Tensor cross interpolation approach for the quantum impurity problem based on the weak-coupling expansion

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Phys. Rev. B **111**, 155150 (2025)

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Outline

- Introduction
  - Quantum impurity problem and DMFT
  - Impurity solver
- Application of TCI to the impurity problem
  - Evaluation of the partition function
  - Evaluation of the Green's function
- Result
  - Exactly solvable impurity model
  - DMFT for the Hubbard model
- Summary and Outlook

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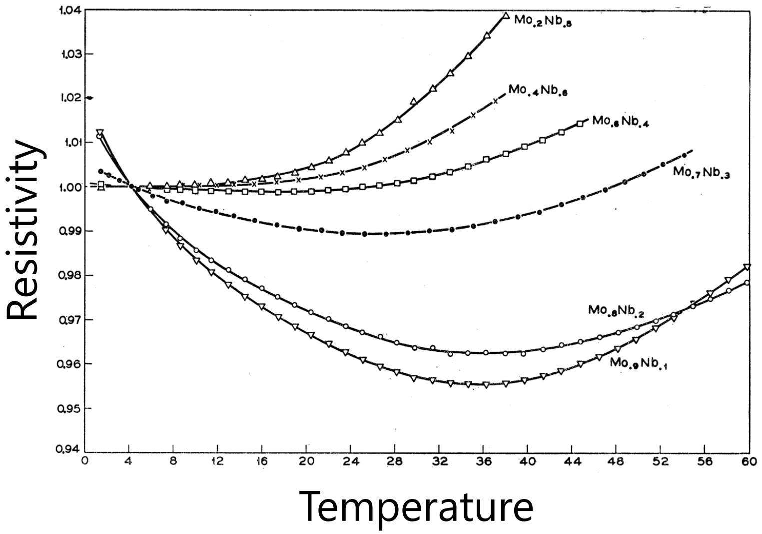
Quantum impurity problem and DMFT

$$H=\sum_{\sigma}\varepsilon_\sigma c_\sigma^\dagger c_\sigma + U\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)+\sum_{k,\sigma}\varepsilon_{k\sigma}b_{k\sigma}^\dagger b_{k\sigma}+\sum_{k,\sigma}(V_{k\sigma}b_{k\sigma}^\dagger c_\sigma + V_{k\sigma}^* c_\sigma^\dagger b_{k\sigma})$$

- Kondo effect

J. Kondo, Prog. Theor. Phys. **32**, 37 (1964)

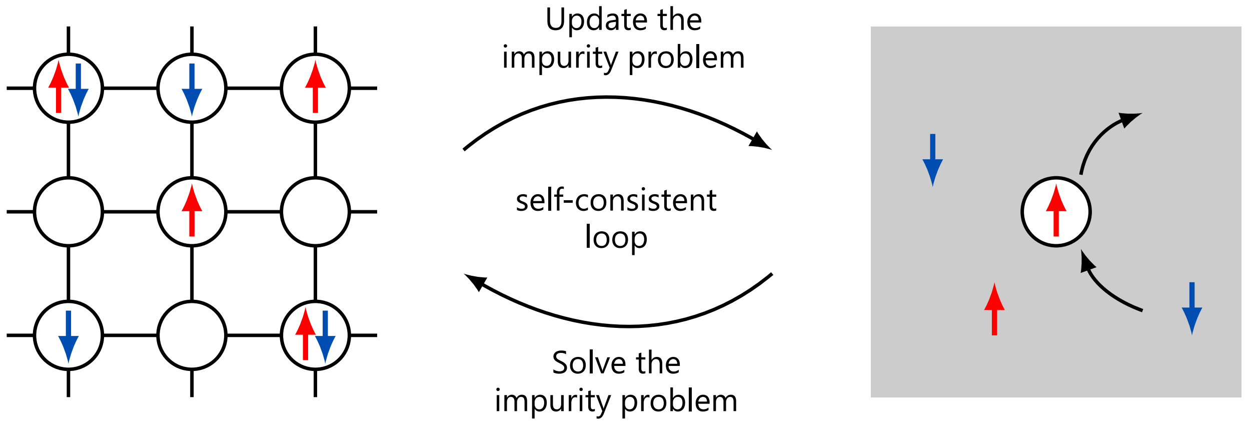


  - Resistance minimum
  - Formation of the Kondo-singlet

Nontrivial many-body phenomena

- Dynamical mean-field theory (DMFT)

A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996)



Hubbard model

Quantum impurity model

  - Hubbard model is mapped to the impurity model.

The important model for understanding
the strongly correlated system

How to solve the impurity problem

- Perturbative expansion
  - The perturbative expansion (weak-coupling or strong-coupling expansion) provides a systematic way to analyze the impurity model.
  - The high-order terms involve high-dimensional integrals, whose evaluation becomes the bottleneck.

Approach 1 : Continuous-time Quantum Monte Carlo method (CT-QMC)

E. Gull *et al.*, Rev. Mod. Phys. **83**, 349 (2011)

- The efficient method to evaluate high-dimensional integrals.
- In some cases, it suffers from the negative sign problem.

Approach 2 : Tensor Cross Interpolation (TCI)

- Sign-problem-free integration
- There are several papers on the TCI impurity solver:
  - nonequilibrium impurity problem (weak-coupling expansion)
  - nonequilibrium impurity problem (strong-coupling expansion)
  - equilibrium impurity problem (strong-coupling expansion)

Y. N. Fernández *et al.*, Phys. Rev. X **12**, 041018 (2022)
M. Jeannin *et al.*, arXiv:2502.16306 (2025)

M. Eckstein, arXiv:2410.19707 (2024)
A. J. Kim *et al.*, Phys. Rev. B **111**, 125120 (2025)
L. Geng *et al.*, arXiv:2507.20385 (2025)

A. Erpenbeck *et al.*, Phys. Rev. B **107**, 245135 (2023)
Y. Yu *et al.*, Phys. Rev. B **112**, 085120 (2025)

Can we solve the equilibrium impurity problem with weak-coupling expansion + TCI ?

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Weak-coupling expansion

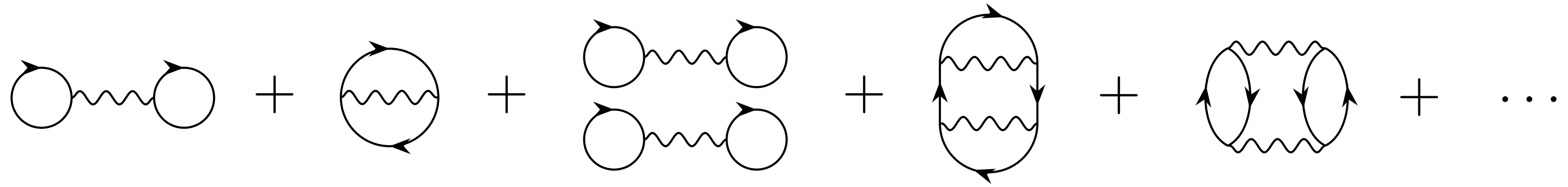
$$H = \sum_{\sigma} \varepsilon_\sigma c_\sigma^\dagger c_\sigma + U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) + \sum_{k,\sigma} \varepsilon_{k\sigma} b_{k\sigma}^\dagger b_{k\sigma} + \sum_{k,\sigma}(V_{k\sigma} b_{k\sigma}^\dagger c_\sigma + V_{k\sigma}^* c_\sigma^\dagger b_{k\sigma})$$

- weak-coupling expansion

$$G_\uparrow(\tau) = -\left\langle T_\tau [c_{\mathrm{H}\uparrow}(\tau) c_{\mathrm{H}\uparrow}^\dagger(0)] \right\rangle = -\frac{\left\langle T_\tau \left[c_{\mathrm{I}\uparrow}(\tau) c_{\mathrm{I}\uparrow}^\dagger(0) \exp\left(-\int_0^\beta d\tau'\, H_{\mathrm{int}}(\tau')\right)\right]\right\rangle_0}{\left\langle T_\tau \exp\left(-\int_0^\beta d\tau'\, H_{\mathrm{int}}(\tau')\right)\right\rangle_0} \qquad H_{\mathrm{int}} = U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right)$$

