} e^{-\beta H} \\
&= -\left[e^{+\beta H_0} H_{\text{hyb}} e^{-\beta H_0}\right] A(\beta)
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&= -e^{\beta H_0}(H_{\text{hyb}}) e^{-\beta H_0} \times e^{\beta H_0} e^{-\beta H} \\
&= -\left[e^{+\beta H_0} H_{\text{hyb}} e^{-\beta H_0}\right] A(\beta) \\
&= -\left[H_{\text{hyb}}(\beta)\right] A(\beta)
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$$\begin{aligned}
\frac{dA(\beta)}{d\beta} &= H_0 e^{\beta H_0} e^{-\beta H} - e^{\beta H_0} H e^{-\beta H} \\
&= -e^{\beta H_0}(H - H_0)e^{-\beta H} \\
&= -e^{\beta H_0}(H_{\text{hyb}})e^{-\beta H} \\
&= -e^{\beta H_0}(H_{\text{hyb}})e^{-\beta H_0} \times e^{\beta H_0} e^{-\beta H} \\
&= -\left[e^{+\beta H_0} H_{\text{hyb}} e^{-\beta H_0}\right] A(\beta) \\
&= -\left[H_{\text{hyb}}(\beta)\right] A(\beta)
\end{aligned}$$

(Heisenberg representation (cf lecture par X. Blase) but for imaginary time)

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

$$\frac{df(x)}{dx} = -V(x)f(x)$$

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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

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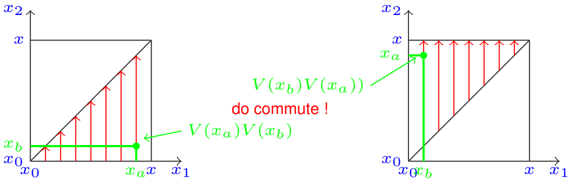

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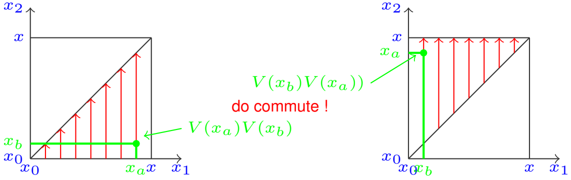

We end with an infinite summation such as:

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

Hybridization expansion

This demonstration can be generalized to the case of matrices

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

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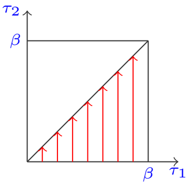

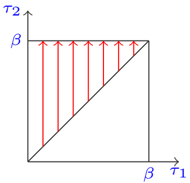

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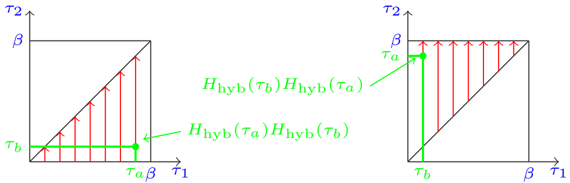

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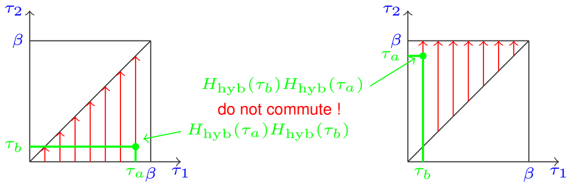

Hybridization expansion and time ordering

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It solves the commutation issue and thus:

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One can thus write the whole serie as

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

Hybridization hamiltonian

H_{hyb} is defined by:

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

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Hybridization hamiltonian

H_{hyb} is defined by:

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

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

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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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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:

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

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

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

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

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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

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

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

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

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

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* $\frac{(2n)!}{(n!)^2}$

$$Z = \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 \ldots \int_0^\beta d\bar{\tau}_n \mathrm{Tr} \left[\mathcal{T} e^{-\beta H_0} H_h(\tau_1) H_h^\dagger(\bar{\tau}_1) \ldots . H_h(\tau_n) H_h^\dagger(\bar{\tau}_n) \right]$$

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

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

$$Z_n = \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \int_0^\beta d\bar{\tau}_1 \ldots \int_0^\beta d\bar{\tau}_n V_{k_1}^{\sigma_1} V_{\bar{k}_1}^{\bar{\sigma}_1 *} \ldots . V_{k_n}^{\sigma_n} V_{\bar{k}_n}^{\bar{\sigma}_n *} \mathrm{Tr} \left[\mathcal{T} e^{-\beta H_0} \right.$$

$$\left. \sum_{k_1..k_n, \bar{k}_1..\bar{k}_n} \sum_{\sigma_1..\sigma_n, \bar{\sigma}_1..\bar{\sigma}_n} c_{k_n}^\dagger(\tau_n) d_{\sigma_n}(\tau_n) d_{\bar{\sigma}_n}^\dagger(\bar{\tau}_n) c_{\bar{k}_n}(\bar{\tau}_n) \ldots c_{k_1}^\dagger(\tau_1) d_{\sigma_1}(\tau_1) d_{\bar{\sigma}_1}^\dagger(\bar{\tau}_1) c_{\bar{k}_1}(\bar{\tau}_1) \right]$$

Separation of Trace over bath and impurity

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

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.

