Sherbrooke, June 2014

Continuous-time impurity solvers

Single-orbital Anderson Impurity Model:

$$H = H_{loc} + H_{bath} + H_{mix}$$

$H_{loc} = U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow)$ ← correlated "d" orbital (impurity)

$H_{bath} = \sum_{p,\sigma} \varepsilon_p c^\dagger_{p,\sigma} c_{p,\sigma}$ ← noninteracting "s" electrons

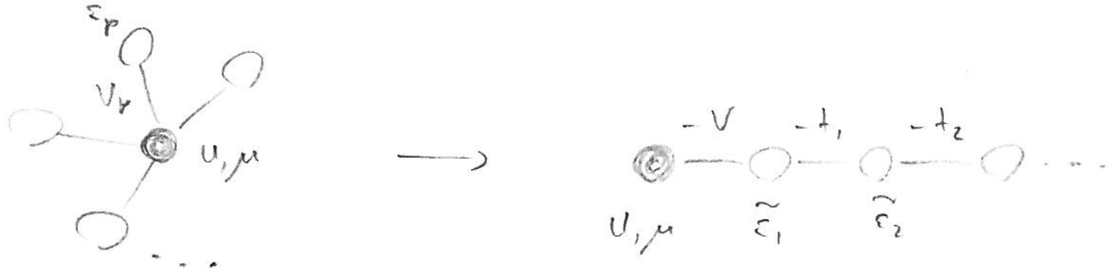
$H_{mix} = \sum_{p,\sigma} (V_{p,\sigma} d^\dagger_\sigma c_{p,\sigma} + h.c.)$ ← s-d hybridization

$H_{loc} = H_U + H_\mu \qquad (H_U = U n_\uparrow n_\downarrow,\ H_\mu = -\mu(n_\uparrow + n_\downarrow))$

Tridiagonalization of $H_\mu + H_{bath} + H_{mix}$

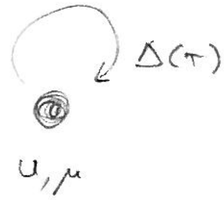
$$\begin{pmatrix} -\mu & V_{p_1} & V_{p_2} & \cdots \\ V^*_{p_1} & \varepsilon_{p_1} & & 0 \\ V^*_{p_2} & & \varepsilon_{p_2} & \\ \vdots & 0 & & \ddots \end{pmatrix} \longrightarrow \begin{pmatrix} -\mu & -V & & 0 \\ -V & \tilde{\varepsilon}_1 & -t_1 & \\ & -t_1 & \tilde{\varepsilon}_2 & -t_2 \\ 0 & & \ddots & \ddots \end{pmatrix}$$

maps the model to a semi-infinite chain



Can choose $V, t_i \geq 0 \quad \forall i$

Action formulation: by integrating out the noninteracting bath we obtain the impurity action $S = S_{loc} + S_{mix}$



$$S_{loc} = \int_0^\beta d\tau \left[U n_\uparrow(\tau) n_\downarrow(\tau) - \mu(n_\uparrow(\tau) + n_\downarrow(\tau)) \right]$$

$$S_{mix} = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d^\dagger_\sigma(\tau) \Delta_\sigma(\tau - \tau') d_\sigma(\tau')$$

Δ is the hybridization function, defined as

$$\Delta(i\omega_n) = \sum_r \frac{|V_{p,r}|^2}{i\omega_n - \varepsilon_r}$$

It is related to the "bath Green's function" $\mathcal{G}_0$ by

$$\mathcal{G}_{0,\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \Delta_\sigma(i\omega_n)$$

Partition function: $\quad Z = \mathrm{Tr}_{d,c}\left[e^{-\beta H}\right] = \mathrm{Tr}_d\left[T e^{-S}\right]$

Green's function: $\quad G_\sigma(\tau) = -\frac{1}{Z}\mathrm{Tr}_{d,c}\left[T e^{-\beta H} d_\sigma(\tau) d^\dagger_\sigma(0)\right]$

$$= -\frac{1}{Z}\mathrm{Tr}_d\left[T e^{-S} d_\sigma(\tau) d^\dagger_\sigma(0)\right]$$

Monte Carlo simulation

Express Z as a sum over "configurations" c with weight w_c:

$$Z = \sum_{c \in \mathcal{C}} w_c$$

Implement a random walk in $\mathcal{C}$ which satisfies

i) ergodicity (all c accessible)

ii) detailed balance

$|w_{c_1}| p(c_1 \to c_2) = |w_{c_2}| p(c_2 \to c_1)$

GF measurement:

$$G \approx \frac{\sum_c w_c G_c}{\sum_c w_c} = \frac{\sum_c |w_c| \mathrm{sign}_c G_c}{\sum_c |w_c| \mathrm{sign}_c} = \frac{\langle \mathrm{sign} \cdot G \rangle}{\langle \mathrm{sign} \rangle}$$

if c is generated with probability $\sim |w_c|$

Continuous-time Monte Carlo

1. Split H into two parts $H = H_1 + H_2$ and switch to the interaction representation $O(\tau) = e^{\tau H_1}\, O\, e^{-\tau H_1}$

$$\rightarrow \quad Z = \mathrm{Tr}\left[e^{-\beta H_1}\, T\, e^{-\int_0^\beta d\tau\, H_2(\tau)} \right]$$