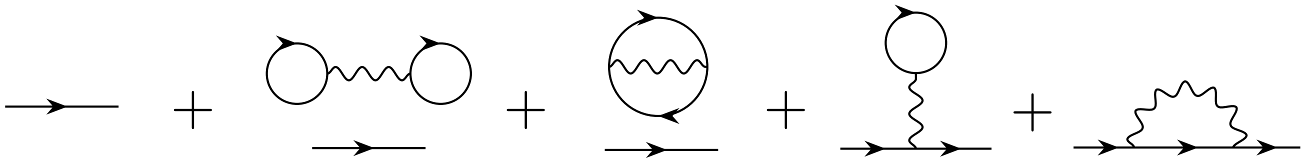
<u>denominator</u>

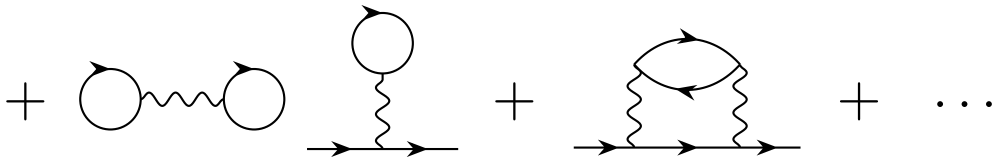
$$\left\langle T_\tau \exp\left(-\int_0^\beta d\tau'\, H_{\mathrm{int}}(\tau')\right)\right\rangle_0 = 1 +$$



<u>numerator</u>

$$-\left\langle T_\tau \left[c_{\mathrm{I}\uparrow}(\tau) c_{\mathrm{I}\uparrow}^\dagger(0) \exp\left(-\int_0^\beta d\tau'\, H_{\mathrm{int}}(\tau')\right)\right]\right\rangle_0 =$$





Weak-coupling expansion

$$H=\sum_{\sigma}\varepsilon_{\sigma}c_{\sigma}^{\dagger}c_{\sigma}+U\left(n_{\uparrow}-\frac{1}{2}\right)\left(n_{\downarrow}-\frac{1}{2}\right)+\sum_{k,\sigma}\varepsilon_{k\sigma}b_{k\sigma}^{\dagger}b_{k\sigma}+\sum_{k,\sigma}(V_{k\sigma}b_{k\sigma}^{\dagger}c_{\sigma}+V_{k\sigma}^{*}c_{\sigma}^{\dagger}b_{k\sigma})$$

- weak-coupling expansion

$$G_{\uparrow}(\tau)=-\left\langle T_{\tau}[c_{\mathrm{H}\uparrow}(\tau)c_{\mathrm{H}\uparrow}^{\dagger}(0)]\right\rangle=-\frac{\left\langle T_{\tau}\left[c_{\mathrm{I}\uparrow}(\tau)c_{\mathrm{I}\uparrow}^{\dagger}(0)\exp\left(-\int_0^{\beta}d\tau'\,H_{\mathrm{int}}(\tau')\right)\right]\right\rangle_0}{\left\langle T_{\tau}\exp\left(-\int_0^{\beta}d\tau'\,H_{\mathrm{int}}(\tau')\right)\right\rangle_0}$$

$$H_{\mathrm{int}}=U\left(n_{\uparrow}-\frac{1}{2}\right)\left(n_{\downarrow}-\frac{1}{2}\right)$$

denominator

$$\left\langle T_{\tau}\exp\left(-\int_0^{\beta}d\tau'\,H_{\mathrm{int}}(\tau')\right)\right\rangle_0=\sum_{n=0}^{\infty}\frac{(-U)^n}{n!}\int_0^{\beta}d\tau_1\cdots d\tau_n\,(\det\boldsymbol{D}_n^{\uparrow})(\det\boldsymbol{D}_n^{\downarrow})$$

TCI can be used to evaluate these integrals.

numerator

$$-\left\langle T_{\tau}\left[c_{\mathrm{I}\uparrow}(\tau)c_{\mathrm{I}\uparrow}^{\dagger}(0)\exp\left(-\int_0^{\beta}d\tau'\,H_{\mathrm{int}}(\tau')\right)\right]\right\rangle_0=\sum_{n=0}^{\infty}\frac{(-U)^n}{n!}\int_0^{\beta}d\tau_1\cdots d\tau_n\,(\det\tilde{\boldsymbol{D}}_n^{\uparrow})(\det\boldsymbol{D}_n^{\downarrow})$$

$$\boldsymbol{D}_n^{\sigma}=\begin{pmatrix}\mathcal{G}_{\sigma}(0^-)-1/2 & \mathcal{G}_{\sigma}(\tau_1-\tau_2) & \cdots & \mathcal{G}_{\sigma}(\tau_1-\tau_n)\\ \mathcal{G}_{\sigma}(\tau_2-\tau_1) & \mathcal{G}_{\sigma}(0^-)-1/2 & \cdots & \mathcal{G}_{\sigma}(\tau_2-\tau_n)\\ \vdots & \vdots & \ddots & \vdots\\ \mathcal{G}_{\sigma}(\tau_n-\tau_1) & \mathcal{G}_{\sigma}(\tau_n-\tau_1) & \cdots & \mathcal{G}_{\sigma}(0^-)-1/2\end{pmatrix}\qquad \tilde{\boldsymbol{D}}_n^{\sigma}=\begin{pmatrix}\mathcal{G}_{\sigma}(\tau) & \mathcal{G}_{\sigma}(\tau-\tau_1) & \cdots & \mathcal{G}_{\sigma}(\tau-\tau_n)\\ \mathcal{G}_{\sigma}(\tau_1) & \mathcal{G}_{\sigma}(0^-)-1/2 & \cdots & \mathcal{G}_{\sigma}(\tau_1-\tau_n)\\ \vdots & \vdots & \ddots & \vdots\\ \mathcal{G}_{\sigma}(\tau_n) & \mathcal{G}_{\sigma}(\tau_n-\tau_1) & \cdots & \mathcal{G}_{\sigma}(0^-)-1/2\end{pmatrix}$$

$\mathcal{G}_{\sigma}(\tau)$: noninteracting Green's function

Integration by TCI

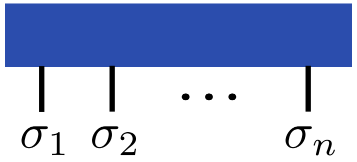
- Gauss–Kronrod quadrature + Tensor-train decomposition

$$\int_{[0,1]^n} dx_1 \cdots dx_n \, f(x_1, \cdots, x_n) \simeq \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_n=1}^{d} w_{\sigma_1} \cdots w_{\sigma_n} f(\tilde{x}_{\sigma_1}, \cdots, \tilde{x}_{\sigma_n})$$

$\tilde{x}_{\sigma_i}$: zeros of the Legendre poly.

w_{σ_i} : suitable weights

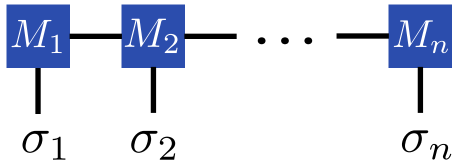
$$= \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_n=1}^{d}$$



n-fold sum

cost : $\mathcal{O}(d^n)$

$$\simeq \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_n=1}^{d}$$



$$= \left(\sum_{\sigma_1=1}^{d} M_1^{\sigma_1} \right) \left(\sum_{\sigma_2=1}^{d} M_2^{\sigma_2} \right) \cdots \left(\sum_{\sigma_n=1}^{d} M_n^{\sigma_n} \right)$$

n single fold sums

cost : $\mathcal{O}(nd\chi^2)$

The high-dimension integrals can be calculated in this way if
(1) the integration domain is a hypercube,
and
(2) the integrand is a smooth function.

