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

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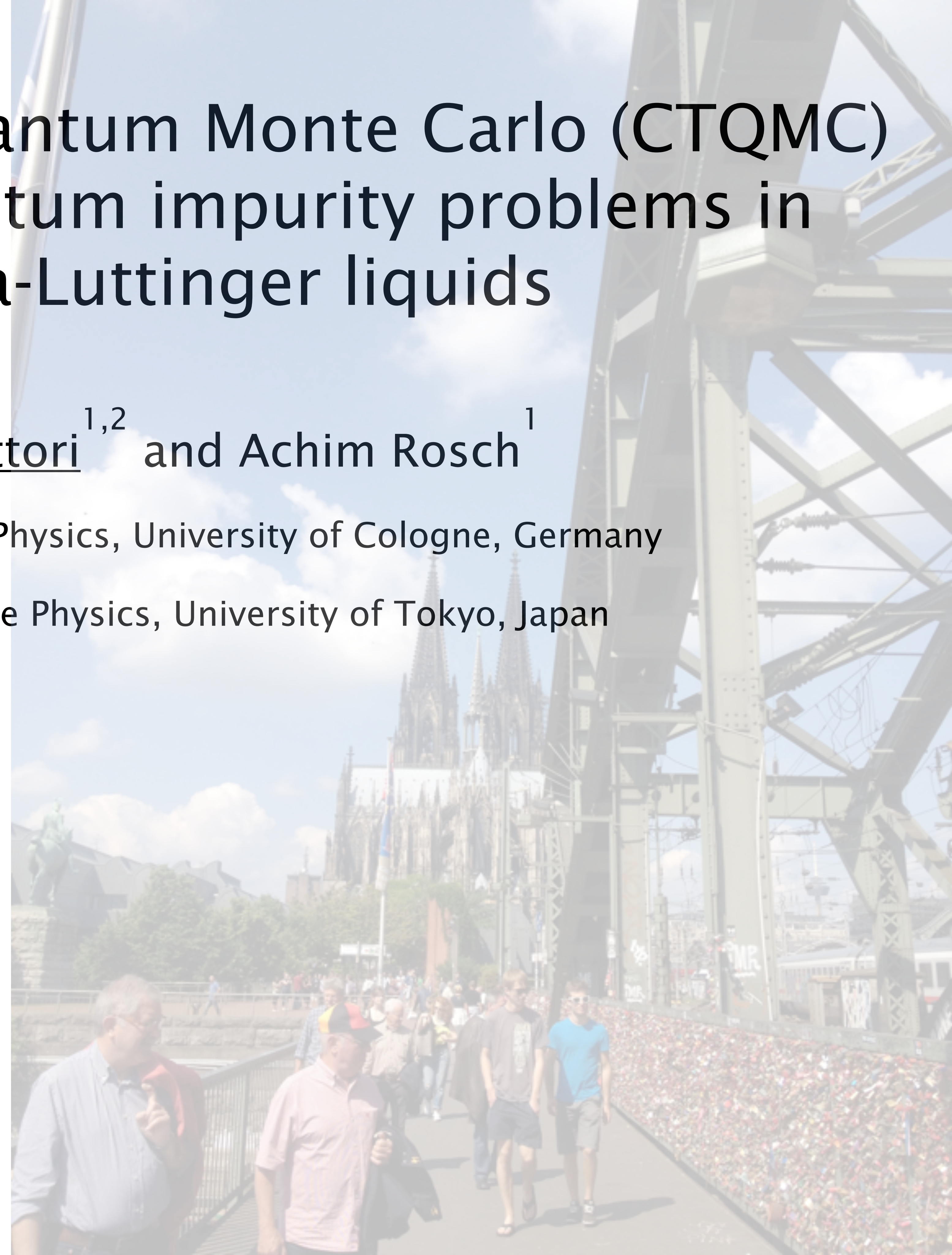
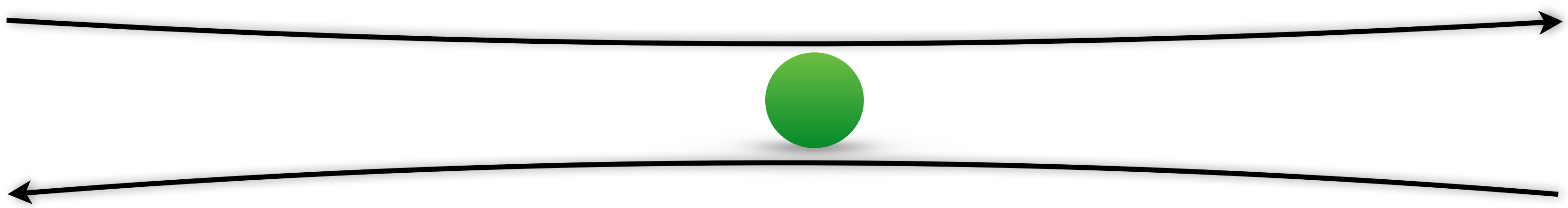


Outline of this talk

- Introduction
  - Bosonization (for beginners)
  - CTQMC for 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

Single impurity in a quantum wire

- even a single impurity in 1d has significant impact
  Kane&Fisher (1992)



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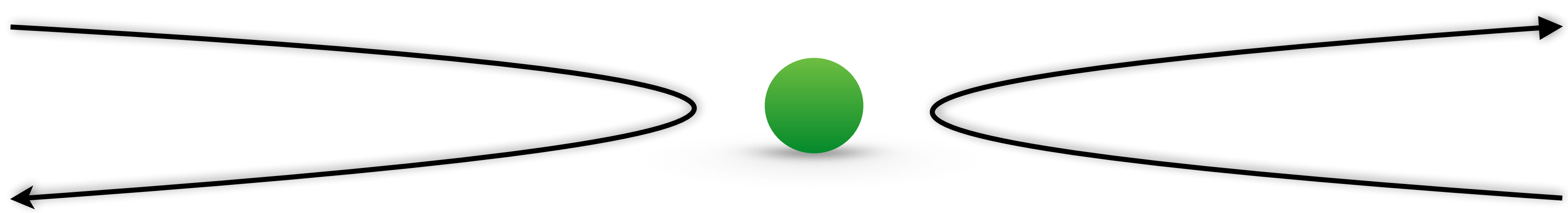

- Cutting the wire @T=0

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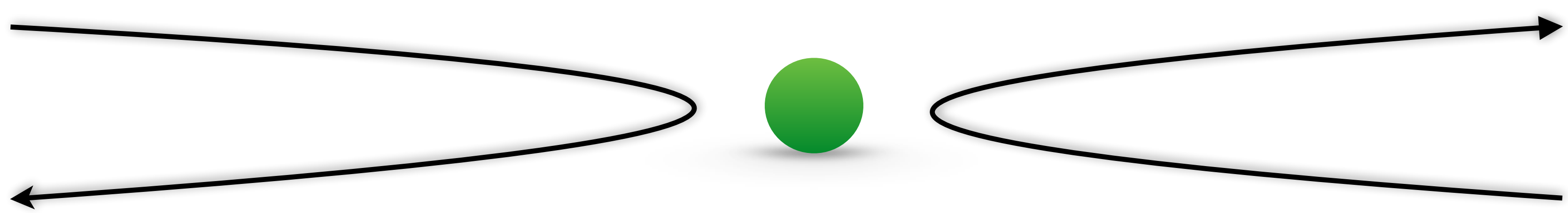

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- most of the theoretical language is based on bosonization

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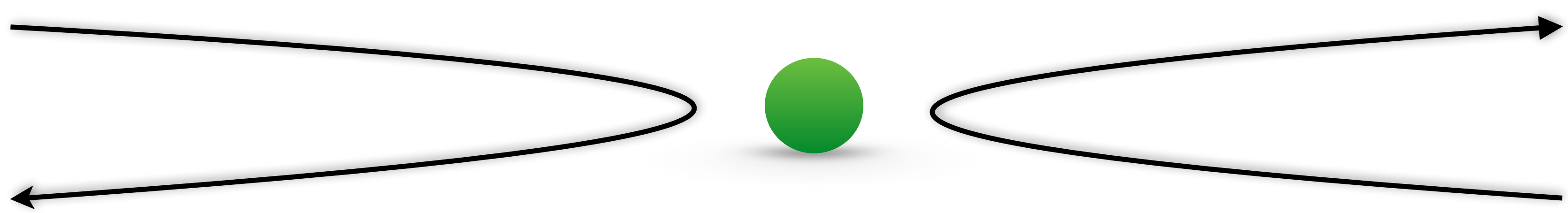

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- Some numerical simulations have been done by Path-integral Monte Carlo   Moon et al (1993), Leung et al (1995), Hamamoto et al (2008)

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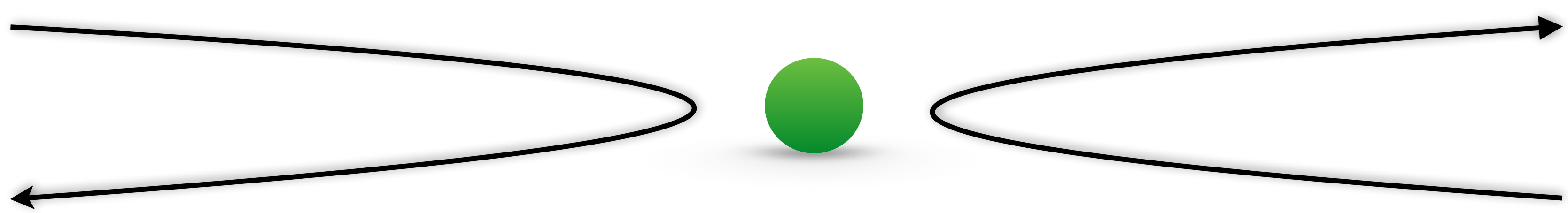


- Cutting the wire @T=0
- most of the theoretical language is based on bosonization
- Some numerical simulations have been done by Path-integral Monte Carlo   Moon et al (1993), Leung et al (1995), Hamamoto et al (2008)
- We try to construct algorithm of modern Continuous-time MC for quantum wires in a bosonization formulation

CTQMC for impurity models

see, a review: Gull et al (2011)

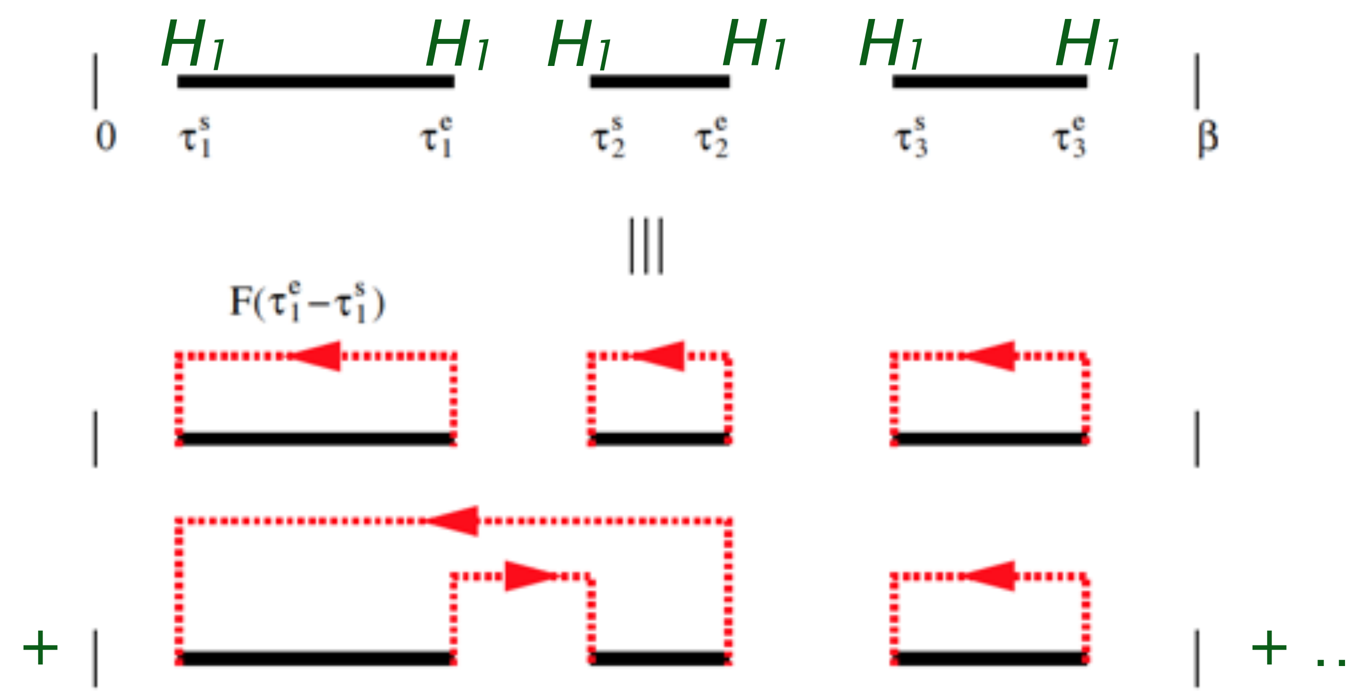
- CTQMC for impurity problems: Rubtsov (2005), Werner (2006), Otsuki (2007)
- Applied to strongly correlated electron systems combined with DMFT
- No negative sign problem [Werner (2006), Otsuki (2007)] for simple models
- Bosonic versions are also developed by Anders (2010), Otsuki (2012)

CTQMC: Infinite series of diagrams are summed efficiently

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

$$Z_0 = \mathrm{Tr}\ e^{-\beta H_0}$$

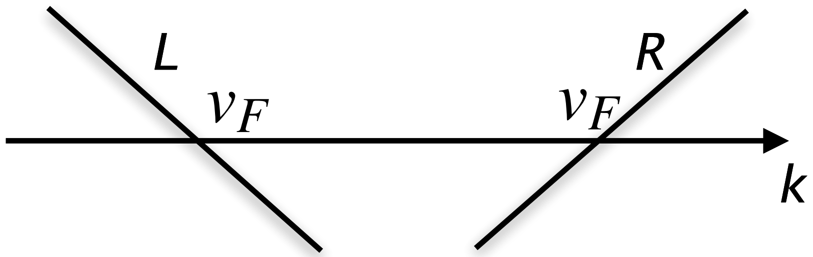
$$\langle A \rangle_0 = \frac{\mathrm{Tr}(e^{-\beta H_0} A)}{Z_0}$$



Werner et al.(2006)

CTQMC for impurity models

- Our purpose here is to develop a "bosonization" version of CTQMC in 1d TLL

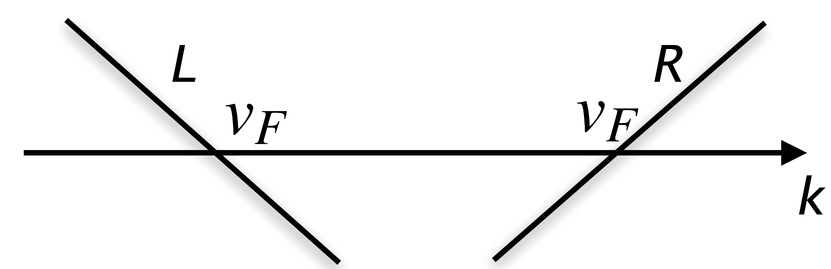


CTQMC for impurity models

- 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

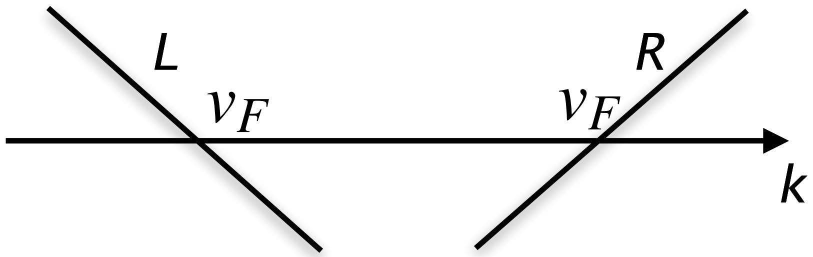
CTQMC for impurity models

- 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]