2. Expand time-ordered exponential into a power-series

$$Z = \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n\, \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)\, e^{-\tau_1 H_1}\right]$$

$$\Leftrightarrow \quad Z = \sum_c w_c \qquad w_c = \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1}(-H_2)\ldots(-H_2)\, e^{-\tau_1 H_1}\right](d\tau)^n$$

$$c = \{\tau_1, \tau_2, \ldots, \tau_n\}, \quad \tau_i \in [0,\beta]$$

Weak-coupling approach: expand Z in powers of U

$$H_1 = H_\mu + H_{bath} + H_{mix} \quad \text{(quadratic part of } H\text{)}$$

"Strong-coupling" approach: expand Z in powers of V

$$H_1 = H_{loc} + H_{bath}$$

Weak-coupling approach

$H_2 = H_U$, $H_1 = H - H_2$ quadratic

$c = \{\tau_1, \ldots, \tau_n\}$ collection of interaction vertices

$$w_c = (-U\, d\tau)^n\, \mathrm{Tr}\left[e^{-(\beta-\tau_n)H_1}\, n_\uparrow n_\downarrow \ldots e^{-(\tau_2-\tau_1)H_1}\, n_\uparrow n_\downarrow\, e^{-\tau_1 H_1}\right]$$

$$= (-U\, d\tau)^n \det \underline{G_{0\uparrow}} \det \underline{G_{0\downarrow}}\, Z_0$$

Wick

Partition function of the $U=0$ impurity

$$n\times n \text{ matrix } \underline{G_{0\sigma}} = \begin{pmatrix} g_{0\sigma}(0^+) & g_{0\sigma}(\tau_1-\tau_2) & \ldots \\ g_{0\sigma}(\tau_2-\tau_1) & g_{0\sigma}(0^+) & \\ \vdots & & \ddots \end{pmatrix}$$

Problem: in the paramagnetic state, $\underline{G_{0\uparrow}} = \underline{G_{0\downarrow}}$

$\Rightarrow$ $(-U)^n$ will lead to a sign problem

Solution: introduce auxiliary fields

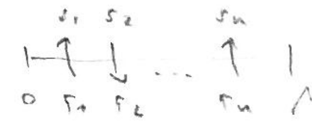
$$H_U = U n_\uparrow n_\downarrow = \frac{U}{2} \sum_{s=\pm 1} \underbrace{\left(n_\uparrow - \tfrac{1}{2} - s\left(\tfrac{1}{2}+\delta\right)\right)\left(n_\downarrow - \tfrac{1}{2} + s\left(\tfrac{1}{2}+\delta\right)\right)}_{\text{some constant} \geq 0 \text{ (away from half-filling)}} + \underbrace{\frac{U}{2}(n_\uparrow + n_\downarrow)}_{\text{shift of chemical potential}} + \text{const}$$

some constant ≥ 0 (away from half-filling)

shift of chemical potential $\mu \to \tilde{\mu} = \mu - \frac{U}{2}$

Exponential enlargement of the configuration space $\left(\sum_{s_1} \cdots \sum_{s_n}\right)$

$c = \{(\tau_1, s_1), (\tau_2, s_2), \dots (\tau_n, s_n)\}$ collection of Ising spins



shifted $\tilde{\mu}$

$$w_c = \left(-\frac{U}{2} d\tau\right)^n \underbrace{\mathrm{Tr}\left[e^{-(\beta-\tau_n)\tilde{H}_1} \left(n_\uparrow - \tfrac{1}{2} - s\left(\tfrac{1}{2}+\delta\right)\right)\left(n_\downarrow - \tfrac{1}{2} + s\left(\tfrac{1}{2}+\delta\right)\right) \dots e^{-\tau_1 \hat{H}_1}\right]}_{\det \tilde{G}_{0\uparrow} \det \tilde{G}_{0\downarrow}}$$

$\det \tilde{G}_{0\uparrow} \det \tilde{G}_{0\downarrow}$

shifted $\tilde{\mu}$

$n \times n$ matrix
$$\tilde{G}_{0\sigma} = \begin{pmatrix} \tilde{g}_{0\sigma}(0^+) - \frac{1}{2} - s_1\sigma\left(\frac{1}{2}+\delta\right) & \tilde{g}_{0\sigma}(\tau_1 - \tau_2) & \cdots \\ \tilde{g}_{0\sigma}(\tau_2 - \tau_1) & \tilde{g}_{0\sigma}(0^+) - \frac{1}{2} - s_2\sigma\left(\frac{1}{2}+\delta\right) & \\ & & \ddots \end{pmatrix}$$

$$\frac{Z}{\tilde{Z}_0} = \sum_n \int_0^\beta d\tau_1 \dots \int_{\tau_{n-1}}^\beta d\tau_n \sum_{s_1 \dots s_n} \left(-\frac{U}{2} d\tau\right)^n \det \underline{\tilde{G}_{0\uparrow}} \det \underline{\tilde{G}_{0\downarrow}}$$