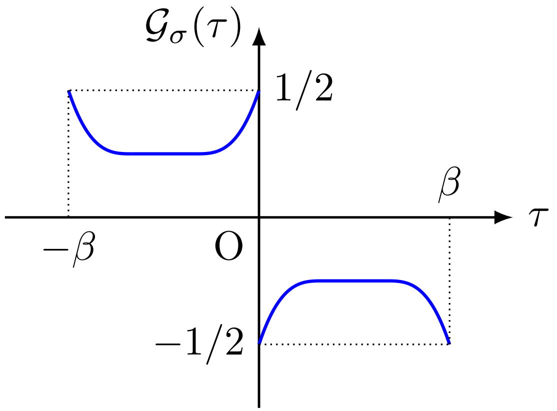
Evaluation of the denominator

$$\mathcal{I}_n = \frac{(-U)^n}{n!}\int_0^\beta d\tau_1\cdots d\tau_n\, P(\tau_1,\cdots,\tau_n)$$

where $P(\tau_1,\cdots,\tau_n) \coloneqq (\det \boldsymbol{D}_n^{\uparrow})(\det \boldsymbol{D}_n^{\downarrow})$

$$\boldsymbol{D}_n^{\sigma} = \begin{pmatrix} \mathcal{G}_\sigma(0^-)-1/2 & \mathcal{G}_\sigma(\tau_1-\tau_2) & \cdots & \mathcal{G}_\sigma(\tau_1-\tau_n) \\ \mathcal{G}_\sigma(\tau_2-\tau_1) & \mathcal{G}_\sigma(0^-)-1/2 & \cdots & \mathcal{G}_\sigma(\tau_2-\tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_\sigma(\tau_n-\tau_1) & \mathcal{G}_\sigma(\tau_n-\tau_1) & \cdots & \mathcal{G}_\sigma(0^-)-1/2 \end{pmatrix}$$

- Removal of discontinuities



  - The noninteracting Green's function $\mathcal{G}_\sigma(\tau)$ has discontinuity at $\tau = 0$.

  ➡ Since the integrand includes $\mathcal{G}_\sigma(\tau_i-\tau_j)$, it has discontinuities at $\tau_i = \tau_j$.

  - To remove the discontinuities, we can use the permutation symmetry $P(\tau_1,\cdots,\tau_n) = P(\tau_{\sigma(1)},\cdots,\tau_{\sigma(n)})$.

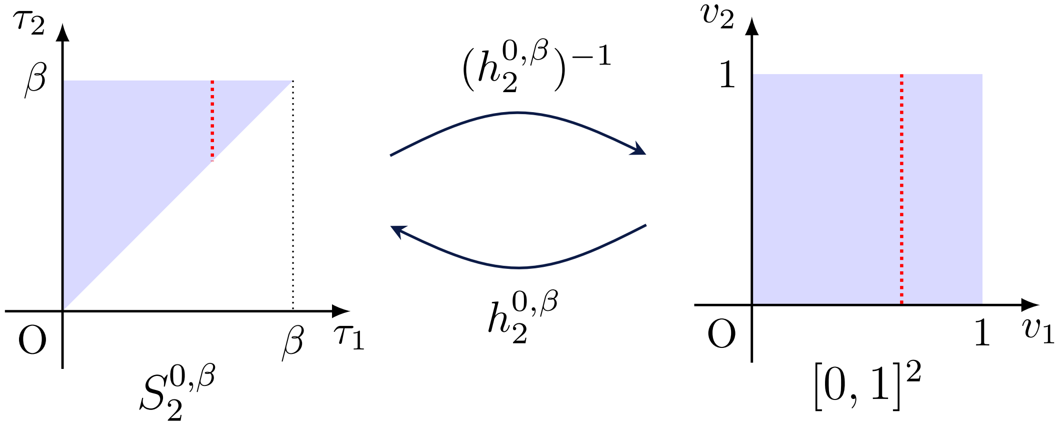
$$\mathcal{I}_n = (-U)^n \int_{S_n^{0,\beta}} d\tau_1\cdots d\tau_n\, P(\tau_1,\cdots,\tau_n) \qquad S_n^{a,b} \coloneqq \{(\tau_1,\cdots,\tau_n)\in\mathbb{R} \mid a\le\tau_1\le\tau_2\le\cdots\le\tau_n\le b\}$$

The integrand $P(\tau_1,\cdots,\tau_n)$ is a smooth function on the simplex $S_n^{0,\beta}$.

Evaluation of the denominator

- Variable transformation
  - The integration domain has to be mapped from the simplex back to the hypercube.
  - To this end, we can use the variable transformation $h_n^{0,\beta} : [0,1]^n \to S_n^{0,\beta}; (v_1, \cdots, v_n) \mapsto (\tau_1, \cdots, \tau_n)$.

$$\begin{aligned}
\tau_1 &= \beta(1-(1-v_1)) \\
\tau_2 &= \beta(1-(1-v_1)(1-v_2)) \\
&\vdots \\
\tau_n &= \beta(1-(1-v_1)(1-v_2)\cdots(1-v_n))
\end{aligned}$$



  - The integral can be written in terms of the new variables as

$$\mathcal{I}_n = (-U)^n \int_{S_n^{0,\beta}} d\tau_1 \cdots d\tau_n \, P(\tau_1, \cdots, \tau_n) = (-U)^n \int_{[0,1]^n} dv_1 \cdots dv_n \, J_{h_n^{0,\beta}}(v_1, \cdots, v_n) P(h_n^{0,\beta}(v_1, \cdots, v_n))$$

The integrand $J_{h_n^{0,\beta}}(v_1, \cdots, v_n) P(h_n^{0,\beta}(v_1, \cdots, v_n))$ is a smooth function on the hypercube $[0,1]^n$.

Evaluation of the numerator

$$\mathcal{J}_n(\tau) = \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n \, Q(\tau_1, \cdots, \tau_n; \tau)$$

where $Q(\tau_1, \cdots, \tau_n; \tau) := (\det \tilde{\boldsymbol{D}}_n^{\uparrow})(\det \boldsymbol{D}_n^{\downarrow})$

$$\tilde{\boldsymbol{D}}_n^{\sigma} = \begin{pmatrix} \mathcal{G}_\sigma(\tau) & \mathcal{G}_\sigma(\tau - \tau_1) & \cdots & \mathcal{G}_\sigma(\tau - \tau_n) \\ \mathcal{G}_\sigma(\tau_1) & \mathcal{G}_\sigma(0^-) - 1/2 & \cdots & \mathcal{G}_\sigma(\tau_1 - \tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_\sigma(\tau_n) & \mathcal{G}_\sigma(\tau_n - \tau_1) & \cdots & \mathcal{G}_\sigma(0^-) - 1/2 \end{pmatrix}$$

- Removal of discontinuities
  - The discontinuities at $\tau_i = \tau_j$ can be removed in the same way as the denominator:

$$\mathcal{J}_n(\tau) = (-U)^n \int_{S_n^{0,\beta}} d\tau_1 \cdots d\tau_n \, Q(\tau_1, \cdots, \tau_n; \tau)$$

  - The integrand of the numerator also has discontinuities at $\tau = \tau_i$.

➡ We first divide the integration domain to $n+1$ smaller regions, which is labeled by k.

$$\mathcal{J}_n(\tau) = (-U)^n \sum_{k=0}^{n} \int_{S_k^{0,\tau}} d\tau_1 \cdots d\tau_k \int_{S_{n-k}^{\tau,\beta}} d\tau_{k+1} \cdots d\tau_n \, Q(\tau_1, \cdots, \tau_n; \tau)$$

$$S_n^{a,b} := \{(\tau_1, \cdots, \tau_n) \mid a \le \tau_1 \le \cdots \le \tau_n \le b\}$$

$$\begin{aligned} k = 0 &: \tau \le \tau_1 \le \tau_2 \le \cdots \le \tau_n, \\ k = 1 &: \tau_1 \le \tau \le \tau_2 \le \cdots \le \tau_n, \\ &\vdots \\ k = n &: \tau_1 \le \tau_2 \le \cdots \le \tau_n \le \tau. \end{aligned}$$

The integrand $Q(\tau_1, \cdots, \tau_n; \tau)$ is a smooth function on each smaller regions.

Evaluation of the numerator

- Variable transformation
  - We can use the variable transformations

$$h_k^{0,\tau} : [0,1]^k \to S_k^{0,\tau}\,;\,(v_1,\cdots,v_k) \mapsto (\tau_1,\cdots,\tau_k) \quad \text{and} \quad h_{n-k}^{\tau,\beta} : [0,1]^{n-k} \to S_{n-k}^{\tau,\beta}\,;\,(v_{k+1},\cdots,v_n) \mapsto (\tau_{k+1},\cdots,\tau_n)$$

to map each small region to a hypercube.