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

Idem for Z_n

Let's now focus on the Bath part:

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

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

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

- For a two particle hamiltonian

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

Separation of Trace over bath and impurity

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

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Let's now focus on the Bath part:

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

and we just start with

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

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

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

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

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

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

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

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

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)

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

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)

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

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

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

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

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

Trace over bath

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

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

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

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

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

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

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

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

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

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

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)

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

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

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

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

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

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)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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)

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

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

Let's gather the terms.

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

and

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

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.

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

and

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

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

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

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

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

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

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 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.

From

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

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

and using definition of F, we have

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

From

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

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

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:

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

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

Bath for more operators (2)

From

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

and using definition of F, we have

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

So that:

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

So the full partition functions writes as:

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

Integration over bath states general case

In the equation:

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

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

In the equation:

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

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

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

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

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

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 ...

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

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

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

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

Let's 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 $\beta < \bar{\tau}_1 < \tau_1 < 0$.

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

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

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

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

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

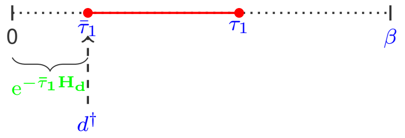
$$\text{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar{\tau}_n) ... d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar{\tau}_1) \right]$$

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

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

So only non zero term in the Tr is:

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



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

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

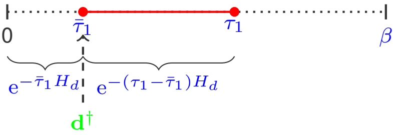
Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

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

So only non zero term in the Tr is:

$$\mathrm{Tr}_d \left[\mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1) \right] = \langle 0 | \mathrm{e}^{-(\beta H_d)} d_{\sigma_1}(\tau_1) d^{\dagger}_{\sigma_1}(\bar{\tau}_1) | 0 \rangle$$

$$= \langle 0 | \mathrm{e}^{-(\beta H_d)} \mathrm{e}^{\tau_1 H_d} d_{\sigma_1} \mathrm{e}^{-\tau_1 H_d} \mathrm{e}^{\bar{\tau}_1 H_d} \mathbf{d}^{\dagger}_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 H_d} | 0 \rangle$$



Let's forget spin and try to understand the Tr_d

We have $\tau_1 < \tau_2 < \ldots < \tau_n$ and $\bar\tau_1 < \bar\tau_2 < \ldots < \bar\tau_n$. Let's now focus on

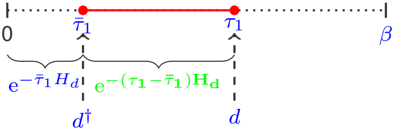
$$\mathrm{Tr}_d \left[\mathcal{T} \mathrm{e}^{-(\beta H_d)} d_{\sigma_n}(\tau_n) d^\dagger_{\sigma_n}(\bar\tau_n) \ldots d_{\sigma_1}(\tau_1) d^\dagger_{\sigma_1}(\bar\tau_1)\right]$$

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 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

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

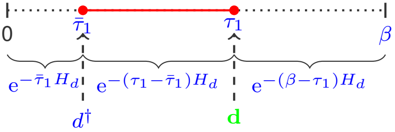
Let's start with $n = 1$ with $\beta < \bar{\tau}_1 < \tau_1 < 0$.

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

So only non zero term in the Tr is:

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

$$= \langle 0 | \mathrm{e}^{-(\beta H_d)} \mathrm{e}^{\tau_1 H_d} \mathbf{d}_{\sigma_1} \mathrm{e}^{-\tau_1 H_d} \mathrm{e}^{\bar{\tau}_1 H_d} d^\dagger_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 H_d} | 0 \rangle$$



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

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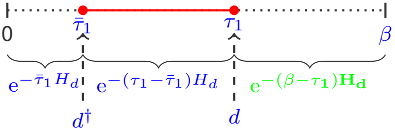
$$= \langle 0 | \mathrm{e}^{-(\beta \mathbf{H_d})} \mathrm{e}^{\tau_1 \mathbf{H_d}} d_{\sigma_1} \mathrm{e}^{-\tau_1 H_d} \mathrm{e}^{\bar{\tau}_1 H_d} d^\dagger_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 H_d} | 0 \rangle$$



Let's forget spin and try to understand the Tr_d

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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 $\beta < \bar{\tau}_1 < \tau_1 < 0$.

