Continuous-time Quantum Monte Carlo (CTQMC) approach for quantum impurity problems in Tomonaga-Luttinger liquids

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Outline of this talk

- Introduction
  - Bosonization (for beginners)
  - CTQMC for fermionic systems

- CTQMC for Tomonaga-Luttinger liquid (TLL)
  - Kane-Fisher’s backscattering problem in a quantum wire
  - XXZ Kondo problem in a herical liquid

- Summary
Single impurity in a quantum wire

- even a single impurity in 1d has significant impact
  Kane&Fisher (1992)
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- Cutting the wire @T=0
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- Some numerical simulations have been done by Path-integral Monte Carlo
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- Most of the theoretical language is based on bosonization

- Some numerical simulations have been done by Path-integral
  Monte Carlo

- We try to construct algorithm of modern Continuous-time MC for
  quantum wires in a bosonization formulation

- Applied to strongly correlated electron systems combined with DMFT
- No negative sign problem [Werner (2006), Otsuki (2007)] for simple models
- Bosonic versions are also developed by Anders (2010), Otsuki (2012)

**CTQMC:** Infinite series of diagrams are summed efficiently

\[
\frac{Z}{Z_0} = \left\langle T_\tau \exp \left[ - \int_0^\beta d\tau H_1(\tau) \right] \right\rangle_0
\]

\[
Z_0 = \text{Tr} \ e^{-\beta H_0}
\]

\[
\langle A \rangle_0 = \frac{\text{Tr}(e^{-\beta H_0} A)}{Z_0}
\]

Werner et al. (2006)
CTQMC for impurity models

- Our purpose here is to develop a “bosonization” version of CTQMC in 1d TLL
CTQMC for impurity models

- Our purpose here is to develop a “bosonization” version of CTQMC in 1d TLL
  - Interaction in the bulk part is “exactly” treated by bosonization

Bosonization — 1d spineless fermion system \([-L/2, L/2]\)

\[
\psi_{L,R}(x) = \frac{1}{\sqrt{a}} F_{L,R} e^{-i \phi_{L,R}(x)}
\]

- \(a\) : cutoff
- \(F_L, F_R\) : Klein factor
CTQMC for impurity models

- Our purpose here is to develop a “bosonization” version of CTQMC in 1d TLL
  - Interaction in the bulk part is “exactly” treated by bosonization
  - It can be proven analytically there is no negative signs (low T: welcome!)

We will show that the CTQMC works very well in several models, as examples

Bosonization — 1d spineless fermion system [-L/2,L/2]

\[ \psi_{L,R}(x) = \frac{1}{\sqrt{a}} F_{L,R} e^{-i\phi_{L,R}(x)} \]

- \( a \): cutoff
- \( F_L, F_R \): Klein factor
Here, we just start letting you know our notations for bosonization, since one can easily be confused in almost all textbook of bosonization, when one studies it at first! (even experts sometimes make mistakes…)


Bosonization for beginners — refermionization for experts

Jan von Delft and Herbert Schoeller

“we hope that experts too might find useful our explicit treatment of certain subtleties that can often be swept under the rug, but are crucial for some applications, such as the calculation of $Q_{dos}(\omega)$ — these include the proper treatment of the so-called Klein factors”
Klein factors

Bosonization (a la Shankar)

\[
H = \frac{1}{2} \int_{-\infty}^{\infty} dx \left[ (\partial_x \phi_{Sha}(t, x))^2 + \Pi_{Sha}(t, x)^2 \right] = \partial_t \phi_{Sha}(t, x)
\]

\[
[\phi_{Sha}(t, x), \Pi_{Sha}(t, x')] = i \delta(x - x')
\]

\[
\psi_{\pm Sha}(t, x) = (2\pi a)^{-1/2} e^{\pm i \sqrt{4\pi} \phi_{\pm Sha}(t, x)}
\]

with

\[
\phi_{\pm Sha}(t, x) = \lim_{x_0 \to -\infty} \frac{1}{2} \left[ \phi_{Sha}(t, x) + \int_{x_0}^{x} dx' \Pi_{Sha}(t, x') \right]
\]

Anticommutation relations are reproduced without Klein factors.

When one consider, e.g., one-particle fermion Green’s function, the bosonization formula without Klein factors makes no sense.

Constructive bosonization:

\[
\psi_{L,R}(x) = \frac{1}{\sqrt{a}} F_{L,R} e^{-i\phi_{L,R}(x)}
\]

Note also \( F_\rho F_\rho \neq 1 \)

Shankar RMP (1994)

\[
\{ F_\rho, F_{\rho'}^\dagger \} = 2\delta_{\rho\rho'} \quad \quad F_\rho F_{\rho'}^\dagger = 1
\]

\[
\{ F_\rho, F_{\rho'} \} = 0, \quad \text{for } \rho \neq \rho'
\]

\( \phi_L \) and \( \phi_R \) are independent
Preparation: 1D TLL

Hamiltonian with interaction U:

\[ H_0 = H_L^0 + H_R^0 + H_U = \frac{\nu}{4} \int_{-L/2}^{L/2} \frac{dx}{2\pi} \left[ \frac{1}{g} \left( \partial_x \phi_-(x) \right)^2 + g \left( \partial_x \phi_+(x) \right)^2 \right] \]

\[ \phi_\pm(x) = \phi_L(x) \pm \phi_R(x) \quad \nu = \frac{\nu_F}{g} \quad g = \frac{1}{\sqrt{1 + 2U/\nu_F}} : \text{TL parameter} \]

We can define two left-moving bosons:

\[ \Phi_\pm(x) = \frac{1}{2\sqrt{2}} \left\{ \left( \frac{1}{\sqrt{g}} + \sqrt{g} \right) \left[ \phi_L(x) \mp \phi_R(-x) \right] \pm \left( \frac{1}{\sqrt{g}} - \sqrt{g} \right) \left[ \phi_L(-x) \mp \phi_R(x) \right] \right\} \]