  - After the variable transformation, the integral can be written as

$$\begin{aligned}\mathcal{J}_n(\tau) &= (-U)^n \sum_{k=0}^{n} \int_{S_k^{0,\tau}} d\tau_1 \cdots d\tau_k \int_{S_{n-k}^{\tau,\beta}} d\tau_{k+1} \cdots d\tau_n \, Q(\tau_1,\cdots,\tau_n;\tau) \\ &= (-U)^n \sum_{k=0}^{n} \int_{[0,1]^n} dv_1 \cdots dv_n \, J_{h_k^{0,\tau}}(v_1,\cdots,v_k;\tau) J_{h_{n-k}^{\tau,\beta}}(v_{k+1},\cdots,v_n;\tau) \tilde{Q}(v_1,\cdots,v_n;\tau)\end{aligned}$$

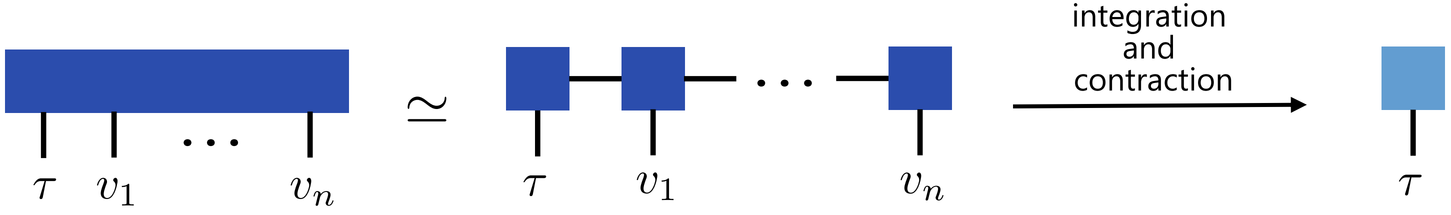
The integrand $J_{h_k^{0,\tau}}(v_1,\cdots,v_k;\tau)J_{h_{n-k}^{\tau,\beta}}(v_{k+1},\cdots,v_n;\tau)\tilde{Q}(v_1,\cdots,v_n;\tau)$ is a smooth function on the hypercube.

Evaluation of the numerator

$$J_n(\tau) = (-U)^n \sum_{k=0}^{n} \int_{[0,1]^n} dv_1 \cdots dv_n \, J_{h_k^{0,\tau}}(v_1, \cdots, v_k; \tau) J_{h_{n-k}^{\tau,\beta}}(v_{k+1}, \cdots, v_n; \tau) \tilde{Q}(v_1, \cdots, v_n; \tau)$$

- How to take the summation over k ?
  - (1) Perform TCI algorithm to $\sum_{k=0}^{n} J_{h_k^{0,\tau}}(v_1, \cdots, v_k; \tau) J_{h_{n-k}^{\tau,\beta}}(v_{k+1}, \cdots, v_n; \tau) \tilde{Q}(v_1, \cdots, v_n; \tau)$.
  - (2) Perform TCI algorithm to $J_{h_k^{0,\tau}}(v_1, \cdots, v_k; \tau) J_{h_{n-k}^{\tau,\beta}}(v_{k+1}, \cdots, v_n; \tau) \tilde{Q}(v_1, \cdots, v_n; \tau)$ for each k and sum after that.

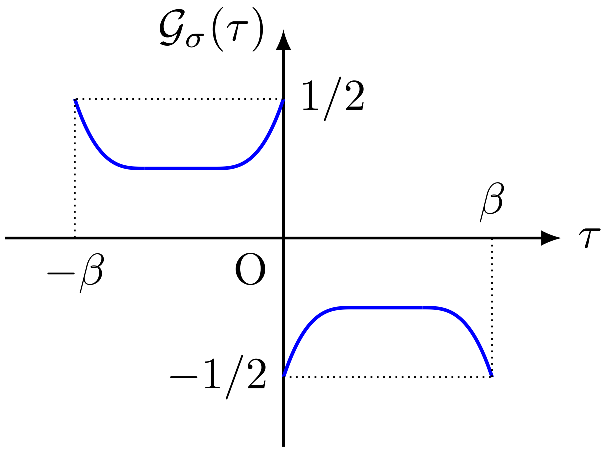
- How to take calculate the τ-dependence?
  - (1) Perform TCI algorithm for each τ .
  - (2) Regard τ as an additional leg of the tensor and perform TCI algorithm.



Structure of the weak-coupling expansion

- How to set the maximum order $n_{\max}$?

$$G_\uparrow(\tau) = \left(\sum_{n=0}^{\infty} \mathcal{J}_n(\tau)\right) \Big/ \left(\sum_{n=0}^{\infty} \mathcal{I}_n\right) \simeq \left(\sum_{n=0}^{n_{\max}} \mathcal{J}_n(\tau)\right) \Big/ \left(\sum_{n=0}^{n_{\max}} \mathcal{I}_n\right)$$



  - Let us approximate the noninteracting Green's function as $\mathcal{G}_\sigma(\tau) \simeq -1/2$.

$$\mathcal{G}_\sigma(\tau) \simeq -1/2 \quad \Rightarrow \quad \mathcal{I}_n = \frac{1}{n!}\left(\frac{\beta U}{4}\right)^n$$

proportional to the Poisson distribution with mean and variance $\dfrac{\beta U}{4}$.

$\wr\wr$

Gaussian distribution

  - One can obtain the accurate result by setting the maximum order as $n_{\max} \simeq \dfrac{\beta U}{4} + 3\sqrt{\dfrac{\beta U}{4}}$.

example. $\beta = 20,\ U = 5$

$$\frac{\beta U}{4} + 3\sqrt{\frac{\beta U}{4}} = 40 \quad \Rightarrow$$ Accurate result is expected when summing up to the 40th order.