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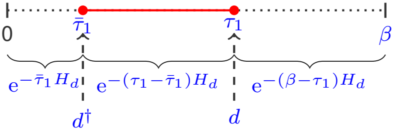

We have $\tau_1 < \tau_2 < ... < \tau_n$ and $\bar{\tau}_1 < \bar{\tau}_2 < ... < \bar{\tau}_n$. Let's now focus on

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

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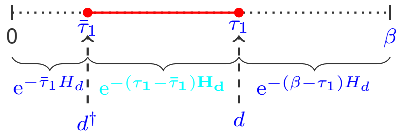
$$= \langle 0 | \mathrm{e}^{-(\beta H_d)} \mathrm{e}^{\tau_1 H_d} d_{\sigma_1} \mathrm{e}^{-\tau_1 H_d} \mathrm{e}^{\bar{\tau}_1 H_d} d^\dagger_{\sigma_1} \mathrm{e}^{-\bar{\tau}_1 H_d} | 0 \rangle = \mathrm{e}^{-(\tau_1 - \bar{\tau}_1)\epsilon_0}$$

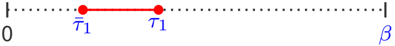


Role of τ versus $\bar{\tau}$?

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

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

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

n=0

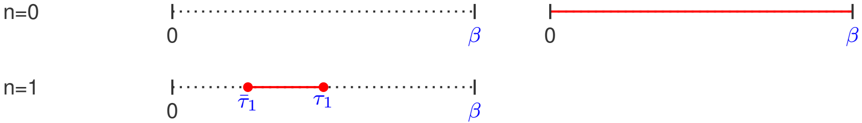
More operators

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

n=0

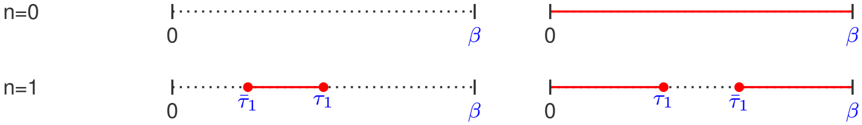
More operators

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



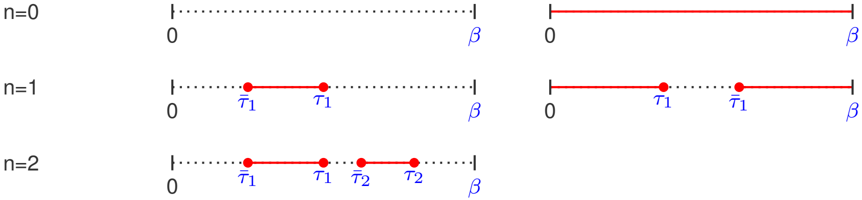
More operators

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



More operators

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



More operators

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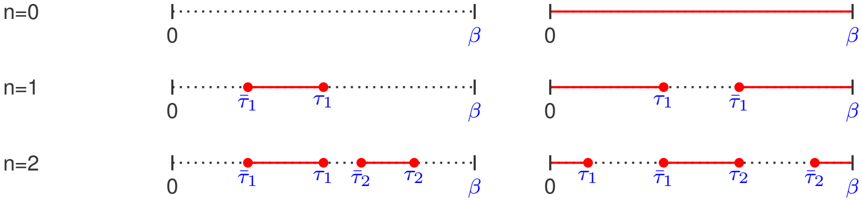


Calculation of trace: need spins

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

$\sigma = \uparrow$

$\sigma = \downarrow$

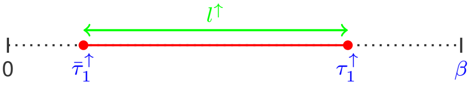
$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

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

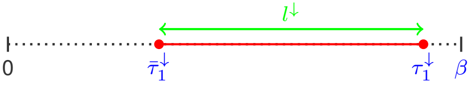
Calculation of trace: need spins

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

$\sigma = \uparrow$



$\sigma = \downarrow$

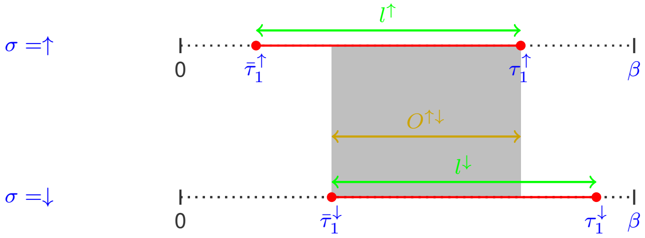


$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

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

Calculation of trace: need spins

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

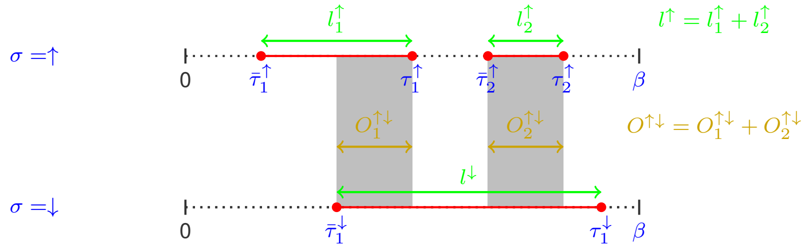


$$H_d = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_d^\uparrow n_d^\downarrow$$