Now, Hamiltonian consists of two independent left-moving bosons

\[ H_0 = \frac{\nu}{2} \int_{-L/2}^{L/2} \frac{dx}{2\pi} \left[ \left( \partial_x \Phi_+(x) \right)^2 + \left( \partial_x \Phi_-(x) \right)^2 \right] \]
One important formula is a multi-point correlator expression:

\[
\mathcal{A}^2 - \sum_i \frac{\lambda_i^2}{2} \langle T_\tau e^{i\lambda_1 \phi(\tau_1)} e^{i\lambda_2 \phi(\tau_2)} \cdots e^{i\lambda_N \phi(\tau_N)} \rangle = \left( \frac{2\pi}{L} \right)^{\frac{1}{2}} \left( \sum_{i=1}^{N} \lambda_i \right)^2 \prod_{i<j} \left( \frac{\beta}{\pi} \sin \left[ \pi T(|\tau_i - \tau_j| \pm a/v) \right] \right) \lambda_i \lambda_j
\]

For thermodynamic limit, neutral condition emerges:

\[
\sum_{i=1}^{N} \lambda_i = 0
\]

This expression serves as “Wick’s theorem” and will be extensively used in our CTQMC.

local boson field: \( \phi(\tau) = \phi(x = 0, \tau) \)

sign for cutoff is chosen as

\[+a/v \quad \text{for} \quad \tau_i - \tau_j \sim 0\]

\[-a/v \quad \text{for} \quad \tau_i - \tau_j \sim \beta\]
Fermionic CTQMC

Let us consider Kane-Fisher model for $g=1$ i.e., non-interacting wire

$$ H = H_0 + (\lambda_B \psi_L^\dagger(0) \psi_R(0) + \text{h.c.}) $$

A general term in perturbation series of $Z$ is

$$ \frac{Z}{Z_0} = \lambda_B^{2k} \int d\tau_1 \cdots d\tau_{2k} \left< T_\tau \psi_L^\dagger(\tau_1) \psi_R(\tau_1) \cdots \psi_R^\dagger(\tau_{2k}) \psi_R(\tau_{2k}) \right> $$

snap shot  $\rightarrow \lambda_B^{2k} \left< \psi_L^\dagger(\tau_1) \psi_L(\tau_2) \psi_L(\tau_3) \cdots \right> \left< \psi_R(\tau_1) \psi_R^\dagger(\tau_2) \psi_R^\dagger(\tau_3) \cdots \right> $

$= \lambda_B^{2k} \det \hat{G} \cdot \det (\hat{G}^T)$

$= \lambda_B^{2k} (\det \hat{G})^2 \rightarrow \text{“weight” for the snapshot configuration (=} \mathcal{W})$

Green’s func matrix: $\left( \hat{G} \right)_{ij} = G_0(\tau_i - \tau_j)$
Updates

Insertion

Metropolis

\[ R = \frac{W_{\text{new}}}{W_{\text{old}}} F \]

accept if

\[ \min(R, 1) > r, \quad 0 \leq r \leq 1 \]

deny otherwise

for insertion

\[ F = \frac{\beta^2}{(k+1)^2} \]

for removal

\[ F = \frac{k^2}{\beta^2} \]
Introduction

- bosonization (for beginners)
- CTQMC for fermonic systems

CTQMC for Tomonaga-Luttinger liquid (TLL)

- Kane-Fisher’s backscattering problem in a quantum wire
- XXZ Kondo problem in a herical liquid

Summary
We consider back scattering processes due to an impurity at \( x=0 \)

Impurity operator (we will consider):

- **Kane-Fisher model**
  \[
  \hat{X}_B = 1
  \]

- **XY-Kondo model in Helical TL liquid**
  \[
  \hat{X}_B = S^-
  \]

**XXZ-type**: always reduced to this form
We consider back scattering processes due to an impurity at x=0

\[
V = V_B + V_B^\dagger = \lambda_B \psi_L^\dagger(0) \psi_R(0) \hat{X}_B + \lambda_B^* \psi_R^\dagger(0) \psi_L(0) \hat{X}_B^\dagger,
\]

\[
= a^{g-1} \lambda_B F_L^\dagger F_R \left( a^{-g} e^{i\sqrt{2g}\phi_+} \right) \hat{X}_B + a^{g-1} \lambda_B^* F_R^\dagger F_L \left( a^{-g} e^{-i\sqrt{2g}\phi_+} \right) \hat{X}_B^\dagger
\]

\[
\equiv V_{\sqrt{2g}} \quad \equiv V_{-\sqrt{2g}}
\]

Here, we have defined

\[
\phi_\pm \equiv \phi_\pm(0) = g^{\mp\frac{1}{2}} \frac{1}{\sqrt{2}} \left[ \phi_L(0) \mp i \phi_R(0) \right]
\]

Only “+” boson appears in V “−” boson is decoupled and can be ignored

Impurity operator (we will consider):

Kane-Fisher model

\[
\hat{X}_B = 1
\]

XY-Kondo model in Helical TL liquid

\[
\hat{X}_B = S^-
\]

XXZ-type: always reduced to this form
\[ Z / Z_0 = \left\langle T_\tau \exp \left[ -\int_0^\beta d\tau H_1(\tau) \right] \right\rangle_0 \]

\[ \frac{(-1)^N}{N!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_N \langle T_\tau V_B(\tau_1) V_B^\dagger(\tau_2) \cdots V_B^\dagger(\tau_N) \rangle_0 \]

\[ \lambda_B(g) \equiv \alpha^{g-1} \lambda_B \]

\[ \lambda = \sqrt{2g} \quad \tau_i > \tau_{i+1} \quad = 1 \quad \text{calculable (}=1,0) \]

\[ \langle S^+ S^- S^+ S^- \cdots S^+ S^- \rangle \]

\[ s_{0ij} \equiv \frac{v\beta}{\pi} \sin \left[ \frac{\pi}{v\beta} (v|\tau_i - \tau_j| \pm a) \right] \]

\[ \lambda_{i,j} = \pm \sqrt{2g} \]

\[ a \quad \text{___} \quad \beta \\
0 \quad \text{_____} \quad -a \]
CTQMC in TLL

\[ Z/Z_0 = \langle T_\tau \exp \left[ - \int_0^\beta d\tau H_1(\tau) \right] \rangle_0 \]

\[ (\frac{(-1)^N}{N!}) \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_N \langle T_\tau V_B(\tau_1) V_B^\dagger(\tau_2) \cdots V_B^\dagger(\tau_N) \rangle_0 \]

\[ \longrightarrow |\lambda_B(g)|^{2k} \langle V_\lambda(\tau_1) \cdots V_{-\lambda}(\tau_{2k}) \rangle_b |F_L^\dagger F_R \cdots F_R^\dagger F_L\rangle_f \langle \hat{X}_B(\tau_1) \cdots \hat{X}_B^\dagger(\tau_{2k}) \rangle_{loc} \]

\[ \lambda = \sqrt{2g} \quad \tau_i > \tau_{i+1} \quad = 1 \]

\[ \langle S^+ S^- S^+ S^- \cdots S^+ S^- \rangle \]

\[ = |\lambda_B(g)|^{2k} \prod_{i<j}^{2k} \lambda_i \lambda_j > 0 \]

\[ \lambda_{i,j} = \pm \sqrt{2g} \]