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



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Bosonization

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…)

Ann. Phys. (Leipzig) **7** (1998) 4, 225 – 306

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 $\varrho_{dos}(\omega)$ – these include the proper treatment of the so-called Klein factors"

Klein factors

Bosonization (*a la* Shankar)

Shankar RMP (1994)

$$H = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}x \left[(\partial_x \phi_{\mathrm{Sha}}(t,x))^2 + \Pi^2_{\mathrm{Sha}}(t,x) \right]$$

$$\Pi_{\mathrm{Sha}}(t,x) \equiv \partial_t \phi_{\mathrm{Sha}}(t,x)$$

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

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

with $\phi_{\pm\mathrm{Sha}}(t,x) \equiv \lim_{x_0\to-\infty} \frac{1}{2}\left[\phi_{\mathrm{Sha}}(t,x) \mp \int_{x_0}^{x} \mathrm{d}x'\, \Pi_{\mathrm{Sha}}(t,x') \right]$

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:

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

$$\{F_\rho, F^\dagger_{\rho'}\} = 2\delta_{\rho\rho'} \qquad F_\rho F^\dagger_\rho = 1$$

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

Note also $F_\rho F_\rho \neq 1$

ϕ_L and ϕ_R are independent

Preparation: 1D TLL

Hamiltonian with interaction U:

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

$$\phi_\pm(x) = \phi_L(x) \pm \phi_R(x) \qquad v = \frac{v_F}{g} \qquad g = \frac{1}{\sqrt{1+2U/v_F}}$$: 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

$$H_0 = \frac{v}{2}\int_{-L/2}^{L/2}\frac{dx}{2\pi} : \left[\Big(\partial_x\Phi_+(x)\Big)^2 + \Big(\partial_x\Phi_-(x)\Big)^2\right] :$$

Multi-point correlator

One important formula is a multi-point correlator expression:

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

$$= \prod_{i<j}\left(\frac{\beta}{\pi}\sin\left[\pi T(|\tau_i-\tau_j| \pm a/v)\right]\right)^{\lambda_i\lambda_j}$$

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

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

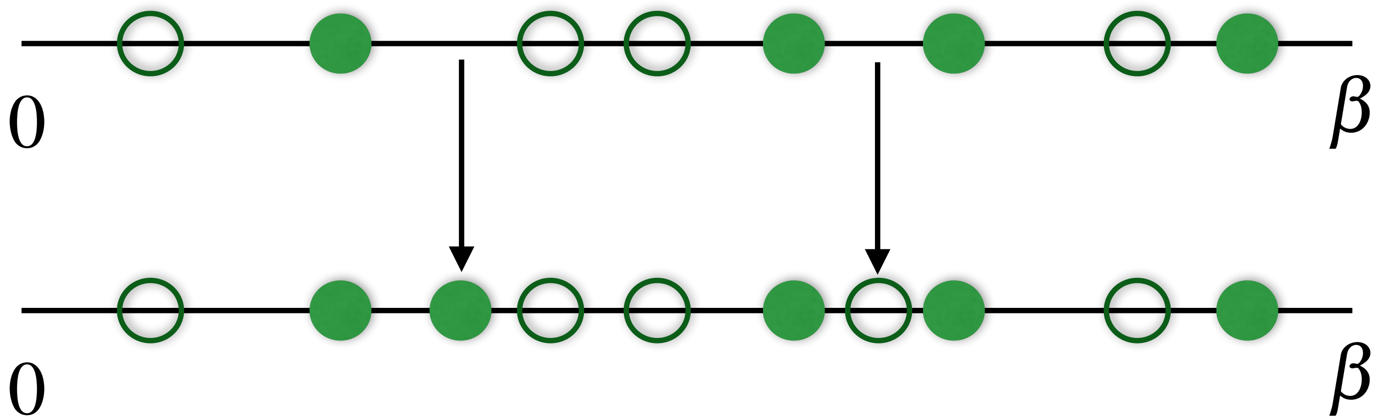
A general term in perturbation series of Z is

$$\begin{aligned}
\frac{Z}{Z_0} &= \lambda_B^{2k} \int_{\tau_1>\tau_2>\cdots>\tau_{2k}} d\tau_1 \cdots d\tau_{2k} \left\langle T_\tau \psi_L^\dagger(\tau_1)\psi_R(\tau_1)\cdots\psi_R^\dagger(\tau_{2k})\psi_R(\tau_{2k})\right\rangle \\
\text{snap shot} &\rightarrow \lambda_B^{2k} \left\langle \psi_L^\dagger(\tau_1)\psi_L(\tau_2)\psi_L(\tau_3)\cdots\right\rangle \left\langle \psi_R(\tau_1)\psi_R^\dagger(\tau_2)\psi_R^\dagger(\tau_3)\cdots\right\rangle \\
&= \lambda_B^{2k} \det\hat{G}\cdot\det\left(\hat{G}^T\right) \\
&= \lambda_B^{2k}\left(\det\hat{G}\right)^2 \quad \text{—> “weight” for the snapshot configuration (= } W\text{)}
\end{aligned}$$

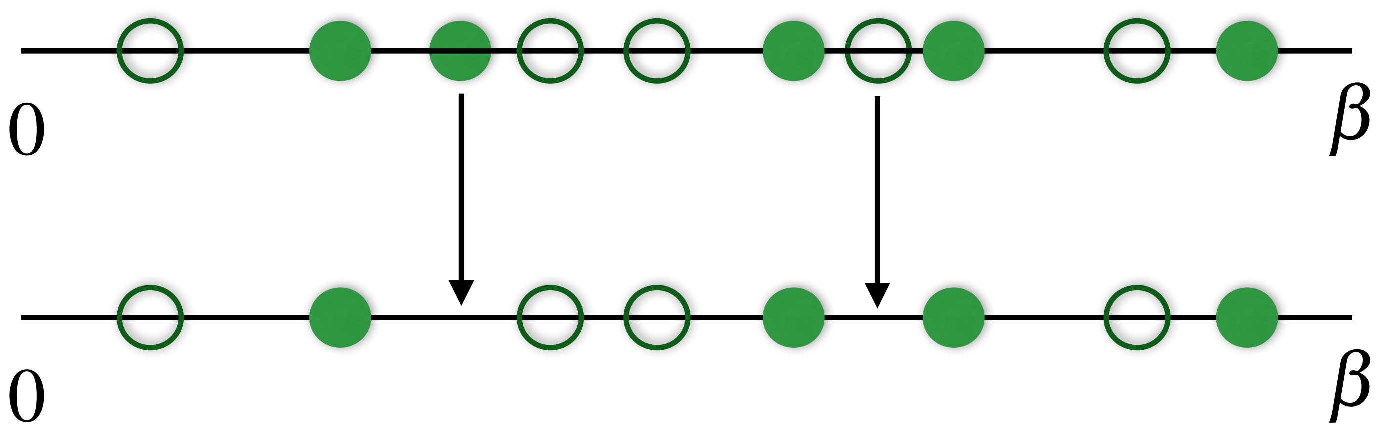
Green’s func matrix: $\left(\hat{G}\right)_{ij} = G_0(\tau_i - \tau_j)$

Updates

Insertion



Remove



Metropolis

$$R = \frac{W_{\text{new}}}{W_{\text{old}}} \, F$$

accept if

$$\text{min}\,(R, 1) > r, \quad 0 \leq r \leq 1$$

deny otherwise

$$F = \frac{\beta^2}{(k+1)^2}$$ for insertion

$$F = \frac{k^2}{\beta^2}$$ for removal

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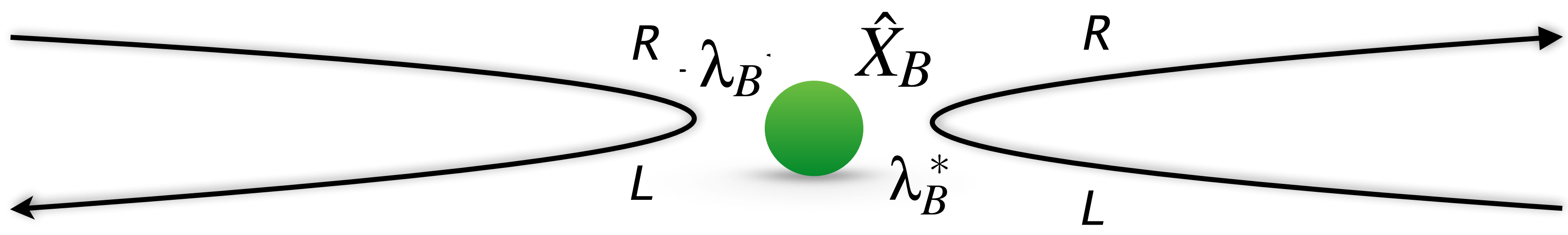
Interaction part

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

Interaction part

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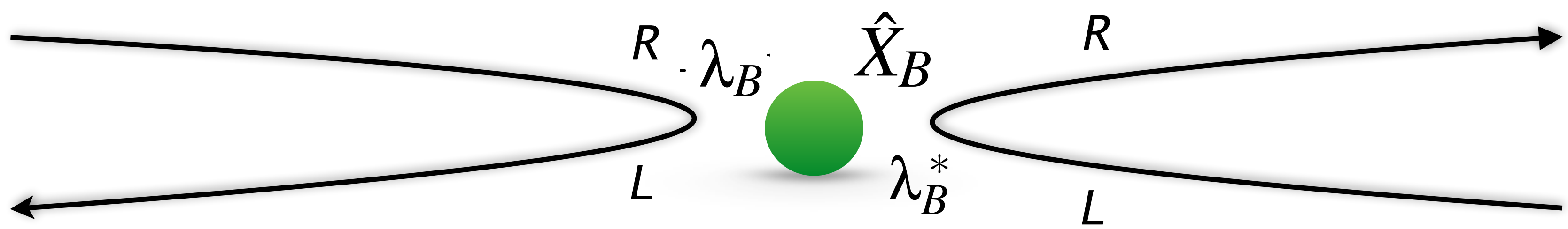

$$V = V_B + V_B^\dagger = \lambda_B \psi_L^\dagger(0)\psi_R(0)\hat{X}_B + \lambda_B^* \psi_R^\dagger(0)\psi_L(0)\hat{X}_B^\dagger$$

$$= a^{g-1}\lambda_B F_L^\dagger F_R \underbrace{\left(a^{-g} e^{i\sqrt{2g}\Phi_+}\right)}_{\equiv V_{\sqrt{2g}}} \hat{X}_B + a^{g-1}\lambda_B^* F_R^\dagger F_L \underbrace{\left(a^{-g} e^{-i\sqrt{2g}\Phi_+}\right)}_{\equiv V_{-\sqrt{2g}}} \hat{X}_B^\dagger$$

Here, we have defined

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

only "+" boson appears in *V*
"–" boson is decoupled and can be ignored

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CTQMC in TLL

N=2k order term in $Z/Z_0 = \left\langle T_\tau \exp\left[- \int_0^\beta d\tau \, H_1(\tau) \right] \right\rangle_0$

$$\lambda_B(g) \equiv a^{g-1} \lambda_B$$

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

$$\xrightarrow[\text{snapshot}]{} |\lambda_B(g)|^{2k} \langle V_\lambda(\tau_1) \cdots V_{-\lambda}(\tau_{2k}) \rangle_b \underbrace{\langle F_L^\dagger F_R \cdots F_R^\dagger F_L \rangle_f}_{=1} \underbrace{\langle \hat{X}_B(\tau_1) \cdots \hat{X}_B^\dagger(\tau_{2k}) \rangle_{loc}}_{\text{calculable } (=1,0)}$$

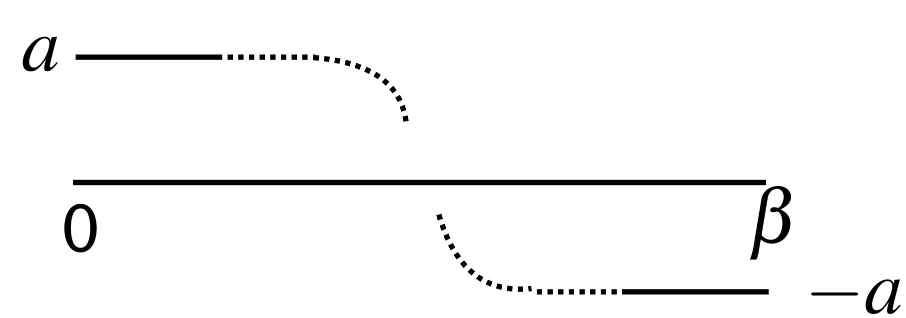
$\lambda = \sqrt{2g} \quad \tau_i > \tau_{i+1}$

$\langle S^+ S^- S^+ S^- \cdots S^+ S^- \rangle$

$$= |\lambda_B(g)|^{2k} \prod_{i<j}^{2k} s_{0ij}^{\lambda_i \lambda_j}$$

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

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



CTQMC in TLL

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$\langle S^+ S^- S^+ S^- \cdots S^+ S^- \rangle$

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

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

❖ 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 order term in $Z/Z_0 = \left\langle T_\tau \exp\left[- \int_0^\beta d\tau\, H_1(\tau) \right] \right\rangle_0$

$$\lambda_B(g) \equiv a^{g-1} \lambda_B$$

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

$\langle S^+ S^- S^+ S^- \cdots S^+ S^- \rangle$

$$= |\lambda_B(g)|^{2k} \prod_{i<j}^{2k} s_{0ij}^{\lambda_i \lambda_j} \rightarrow |\lambda_B(g)|^{2k} \left| \det \hat{S} \right|^{2g} > 0 \quad \text{for } a \rightarrow 0$$

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

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

non-int. *"electron"* Green's func.:

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

$$\left[\hat{S}\right]_{lm} = -\mathrm{sgn}(\tau_l^- - \tau_m^+)/s_{0lm}$$

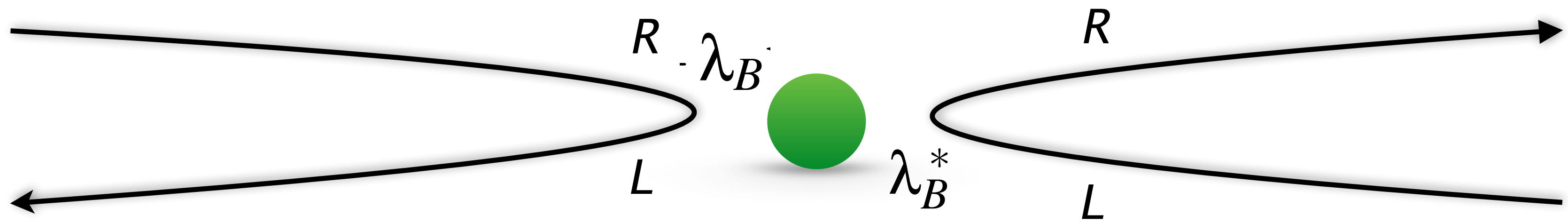
$$\tau^\pm : \tau \text{ for } \pm\lambda$$

Kane-Fisher model

Kane & Fisher PRL (1992)