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

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:

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

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

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

We now have

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

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

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

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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

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

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

- 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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- A Necessary condition for stationarity is

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

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- The detailed balance condition is a sufficient condition for stationarity

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

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- The detailed balance condition is a sufficient condition for stationarity

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

- 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

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

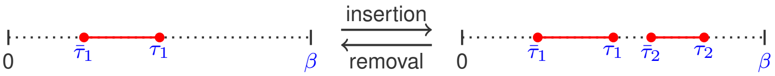
- Metropolis algorithm

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

Monte Carlo moves

Basic moves

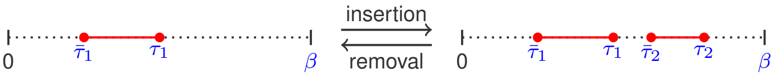
- insertion/removal of a segment



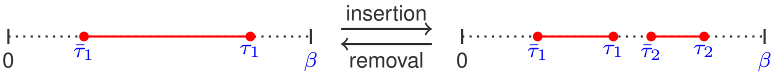
Monte Carlo moves

Basic moves

- insertion/removal of a segment

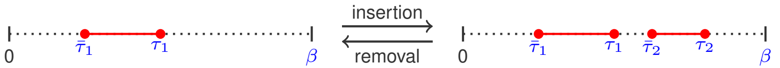


- insertion/removal of a anti-segment



Description of the insertion/removal of a segment

- For a segment insertion:



(a)

Description of the insertion/removal of a segment

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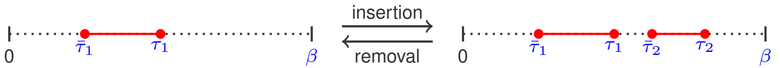
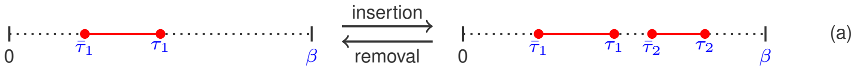


(a)

- 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).

Description of the insertion/removal of a segment

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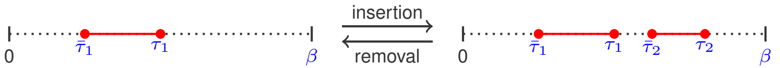

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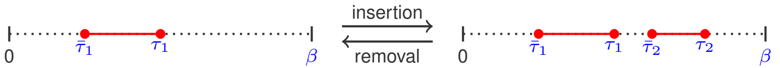

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- If move is accepted, choose a time τ_2. Two general case are possible (a) and (b)

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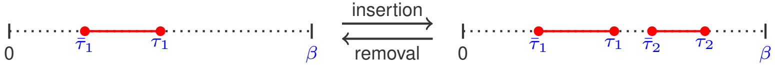

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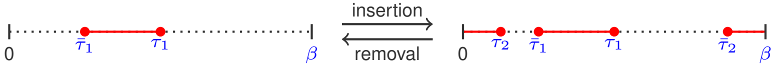
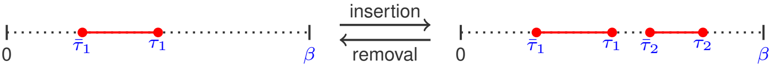


(b)

Description of the insertion/removal of a segment

- For a segment insertion:



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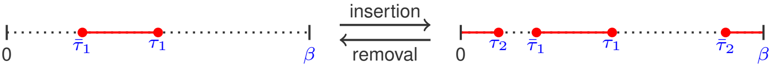

(b)

- The proposal probability of the insertion is ($l_{\max}$ is the length available for the insertion).

$$p_{\text{prop}}(x \rightarrow x') = \frac{1}{2}\frac{d\tau}{\beta}\frac{d\tau}{l_{\max}}$$

Description of the insertion/removal of a segment

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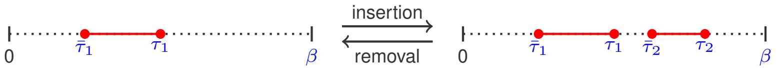

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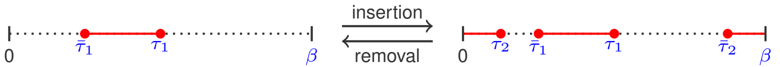