• Weight is positive definite

\[ s_{0ij} \equiv \frac{v\beta}{\pi} \sin \left[ \frac{\pi}{v\beta} (v|\tau_i - \tau_j| \pm a) \right] > 0 \]
CTQMC in TLL

\[ N=2k \text{ order term in } Z/Z_0 = \left< T_\tau \exp \left[ -\int_0^\beta d\tau H_1(\tau) \right] \right>_0 \]

\[ \frac{(-1)^N}{N!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_N \left< T_\tau V_B(\tau_1)V_B^\dagger(\tau_2) \cdots V_B^\dagger(\tau_N) \right>_0 \]

\[ \longrightarrow \left| \lambda_B(g) \right|^{2k} \left< V_{\lambda}(\tau_1) \cdots V_{-\lambda}(\tau_{2k}) \right>_b \left< F_L^\dagger F_R \cdots F_R^\dagger F_L \right>_f \left< \hat{X}_B(\tau_1) \cdots \hat{X}_B^\dagger(\tau_{2k}) \right>_{\text{loc}} \]

\[ \lambda = \sqrt{2g} \quad \tau_i > \tau_{i+1} \quad = 1 \quad \text{calculable (}=1,0) \]

\[ \left< S^+ S^- S^+ S^- \cdots S^+ S^- \right> \]

\[ = \left| \lambda_B(g) \right|^{2k} \prod_{i<j}^{2k} s_{0ij} \longrightarrow \left| \lambda_B(g) \right|^{2k} \left| \det \hat{S} \right|^{2g} > 0 \quad \text{for } a \to 0 \]

\[ \lambda_{i,j} = \pm \sqrt{2g} \]

- **Weight is positive definite**
- **This simple form represents all the interaction effects in the bulk part**

\[ s_{0ij} \equiv \frac{v\beta}{\pi} \sin \left[ \frac{\pi}{v\beta} (v |\tau_i - \tau_j| \pm a) \right] > 0 \]

\[ [\hat{S}]_{lm} = -\text{sgn}(\tau_i^- - \tau_m^+) / s_{0lm} \]

\[ \tau^\pm : \tau \text{ for } \pm \lambda \]
Kane-Fisher model
Kane-Fisher model

Potential barrier for spin-less fermion in 1D

\[ H = H_0 + a^{g-1} \lambda_B F_L^\dagger F_R V_+ + a^{g-1} \lambda_B^* F_R^\dagger F_L V_- \]

Kane & Fisher PRL (1992)
Kane-Fisher model

Potential barrier for spin-less fermion in 1D

\[ H = H_0 + a^{g-1} \lambda_B F_L^\dagger F_R V_+ \lambda + a^{g-1} \lambda_B^* F_R^\dagger F_L V_- \lambda \]

RG eq.:

\[ \partial \lambda_B = (1 - g)\lambda_B \quad \lambda_B \to \infty \quad (g < 1) \]

Completely decoupled chains at low-energy for repulsive int. \( g < 1 \)

This model is intensively analyzed so far, here we will show

- electron Green’s function (1st numerically exact data in our knowledge)
- Conductance \( G \to 0 \) at \( T=0 \) (compare exact result @\( g=0.5 \) → check)

Both consistent with RG result.  

Kane & Fisher PRL (1992)
Electron Green’s functions

Fermion operator:

\[ \psi_L(x = 0) = \frac{1}{\sqrt{a}} F_L e^{-i\phi_L(x=0)} \]

\[ = a^{\frac{g}{4} + \frac{1}{4g} - \frac{1}{2}} \left( a^{-\frac{1}{4g}} e^{-i\sqrt{\frac{g}{2}}\Phi_-} \right) F_L \left( a^{-\frac{g}{4}} e^{-i\sqrt{\frac{g}{2}}\Phi_+} \right) \]

Green’s function:

\[ -G(\tau) = \langle T_\tau \psi_L(\tau, 0) \psi_L^\dagger(0, 0) \rangle \]

\[ = a^{\frac{g}{4} + \frac{1}{4g} - \frac{1}{2}} \langle T_\tau V_-^{-\frac{1}{\sqrt{2g}}} (\tau) V_-^{-\frac{1}{\sqrt{2g}}} (0) \rangle \langle T_\tau F_L V_+^{-\sqrt{\frac{g}{2}}} (\tau) F_L^\dagger V_+^{\sqrt{\frac{g}{2}}} (0) \rangle \]

\[ = a^{\frac{g}{4} + \frac{1}{4g} - \frac{1}{2}} \left[ \frac{1}{s(\tau)} \right]^{\frac{1}{2g}} \left[ -G^+(\tau) \right] \]

Direct sampling of \( G^+ \) (\( P_{ij} \): No. of vertices between \( i \) and \( j \) in a snapshot) @2nth order

\[ \mathcal{G}^{(2n)}_{i,j} = -\left\langle F_L(\tau_i) V_-^{\frac{g}{2}} (\tau_i) F_L^\dagger (\tau_j) V_+^{\frac{g}{2}} (\tau_j) \right\rangle_{MC} \]

\[ = \left\langle \left( -1 \right)^{P_{ij} s^{g}_{0ij}} \left| \frac{\det \hat{S}_n \oplus i j}{\det \hat{S}_n} \right|^{g} \right\rangle_{MC} \]

Indirect sampling (fast)

\[ \tilde{\mathcal{G}}^{(2k)}_{i,j} = \left\langle \left( -1 \right)^{P_{ij} s^{g}_{0ij}} \frac{\det \hat{S}_n \oplus i j}{|\lambda_B(g)|^2 s^{g}_{0ij}} \frac{\det \hat{S}_n}{\det \hat{S}_n} \right|^{g} \right\rangle_{MC} \]
Bench mark for $g=1$

Let us check the Green's function for non-interacting case ($g=1$)