Sampling procedure

Sample c using local updates (random insertion / removal of spins)

ergodicity: ✓

detailed balance: $|w(n)|\, p(n \to n+1) = |w(n+1)|\, p(n+1 \to n)$

$p^{prop}(n \to n+1)\, p^{acc}(n \to n+1)$ $\qquad$ $p^{prop}(n+1 \to n)\, p^{acc}(n+1 \to n)$

i) insertion: pick random orientation and random time for the new spin

$$p^{prop}(n \to n+1) = \frac{1}{2} \frac{d\tau}{\beta}$$

ii) removal: pick random spin

$$p^{prop}(n+1 \to n) = \frac{1}{n+1}$$

$$\Rightarrow \frac{p^{acc}(n \to n+1)}{p^{acc}(n+1 \to n)} = \left| \frac{-\beta u}{n+1} \prod_{\sigma} \frac{\det \tilde{\underline{g}}_{0\sigma}^{(n+1)}}{\det \tilde{\underline{g}}_{0\sigma}^{(n)}} \right|$$

insertion/removal of one spin adds/removes one row and column to/from the matrix $\tilde{\underline{g}}_{0\sigma}$

$$\underset{n \times n}{\left(\underline{g}_{0\sigma}^{(n)} \right)} \xrightarrow{\text{insertion}} \underset{(n+1)\times(n+1)}{\left(\begin{array}{c|c} \underline{g}_{0\sigma}^{(n)} & Q \\ \hline R & S \end{array} \right)} \equiv \tilde{\underline{g}}_{0\sigma}^{(n+1)}$$

$$\underset{n \times n}{\left(\left(\tilde{\underline{g}}_{0\sigma}^{(n)} \right)^{-1} \right)} \longrightarrow \left(\begin{array}{c|c} \tilde{P} & \tilde{Q} \\ \hline \tilde{R} & \tilde{S} \end{array} \right) \equiv \left(\tilde{\underline{g}}_{0\sigma}^{(n+1)} \right)^{-1}$$

$$\frac{\det \tilde{\underline{g}}_{0\sigma}^{(n+1)}}{\det \tilde{\underline{g}}_{0\sigma}^{(n)}} = \frac{1}{\det \tilde{S}} = \underset{1\times 1}{S} - \underset{1\times n}{R} \left[\underset{n \times n}{\left(\tilde{\underline{g}}_{0\sigma}^{(n)} \right)^{-1}} \underset{n \times 1}{Q} \right] \qquad O(n^2)$$

$$\frac{\det \tilde{\underline{g}}_{0\sigma}^{(n)}}{\det \tilde{\underline{g}}_{0\sigma}^{(n+1)}} = \det \tilde{S} = \left[\left(\tilde{\underline{g}}_{0\sigma}^{(n+1)} \right)^{-1} \right]_{n+1,n+1} \qquad O(1)$$

$\Rightarrow$ In the simulation, we store and manipulate $\left(\tilde{\underline{g}}_{0\sigma}^{(n)} \right)^{-1}$

GF measurement

Contribution of a configuration $c = \{(\tau_1, s_1), \ldots (\tau_n, s_n)\}$ in

$$G_\sigma^c(\tau) = \frac{1}{w_c} \mathrm{Tr}\Big[\ldots e^{-(\tau_2-\tau)\hat{H}_n} \underset{\tau}{d_\sigma} \ldots \big(n_\uparrow - \tfrac{1}{2} - s(\tfrac{1}{2}+\delta)\big)\big(n_\downarrow - \tfrac{1}{2} + s(\tfrac{1}{2}+\delta)\big) e^{-\tau_1 \hat{H}_1} \underset{0}{d_\sigma^\dagger}\Big]\left(-\frac{U d\tau}{2}\right)^n$$

$$= \frac{w\big[\uparrow\ \overset{d_\sigma}{\circ}\ \downarrow\ \overset{d_\sigma^\dagger}{\bullet}\big]}{w\big[\uparrow\ \ \downarrow\ \ \big]}$$

$$= \frac{1}{\det \underline{\tilde{g}_{0\sigma}} \det \underline{\tilde{g}_{0\bar\sigma}}} \det \underline{\tilde{g}_{0\bar\sigma}} \det \begin{pmatrix} \underline{\tilde{g}_{0\sigma}} & \tilde{g}_{0\sigma}(\tau_i) \\ \tilde{g}_{0\sigma}(\tau - \tau_j) & \tilde{g}_{0\sigma}(\tau) \end{pmatrix}$$

$$= \tilde{g}_{0\sigma}(\tau) + \underbrace{[g_{0\sigma}(\tau-\tau_j)]}_{1\times n}\underbrace{[\underline{\tilde{g}_{0\sigma}}^{-1}]}_{n\times n}\underbrace{[\tilde{g}_{0\sigma}(\tau_i)]}_{n\times 1}$$