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- The proposal probability of the removal is

$$p_{\mathrm{prop}}(x \to x') = \frac{1}{2}\frac{1}{n_\sigma}$$

Description of the insertion/removal of a segment

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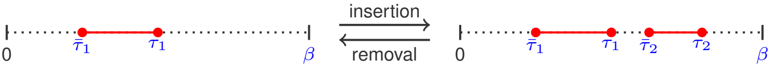

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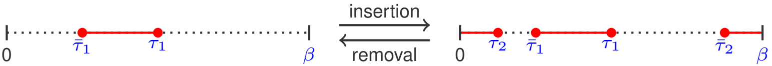

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- The proposal probability of the removal is

$$p_{\text{prop}}(x \to x') = \frac{1}{2}\frac{1}{n_\sigma}$$

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

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

Acceptance probability

- The proposal probability of the insertion is: $p_{\mathrm{prop}}(x \to x') = \frac{1}{2} \frac{d\tau}{\beta} \frac{d\tau}{l_{\mathrm{max}}}$

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Acceptance probability

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- The proposal probability of the removal is: $p_{\text{prop}}(x \to x') = \frac{1}{2n_\sigma}$
- Then we use the Metropolis expression for the acceptance probability of the insertion

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

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

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

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

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

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- similar expression can be obtained for other moves.

Measurements

- Occupations

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

- 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

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

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

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 ?

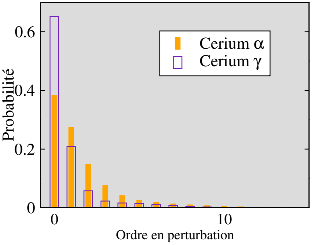
$$\langle A \rangle_{f(x)} = \frac{\int dx f(x) A(x)}{\int dx f(x)} = \frac{\int dx f(x) A(x)}{\int dx f(x)} = \frac{\int dx |f(x)| \mathrm{sgn}(f(x)) A(x)}{\int dx |f(x)| \mathrm{sgn}(f(x))}$$

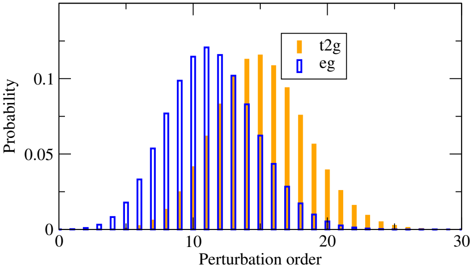
$$\langle A \rangle_{f(x)} = \frac{\langle \mathrm{sgn}(f(x)) A(x) \rangle_{|f(x)|}}{\langle \mathrm{sgn}(f(x)) \rangle_{|f(x)|}}$$

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.

Thanks to Jordan Bieder, Jules Denier, Valentin Planes.

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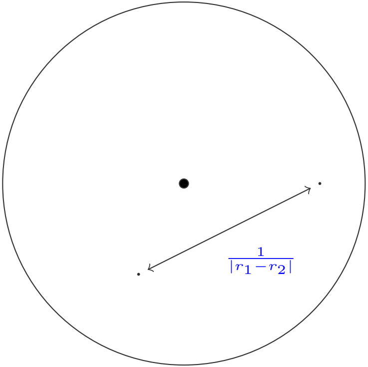
PhD A.R Flesch, "Electronic structure of strongly correlated materials "
E. Gull *et al* RMP 2011 "Continuous-time Monte Carlo methods for quantum impurity models"

How to compute the effective interaction ?



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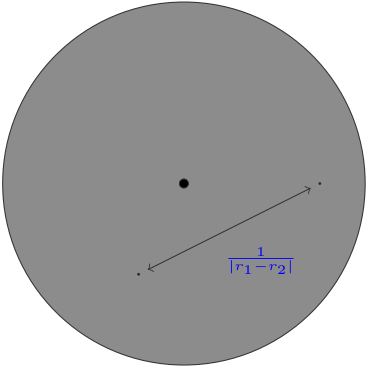

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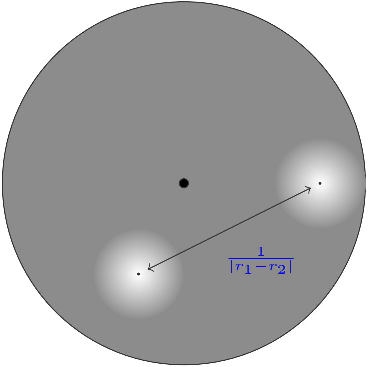