Exact $G$ can be obtained via EOM as

$$G^+_{L,\text{ex}}(\tau) = \frac{[s(\tau)]^{-\frac{1}{2}}}{1 + \pi^2 \lambda_B^2 / v^2}$$

for $a \to 0$
Nontrivial part:

\[ G_L^+(\tau) = \langle F_L(\tau) \hat{\mathcal{V}} - \sqrt{\frac{g}{2}}(\tau) F_L(0) \hat{\mathcal{V}} \sqrt{\frac{g}{2}}(0) \rangle \Phi_+ \]

We found:

\[ G_L^+(\tau) \sim \tau^{-\frac{1}{2g}} \text{ for } \tau \to \infty \]

consistent with result by Furusaki (1997)

reflecting vanishing DOS \( \omega^{1/g-1} \) at \( x=0 \)
Universal function @ $T=0$

Green's function is expressed as

$$G_{L}^{+}(\tau) \approx [s(\tau)]^{-g/2} \mathcal{F}_{g}(T^* \tau, T/T^*)$$

$$T^* = \frac{v}{a} \left( \frac{\lambda_B}{\nu} \right)^{1/(1-g)}$$

Universal part has two obvious limits:

$$\mathcal{F}_{g}(x \to \infty, 0) \propto x^{(g-1/g)/2}$$

$$\mathcal{F}_{g}(x \to 0, 0) = 1$$

$T=0$ universal func. is drawn from our $T>0$ data by using data for $\tau/\beta < 1/6$
Green's function is expressed as

\[ G^+_L(\tau) \approx [s(\tau)]^{-g/2} \mathcal{F}_g(T^*\tau, T/T^*) \]

For \( T > 0 \), universal func. depends only \( T/T^* \).

This can be checked by examining data with fixed \( T/T^* \).

\[ T^* \tau = \frac{T^*}{T} \cdot \frac{\tau}{\beta} \]
Kubo formula:

\[ G(x, y) = \lim_{\omega \to 0} \frac{1}{\omega} \int dt e^{i\omega t} \langle [j(x, t), j(y, 0)] \rangle \Theta(t) \]

In the bosonization language, the current operator is:

\[ j(x, \tau) = \frac{ev}{2\pi} \partial_x (\phi_L(x, \tau) + \phi_R(x, \tau)) \]

In our basis @x=0,

\[ j(0, \tau) = i \frac{e\sqrt{g}}{\sqrt{2\pi}} \partial_\tau \Phi_+(\tau) \]

we can calculate G in our CTQMC

c.f., PIMC, Moon et al (1993),

There are some complicated things... about G in TLL wire:

\[ G = \frac{e^2 g}{h} \quad \text{or} \quad \frac{e^2}{h} \]

With leads:
Feed-back effect of interactions:
Kawabata (1996)

without leads: Apel-Rice (1982)
Conductance for $g=0.5$

For small cutoff $a$, results are consistent with the exact one by Kane&Fisher (1992)

$$
\frac{G}{G_0} = -\lim_{\omega \to 0} \frac{g}{\pi \omega} \text{Im} \left( D(i\omega_n) \bigg|_{i\omega_n \to \omega + i0} \right), \quad D(\tau) = -\langle T_\tau \partial_\tau \Phi_+(\tau) \partial_\tau \Phi_+(0) \rangle
$$

In CTQMC, $D(\tau)$ is calculated by

$$
-\mathcal{D}(\tau_l - \tau_m) = v^2 s_{0lm}^2 + (\pi T)^2 Q(\tau_l) Q(\tau_m)
$$

$$
Q(\tau) = \sum_{p=\pm,i} q_i^p(\tau) \cot \left[ \frac{\pi}{\beta} \left( |\tau - \tau_i^p| \pm \frac{a}{v} \right) \right]
$$

$$
q_i^\pm(\tau) = \pm \sqrt{2g} \text{ sgn}(\tau - \tau_i^\pm)
$$

Analytic continuation is done by fitting $D(i\omega_n)$ for low frequency by

$$
f(\omega_n) = a - b \omega_n + c \omega_n^2 + d \omega_n^2 \log(\omega_n)
$$
Helical Kondo problem
Impurities in a helical liquid

What kinds of impurities are interesting in a helical liquid (e.g., on the edge of 2d topological insulator)?

- Non-magnetic impurity (like Kane-Fisher): impossible due to TRS
  \( \sim u \psi_{\uparrow}^{\dagger}(0) \psi_{\downarrow}(0) \)

- Two-particle backward scattering: possible and relevant for \( g < 1/4 \)
  \( \sim u' \psi_{\uparrow}^{\dagger}(0) \psi_{\uparrow}^{\dagger}(a) \psi_{\downarrow}(a) \psi_{\downarrow}(0) \)

- Magnetic impurity: possible

Since general Kondo interactions are highly anisotropic due to the SO interaction (Eriksson et al., 2012), we here analyze a simpler XXZ model (Maciejko, 2012) by CTQMC

Wu et al., PRL (2006)
**Helical Kondo problem**

A magnetic impurity on the edge of 2d topological insulator (without Rashba term)

\[ H = H_0 + \lambda_F \sqrt{\frac{2}{g}} \partial_x \Phi_+(0) S^z + a^{-g} e^{i \sqrt{2g} \Phi_+} \lambda_B F_L^\dagger F_R S^- + a^{-g} \lambda_B^* F_R^\dagger F_L S^+ \]

Remove forward scattering term via

\[ U \equiv \exp \left[ i \frac{\sqrt{2g} \lambda_F}{gv} \Phi_+(0) S^z \right] \]

\[ U H U^\dagger = H_0 + a^{-1} \tilde{g} \lambda_B F_L^\dagger F_R S^- + a^{-1} \lambda_B^* F_R^\dagger F_L S^+ \]

Now, exponent is shifted:

\[ \sqrt{2\tilde{g}} \equiv \sqrt{2g} (1 - \lambda_F / gv) \]

\[ \lambda_F = gv : \text{decoupled point (dP)} \]

Maciejko PRB (2012)
Interactions:

\[ V = \frac{J^z a}{\sqrt{2g}} \partial_x \Phi_+(0) S^z + \frac{J^\pm a^g}{2} \left( F'^{\dagger}_L F' R V_\lambda S^- + F'^{\dagger}_R F' L V_{-\lambda} S^+ \right) \]