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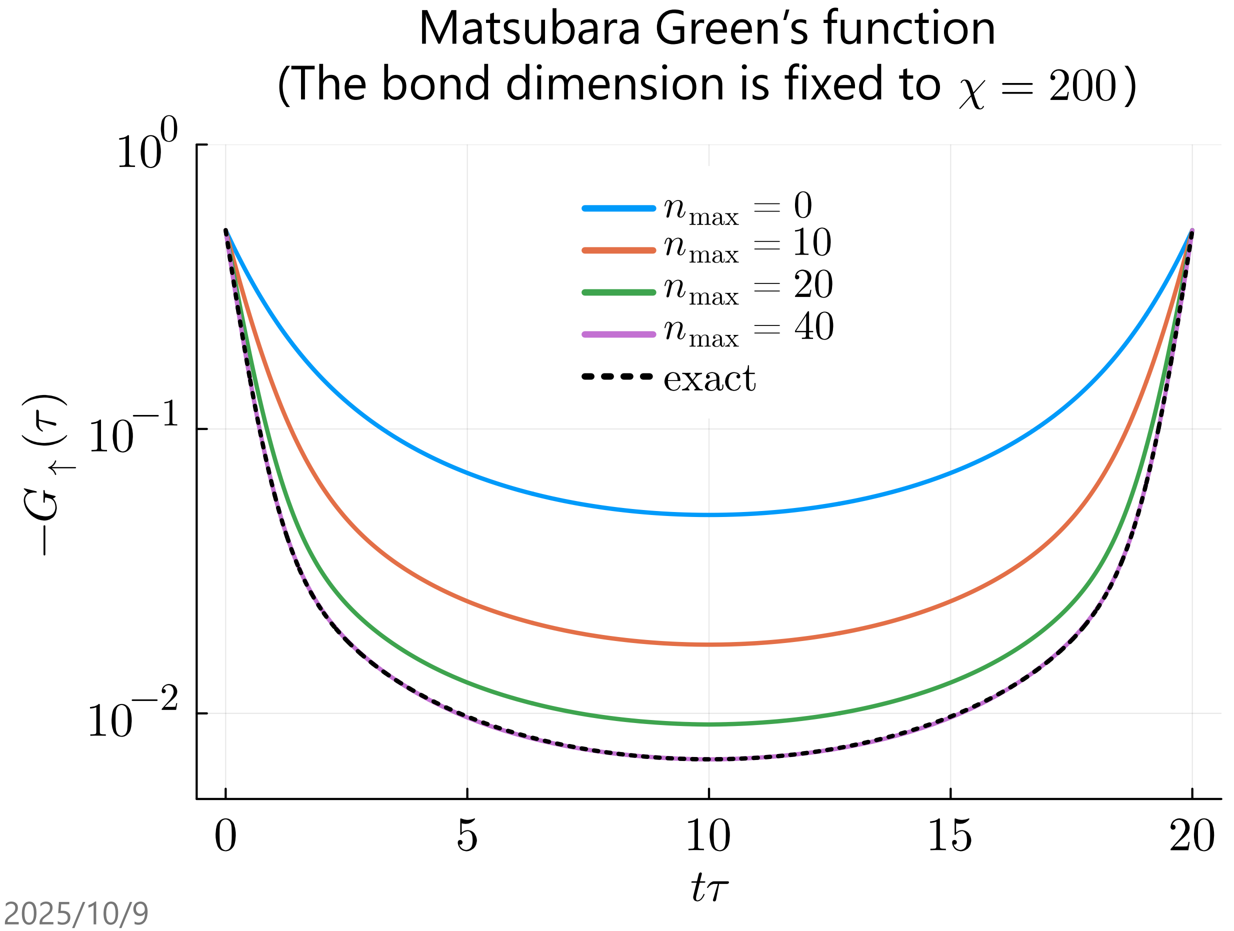
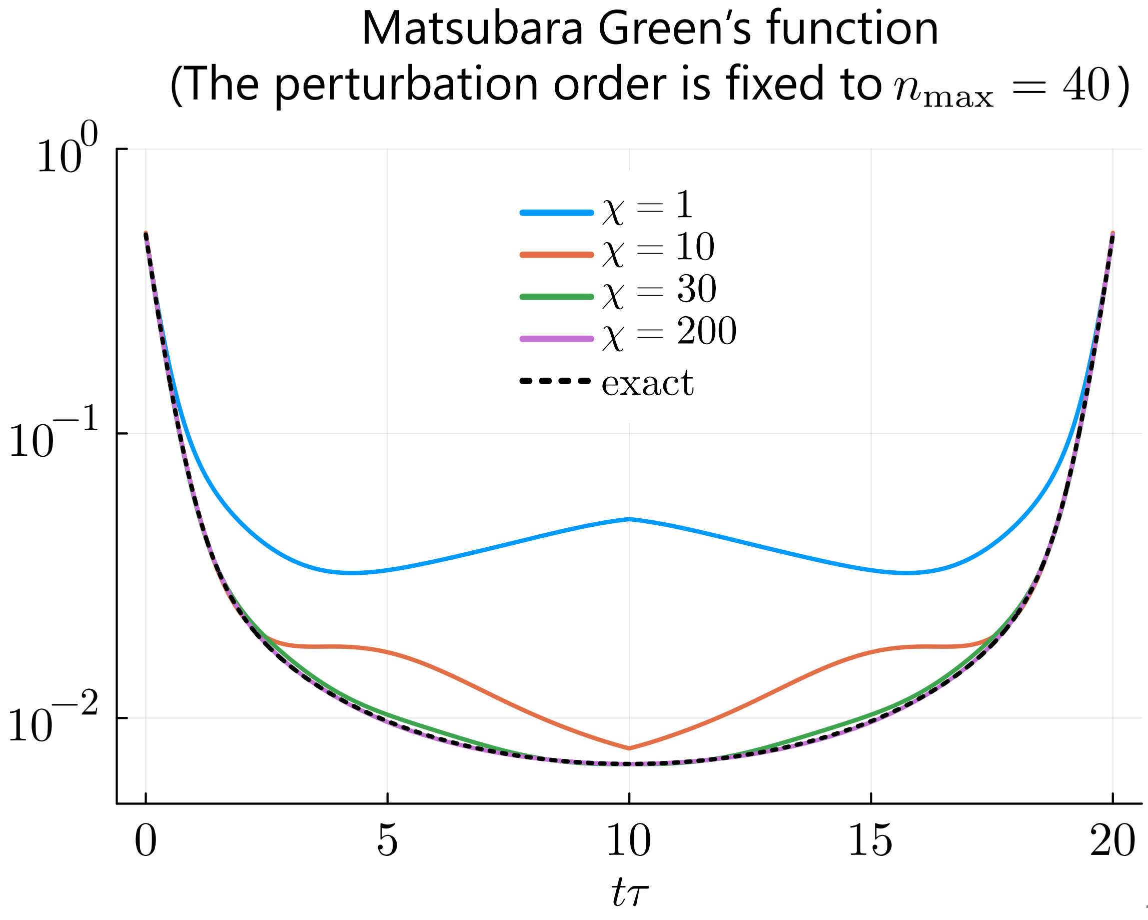
Exactly solvable impurity model

$$H = \sum_{\sigma} \varepsilon_\sigma c_\sigma^\dagger c_\sigma + U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) + \sum_{k,\sigma} \varepsilon_{k\sigma} b_{k\sigma}^\dagger b_{k\sigma} + \sum_{k,\sigma}(V_{k\sigma} b_{k\sigma}^\dagger c_\sigma + V_{k\sigma}^* c_\sigma^\dagger b_{k\sigma})$$ with $V_{k\downarrow} = 0$