To avoid the evaluation of this formula for each τ, we rewrite

$$G_\sigma^c(\tau) = \tilde{g}_{0\sigma}(\tau) + \int_0^\beta d\tilde{\tau}\, \tilde{g}_{0\sigma}(\tau - \tilde{\tau}) \underbrace{\sum_{k=1}^n \delta(\tilde{\tau} - \tau_k) \sum_{l=1}^n [\underline{\tilde{g}_{0\sigma}}^{-1}]_{kl}\, \tilde{g}_{0\sigma}(\tau_l)}_{\equiv\, S_\sigma(\tilde{\tau})}$$

and compute the MC average of S (Dyson-Eq. $\to \langle S \rangle = \Sigma * G$)

Average expansion order

$$H_2 = \tilde{H}_U = \frac{U}{2}\sum_s \big(n_\uparrow - \tfrac{1}{2} - s(\tfrac{1}{2}+\delta)\big)\big(n_\downarrow - \tfrac{1}{2} + s(\tfrac{1}{2}+\delta)\big) = U n_\uparrow n_\downarrow - \frac{U}{2}(n_\uparrow + n_\downarrow) + \text{const}$$

this gives e^{const} in Z

$$\langle -H_2 \rangle = \frac{1}{\beta}\int_0^\beta d\tau \, \langle -H_2(\tau)\rangle$$

$$= \frac{1}{\beta}\frac{1}{Z}\sum_{n=0}^\infty \underset{\uparrow \ \frac{n+1}{(n+1)!}}{\frac{1}{n!}} \int_0^\beta d\tau \Big[\int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n\Big] \mathrm{Tr}\Big[e^{-\beta H_1}\, T\, (-H_2(\tau))(-H_2(\tau_n))\ldots(-H_2(\tau_1))\Big]$$

$$= \frac{1}{\beta}\frac{1}{Z}\sum_c n(c)\, w_c = \frac{1}{\beta}\langle n \rangle$$

$$\Rightarrow \langle n \rangle = -\beta U \langle n_\uparrow n_\downarrow \rangle + \frac{\beta U}{2}\langle n_\uparrow + n_\downarrow \rangle$$

Weak-coupling values: $\langle n \rangle \sim U\beta$

For $T>0$: $\langle n \rangle < \infty$, distribution with finite variance

$\downarrow$

compute $\langle (-H_c)(-H_c) \rangle$

Absence of sign problem:

$$w_c = \mathrm{Tr}\left[e^{-(\beta-\tau_n)\tilde{H}_1} A(s_n) \dots A(s_1) e^{-\tau_1 \tilde{H}_1} \right] (d\tau)^n$$

$$A(s) = (-U/2)\left[n_\uparrow - \tfrac{1}{2} - s\left(\tfrac{1}{2}+\delta\right)\right]\left[n_\downarrow - \tfrac{1}{2} + s\left(\tfrac{1}{2}+\delta\right)\right]$$

Evaluate trace in the chain basis

$$\rightarrow \tilde{H}_1 = \sum_\sigma \sum_{j=0}^{\infty} \left[\tilde{\varepsilon}_j c^\dagger_{j,\sigma} c_{j,\sigma} - t_j \left(c^\dagger_{j+1,\sigma} c_{j\sigma} + c^\dagger_{j,\sigma} c_{j+1,\sigma} \right) \right] \qquad t_j \geq 0$$

by adding an appropriate term $\Lambda(N_\uparrow + N_\downarrow)$ with $\Lambda \geq 0$, $N_\sigma = \sum_j c^\dagger_{j\sigma} c_{j\sigma}$

we can ensure that all diagonal elements of $\tilde{H}_1 - \Lambda(N_\uparrow + N_\downarrow)$ are ≤ 0

$\Rightarrow$ all elements of the matrix $\exp\left[-\tilde{H}_1 - \Lambda(N_\uparrow + N_\downarrow)\right]$ are ≥ 0

since $\tilde{H}_1$ conserves N_σ: $$e^{-\tau \tilde{H}_1} = \underbrace{e^{-\tau(\tilde{H}_1 - \Lambda(N_\uparrow + N_\downarrow))}}_{\text{elements} \geq 0} \underbrace{e^{-\tau\Lambda(N_\uparrow + N_\downarrow)}}_{\text{elements} \geq 0}$$

has all elements ≥ 0

Matrix elements of $A(s)$: $\leftarrow$ non-zero only on the impurity site

for $\delta > 0$ and $U > 0$

$$s=1: \quad \underbrace{(-U/2)}_{<0}\underbrace{(n_\uparrow - 1 - \delta)}_{<0}\underbrace{(n_\downarrow + \delta)}_{>0} \quad > 0$$

$$s=-1: \quad \underbrace{(-U/2)}_{<0}\underbrace{(n_\uparrow + \delta)}_{>0}\underbrace{(n_\downarrow - 1 - \delta)}_{<0} \quad > 0$$