2nd order perturbation for partition func. (only \( S^z \) terms shown):

\[-(J^\pm)^2 \frac{a^{2g}}{4} \int_0^\infty d\tau_1 \int_0^{\tau_1} d\tau_2 \left\langle \left( V_\lambda(\tau_1) V_{-\lambda}(\tau_2) - V_{-\lambda}(\tau_1) V_\lambda(\tau_2) \right) S^z \right\rangle \]

OPE:

\[ V_\lambda(z) V_{-\lambda}(z') \sim \frac{1}{(z-z'+a)^2} + \lambda \frac{\partial_x \Phi(z)}{(z-z'+a)^2 - 1} + \ldots \]

Thus, we have effective interaction correction to \( J^z \) as

\[-g(J^\pm)^2 \frac{a \Delta \tau}{\sqrt{2g}} \int_0^\infty d\tau_1 \left\langle \partial_x \Phi(\tau_1) S^z \right\rangle \]

1-loop RG eqs. are given as (with adding trivial part):

\[ \partial_l J^\pm = (1-g) J^\pm + \rho J^\pm J^z, \]

\[ \partial_l J^z = \rho g J^{\pm 2}. \]
Exchange up and down local spin indices:

\[ S^z \rightarrow -S^z, \ S^\pm \rightarrow S^\mp \]

Then, Hamiltonian reads,

\[
UHU^\dagger \rightarrow H_0 + \left[ a^{g-1} \lambda_B F_L^\dagger F_R \left( a^{-g} e^{-i\sqrt{2g(\lambda_F/gv-1)\Phi_+}} \right) S^+ + h.c. \right]
\]

Equivalent

\[
\frac{\lambda_F}{gv} \quad \leftrightarrow \quad (2 - \frac{\lambda_F}{gv})
\]

Trajectories based on Anderson-Yuval-Hamann’s method
Spin-spin correlations

Sampling transverse spin-spin correlations is similar to that of G in Kane-Fisher model

\[ \chi^{+-}(\tau_{ij}) \equiv \langle T_{\tau} \hat{S}^+ (\tau_i) \hat{S}^- (\tau_j) \rangle \]

but note that we are in a transformed system:

\[ \hat{U} \hat{S}^\pm \hat{U}^\dagger = e^{\pm i \sqrt{2g} \lambda_F/(gv) \Phi_+(0)} \hat{S}^\pm \]

Indirect sampling of transverse spin susceptibility:

\[ \chi^{+-}(\tau) = \frac{1}{\beta} \left\langle \sum_{ij}^k \mathcal{M}_{ij} \left[ \delta(\tau - \tau_{ij}) + \delta(\beta + \tau_{ij} - \tau) \right] \right\rangle \]

with

\[ \mathcal{M}_{ij} = \frac{a^2 g (\frac{\lambda_F}{gv})^2}{|\chi_B'|^2} \left[ S(\tau_{ij}) \right] - \frac{2 \lambda_F}{v} \left| \frac{\det \hat{S}_{k-1} \{ \tau \ominus \tau_{ij}^- , \tau_{ij}^+ \}}{\det \hat{S}_k \{ \tau \}} \right|^{2g'} \]

\[ g' = g - \frac{\lambda_F}{v} \]

direct sampling of longitudinal spin susceptibility:

\[ \chi^z(\tau_i - \tau_j) = \frac{\langle S^\pm(\tau_1) \cdots S^z(\tau_i) \cdots S^z(\tau_j) \cdots \rangle}{\langle S^\pm(\tau_1) \cdots \cdots \rangle} \]
Phase diagram

Phase boundary is well described by RG calculation (Maciejko, 2012)

SC: screened phase ("strong coupling")
LM: local-moment phase (Ferro Kondo)

Typical T-dependence of spin correlation:

\[ g = 0.3 \]
\[ \lambda_F = -0.5 \quad (LM) \]
\[ \beta = 800, 1600, 3200, 6400 \]

\[ \lambda_F = -0.2 \quad (SC) \]
"Strong-coupling" Fixed Point

Dynamical impurity spin-spin correlations

\[ g_{ij}^{(2k)} = a^2 g^2 (\frac{\lambda F}{g})^2 |\lambda_B'(g)|^{-2} [s_{0ij}]^{-2} |\hat{S}_{ji}|^{-2} (g - \frac{\lambda F}{g}) \]

\[ \lambda_B'(g) = \lambda_B a^g (1 - \frac{\lambda F}{g})^2 - 1 \]

\( \lambda_B = \lambda_F = 0.2, \ a = 1 \)

\( \beta = 3200 \)

\[ g = 0.3 \]
\[ g = 0.5 \]
\[ g = 0.7 \]
\[ g = 1 \]

dotted lines: \( \sim \tau^{2g} \)

\[ \frac{1}{\tau^{2g}} : \text{The exponent is precisely the exponent @ dP} \]

\[ \frac{1}{\tau^2} : \text{dP+ perturbation ; dP@g=0.2} \]

Spin susceptibility \( \chi^\perp \propto \frac{1}{T^{1-2g}} \) diverges for \( g < 1/2 \), log corrections for \( g = 1/2 \)
Spin susceptibility

\[ \chi_0(\tau) \equiv \langle O(\tau)O(0) \rangle \sim \tau^{-2\Delta_0} \]

in our case, \( \Delta_0 = g \) for \( \chi^\perp \)

\[ \chi_0(T) = \int_0^\beta d\tau \chi_0(\tau) \sim T^{2\Delta_0-1} \]

\[ \chi_0(T) \sim -\ln T \quad \text{for} \quad \Delta_0 = \frac{1}{2} \]
Summary

- CTQMC applied to TLL successfully **without negative sign** in several models (also applicable to other models → future studies).

- **Kane-Fisher model**
  - Green’s functions for all TL parameters $g$
  - Confirmed approx. exponent $1/(2g)$ by Furusaki (1997)
    
    $$G_L^+(\tau) \sim \tau^{-1/2g}$$
  - Conductance is also calculable

- **Helical Kondo model**
  - Phase diagram
    
    $$\chi^- \sim \tau^{-2g}, \ \chi^z \sim \tau^{-2}$$
  - Spin-spin correlation functions
Other applications

❖ Two-particle backward scattering problem

✶ Almost the same as Kane-Fisher model
✶ But there needs a special care for electron Green’s func.