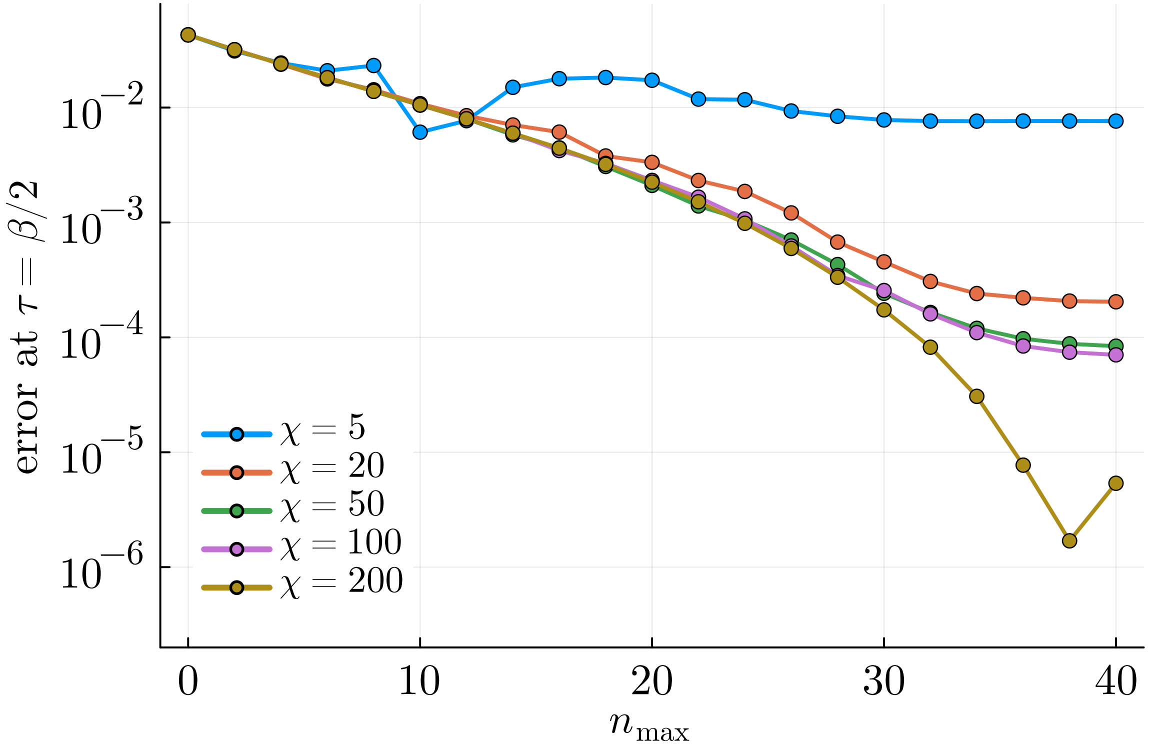
$\beta = 20,\ U = 5$

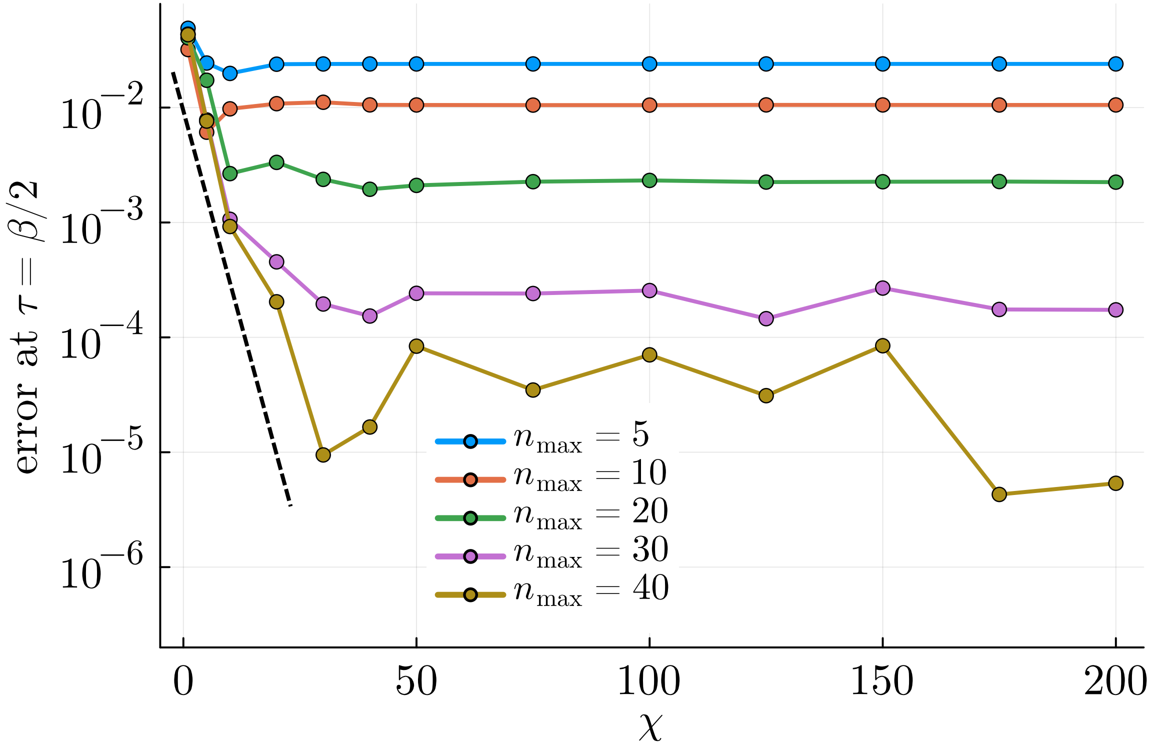




Exactly solvable impurity model

- Convergence



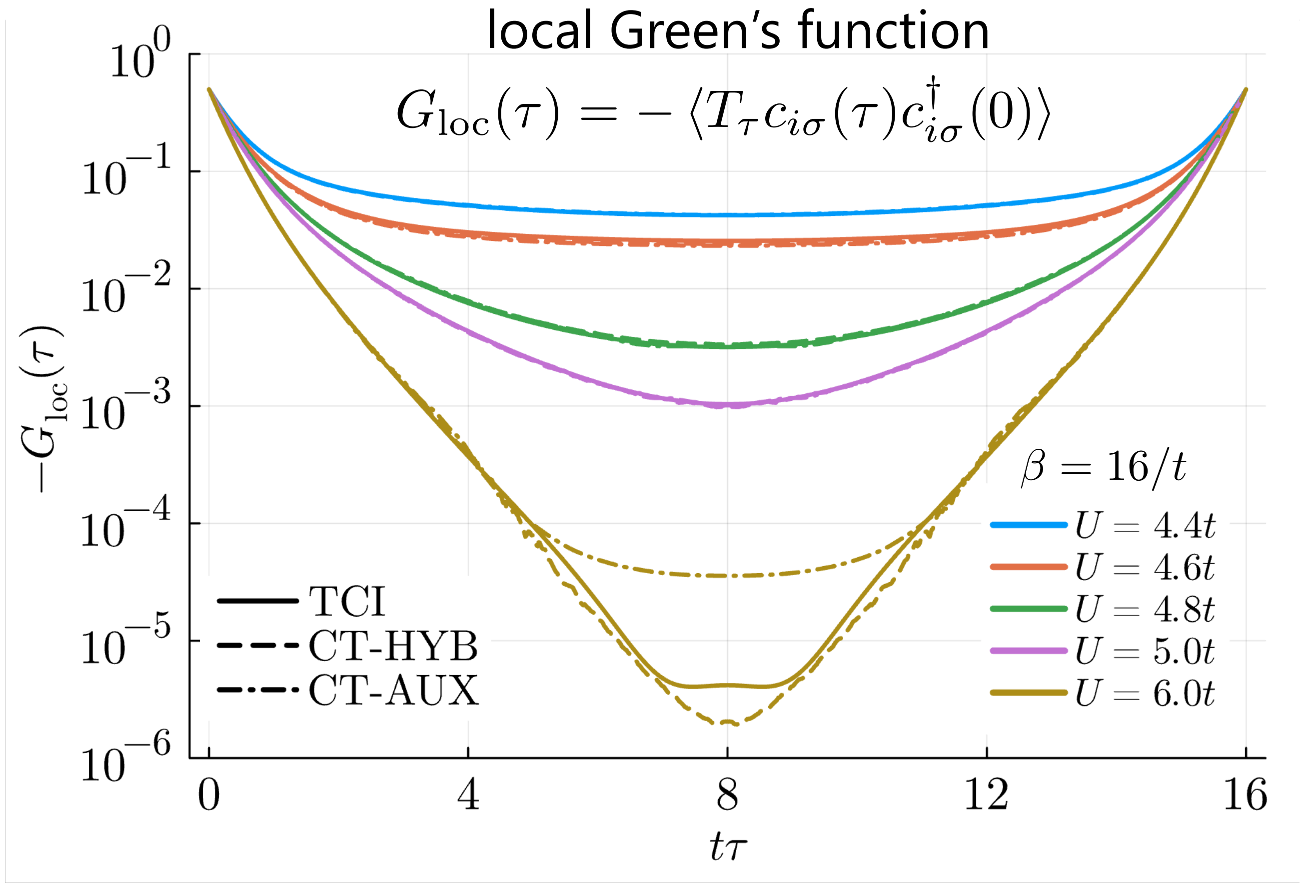


- If the bond dimension is high-enough, the error decreases as the maximum order become larger.
- The error decreases exponentially as we increase the bond dimension χ in the range of $1 \leq \chi \leq 20$.

➡ The integrand of the weak-coupling expansion has the low-rank structure.

DMFT for the Hubbard model

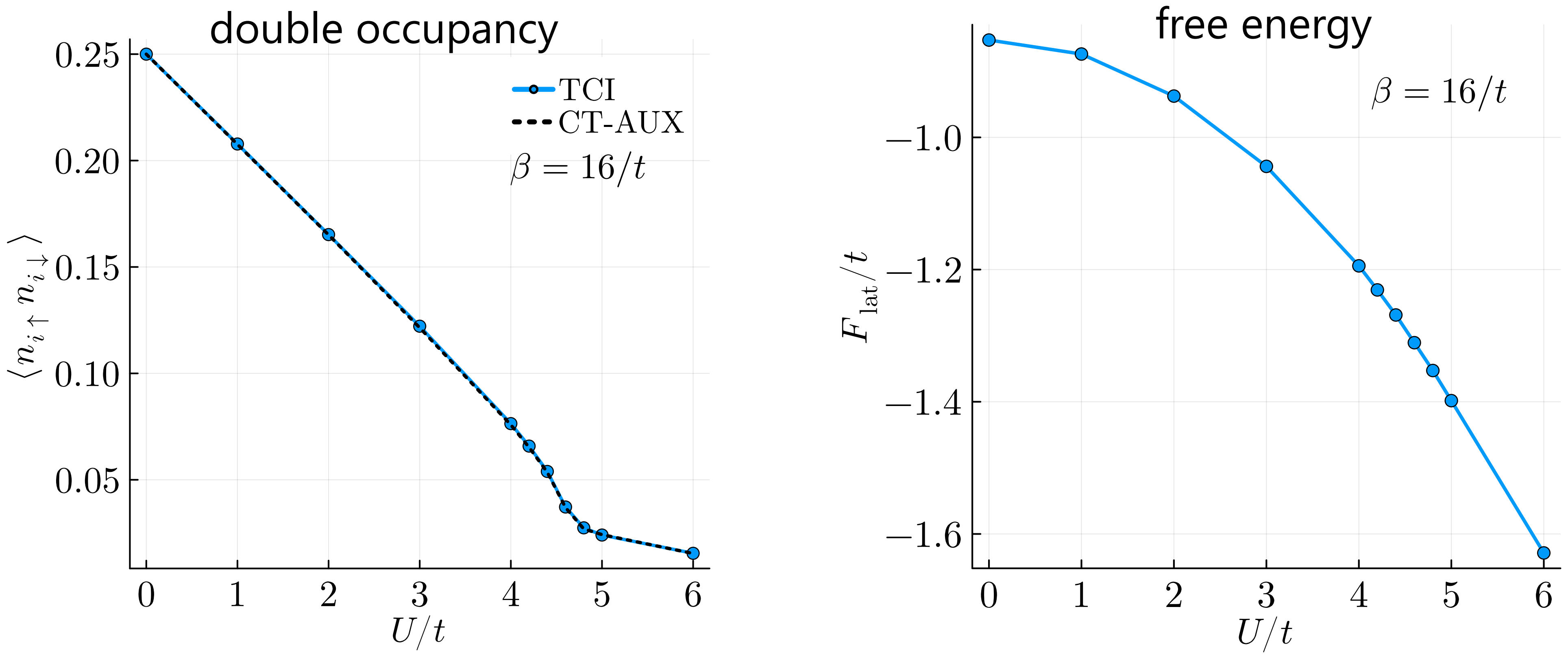
$H = -\frac{t}{\sqrt{z}} \sum_{\langle i,j \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + \sum_i U \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)$ on the Bethe lattice with the connectivity