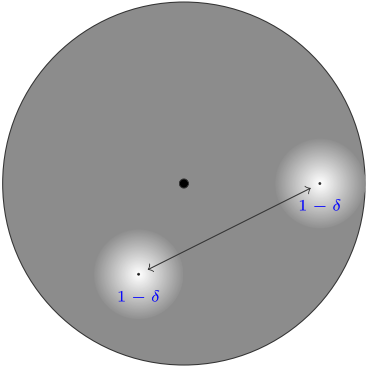
$1-\delta$
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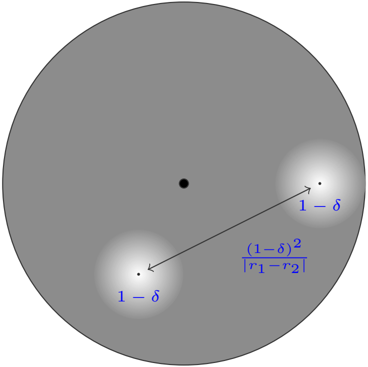


Screening

How to compute U ?

U is the screened interaction between electrons:

$$U = \langle\chi(\mathbf{r})\chi(\mathbf{r}')|W_r(\mathbf{r},\mathbf{r}',w=0)|\chi(\mathbf{r}')\chi(\mathbf{r}')\rangle$$

where W is the screened interaction between correlated electrons.

- Direct calculation in LDA by constraint LDA [1]
  - The coupling between d electrons and others is removed for the calculation.
- Direct approach by linear response theory [3]
  - The d local potential is modified.
- Calculation using the screening from LDA (GW formalism [2])
  - Frequency dependent interaction.

(1) Anisimov and Gunnarsson PRB **43** 7570 (1991)
(2) Aryasetiawan, *et al* PRB **70** 195104 (2004)
(3) Cococcioni and de Gironcoli PRB **71** 035105 (2006)

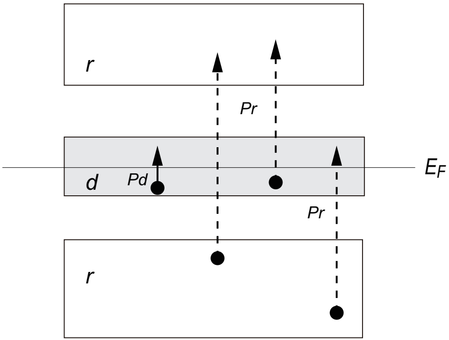
The constrained RPA method cRPA

- Screening is an essential part in the determination of U
- The screening is completely expressed in the dielectric function.
  - $W(\mathbf{r}, \mathbf{r}', \omega) = \int \epsilon^{-1}(\omega, \mathbf{r}, \mathbf{r}'') v(\mathbf{r}'' - \mathbf{r}') d\mathbf{r}'$
- The screening in response to a potential can be expressed through perturbation theory as electron hole excitations: Usual perturbation theory in quantum mechanics gives:

$$|\Psi_n^{(1)}\rangle = |\Psi_n^{(0)}\rangle + \sum_{n' \neq n} \frac{\langle \Psi_{n'}^{(0)} | V_{\text{pert}} | \Psi_n^{(0)} \rangle}{E_n^0 - E_{n'}^0} |\Psi_{n'}^{(0)}\rangle$$

The cRPA approach.

Polarisation: $P = Pd + Pr$



- In cRPA, all excitations are taken into account except the one belonging to the correlated subshell.

Picture from F. Aryasetiawan, The LDA+DMFT approach to strongly correlated materials E. Pavarini, E. Koch, D. Vollhardt, A. Lichtenstein (Eds.), Forschungszentrum Jülich (2011).
F. Aryasetiawan, Imada, Georges, Kotliar, Biermann et Lichtenstein PRB 2004.

The cRPA approach.

We call here χ_0 the non interacting (Kohn-Sham) polarizability of the system. Let's now separate the correlated states (They could be d states but the method is more general and correlated orbitals could gather several orbitals from e.g different atoms) from the rest (r). We thus have:

$$\chi_0 = \chi_0^{\text{correl}} + \chi_0^r$$

thus, we can rewrite the inverse dielectric matrix as:

$$\epsilon^{-1} = \frac{1}{1 - v(\chi_0^{\text{correl}} + \chi_0^r)}$$

We now define the dielectric function due to correlated electrons as

The cRPA approach.

$$\epsilon_{\text{correl}}^{-1} \hat{=} \frac{1}{1 - W_r \chi_0^{\text{correl}}},$$

the dielectric function of the other electrons as

$$\epsilon_r^{-1} \hat{=} \frac{1}{1 - v\chi_0^r},$$

and the interaction screened only by the other (r) electrons as:

$$W_r = \frac{v}{1 - v\chi_0^r}$$

The cRPA approach.