❖ Topological Kondo problem(s)

✶ Majorana fermions in SC island coupled with leads
✶ negative-sign free CTQMC is applicable (with odd-order perturbations present)
Two-particle backward scattering problem

\[ H = H_0 + a^{2g-1} \lambda_B (F_L^\dagger F_R)^2 V_\lambda + a^{2g-1} \lambda_B (F_R^\dagger F_L)^2 V_{\lambda^c} \]
\[ \sim H_0 + 2 a^{2g-1} \lambda_B \cos(\lambda \Phi_+) \]

RG eq.:
\[ \partial \lambda_B = (1 - 4g) \lambda_B \]
\[ \lambda_B \rightarrow \infty \quad (g < 1/4) \]

Kane & Fisher PRB (1992)

Completely decoupled chains at low-energy for \( g < 1/4 \)

Is this the full story? & Is there any quantitative difference from Kan-Fisher model?

There is a difference in electron Green’s function!, which is closely related to Klein factors
Green’s function

Let us consider “fermion sign” in G, i.e. Klein factor part

For any terms in perturbation series, we have something like

\[ F_L(\tau)[(F_{L,R}^\dagger F_{R,L})^q \cdots]F_L^\dagger(\tau = 0) \quad q = 1(KFM), \ 2(2PBM) \]

For even No. of vertices in [ ]:

\[ \rightarrow (-1)^p F_L(\tau)[(F_{L,R}^\dagger)^n(F_{R,L})^n]F_L^\dagger(\tau = 0) \rightarrow (-1)^p [(F_{L,R}^\dagger)^n(F_{R,L})^n] \]

For odd No. of vertices in [ ]:

\[ \rightarrow (-1)^p F_L(\tau)[(F_{L,R}^\dagger)^n(F_{R,L})^n(F_{L,R}^\dagger F_{R,L})^q]F_L^\dagger(\tau = 0) \]
\[ \rightarrow (-1)^{p+q} [(F_{L,R}^\dagger)^n(F_{R,L})^n] \]

Note: there is no time dependence in Klein fac.

This clearly indicates difference in the two models

\* No sign in 2-particle backscattering model

\[ \langle T\tau \psi_L(\tau) \psi_L^\dagger(0) \rangle = \langle T\tau e^{-i\sqrt{g/2}\Phi}(\tau)e^{i\sqrt{g/2}\Phi}(0) \rangle \]
\[ \sim \langle e^{-i\sqrt{g/2}\Phi}(0) \rangle \langle e^{i\sqrt{g/2}\Phi}(0) \rangle \quad \text{i.e., no Klein fac.} \]

Finite value remains
Topological Kondo problems

- Robust (~topologically protected) NFL is realized (SO(M) sym.)

- As for CTQMC, no negative sign, but we need to introduce an update operation with cyclic three vertices insertion/removal or equivalent ones.

\[
H = -i \sum_{j=1}^{M} \int_{-\infty}^{\infty} dx \, \psi_j^{\dagger}(x) \partial_x \psi_j(x) + \sum_{j \neq k} \lambda_{jk} \gamma_j \gamma_k \psi_k^{\dagger}(0) \psi_j(0)
\]
Numerical results

5.5.1 \( g = 1 \) case

Figure 1 shows \( \tau \) dependence of \( G_{LL}(\tau) \) for several values of \( \lambda_B \) and \( a \). One can see that the deviations between numerical results and exact one become smaller and smaller as \( a \) decreases. Note also that the results by two methods for calculating \( G_{LL} \) is consistent with each other for all the parameters.

Figure 2 shows distribution of perturbation order \( P(n) \) in the MC samplings. The peak position of \( P(n) \) scales to \( \propto \beta \lambda_B / a \). This (evidently) means, cases for low \( T \), strong coupling, and smaller cutoff, require heavy calculations.
Check SU(2) symmetry for $g=1$

$\lambda_B = \lambda_F = 0.2$, $a = 0.5$

$\beta = 200$

$\beta = 3200$
For small $g$, we succeeded to get the strong-coupling fixed point. But, numerical difficulty appears when we approach $g=1$ for isotropic case.
Effects of cutoff in LM phase

Config. includes many \( \tau_1 \sim a \), which affects SU(2) symmetry: finite cutoff effect

\[
s_{0ij} \equiv \frac{v\beta}{\pi} \sin \left[ \frac{\pi}{v\beta} (v|\tau_i - \tau_j| \pm a) \right]
\]

"data.dat" u 1:2:3
"data.dat" u 1:4:5
"data_fm.dat" u 1:2:3
"data_fm.dat" u 1:4:5
\( \pi \cdot 0.125/200 \)
Decoupled-point Hamiltonian

\[ UHU^\dagger = H_0 + \frac{\lambda_B}{a} \left[ F_L^\dagger F_R S^- + \text{h.c.} \right] \]

\[
\begin{pmatrix}
0 & h & \cdots & \cdots \\
-h & 0 & \cdots & \cdots \\
\vdots & \vdots & \ddots & \cdots \\
\cdots & \cdots & \cdots & 0
\end{pmatrix}
\]

\[
(-1)^{N_R} \begin{pmatrix}
0 & h & \cdots & \cdots \\
-h & 0 & \cdots & \cdots \\
\vdots & \vdots & \ddots & \cdots \\
\cdots & \cdots & \cdots & 0
\end{pmatrix}
\]

\[ |N_R \ N_L; \uparrow > \]

\[ |N_R+1 \ N_L-1; \uparrow > \]

\[ |N_R \ N_L; \downarrow > \]

\[ |N_R-1 \ N_L+1; \downarrow > \]

\[ UHU^\dagger = H_0 + \frac{\lambda_B}{a} (S^+ + S^-) \quad h = \frac{\lambda_B}{a} \]
Decoupled point

@ $\lambda_F = g v$

$$UHU^\dagger = H_0 + \frac{\lambda_B}{a} \left[ F_L^\dagger F_R S^- + \text{h.c.} \right] \Rightarrow UHU^\dagger = H_0 + \frac{\lambda_B}{a} (S^+ + S^-)$$

Klein Factors play no role

Spin-spin correlations are trivial ($T=0$):

$$\chi_{+ -}^{d\text{FP}} = \langle T^\tau S^+ (\tau) S^- (0) \rangle_{d\text{FP}} = \frac{1}{4} (1 + e^{-2h\tau})$$

$$\chi_{zz}^{d\text{FP}} = \langle T^\tau S^z (\tau) S^z (0) \rangle_{d\text{FP}} = \frac{1}{4} e^{-2h\tau}$$