- We first iterate the DMFT loops with $\chi = 50$.
- After that, we iterate additional loops with $\chi = 200$ to obtain the accurate result.

- Even in the strong-coupling regime, the TCI solver is able to reproduce the result by CT-QMC.

DMFT for the Hubbard model

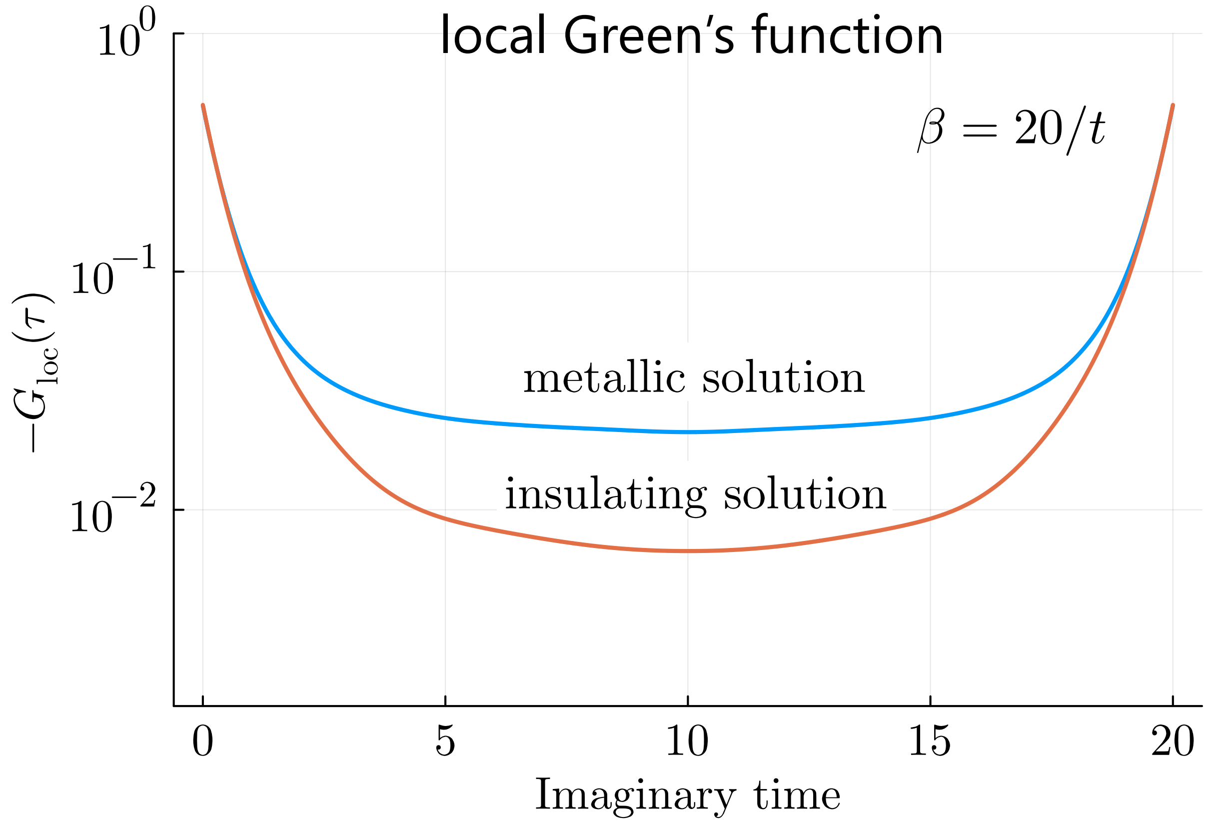


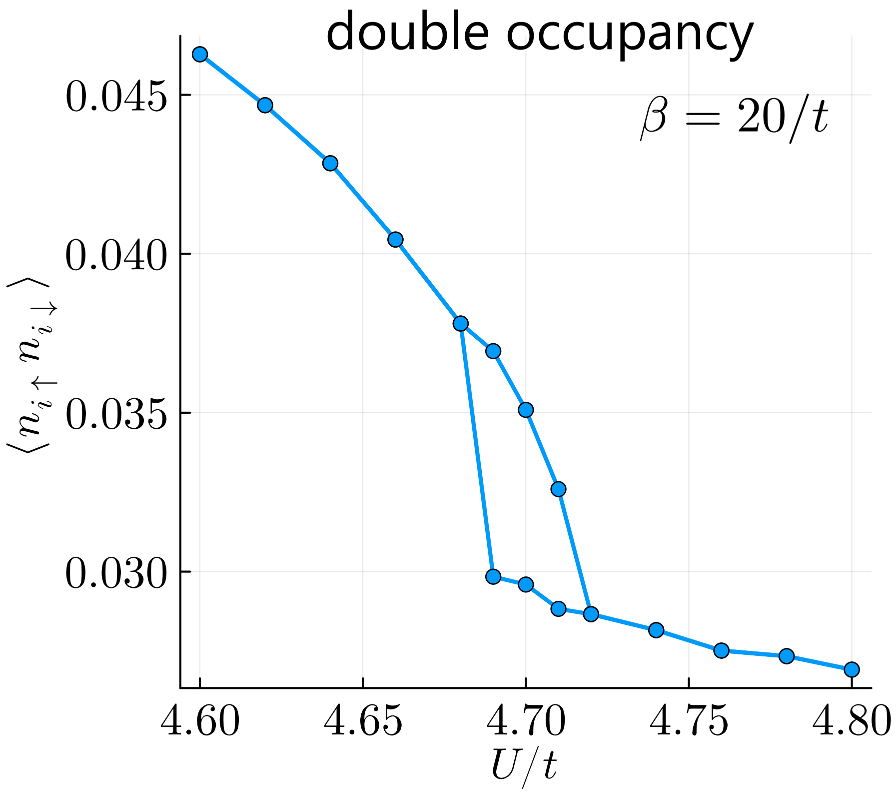
- The double occupancy and the free energy can be calculated directly with no additional cost.
  ($\longleftrightarrow$ CT-QMC methods have difficulty calculating the free energy.)

double occupancy: $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \frac{1}{4} - \frac{1}{\beta U} \left(\sum_{n=0}^{\infty} n \mathcal{I}_n \right) \Big/ \left(\sum_{n=0}^{\infty} \mathcal{I}_n \right)$

free energy: $F_{\text{lat}} = F_{0,\text{lat}} - \frac{1}{\beta} \ln \left(\sum_{n=0}^{\infty} \mathcal{I}_n \right)$

DMFT for the Hubbard model





- At low temperature, we can find two converged solutions and the hysteresis in the double occupancy.
- Weak-coupling expansion + TCI solver can explore the metal-to-insulator transition.