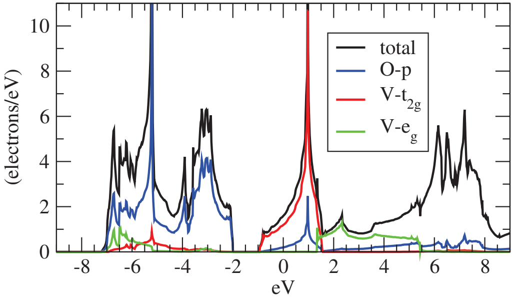
With these definitions, one shows that

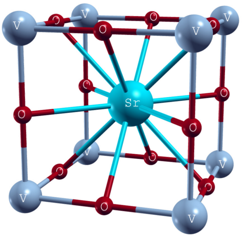
$$\epsilon_{\text{correl}}^{-1}\epsilon_r^{-1} = ... = \frac{1}{1 - v\chi_0^r - v\chi_0^{\text{correl}}} = \frac{1}{1 - v\chi_0} = \epsilon^{-1}$$

Thus, we have

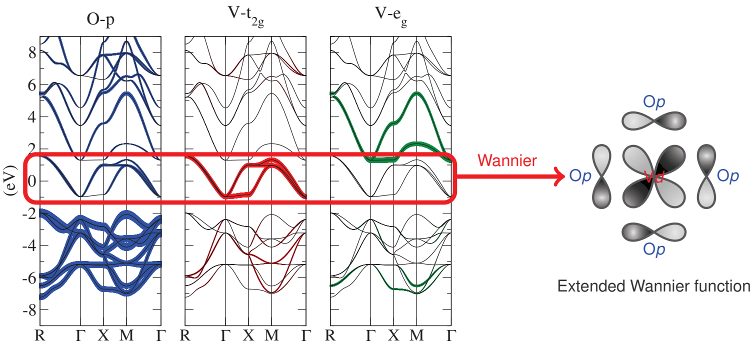
$$W \hat{=} \epsilon^{-1} v = \epsilon_{\text{correl}}^{-1}\epsilon_r^{-1} v$$

We can interpret this result: The fully screened RPA interaction is the combination of two screening processes. First, the bare interaction is screened by non-correlated electrons (r), and it gives rises to a screened interaction W_r. Secondly the screening of this interaction by correlated electrons recovers the fully screened interaction.

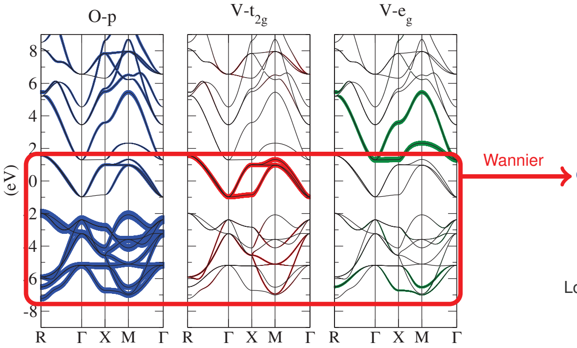


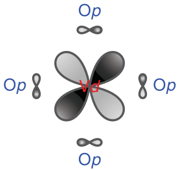


- metallic oxide with one d electron on the correlated atom (Vanadium).
- Hybridization between Oxygen and Vanadium.
- In a cubic environnement, d orbitals are splitted in two subgroups called t_{2g} and e_g.



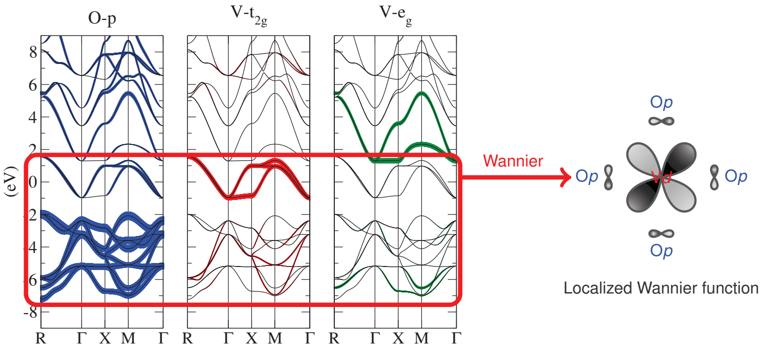
Wannier orbitals are not pure Vd orbitals
No double counting, easier comparison with model studies.





Localized Wannier function

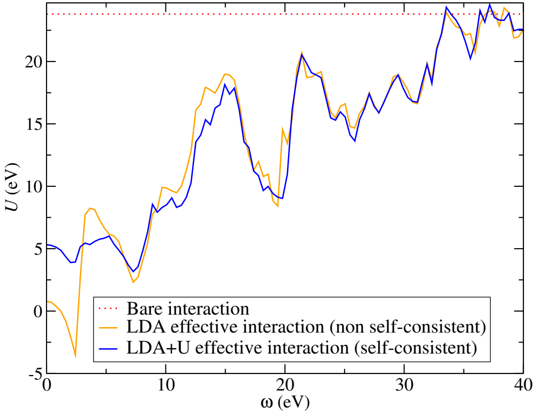
Wannier orbitals are more localized on V.
More realistic description of chemical bonding.