$\rightarrow$ in the chain basis, neither the time evolution operators $e^{-\tau\tilde{H}_1}$ nor the "interaction vertices" $A(s)$ have negative elements

$\rightarrow$ w_c = trace of a product of matrices with positive elements ≥ 0

Strong-coupling approach (hybridization expansion)

$$H_2 = \underbrace{\sum_{p\sigma} V_{p\sigma} d^\dagger_\sigma c_{p\sigma}}_{= H_2^{d^\dagger}} + \underbrace{\sum_{p\sigma} V^*_{p\sigma} c^\dagger_{p\sigma} d_\sigma}_{= H_2^{d}}$$

need equal number of $d^\dagger$ and d $\rightarrow \frac{2n!}{n!\,n!}$ possibilities for order $2n$

$$Z = \sum_{n=0}^{\infty} \frac{1}{(2n)!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_{2n} \, \mathrm{Tr}\left[e^{-\beta H_1} T\, H_2(\tau_{2n}) \ldots H_2(\tau_1) \right]$$

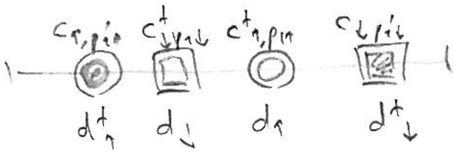
$$= \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \left(\int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \right) \left(\int_0^\beta d\tau_1' \ldots \int_0^\beta d\tau_n' \right) \mathrm{Tr}\left[e^{-\beta H_1} T\, H_2^d(\tau_n) H_2^{d^\dagger}(\tau_n') \ldots H_2^d(\tau_1) H_2^{d^\dagger}(\tau_1') \right]$$

Note that H_2^d, $H_2^{d^\dagger}$ commute

Separating the d and $d^\dagger$ operators into $\sigma = \uparrow, \downarrow$ $\left(n = n_\uparrow + n_\downarrow \rightarrow \frac{n!}{n_\uparrow!\, n_\downarrow!} \text{ combinations} \right)$

and time-ordering the integrals gives

$$Z = \sum_{\{n_\sigma\}} \prod_\sigma \left(\int_0^\beta d\tau_1^\sigma \ldots \int_{\tau_{n-1}^\sigma}^\beta d\tau_n^\sigma \right) \left(\int_0^\beta d\tau_1'^\sigma \ldots \int_0^\beta d\tau_n'^\sigma \right)$$

$$\times \mathrm{Tr}\Big[e^{-\beta H_1} \prod_\sigma \sum_{\{p\}} \sum_{\{p'\}} VV^* \ldots VV^*$$ 

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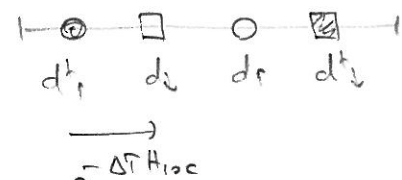
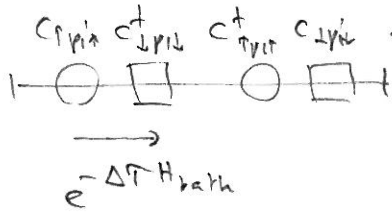
$H = H_{loc} + H_{bath}$ does not mix impurity and bath states

$\rightarrow$ separate $\mathrm{Tr}[\ldots]$ into impurity (d) and bath (c) states

impurity: $\mathrm{Tr}_d \Big[$ 

$\Big]$

bath: $Z_{bath} \frac{1}{Z_{bath}} \mathrm{Tr}_c \Big[\prod_\sigma \sum_{\{p\}} \sum_{\{p'\}} VV^* \ldots VV^*$ 

$\Big]$

H_{bath} is noninteracting $\Rightarrow$ Wick theorem gives

$$\frac{1}{Z_{bath}} \mathrm{Tr}_c [\ldots] = \det(\ldots)$$

What is det (...) ? $\to$ compute lowest order $n_\sigma = 1$, $n_{\bar\sigma} = 1$

$$Z_{bath} = \prod_\sigma \prod_p \big(\underset{\displaystyle |1\rangle_p}{\underset{\downarrow}{e^{-\varepsilon_p \beta}}} + \underset{\displaystyle |0\rangle_p}{\underset{\downarrow}{1}} \big)$$