Kane-Fisher model

Potential barrier for spin-less fermion in 1D



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

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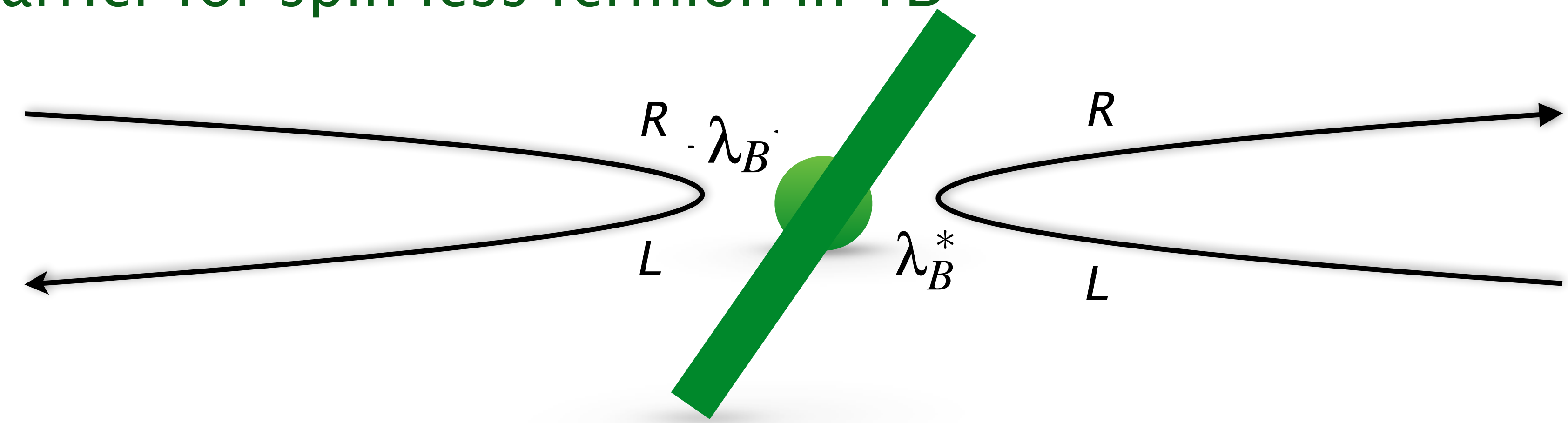


$$H = H_0 + a^{g-1}\lambda_B F_L^\dagger F_R V_{+\lambda} + a^{g-1}\lambda_B^* F_R^\dagger F_L V_{-\lambda}$$

RG eq.:

$$\partial\lambda_B = (1-g)\lambda_B \qquad \lambda_B \to \infty \quad (g<1)$$

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 —> 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:

$$\begin{aligned}
\psi_L(x=0) &= \frac{1}{\sqrt{a}} F_L e^{-i\phi_L(x=0)} \\
&= a^{\frac{g}{4}+\frac{1}{4g}-\frac{1}{2}} \left(a^{-\frac{1}{4g}} e^{-\frac{i}{\sqrt{2g}}\Phi_-}\right) F_L \left(a^{-\frac{g}{4}} e^{-i\sqrt{\frac{g}{2}}\Phi_+}\right) \\
&= a^{\frac{g}{4}+\frac{1}{4g}-\frac{1}{2}} V^-_{-\frac{1}{\sqrt{2g}}} \cdot F_L V^+_{-\sqrt{\frac{g}{2}}}
\end{aligned}$$

Green's function:

$$s(\tau) = \frac{v\beta}{\pi} \sin\left[\frac{\pi}{v\beta}\left(v|\tau| \pm a\right)\right]$$

$$\begin{aligned}
-G(\tau) &= \langle T_\tau \psi_L(\tau,0)\psi_L^\dagger(0,0)\rangle \\
&= a^{\frac{g}{2}+\frac{1}{2g}-1} \langle T_\tau V^-_{-\frac{1}{\sqrt{2g}}}(\tau) V^-_{\frac{1}{\sqrt{2g}}}(0)\rangle \langle T_\tau F_L V^+_{-\sqrt{\frac{g}{2}}}(\tau) F_L^\dagger V^+_{\sqrt{\frac{g}{2}}}(0)\rangle \\
&= a^{\frac{g}{2}+\frac{1}{2g}-1} \left[1/s(\tau)\right]^{\frac{1}{2g}} \left[-G^+(\tau)\right]
\end{aligned}$$

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

$$\begin{aligned}
\mathscr{G}^{(2n)}_{i>j} &= -\left\langle F_L(\tau_i) V_{-\sqrt{\frac{g}{2}}}(\tau_i) F_L^\dagger(\tau_j) V_{\sqrt{\frac{g}{2}}}(\tau_j)\right\rangle_{\mathrm{MC}} \\
&= \left\langle -(-1)^{P_{ij}} s_{0ij}^{\frac{g}{2}} \left|\frac{\det \hat{S}_{n\oplus ij}}{\det \hat{S}_n}\right|^g \right\rangle_{\mathrm{MC}}
\end{aligned}$$

Indirect sampling (fast)

$$\tilde{\mathcal{G}}^{(2k)}_{i>j} = \left\langle -\frac{(-1)^{P_{ij}}}{|\lambda_B(g)|^2} s_{0ij}^{\frac{g}{2}} \left|\frac{\det \hat{S}_{n\ominus ij}}{\det \hat{S}_n}\right|^g \right\rangle_{\mathrm{MC}}$$

Bench mark for g=1

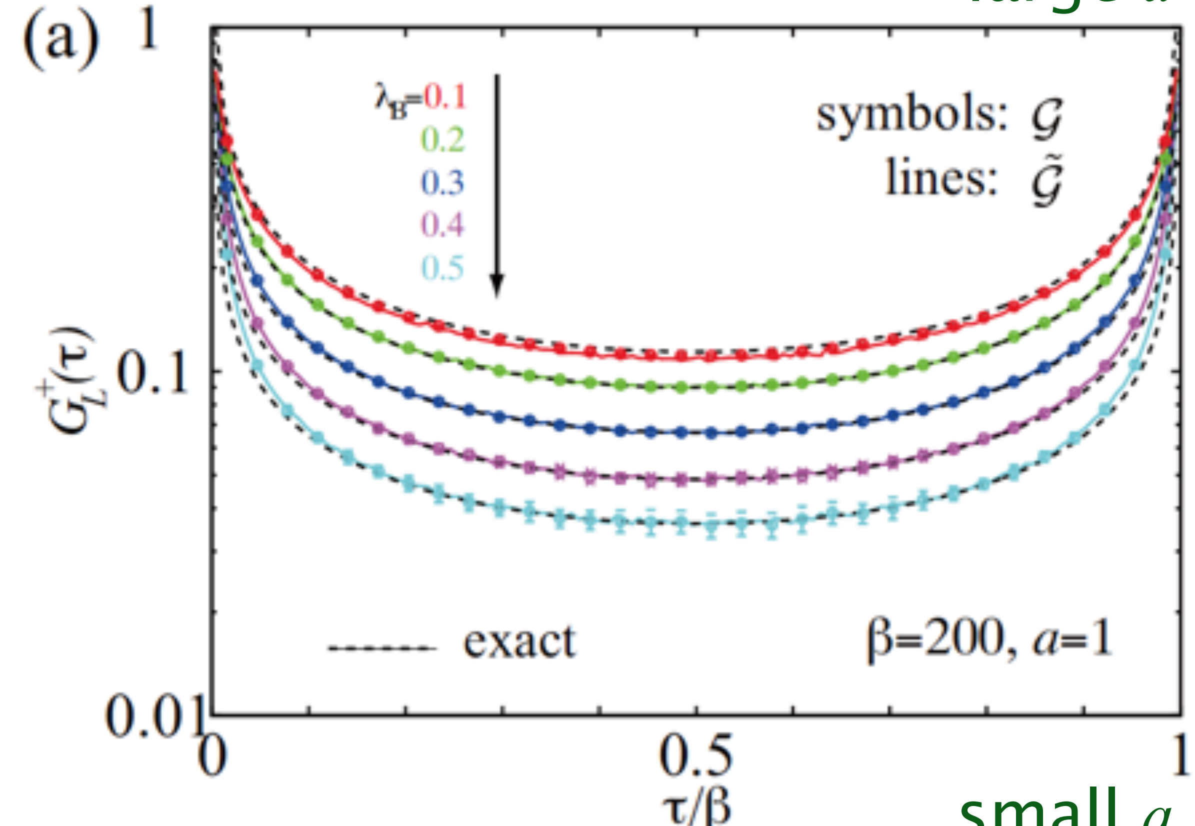
Let us check the Green's function for non-interacting case (g=1)

Exact G can be obtained via EOM as

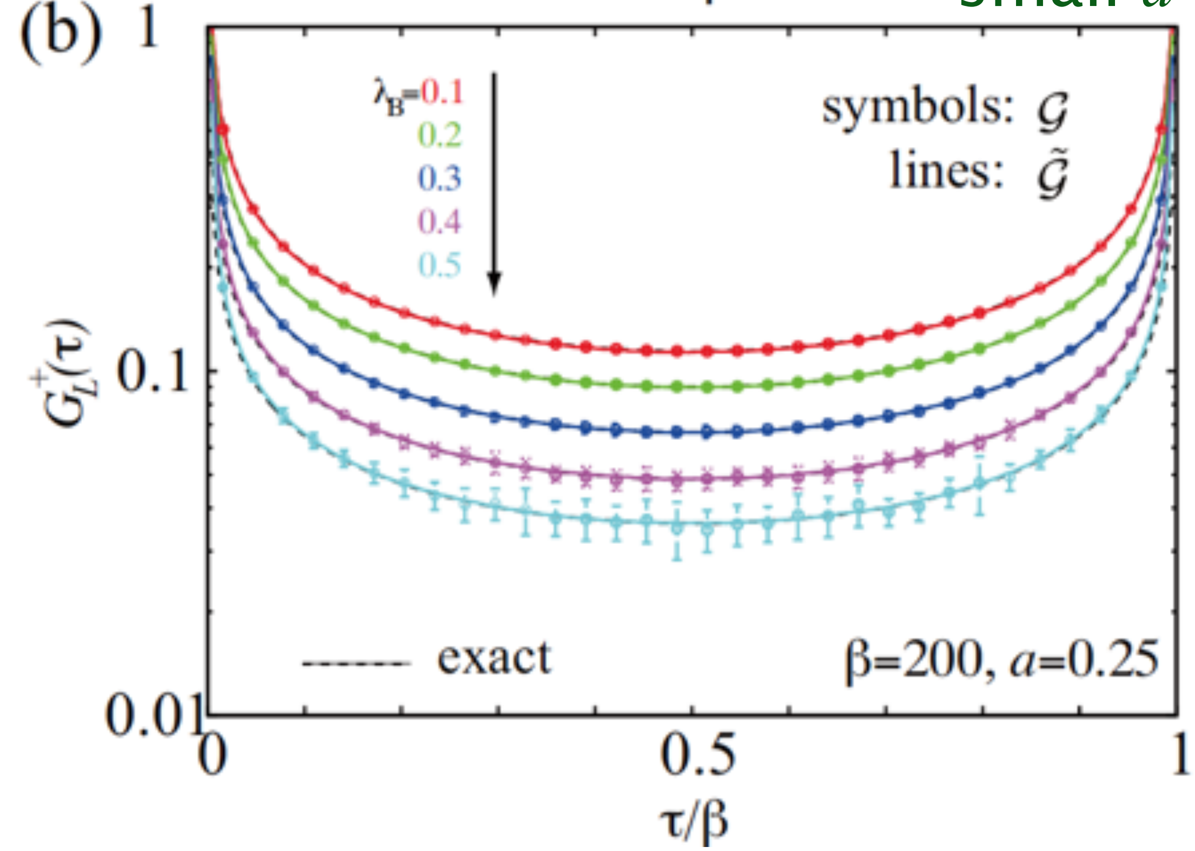
$$G_L^{+,\mathrm{ex}}(\tau) = \frac{\left[s(\tau)\right]^{-\frac{1}{2}}}{1+\pi^2\lambda_B^2/v^2}$$

for a—> 0

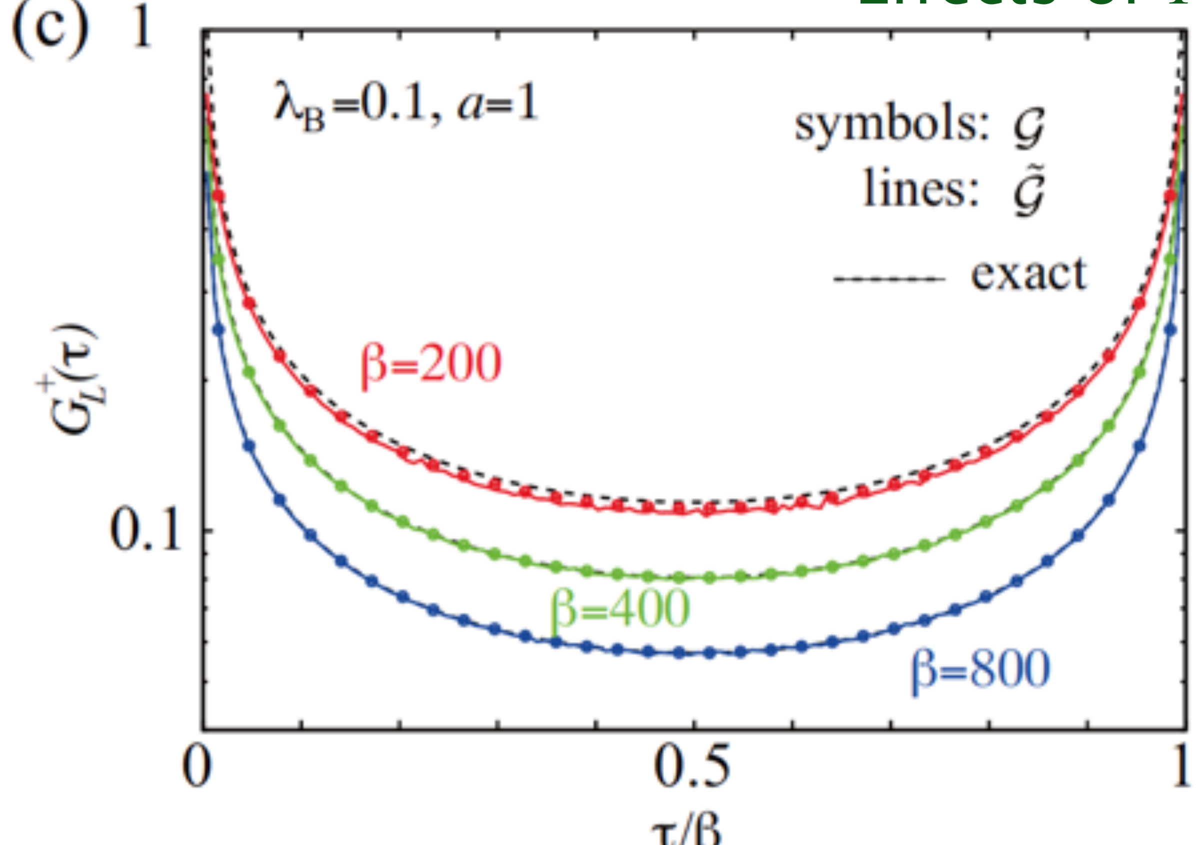
large a



small a



Effects of T



Electron Green's function

Nontrivial part:

$$G_L^+(\tau) = \langle F_L(\tau)\hat{V}_{-\sqrt{\frac{g}{2}}}(\tau)F_L(0)\hat{V}_{\sqrt{\frac{g}{2}}}(0)\rangle_{\Phi_+}$$