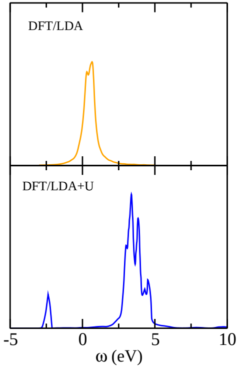


Wannier orbitals are more localized on V.
More realistic description of chemical bonding.

	Vt_{2g} only More extended	Vt_{2g} + Oxygen p More localized
v	16.1 eV	19.4 eV
U	3.2 eV	4.5 eV

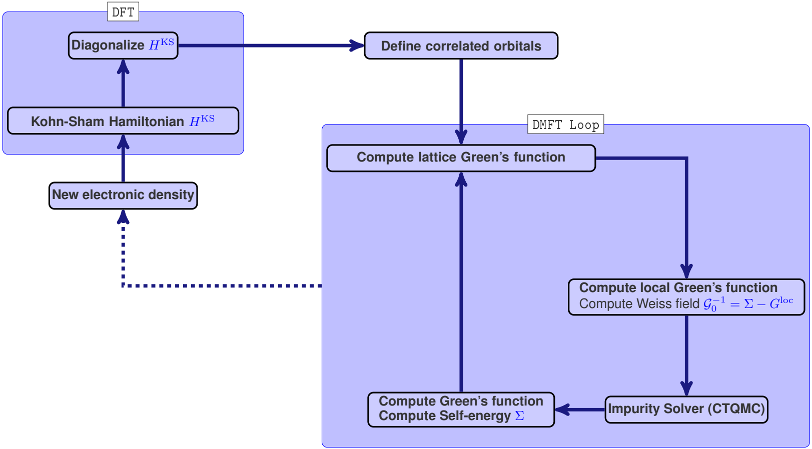
Effective interactions in cerium





- Interaction is frequency dependent.
- The LDA and LDA+U effective interactions are very different.
- The self-consistent calculation of U leads to reasonable values.

DFT+DMFT scheme



Conclusion

- DMFT can improve the description of
  - Paramagnetic Mott insulators
  - Paramagnetic-Ferromagnetic transition
  - Mott transitions
  - Correlated metals
- Spectra, total, free energies and forces can be computed.
- Electronic temperature on energy or spectra.
- Can be computationaly expensive but can use efficiently supercomputers.
- Use imaginary time/frequencies, requires analytical continuation.

[t] For an atomic orbital χ, we have the identity

$$|\chi\rangle = \left[\sum_{\nu} |\Psi_{\mathbf{k}\nu}\rangle\langle\Psi_{\mathbf{k}\nu}|\right] |\chi\rangle = \sum_{\nu} |\Psi_{\mathbf{k}\nu}\rangle\langle\Psi_{\mathbf{k}\nu}|\chi\rangle.$$

If we restrict the number of Kohn Sham states, then the resulting sum needs to be orthonormalized.

$$|\tilde{\chi}\rangle \equiv \sum_{\nu\in\mathcal{W}} |\Psi_{\mathbf{k}\nu}\rangle\langle\Psi_{\mathbf{k}\nu}|\chi\rangle.$$

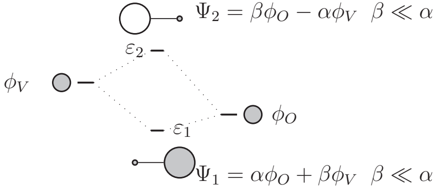
The orthonormalization of $|\tilde{\chi}\rangle$ leads to well defined Wannier functions $|w\rangle$, unitarily related to $|\Psi_{\mathbf{k}\nu}\rangle$ by

$$|w\rangle = \sum_{\nu\in\mathcal{W}} \langle\Psi_{\mathbf{k}\nu}|w\rangle|\Psi_{\mathbf{k}\nu}\rangle$$

A convenient way to define Wannier functions, especially for f electrons systems.

V. I. Anisimov et al., Phys. Rev. B 71, 125119 (2005)

B. Amadon, F. Lechermann, A. Georges, F. Jollet, T. Wehling and A. I. Lichtenstein Phys. Rev. B 77, 205112 (2008)



Two windows of energy are possible to compute wannier functions.

- If only ε_2 is included, the correlated wavefunction is $|\chi\rangle = |\Psi_2\rangle$ and contains an Oxygen contribution
- If only ε_1 and ε_2 is included, the correlated wavefunction is $|\chi\rangle = |\phi_V\rangle$ and is much more localized.