$$\sum_{p_1} \sum_{p_1'} V_{p_1}^\sigma V_{p_1'}^{\sigma *} \frac{1}{Z_{bath}} \mathrm{Tr}_c \left[e^{-\beta H_{bath}} T c^\dagger_{\sigma,p_1}(\tau_1^\sigma) c_{\sigma,p_1'}(\tau_1'^\sigma) \right] \to p_1 = p_1'$$

$$= \sum_p \frac{|V_p|^2}{e^{-\varepsilon_p \beta} + 1} \begin{cases} e^{-\varepsilon_p(\beta - (\tau_1^\sigma - \tau_1'^\sigma))} & \tau_1^\sigma > \tau_1'^\sigma \\ -e^{-\varepsilon_p(\tau_1'^\sigma - \tau_1^\sigma)} & \tau_1^\sigma < \tau_1'^\sigma \end{cases}$$

$\equiv \Delta_\sigma(\tau_1'^\sigma - \tau_1^\sigma)$ hybridization function $\left[\Delta(i\omega_n) = \sum_p \frac{|V_p|^2}{i\omega_n - \varepsilon_p} \right]$

For higher orders, one gets $\frac{1}{Z_{bath}} \mathrm{Tr}_c [\dots] = \prod_\sigma \det M_\sigma^{-1}$, $(M_\sigma^{-1})_{ij} = \Delta(\tau_i'^\sigma - \tau_j^\sigma)$

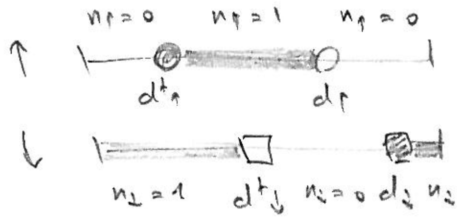
Monte Carlo configurations: $c = \{ \underbrace{\tau_1^\uparrow, \dots, \tau_{n_\uparrow}^\uparrow}_{n_\uparrow \times d_\uparrow} ; \underbrace{\tau_1'^\uparrow \dots \tau_{n_\uparrow}'^\uparrow}_{n_\uparrow \times d^\dagger_\uparrow} \mid \underbrace{\tau_1^\downarrow, \dots, \tau_{n_\downarrow}^\downarrow}_{n_\downarrow \times d_\downarrow} ; \underbrace{\tau_1'^\downarrow \dots \tau_{n_\downarrow}'^\downarrow}_{n_\downarrow \times d^\dagger_\downarrow} \}$

$$w_c = Z_{bath} \underbrace{\mathrm{Tr}_d \left[e^{-\beta H_{loc}} T \prod_\sigma d_\sigma(\tau_{n_\sigma}^\sigma) d^\dagger_\sigma(\tau_{n_\sigma}'^\sigma) \dots d_\sigma(\tau_1^\sigma) d^\dagger_\sigma(\tau_1'^\sigma) \right]}_{\text{impurity contribution}} \underbrace{\prod_\sigma \det M_\sigma^{-1} (d\tau)^{2n}}_{\text{bath contribution}}$$

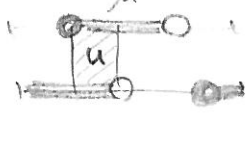
(must be evaluated explicitly)

Simple case: density-density interactions (occupation number basis is eigenbasis of H_{loc})

$\to$ alternating $d^\dagger_\sigma$ and d_σ operators $\Rightarrow$ collection of segments on $[0, \beta]$



Segment picture allows cheap calculation of $\mathrm{Tr}_d [\dots] = e^{\mu(l_\uparrow + l_\downarrow) - U l_{overlap}} \times S$



$\uparrow$ from time-ordering

<u>Sampling procedure</u> Z = sum over all segment configurations

local updates in the segment configurations

insertion / removal of segments and anti-segments

ex: insertion of segment : 

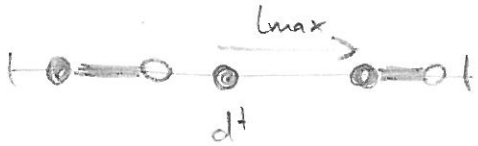
insertion of antisegment : 

<u>detailed balance:</u>

insertion: choose d^+ randomly in $[0,\beta]$

if it falls on a segment $\longrightarrow$ reject move

if it falls on an empty space $\longrightarrow$ compute l_{max}



choose d randomly in interval of length l_{max}:

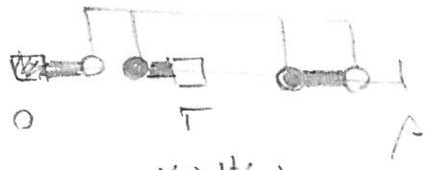
$$p^{prop}(n_\sigma \to n_\sigma+1) = \frac{d\tau}{\beta}\frac{d\tau}{l_{max}}$$

removal: choose a random segment

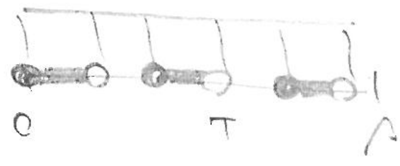
$$p^{prop}(n_\sigma+1 \to n_\sigma) = \frac{1}{n_\sigma+1}$$

$$\frac{p^{acc}(n_\sigma \to n_\sigma+1)}{p^{acc}(n_\sigma+1 \to n_\sigma)} = \underbrace{\frac{p^{prop}(n_\sigma+1 \to n_\sigma)}{p^{prop}(n_\sigma \to n_\sigma+1)}}_{\frac{\beta l_{max}}{(n_\sigma+1)\cancel{(d\tau)^2}}} \underbrace{\frac{|w_c(n_\sigma+1)|}{|w_c(n_\sigma)|}}_{\cancel{(d\tau)^2}\frac{|\det(M_\sigma^{(n+1)})^{-1}|}{|\det(M_\sigma^{(n)})^{-1}|}e^{\mu\Delta l - U\Delta l_{ov.}}}$$

Measurement of the GF



$w_c^{d(\tau)d^+(0)}$



$w_c^{(0,\tau)}$

diagram which appears in the expansion of $G(\tau)$

diagram with d^+ at 0 and d at τ which appears in the expansion of Z

$$G(\tau) = -\frac{1}{Z}\sum_c w_c^{d(\tau)d^+(0)} = -\frac{1}{Z}\sum_c w_c^{(0,\tau)} \underbrace{\frac{w_c^{d(\tau)d^+(0)}}{w_c^{(0,\tau)}}}$$

Tr[...] identical $\Rightarrow \dfrac{\det M_c^{-1}}{\det (M_c^{(0,\tau)})^{-1}}$

$$(\;\;) = (M_c^{(0,\tau)})^{-1}$$

$$= \frac{\det\begin{pmatrix} & | & \\ - & | & - \\ & | & \end{pmatrix}}{\det\begin{pmatrix} & & \end{pmatrix}}$$

d^+ (column j)

$\leftarrow d$ (row i)

$(-1)^{i+j}$

minor ij

$$= (M_c^{(0,\tau)})_{ji}$$

Want to go from $\sum_c w_c^{(0,\tau)} (M_c^{(0,\tau)})_{ji}$ (with fixed operators at $0,\tau$)

to $\sum_{\tilde{c}} w_{\tilde{c}} (M_{\tilde{c}})_{ji} (\dots)$ (no restriction on operator positions)

$\downarrow$

$\sum_{ij} \frac{1}{\beta} \delta(\tau, \tau_i - \tau_j')$ β-antiperiodic δ-function

sum over n^2 (d^+, d) pairs, because we go from $\frac{1}{(n-1)!}\int_0^\beta d\tau_1 \dots d\tau_{n-1} \frac{1}{(n-1)!}\int_0^\beta d\tau_1' \dots d\tau_{n-1}'$

to $\frac{1}{n!}\int_0^\beta d\tau_1 \dots d\tau_n \frac{1}{n!}\int_0^\beta d\tau_1' \dots d\tau_n'$

$\Rightarrow n^2 \delta(\tau, \tau_n - \tau_1')$ or $\sum_{ij} \delta(\tau, \tau_i - \tau_j')$

$$G(\tau) = -\frac{1}{\beta}\left\langle \sum_{ij} \delta(\tau, \tau_i - \tau_j')(M_c)_{ji} \right\rangle$$

Average perturbation order

DMFT: kinetic energy $\quad E_{kin} = \sum_{\sigma} \int_0^{\beta} d\tau\, G_{\sigma}(\tau)\, \Delta_{\sigma}(-\tau)$

$$\int_0^{\beta} d\tau\, G(\tau)\,\Delta(-\tau) = \int_0^{\beta} d\tau \left\langle -\frac{1}{\beta} \sum_{ij} \delta(\tau, \tau_i - \tau_j')\, M_{ji} \right\rangle \Delta(-\tau)$$

$$= -\frac{1}{\beta} \left\langle \sum_{ij} M_{ji}\, \Delta(\tau_j' - \tau_i) \right\rangle$$

$$M_{ji} = (-1)^{i+j} \frac{\det\left(\begin{array}{c|c} & j \\ \hline \quad & \end{array}\right)_i}{\det\left(\;\Delta\;\right)} \longrightarrow \sum_j (-1)^{i+j} \det\left(\begin{array}{c|c} & j \\ \hline \quad & \end{array}\right) \Delta(\tau_j' - \tau_i)$$

is the expansion of the hybridization matrix determinant along row i

$$= \det\left(\;\Delta\;\right)$$

$$\int_0^{\beta} d\tau\, G(\tau)\,\Delta(-\tau) = -\frac{1}{\beta} \left\langle \sum_{i=1}^{n} \frac{\det(\Delta)}{\det(\Delta)} \right\rangle = -\frac{1}{\beta} \langle n \rangle$$

perturbation order

$$\Rightarrow \quad E_{kin} = -\frac{1}{\beta} \sum_{\sigma} \langle n_{\sigma} \rangle$$