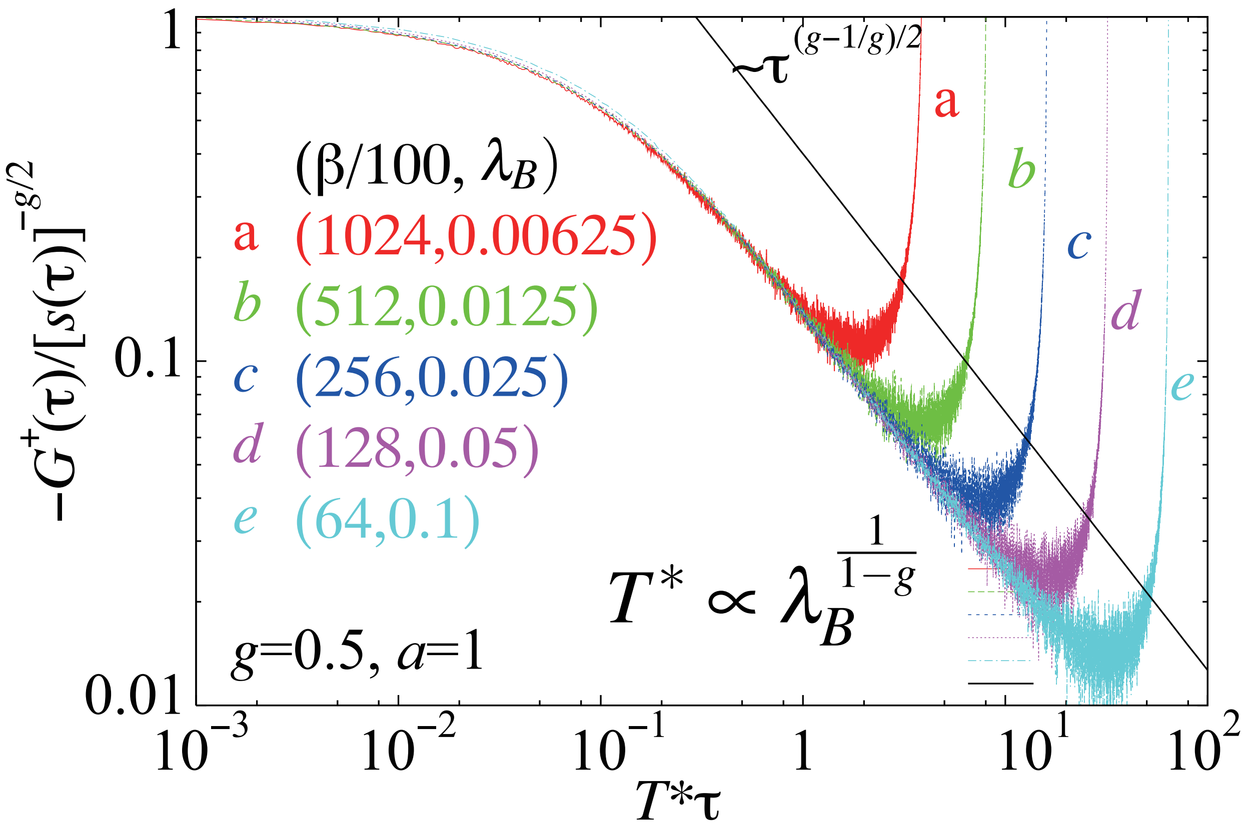
We found:

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

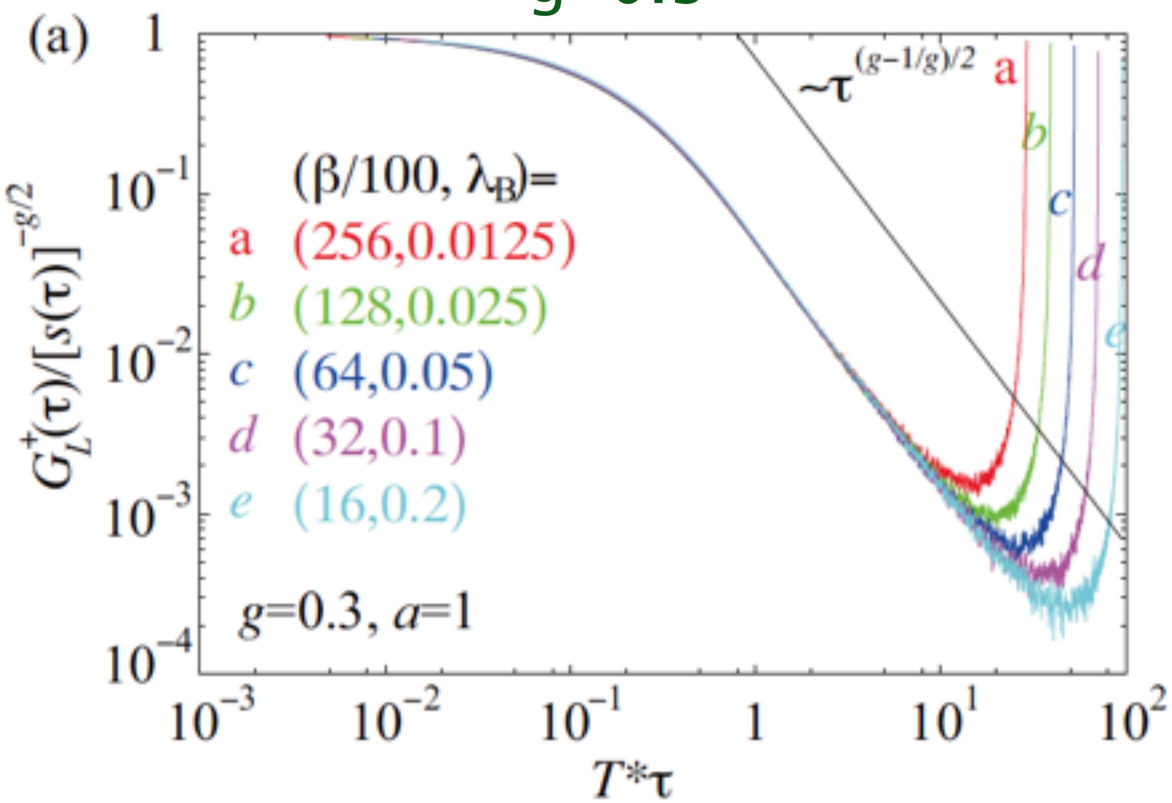
consistent with result by Furusaki (1997)

reflecting vanishing DOS $\omega^{1/g-1}$ at x=0

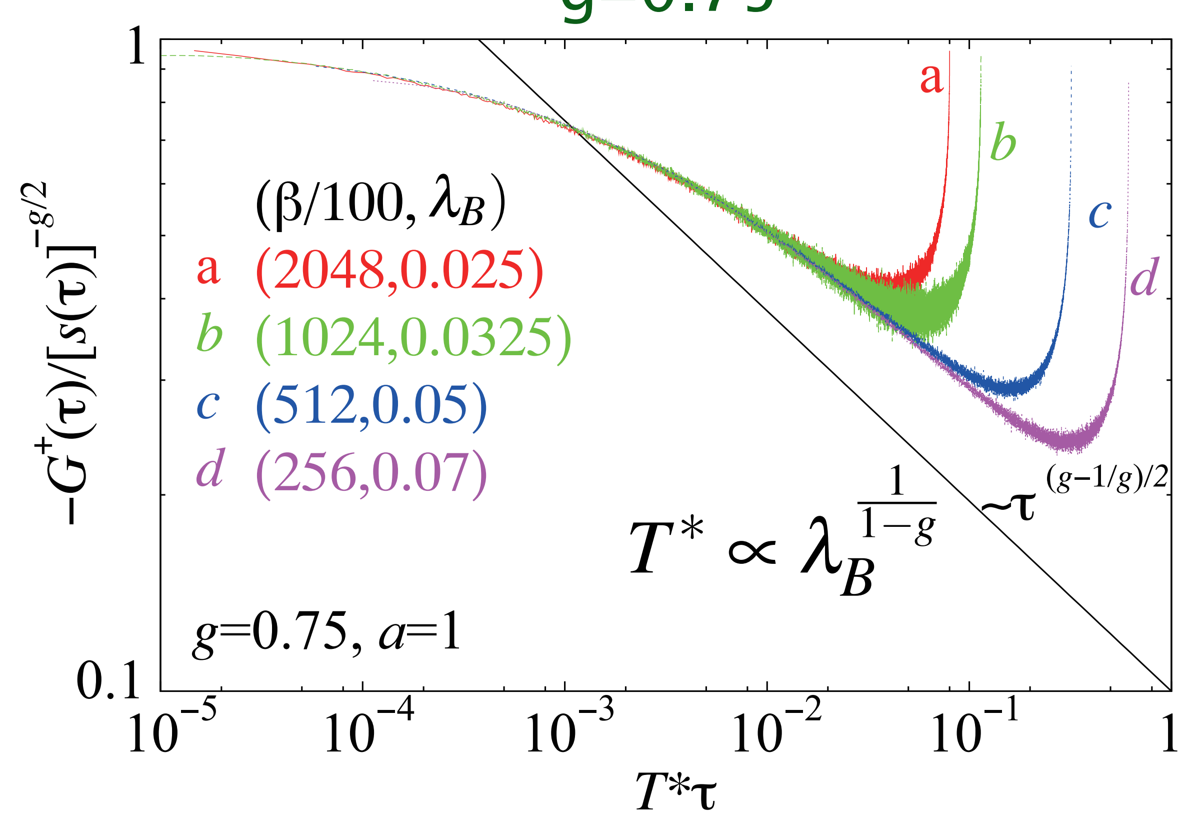
g=0.5



g=0.3



g=0.75



Universal function @ T=0

Green's function is expressed as

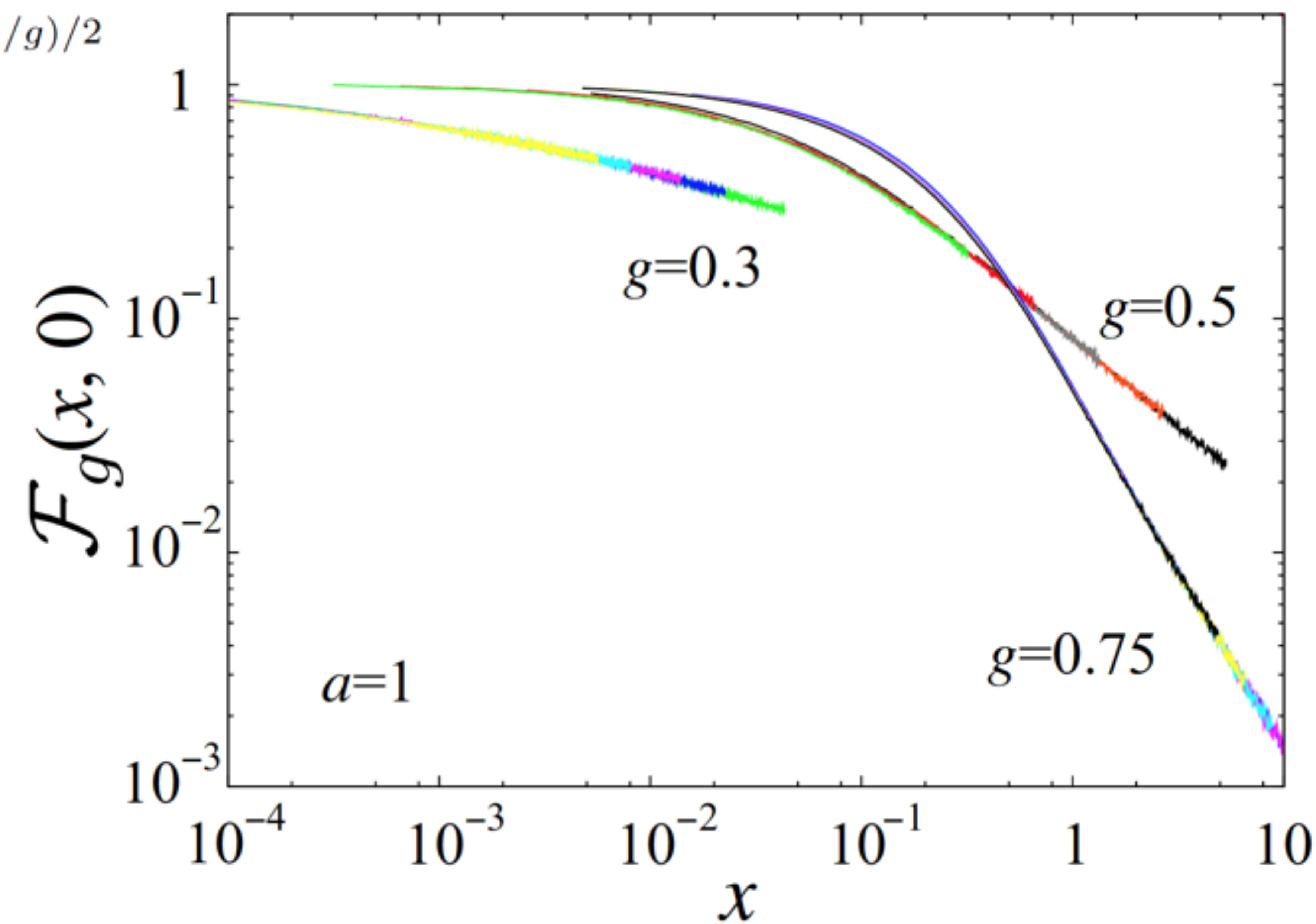
$$G_L^+(\tau) \approx [s(\tau)]^{-g/2} \mathcal{F}_g(T^*\tau\,, T/T^*) \qquad T^* = \frac{v}{a}\left(\frac{\lambda_B}{v}\right)^{1/(1-g)}$$

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 $\tau/\beta < 1/6$



Universal function @ T>0

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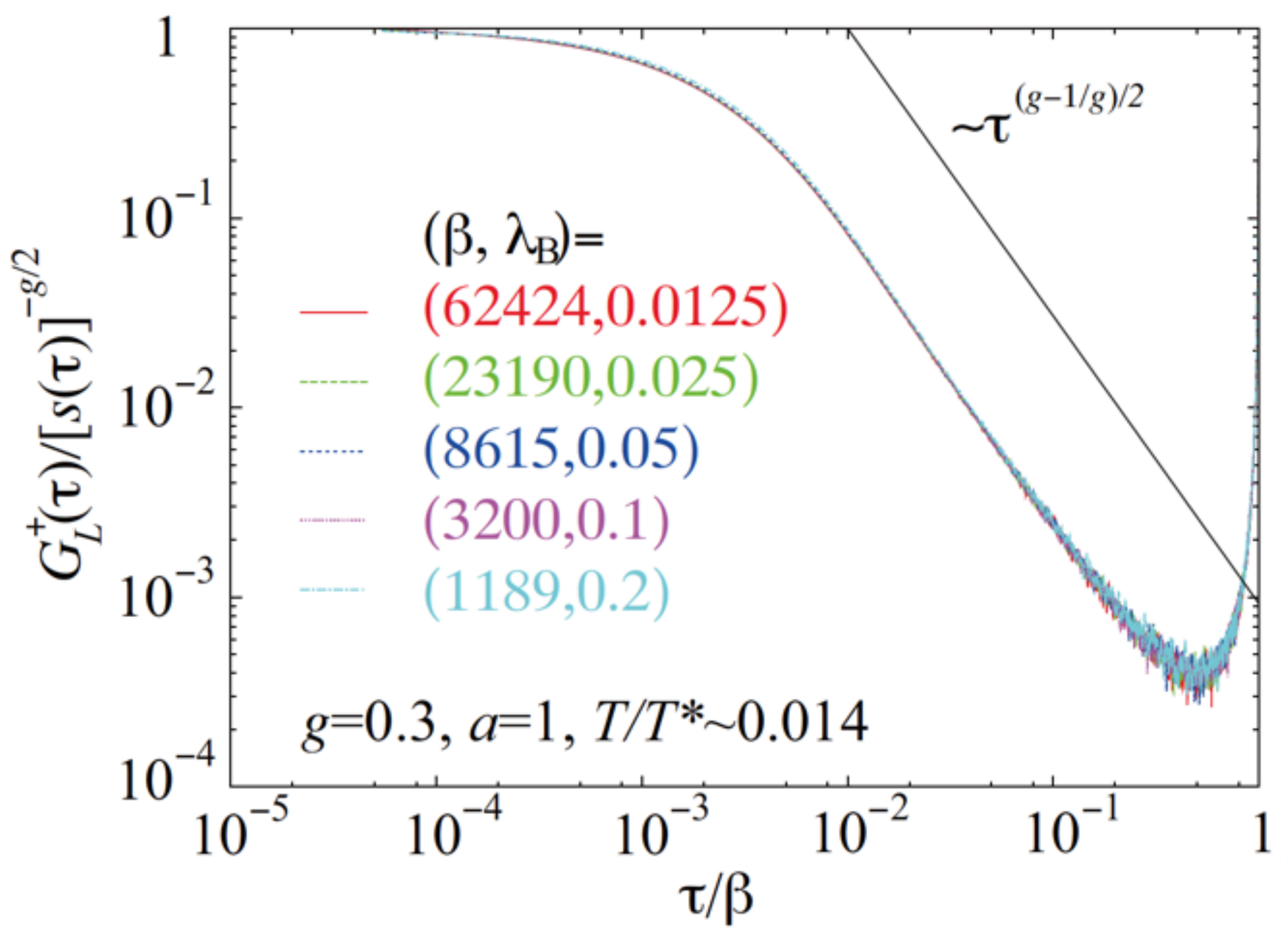
For T>0, universal func. depends only T/T*.