In the original language ($T=0$):

$$US^{\pm} U^\dagger = e^{\pm \sqrt{2g} \Phi} + S^{\pm} \quad US^z U^\dagger = S^z$$

$$\chi_{+ -} = \langle T^\tau S^+ (\tau) S^- (0) \rangle = \frac{1}{4} (1 + e^{-2h\tau}) \left( \frac{a}{\nu \tau} \right)^{2g}$$

$$\chi_{zz} = \langle T^\tau S^z (\tau) S^z (0) \rangle = \frac{1}{4} e^{-2h\tau}$$

Maciejko PRB (2012)
Perturbations from decoupled FP

\[ U \delta V U^\dagger = \delta \lambda_F \sqrt{\frac{2}{g} \partial_x \Phi_+(0) S^z} = \delta \lambda_F \sqrt{\frac{1}{2g} \partial_x \Phi_+(0) (\tilde{S}^+ + \tilde{S}^-)} \]

change quantization axis

\[ \delta \lambda_F = \lambda_F - g\nu. \]

\[ \delta \chi_{zz}^{dFP}(\tau) : \text{power-low decay appears in two diagrams} \]

\[ \langle T_\tau \partial_x \Phi_+(\tau_1) \partial_x \Phi_+(\tau_2) \rangle \]

\[ \tilde{S}^-(\tau), \tilde{S}^+(\tau_1), \tilde{S}^-(\tau_2), \tilde{S}^+(0) \]

\[ \sim \tau^{-2} \]

\[ \delta \chi_{zz}^{dFP}(\tau) \sim \frac{a^2 \delta \lambda_F^2}{16g\nu^2\lambda_B^2} \frac{1}{\tau^2} \]

\[ \delta \chi_{+-}^{dFP}(\tau) : \text{stronger decay than the fixed point susceptibility, i.e., not important} \]
Notations

\[ 2\sqrt{\pi} \phi_{\text{Maciejko}} = \phi_L - \phi_R \]
\[ \frac{J_{\perp,\text{Maciejko}} a_{\text{Maciejko}}}{2\pi \xi} = \frac{\lambda_B}{a} \]
\[ 2\sqrt{\pi} \Pi_{\text{Maciejko}} = \partial_x (\phi_L + \phi_R) \]
\[ \rightarrow \sqrt{\frac{2}{g}} \partial_x \Phi_+(0) \quad (x \rightarrow 0) \]

\[ S^\pm_{\text{Maciejko}} = S^\mp, S^z_{\text{Maciejko}} = -S^z \]
\[ \rho_{\text{Maciejko}} J_{z,\text{Maciejko}}^{d\text{FP}} = 2K = \frac{2\lambda_F}{v} \]
consistent with ours

\[ \frac{J_{z,\text{Maciejko}} a_{\text{Maciejko}}}{\sqrt{\pi}} \times \frac{1}{2\sqrt{\pi}} \sqrt{\frac{2}{g}} (-1) = \lambda_F \sqrt{\frac{2}{g}} \]
\[ J_{z,\text{Maciejko}} a_{\text{Maciejko}} = 2\pi \lambda_F \]

\[ \rho_{\text{Maciejko}} J_{z,\text{Maciejko}}^{*,\pm} = 2(K \pm \sqrt{K}) = 2\pi \lambda_F \rho / a = \frac{2\lambda_F}{v} \]
\[ \lambda_{F,\pm} / v = (g \pm \sqrt{g}) \]
Details of $G$'s

\[
G^{(2n)}_{i>j} = - \langle T_\tau F_L (\tau_i) V_{-\lambda} (\tau_i) F^\dagger (\tau_j) V_{-\lambda} (\tau_j) \hat{P}_{2n} \rangle / \delta Z_{2n}
\]

\[
= - \frac{\langle V_{\lambda_1} (\tau_1) \cdots V_{-\lambda} (\tau_i) \cdots V_{\lambda} (\tau_j) \cdots V_{\lambda_2n} (\tau_{2n}) \rangle + \langle F^\dagger \rangle \langle F^\dagger \rangle \langle F \rangle \langle F \rangle \cdots \langle F \rangle \langle F \rangle \langle \tau_{2n} \rangle}{\langle V_{\lambda_1} (\tau_1) \cdots V_{\lambda_2n} (\tau_{2n}) \rangle + \langle F^\dagger \rangle \langle F^\dagger \rangle \langle F \rangle \langle F \rangle \cdots \langle F \rangle \langle F \rangle \langle \tau_{2n} \rangle}.
\]

\[
= - \frac{\langle V_{\lambda_1} (\tau_1) \cdots V_{-\lambda} (\tau_i) \cdots V_{\lambda} (\tau_j) \cdots V_{\lambda_2n} (\tau_{2n}) \rangle + \langle F_L (\tau_i) F_L^\dagger (\tau_j) F^\dagger \rangle \langle F^\dagger \rangle \langle F \rangle \langle F \rangle \cdots \langle F \rangle \langle F \rangle \langle \tau_{2n} \rangle }{\langle V_{\lambda_1} (\tau_1) \cdots V_{\lambda_2n} (\tau_{2n}) \rangle + \langle F^\dagger \rangle \langle F^\dagger \rangle \langle F \rangle \langle F \rangle \cdots \langle F \rangle \langle F \rangle \langle \tau_{2n} \rangle} (-1)^{P_{ij}}
\]

\[
\lambda = \sqrt{\frac{g}{2}}
\]

\[
\lambda_1, \ldots, \lambda_{2n} = \pm \sqrt{2g}
\]
Details of G's

\[ G_{i>\ j}^{(2n)} = -\langle T_\tau F_L(\tau_i)V_{-\lambda}(\tau_i)\hat{F}_\tau(\tau_i)V_{\lambda}(\tau_i)\hat{F}_{2n}/\delta Z_{2n} \]

\[ = -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_{\lambda}(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle} + \frac{\langle F_{\star}^\dagger F_{\star}(\tau_1)\cdots F_L(\tau_i)\cdots F_{\star}^\dagger F_{\star}(\tau_{2n})\rangle}{\langle F_{\star}^\dagger F_{\star}(\tau_1)\cdots F_{\star}(\tau_{2n})\rangle} \]

\[ G_{i>\ j}^{(2n)} = -(-1)^{P_{ij}} \frac{\prod_{\alpha>\gamma}^{2n+i+j} \lambda_\alpha \lambda_\gamma}{\prod_{\alpha'>\gamma'}^{2n} \lambda_{\alpha'} \lambda_{\gamma'}} \]