Derivation of the kinetic energy formula:

$$E_{kin} = \sum_{k,\sigma} \varepsilon_k\, G_{k,\sigma}(0^-) = \sum_{k,\sigma} \varepsilon_k \frac{1}{\beta} \sum_n e^{-i\omega_n 0^-} G_{k,\sigma}(i\omega_n)$$

$$= \sum_{k,\sigma} \varepsilon_k \frac{1}{\beta} \sum_n e^{i\omega_n 0_+} \frac{1}{i\omega_n + \mu - \varepsilon_k - \Sigma_{\sigma}(i\omega_n)}$$

density of states

$$= \sum_{\sigma} \frac{1}{\beta} \sum_n e^{i\omega_n 0_+} \int d\varepsilon \frac{\varepsilon}{i\omega_n + \mu - \varepsilon - \Sigma_{\sigma}(i\omega_n)} D(\varepsilon)$$

$$= \sum_{\sigma} \frac{1}{\beta} \sum_n e^{i\omega_n 0_+} \int d\varepsilon \frac{-[i\omega_n + \mu - \varepsilon - \Sigma_{\sigma}] + [i\omega_n + \mu - \Sigma_{\sigma}]}{i\omega_n + \mu - \varepsilon - \Sigma_{\sigma}(i\omega_n)} D(\varepsilon)$$

$$= \sum_{\sigma} \frac{1}{\beta} \sum_n e^{i\omega_n 0_+} \left(-1 + [i\omega_n + \mu - \Sigma_{\sigma}]\, G_{\sigma}^{loc}\right) \qquad \text{DMFT: } G_{\sigma}^{loc} = G_{\sigma}$$

$$= \sum_{\sigma} \frac{1}{\beta} \sum_n e^{i\omega_n 0_+} G_{\sigma}(i\omega_n)\, \Delta_{\sigma}(i\omega_n) \qquad G = [i\omega_n + \mu - \Sigma - \Delta]^{-1}$$

Absence of sign problem

$$w_c = \mathrm{Tr}\left[e^{-(\beta-\tau_n)(H_{loc}+H_{bath})} (-H^{d\dagger}_{mix}) \dots (-H^{d}_{mix}) e^{-\tau_1 (H_{loc}+H_{bath})} \right] (d\tau)^{2n}$$

Let us evaluate this trace in the chain basis

$$\underset{c_0 = d}{\bullet} \overset{-V}{—} \underset{c_1}{\circ} \overset{-t_1}{—} \underset{c_2}{\circ} \overset{-t_2}{—} \circ — \circ \dots \qquad V, t_i \geq 0$$

$-H^{d\dagger}_{mix} = V c_0^\dagger c_1$, $-H^{d}_{mix} = V c_1^\dagger c_0$

$\to$ hybridization operators do not produce negative signs ($V \geq 0$)

In the imaginary-time evolution operator, H_{loc} is diagonal, while H_{bath} has off-diagonal elements $-t_i \leq 0$

$$e^{-\tau(H_{loc}+H_{bath})} = \lim_{N\to\infty} \left(1 - \frac{\tau}{N}\left[H_{loc} + H_{bath} \right] \right)^N$$

dominates diagonal terms $\Rightarrow > 0$

off-diagonal terms (originating from $-\frac{\tau}{N} H_{bath}$) also ≥ 0

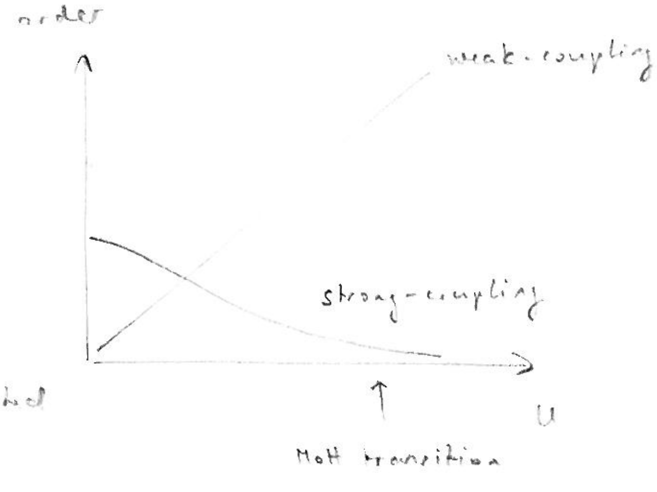
$\to$ imaginary-time evolution operators have no negative elements

$\Rightarrow$ w_c is the trace of a matrix with all elements ≥ 0

Scaling of the algorithms

Weak-coupling: β^3 U^2

Strong-coupling: β^3 ?



single orbital AIM: strong-coupling solver much more efficient in the strongly correlated metal and Mott insulating regime