This can be checked by examining data with fixed T/T*.



$$T^*\tau = \frac{T^*}{T}\cdot\frac{\tau}{\beta}$$

Conductance

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:

$$j(x,\tau) = \frac{ev}{2\pi}\partial_x(\phi_L(x,\tau)+\phi_R(x,\tau)) \longrightarrow j(x,\tau) = i\frac{e}{2\pi}\partial_\tau(\phi_L(x,\tau)-\phi_R(x,\tau))$$

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),
real-time PIMC, Leung et al (1995)

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

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

without leads: Apel-Rice (1982)

With leads:
Maslov-Stone (1995), Ponomarenko (1995)
Feed-back effect of interactions:
Kawabata (1996)

Conductance for g=0.5

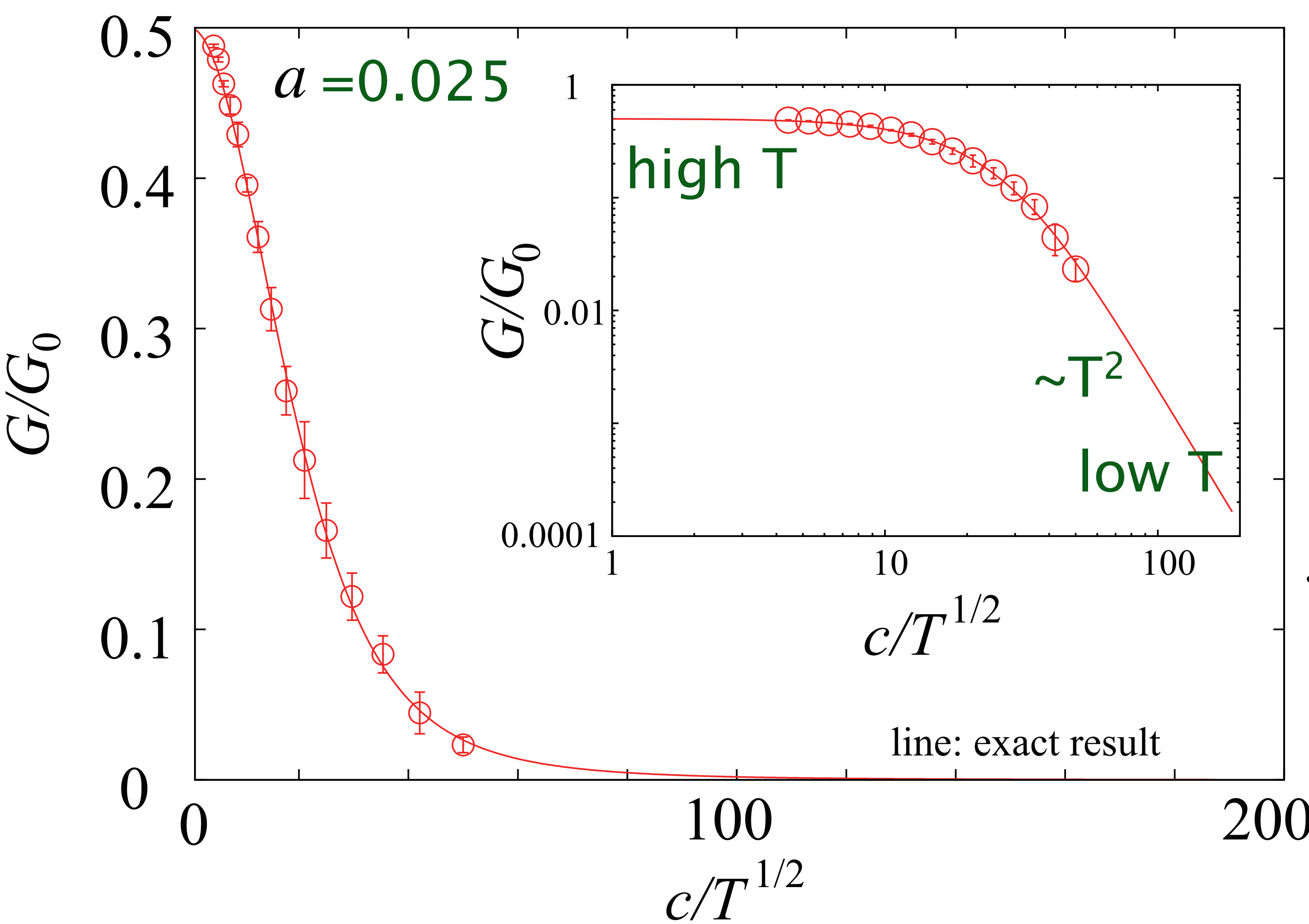
For small cutoff a, results are consistent with the exact one by Kane&Fisher (1992)

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

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

$$-\mathscr{D}(\tau_l-\tau_m) = v^2 s_{0lm}^{-2} + (\pi T)^2 Q(\tau_l)Q(\tau_m) \qquad Q(\tau) = \sum_{p=\pm,i} q_i^p(\tau)\cot\left[\frac{\pi}{\beta}(|\tau-\tau_i^p| \pm \frac{a}{v})\right]$$

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



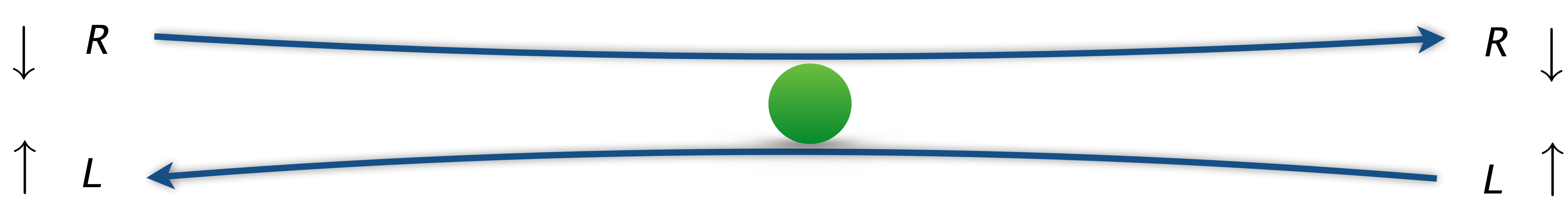
Analytic continuation is done by fitting $D(i\omega_n)$ for low frequency by

$$f(\omega_n) = a - b\omega_n + c\omega_n^2 + d\omega_n^2\log(\omega_n)$$

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

$$\sim u'\psi_\uparrow^\dagger(0)\psi_\uparrow^\dagger(a)\psi_\downarrow(a)\psi_\downarrow(0)$$

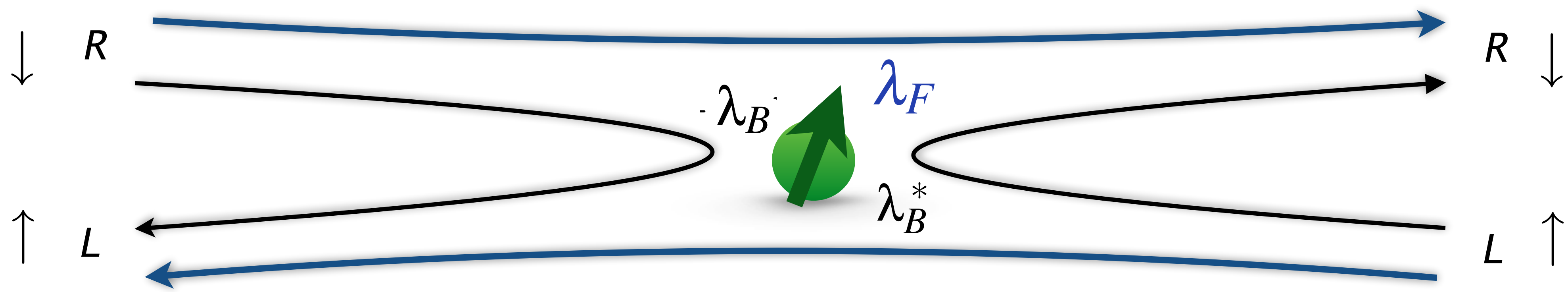
- Magnetic impurity: possible

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)



Wu et al, PRL (2006)

$$H = H_0 + \lambda_F \sqrt{\frac{2}{g}}\partial_x \Phi_+(0) S^z + a^{g-1}\lambda_B F_L^\dagger F_R \left(a^{-g} e^{i\sqrt{2g}\Phi_+}\right) S^- + a^{g-1}\lambda_B^* F_R^\dagger F_L \left(a^{-g} e^{-i\sqrt{2g}\Phi_+}\right) S^+$$

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

$$UHU^\dagger = H_0 + a^{\tilde{g}-1}\lambda_B F_L^\dagger F_R \left(a^{-\tilde{g}} e^{i\sqrt{2\tilde{g}}\Phi_+}\right) S^- + a^{\tilde{g}-1}\lambda_B^* F_R^\dagger F_L \left(a^{-\tilde{g}} e^{-i\sqrt{2\tilde{g}}\Phi_+}\right) S^+$$

now, exponent is shifted:

$\sqrt{2\tilde{g}} \equiv \sqrt{2g}(1-\lambda_F/gv)$ $\quad\quad$ $\lambda_F = gv$: decoupled point (dP)

Maciejko PRB (2012)

Poor man's scaling

Interactions:

$$V = \frac{J^z a}{\sqrt{2g}} \partial_x \Phi_+(0) S^z + \frac{J^\pm a^g}{2} \left(F_L^\dagger F_R V_\lambda S^- + F_R^\dagger F_L V_{-\lambda} S^+ \right)$$

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:

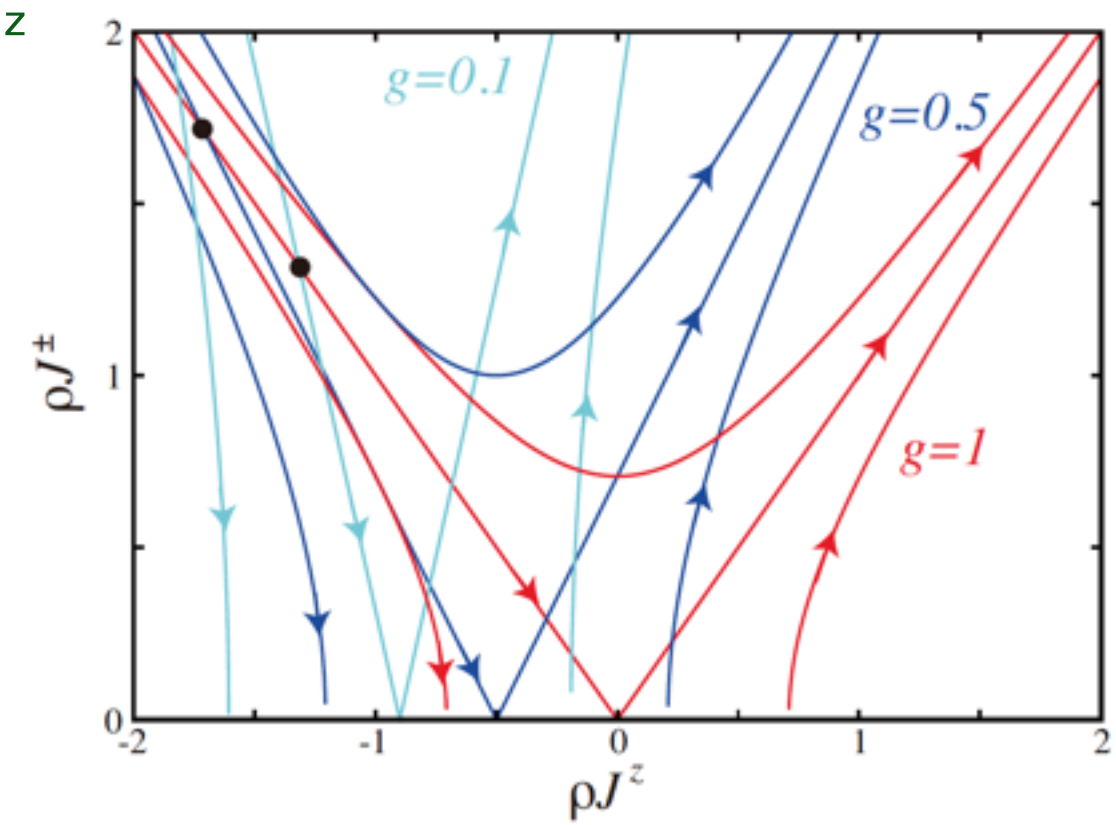
$$V_\lambda(z) V_{-\lambda}(z') \sim \frac{1}{(z - z' + a)^{\lambda^2}} + \lambda \frac{\partial_x \Phi(z)}{(z - z' + a)^{\lambda^2 - 1}} + \cdots$$

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):

$$\begin{aligned} \partial_l J^\pm &= (1-g) J^\pm + \rho J^\pm J^z, \\ \partial_l J^z &= \rho g {J^\pm}^2. \end{aligned}$$



RG flow & decoupled points

Exchange up and down local spin indices:

$$S^z \to -S^z,\ S^\pm \to S^\mp$$

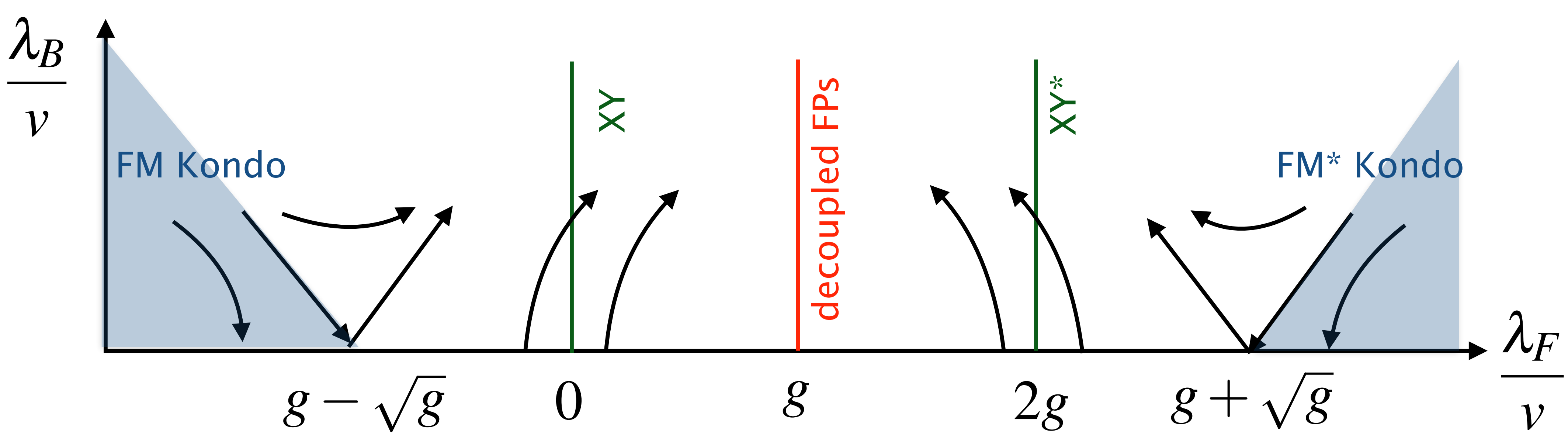
Then, Hamiltonian reads,

originally $F_R^\dagger F_L$　　originally $1-\lambda_F/gv$

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

Equivalent

$$\lambda_F/gv \longleftrightarrow (2-\lambda_F/gv)$$



Trajectories based on Anderson-Yuval-Hamann's method

Maciejko PRB (2012)