Why does the TCI approach work well?

$$\mathcal{I}_n = (-U)^n \int_{S_n^{0,\beta}} d\tau_1 \cdots d\tau_n \, P(\tau_1, \cdots, \tau_n) = (-U)^n \int_{[0,1]^n} dv_1 \cdots dv_n \, J_{h_n^{0,\beta}}(v_1, \cdots, v_n) P(h_n^{0,\beta}(v_1, \cdots, v_n))$$

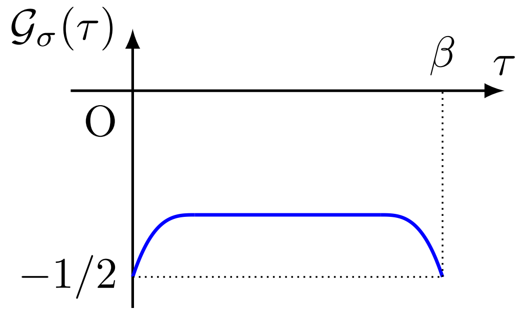
- The Jacobian can be analytically written down as $J_{h_n^{0,\beta}}(v_1, \cdots, v_n) = \beta^n (1-v_1)^{n-1}(1-v_2)^{n-2} \cdots (1-v_{n-1})$.

➡ The Jacobian $J_{h_n^{0,\beta}}(v_1, \cdots, v_n)$ is a separable function.

- In the strong-coupling regime, the Weiss field $\mathcal{G}_\sigma(\tau)$ typically shows a plateau over $0 \le \tau \le \beta$.

$$P(\tau_1, \cdots, \tau_n) \coloneqq (\det \boldsymbol{D}_n^{\uparrow})(\det \boldsymbol{D}_n^{\downarrow})$$

$$\boldsymbol{D}_n^{\sigma} = \begin{pmatrix} \mathcal{G}_\sigma(0^-) - 1/2 & \mathcal{G}_\sigma(\tau_1 - \tau_2) & \cdots & \mathcal{G}_\sigma(\tau_1 - \tau_n) \\ \mathcal{G}_\sigma(\tau_2 - \tau_1) & \mathcal{G}_\sigma(0^-) - 1/2 & \cdots & \mathcal{G}_\sigma(\tau_2 - \tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_\sigma(\tau_n - \tau_1) & \mathcal{G}_\sigma(\tau_n - \tau_1) & \cdots & \mathcal{G}_\sigma(0^-) - 1/2 \end{pmatrix}$$



➡ $P(\tau_1, \cdots, \tau_n) = P(h_n^{0,\beta}(v_1, \cdots, v_n))$ is almost constant over the hypercube.

- The integrand $J_{h_n^{0,\beta}}(v_1, \cdots, v_n) P(h_n^{0,\beta}(v_1, \cdots, v_n))$ is an almost separable function.

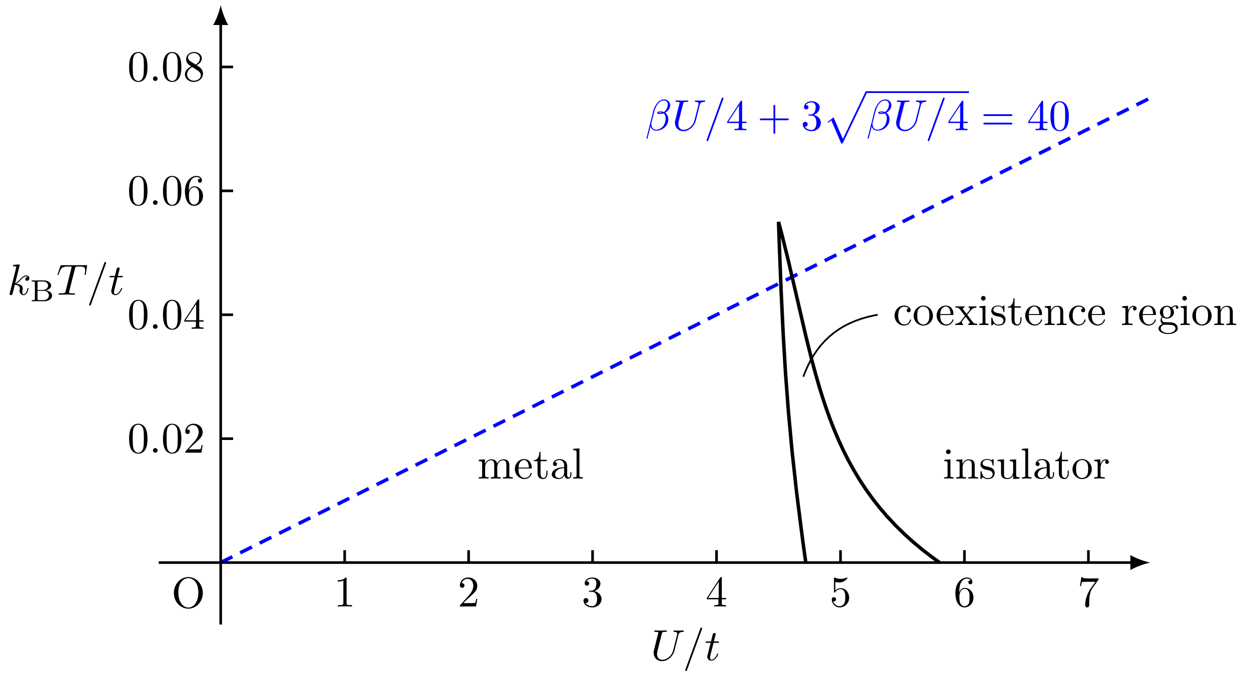
Current limitation

$$J_n(\tau) = (-U)^n \sum_{k=0}^{n} \int_{[0,1]^n} dv_1 \cdots dv_n \, J_{h_k^{0,\tau}}(v_1, \cdots, v_k; \tau) J_{h_{n-k}^{\tau,\beta}}(v_{k+1}, \cdots, v_n; \tau) \tilde{Q}(v_1, \cdots, v_n; \tau)$$

- The summands in $\sum_{k=0}^{n}$ can take both positive and negative values depending on k.

➡ Their cancellation leads to the loss of significance digits.

- The loss of significance leads to the violation of the condition $\mathcal{G}_\sigma(\tau) < 0 \ (0 < \tau < \beta)$ when $n_{\max} \gtrsim 40$.



Room for improvement

- The most time-consuming part of our algorithm is the evaluation of the Wick determinant.

$$\det\begin{pmatrix} \mathcal{G}_\sigma(\tau) & \mathcal{G}_\sigma(\tau-\tau_1) & \cdots & \mathcal{G}_\sigma(\tau-\tau_n) \\ \mathcal{G}_\sigma(\tau_1) & \mathcal{G}_\sigma(0^-)-1/2 & \cdots & \mathcal{G}_\sigma(\tau_1-\tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_\sigma(\tau_n) & \mathcal{G}_\sigma(\tau_n-\tau_1) & \cdots & \mathcal{G}_\sigma(0^-)-1/2 \end{pmatrix} \qquad \det\begin{pmatrix} \mathcal{G}_\sigma(0^-)-1/2 & \mathcal{G}_\sigma(\tau_1-\tau_2) & \cdots & \mathcal{G}_\sigma(\tau_1-\tau_n) \\ \mathcal{G}_\sigma(\tau_2-\tau_1) & \mathcal{G}_\sigma(0^-)-1/2 & \cdots & \mathcal{G}_\sigma(\tau_2-\tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_\sigma(\tau_n-\tau_1) & \mathcal{G}_\sigma(\tau_n-\tau_1) & \cdots & \mathcal{G}_\sigma(0^-)-1/2 \end{pmatrix}$$

- In the CT-QMC solver, the fast update algorithm allows us to calculate these determinants with a cost of $\mathcal{O}\left(n^2\right)$.
- In the TCI solver, we did not use such technique, and thus its cost is $\mathcal{O}\left(n^3\right)$.

- Can we implement the fast update algorithm for the TCI impurity solver?
- Naively thinking, it is difficult due to the variable transformation.
  - In CT-QMC, only a few numbers of entries in the matrix are updated at each Monte Carlo step.
  - In TCI, a variation in any single parameter v_i results in changes of all entries in the matrix.

Summary and outlook

- Summary
  - The integrands of the weak-coupling expansion of the Matsubara Green's function have low-rank structures.
  - The TCI impurity solver + DMFT enables us to study the metal-to-insulator transition.

  - A kind of sign problem which associated with the k-summation restricts the accessible parameter regime.
  - The fast update algorithm may accelerate the calculation.

- Outlook
  - Analyzing the system with a severe sign problem by TCI approach is an important direction.
    - nonequilibrium DMFT
    - cluster impurity problem
    - retarded interaction
    - spin-orbit coupled system