\[ = -(-1)^{P_{ij}} s_{0ij}^{-\lambda_2} \prod_\gamma s_{0i\gamma}^{-\lambda_\lambda_\gamma} \prod_\alpha s_{0\alpha j}^{\lambda_\lambda_\alpha} \]

\[ \lambda_\alpha > 0 \quad \lambda_\alpha < 0 \]

\[ i \rightarrow \lambda_\alpha = t^a \]
Details of G’s

\[G_{i>\cdot j}^{(2n)} = -\langle T^\tau F_L(\tau_i) V^-_\lambda(\tau_i) F^\dagger(\tau_j) V^-_\lambda(\tau_j) \hat{P}_{2n} \rangle / \delta Z_{2n} \]

\[= -\frac{\langle V^-_\lambda(\tau_1) \cdots V^-_\lambda(\tau_i) \cdots V^-_\lambda(\tau_j) \cdots V^-_\lambda(\tau_{2n}) \rangle}{\langle V^-_\lambda(\tau_1) \cdots V^-_\lambda(\tau_{2n}) \rangle + \langle F^\dagger F^\dagger(\tau_1) \cdots F^\dagger F^\dagger(\tau_j) \cdots F^\dagger F^\dagger(\tau_{2n}) \rangle} \frac{\langle F^\dagger F^\dagger(\tau_1) \cdots \cdots F^\dagger F^\dagger(\tau_{2n}) \rangle}{\langle F^\dagger F^\dagger(\tau_1) \cdots \cdots F^\dagger F^\dagger(\tau_{2n}) \rangle} \cdot (-1)^{P_{ij}} \]

\[G_{i>\cdot j}^{(2n)} = -(-1)^{P_{ij}} s_{0ij}^{-\lambda^2} \prod_{\alpha}>\gamma s_{0\alpha\gamma} x_{\alpha} \lambda_{\gamma} \]

\[= -(-1)^{P_{ij}} s_{0ij}^{-\lambda^2} \prod_{\gamma} s_{0\gamma}^{-\lambda_{\gamma}} \prod_{\alpha} s_{0\alpha}^{\lambda_{\alpha}} \]

\[= -(-1)^{P_{ij}} s_{0ij}^{g} \left( \frac{\prod_{\alpha}>\gamma s_{0\alpha\gamma}^{w_\alpha w_\gamma}}{\prod_{\alpha}>\gamma s_{0\alpha\gamma}^{w_\alpha w_\gamma}} \right) \frac{g}{\prod_{\alpha}>\gamma s_{0\alpha\gamma}^{w_\alpha w_\gamma}} \]

\[= -(-1)^{P_{ij}} s_{0ij}^{\frac{g}{2}} \left( \frac{\prod_{\alpha}>\gamma s_{0\alpha\gamma}^{w_\alpha w_\gamma}}{\prod_{\alpha}>\gamma s_{0\alpha\gamma}^{w_\alpha w_\gamma}} \right)^{g} \left( \frac{\det \hat{S}_{n+i}}{\det \hat{S}_{n}} \right)^{g} \]

\[\lambda = \sqrt{\frac{g}{2}} \]

\[\lambda_1, \ldots, \lambda_{2n} = \pm \sqrt{2g} \]

\[w_\alpha, w_\gamma = \text{sgn}(\lambda_\alpha), \text{sgn}(\lambda_\gamma)\]
Basic algorithm of CTQMC

To be specific, let us consider Anderson model [Werner (2006)]

"Non-interacting" part:

\[ H_0 = H_c + H_f \]

\[ H_c = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} \]

\[ H_f = \epsilon_f \sum_{\sigma} n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow} \]

"perturbation" part:

\[ H_1 = \sum_{\sigma} H_{1\sigma}, \quad H_{1\sigma} = v c^\dagger_\sigma f_\sigma + \text{h.c.} \]

Only even-order terms survive \((n=2k)\), and these are something like...

\[ (-)^{2k} \langle H_1(\tau_1) \cdots \rangle = \pm v^{2k} \langle c^\dagger_1(\tau_1) c^\dagger_2(\tau_2) c^\dagger_3(\tau_3) \cdots c^\dagger_{n\uparrow}(\tau_{n\uparrow}) \rangle_{\uparrow,\uparrow} \]

\[ \times \langle f^\dagger_1(\tau_1) f^\dagger_2(\tau_2) f^\dagger_3(\tau_3) \cdots \rangle_f \]

\[ = \pm v^{2k} \det \hat{G}_{\uparrow} \det \hat{G}_{\downarrow} \langle f^\dagger_1(\tau_1) f^\dagger_2(\tau_2) f^\dagger_3(\tau_3) \cdots \rangle_f \equiv W \]

\[ \cdot \cdot \cdot \text{Wick's theorem} \]

\[ \cdot \cdot \cdot \text{"weight" for the config.} \]

\[ \text{with} \quad n_{\uparrow} + n_{\downarrow} = 2k \]
Green’s function matrix:

\[
\left[ \hat{G}_{c\uparrow} \right]_{ij} = \left\langle c_{\uparrow}^{\dagger}(\tau_{2i-1}) c_{\uparrow}(\tau_{2j}) \right\rangle = G_{c\uparrow}^{0}(\tau_{2j} - \tau_{2i-1}) : \text{free electron Green’s function}
\]

Matrix products for local degrees of freedom:

\[
\left\langle f_{\uparrow}(\tau_1) f_{\uparrow}^{\dagger}(\tau_2) f_{\downarrow}(\tau'_1) \cdots \right\rangle_f = \exp\{-\epsilon_f(l_{\uparrow} + l_{\downarrow}) - U l_{\text{doublon}}\} / Z_f
\]

\[
Z_f = 1 + 2e^{-\beta \epsilon_f} + e^{-\beta(2\epsilon_f + U)}
\]

“Segment” representation:

\[\tau = \beta\quad \text{imaginary-time config.}\]

\[\tau = 0\]
Update operations

(i) Insert a vertex pair
(ii) Remove a vertex pair
(iii) Shift a vertex

calculate ratio: \( R = \frac{W_{\text{new}}}{W_{\text{old}}} F \)

accept if \( \min(R, 1) > r, \ 0 \leq r \leq 1 \)

deny otherwise (Metropolis)

\( R \) = empirically positive for Anderson model

\( F \): config. dep.

for (i) and (ii)

\( F = 1 \) for (iii)