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:

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

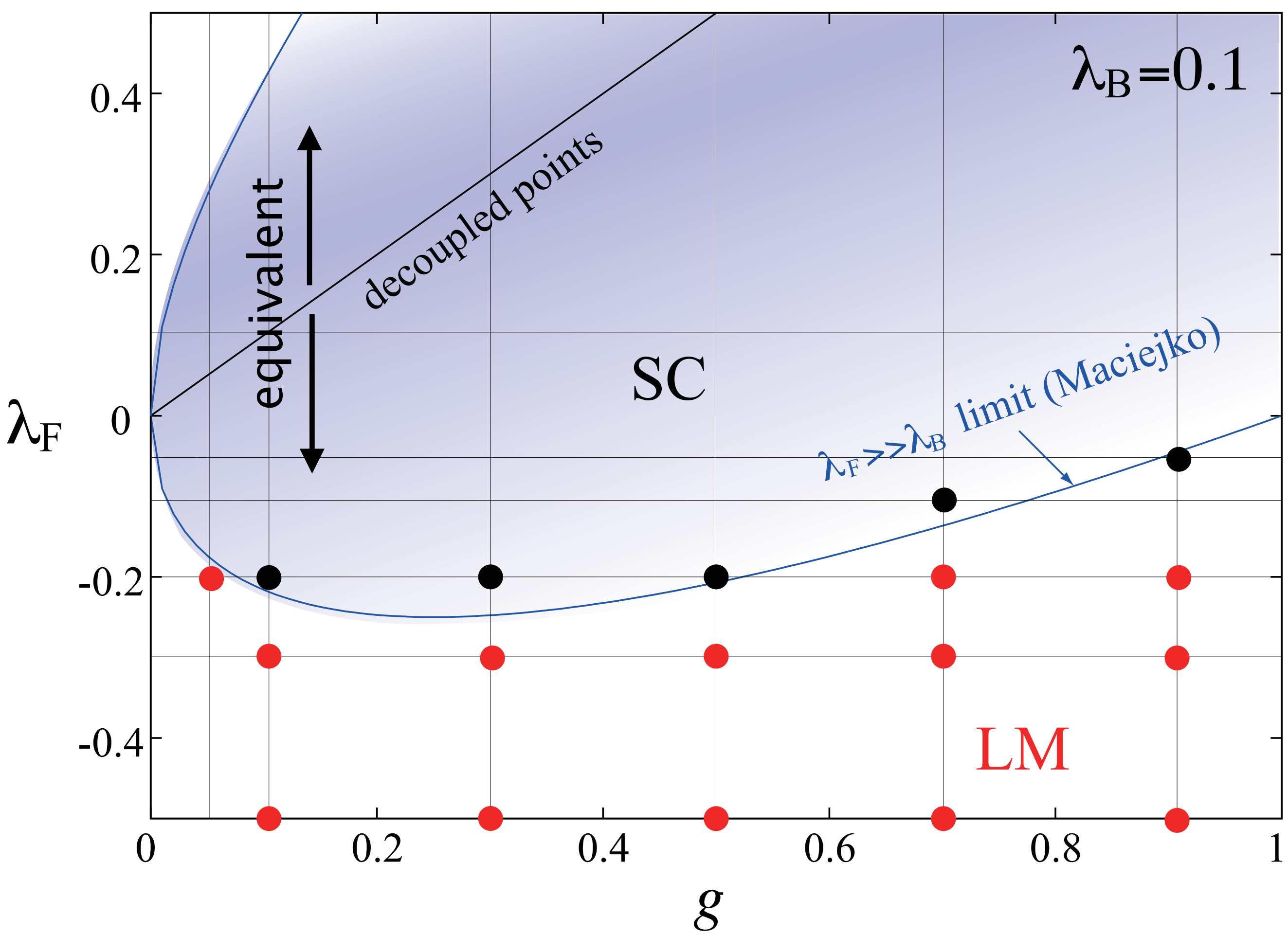
with $\mathcal{M}_{ij} = \dfrac{a^{2g\left(\frac{\lambda_F}{gv}\right)^2}}{|\lambda'_B|^2}\left[s(\tau_{ij})\right]^{-\frac{2\lambda_F}{v}}\left|\dfrac{\det\hat{S}_{k-1}\{\tau\ominus\tau_i^-,\tau_j^+\}}{\det\hat{S}_k\{\tau\}}\right|^{2g'}$ $\quad g' = g - \lambda_F/v$

direct sampling of longitudinal spin susceptibility:

$$\chi^z(\tau_i - \tau_j) = \frac{\langle S^{\pm}(\tau_1)\cdots S^z(\tau_i)\cdots S^z(\tau_j)\cdots\rangle}{\langle S^{\pm}(\tau_1)\cdots\cdots\rangle}$$

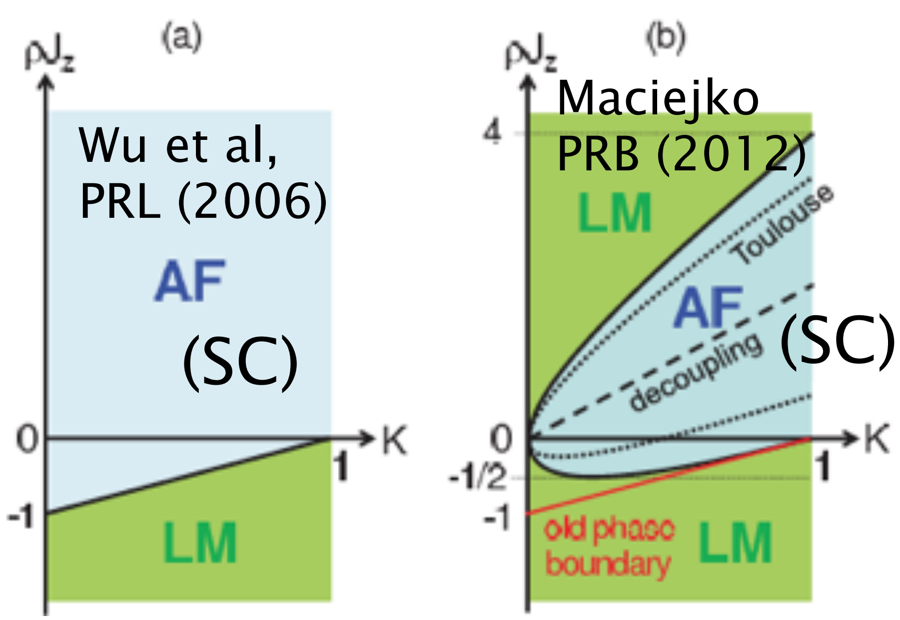
Phase diagram

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

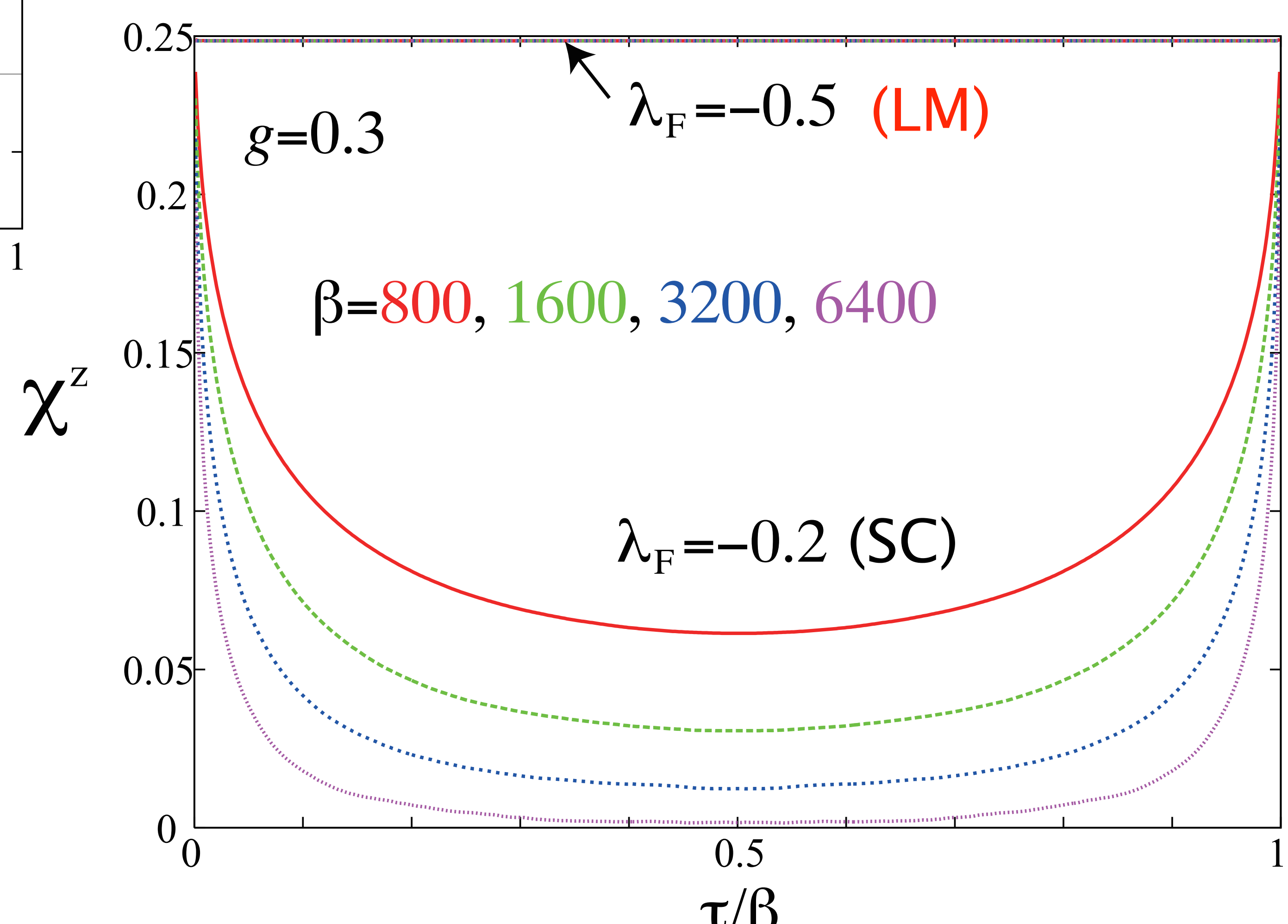


SC: screened phase ("strong coupling")

LM: local-moment phase (Ferro Kondo)



Typical T-dependence of spin correlation

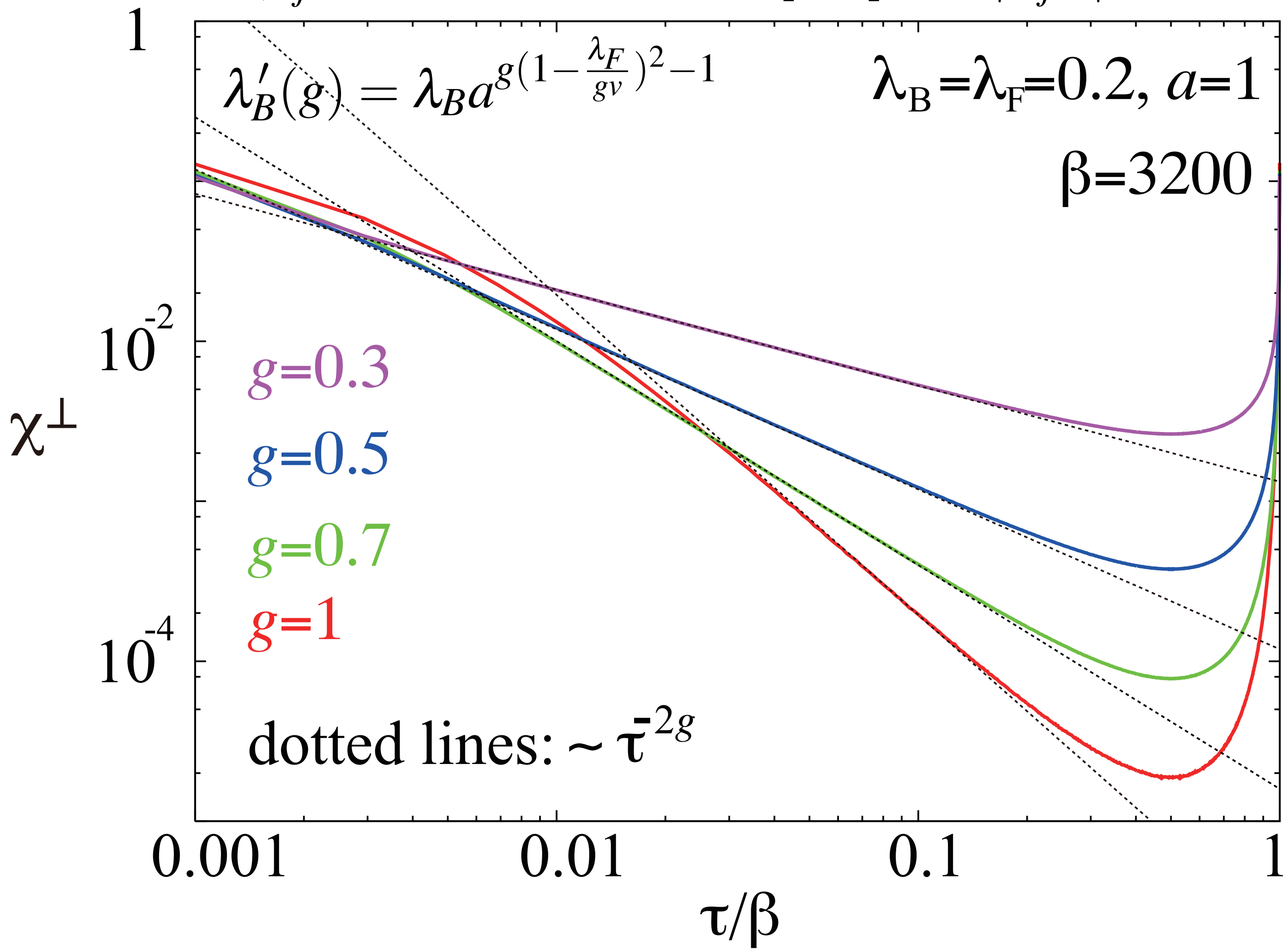


"Strong-coupling" Fixed Point

Dynamical impurity spin-spin correlations

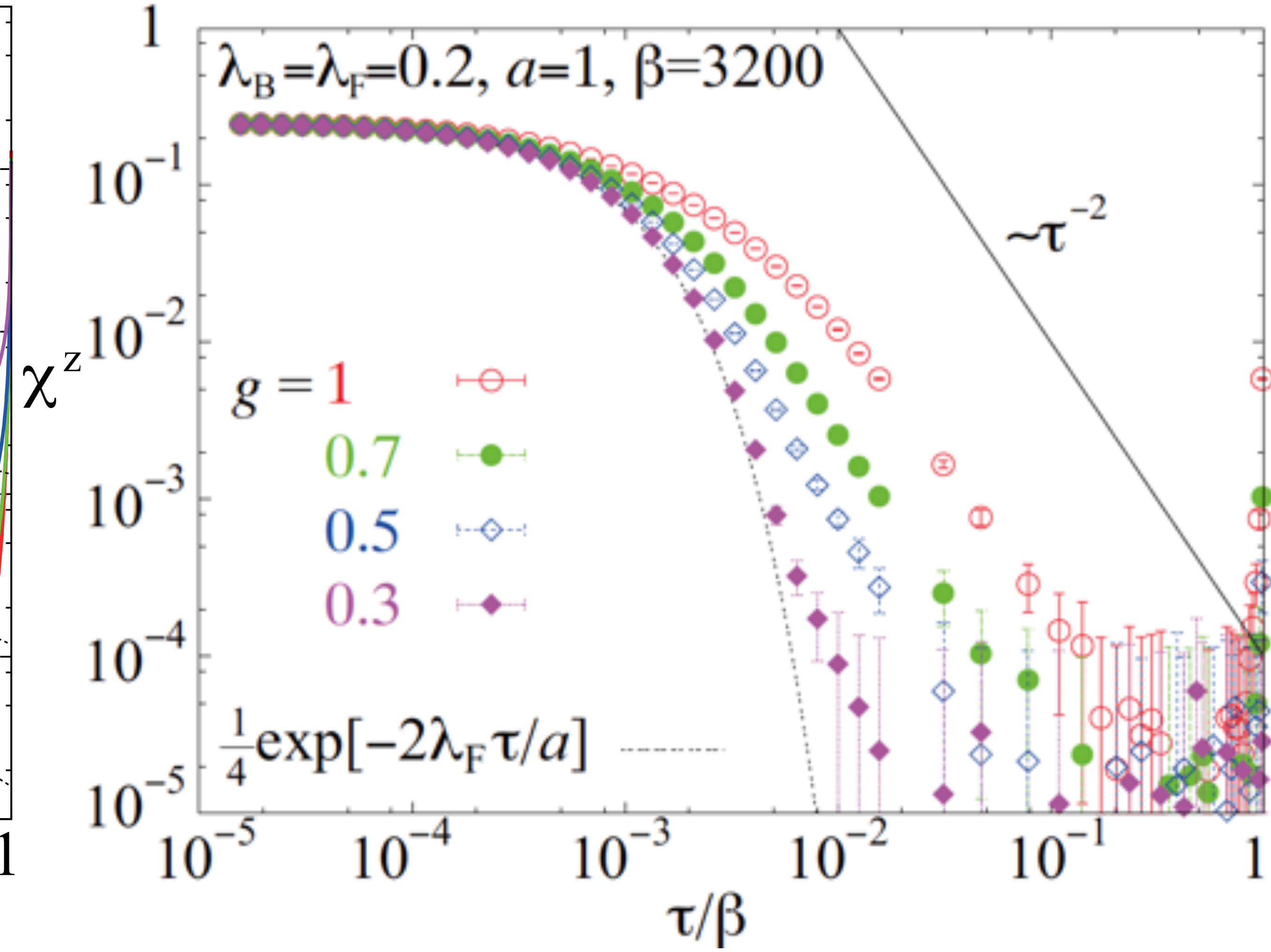
transverse

$$\tilde{\mathscr{G}}^{(2k)}_{i>j} = a^{2g(\frac{\lambda_F}{gv})^2} |\lambda'_B(g)|^{-2} \left[s_{0ij}\right]^{-\frac{2\lambda_F}{v}} \left|\hat{S}^{-1}_{ji}\right|^{2(g-\frac{\lambda_F}{v})}$$



longitudinal

(directly calculated)



$1/\tau^{2g}$: The exponent is precisely the exponent @ dP

$1/\tau^2$: dP+ perturbation ; dP@g=0.2

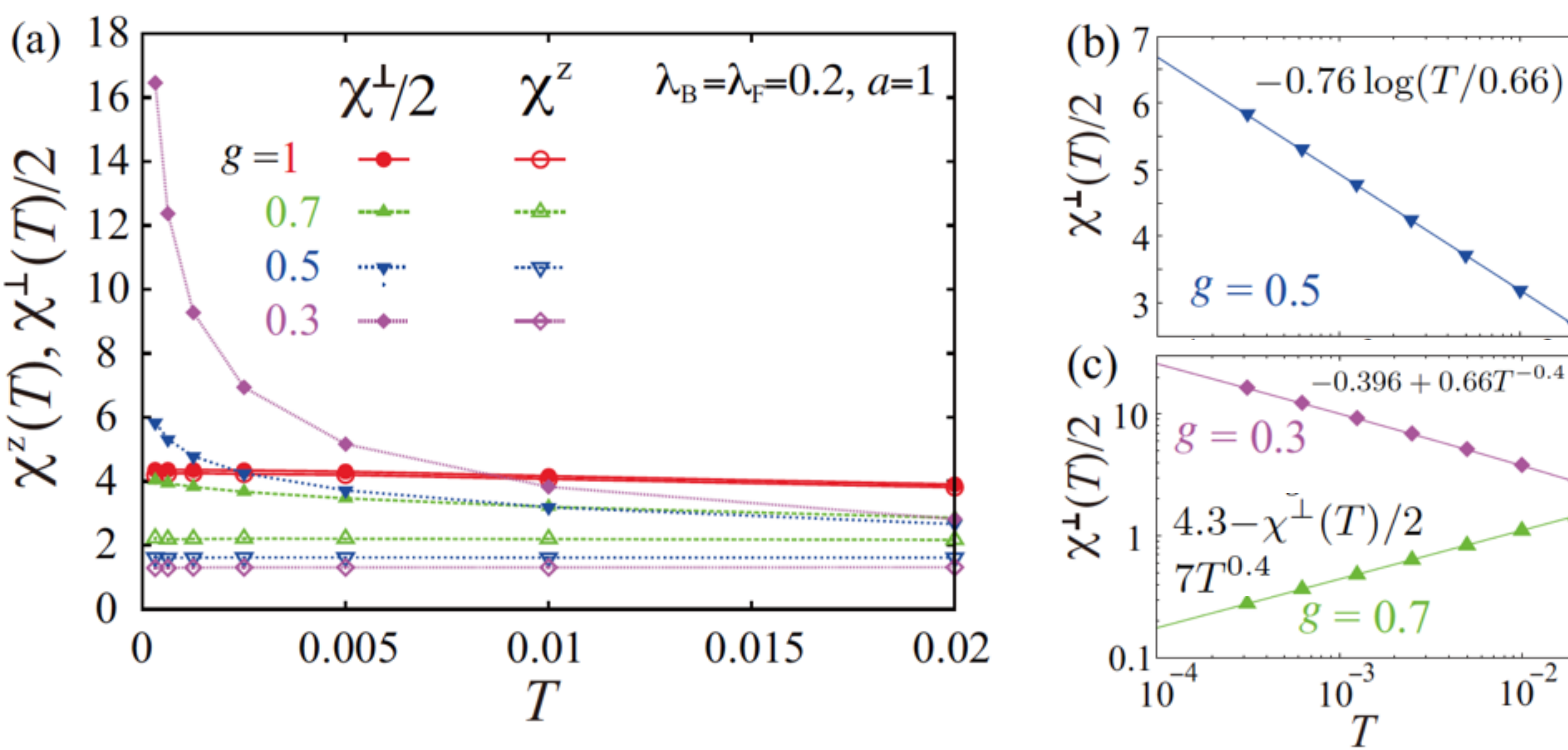
spin susceptibility $\chi^\perp \propto 1/T^{1-2g}$ diverges for g < 1/2, log corrections for g=1/2

Spin susceptibility

$$\chi_O(\tau) \equiv \langle O(\tau)O(0)\rangle \sim \tau^{-2\Delta_O} \longrightarrow \chi_O(T) = \int_0^\beta d\tau \chi_O(\tau) \sim T^{2\Delta_O - 1}$$

$$\chi_O(T) \sim -\ln T \quad \text{for } \Delta_O = \frac{1}{2}$$

in our case, $\Delta_O = g$ for $\chi^\perp$



Summary

- CTQMC applied to TLL successfully without negative sign in several models (also applicable to other models —> future studies):
- <u>Kane-Fisher model</u>
  - Green's functions for all TL parameters g
  - Confirmed approx. exponent 1/(2g) by Furusaki (1997)
  - Conductance is also calculable

$$G_L^+(\tau) \sim \tau^{-1/2g}$$

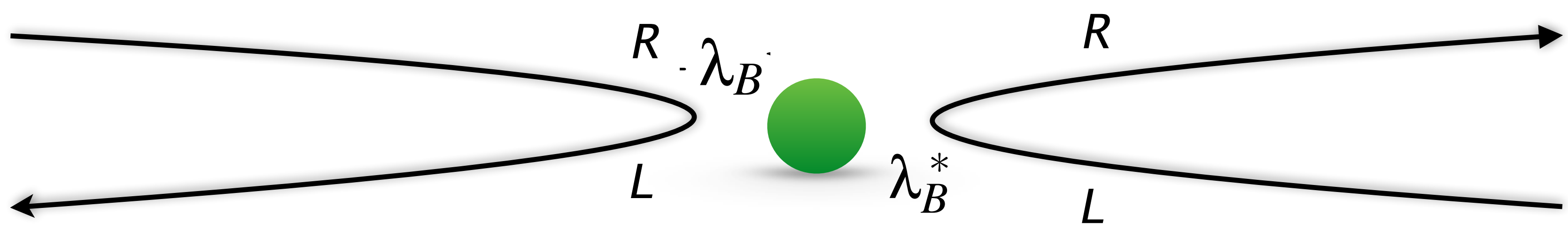
- <u>Helical Kondo model</u>
  - Phase diagram
  - Spin-spin correlation functions

$$\chi^\perp \sim \tau^{-2g}, \;\; \chi^z \sim \tau^{-2}$$

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



$$H = H_0 + a^{2g-1}\lambda_B (F_L^\dagger F_R)^2 V_\lambda + a^{2g-1}\lambda_B (F_R^\dagger F_L)^2 V_{-\lambda}$$

$$\sim H_0 + 2a^{2g-1}\lambda_B \cos(\lambda\Phi_+) \qquad \lambda = \sqrt{8g}$$

RG eq.:

$$\partial\lambda_B = (1-4g)\lambda_B \qquad \lambda_B \to \infty \quad (g < 1/4)$$

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

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

For even No. of vertices in [ ]:

$$\to(-1)^pF_L(\tau)[(F^\dagger_{L,R})^n(F_{R,L})^n]F^\dagger_L(\tau=0)\ \to(-1)^p[(F^\dagger_{L,R})^n(F_{R,L})^n]$$

For odd No. of vertices in [ ]:

$$\to(-1)^pF_L(\tau)[(F^\dagger_{L,R})^n(F_{R,L})^n(F^\dagger_{L,R}F_{R,L})^q]F^\dagger_L(\tau=0)$$

$$\to(-1)^{p+q}[(F^\dagger_{L,R})^n(F_{R,L})^n]$$

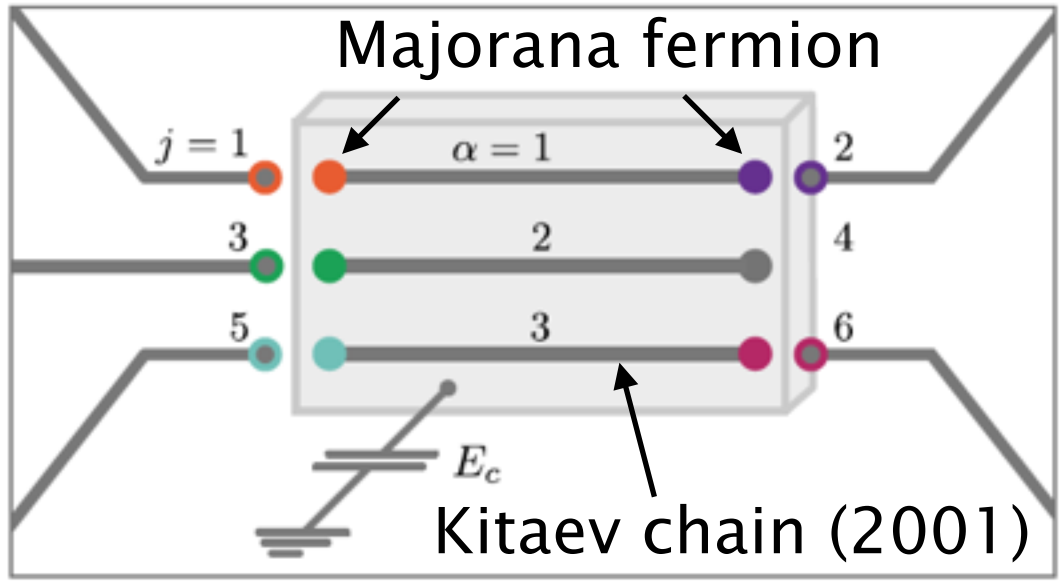
Note: there is no time dependence in Klein fac.

This clearly indicates difference in the two models

✤ No sign in 2-particle backscattering model

$$\begin{aligned}\langle T_\tau\psi_L(\tau)\psi^\dagger_L(0)\rangle &= \langle T_\tau e^{-i\sqrt{g/2}\Phi_+(\tau)}e^{i\sqrt{g/2}\Phi_+(0)}\rangle && \text{i.e., no Klein fac.}\\ &\sim \langle e^{-i\sqrt{g/2}\Phi_+(0)}\rangle\langle e^{i\sqrt{g/2}\Phi_+(0)}\rangle && \text{Finite value remains}\end{aligned}$$

Topological Kondo problems



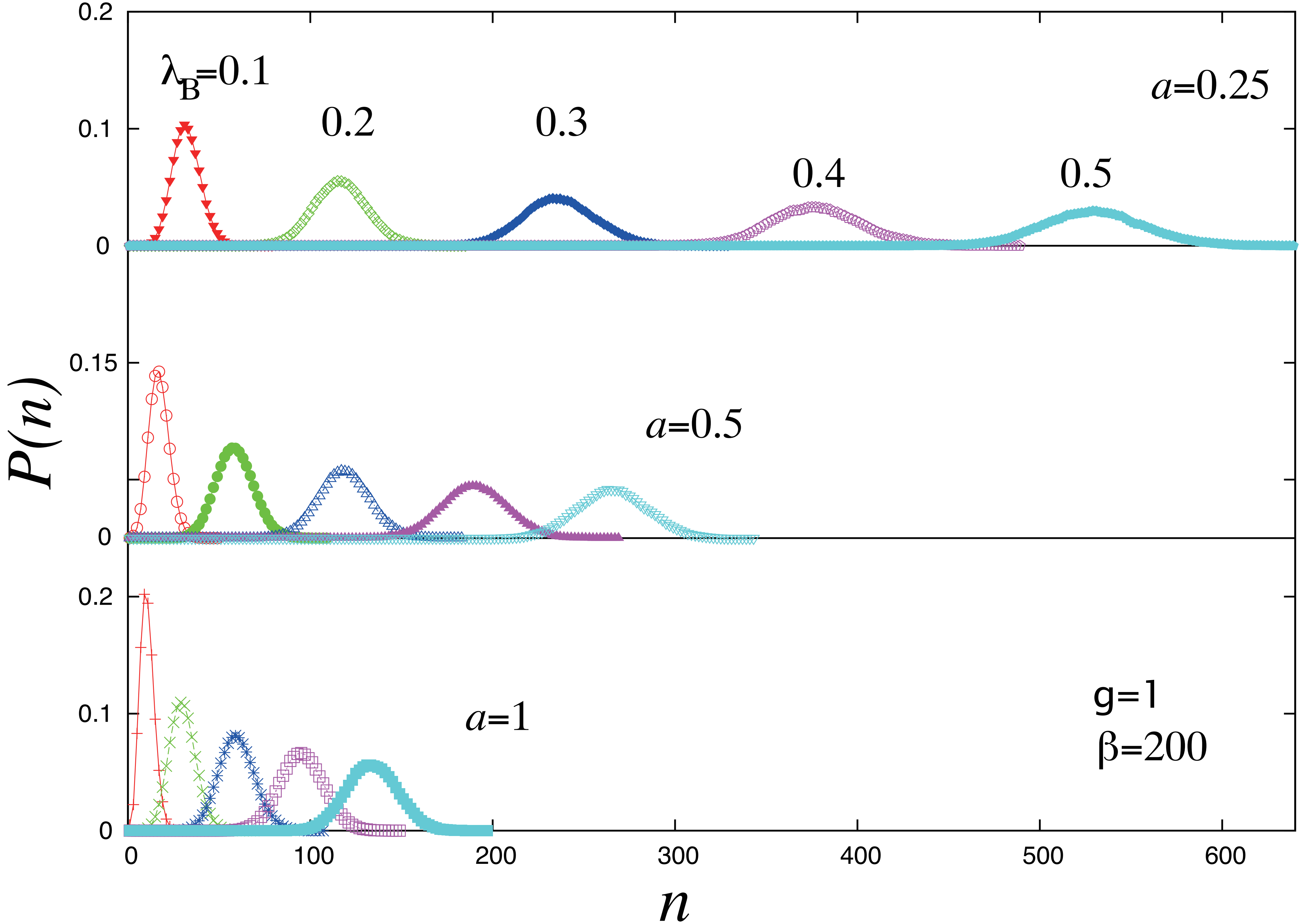
Beri&Cooper (2012)
Altland&Egger (2013)

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

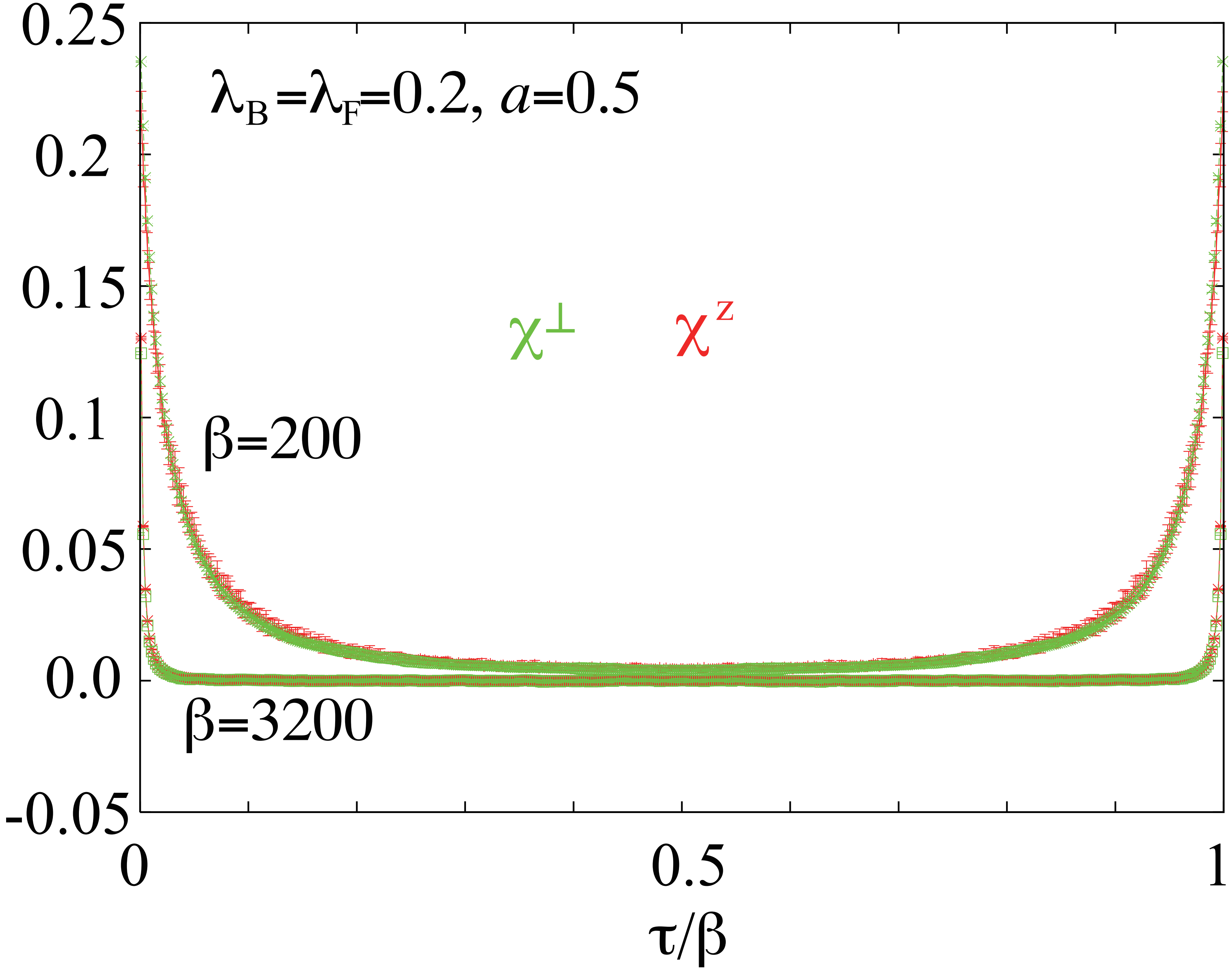
- Robust (~topologically protected) NFL is realized (SO(M) sym.)
- As for CTQMC, no negative sign, but we need to introduce an update operation with cyclic three vertices insertion/removal or equivalent ones.

$$\psi_1^\dagger(\tau)\psi_2(\tau)\psi_2^\dagger(\tau')\psi_3(\tau')\psi_3^\dagger(\tau'')\psi_1(\tau'')$$

Probability density



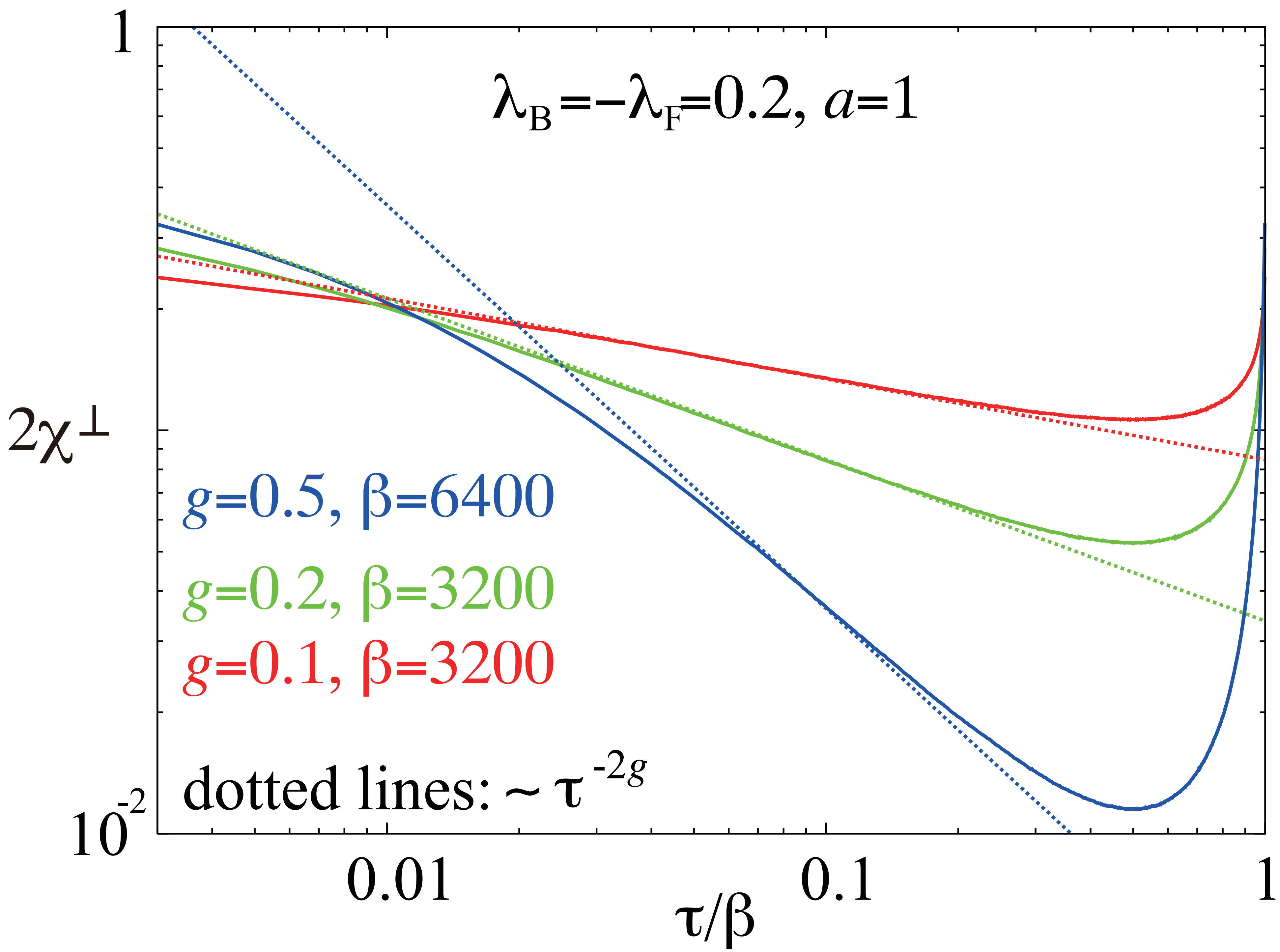
Check SU(2) symmetry for g=1



FM cases

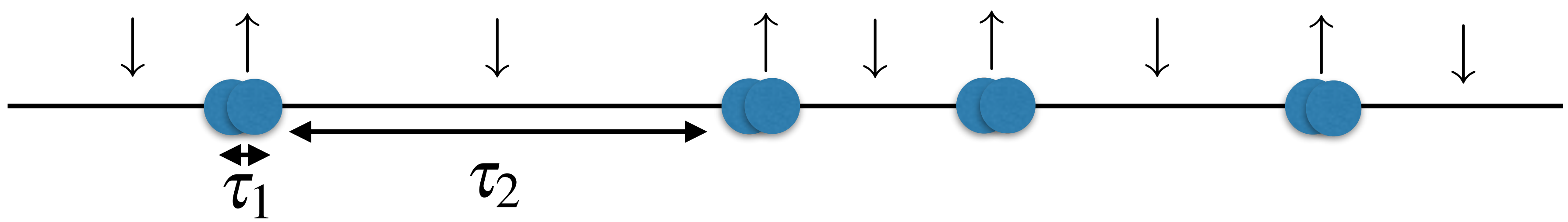
For small g, we succeeded to get the strong-coupling fixed point.

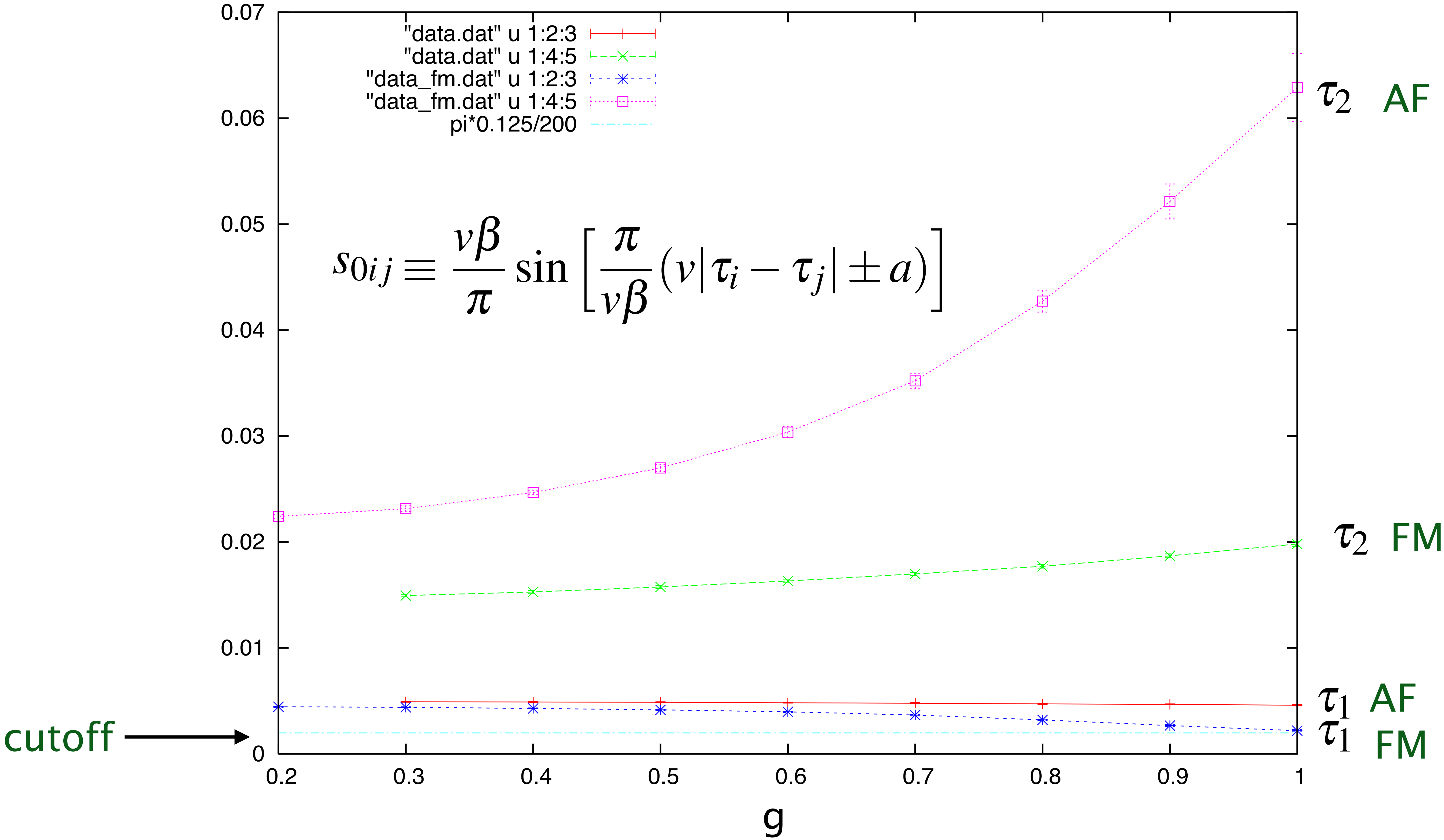
But, numerical difficulty appears when we approach g=1 for isotropic case



Effects of cutoff in LM phase

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





Decoupled-point Hamiltonian

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

$$(-1)^{N_R}\begin{pmatrix} & & & h \\ 0 & & -h & \\ & -h & & 0 \\ h & & & \end{pmatrix}\;\begin{array}{l} |N_R\, N_L\;;\uparrow> \\ |N_R{+}1\;N_L{-}1;\uparrow> \\ |N_R\, N_L;\downarrow> \\ |N_R{-}1\;N_L{+}1;\downarrow> \end{array}$$

$$\rightarrow \quad UHU^\dagger \;=\; H_0 + \frac{\lambda_B}{a}(S^+ + S^-) \qquad\qquad h = \frac{\lambda_B}{a}$$

Decoupled point

@ $\lambda_F = gv$

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

Klein Factors play no role

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

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

$$\chi_{zz}^{\text{dFP}} = \langle T_\tau S^z(\tau) S^z(0)\rangle_{\text{dFP}} = \frac{1}{4}e^{-2h\tau} \qquad h = \frac{\lambda_B}{a}$$

In the original language (T=0):

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

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

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

Maciejko PRB (2012)

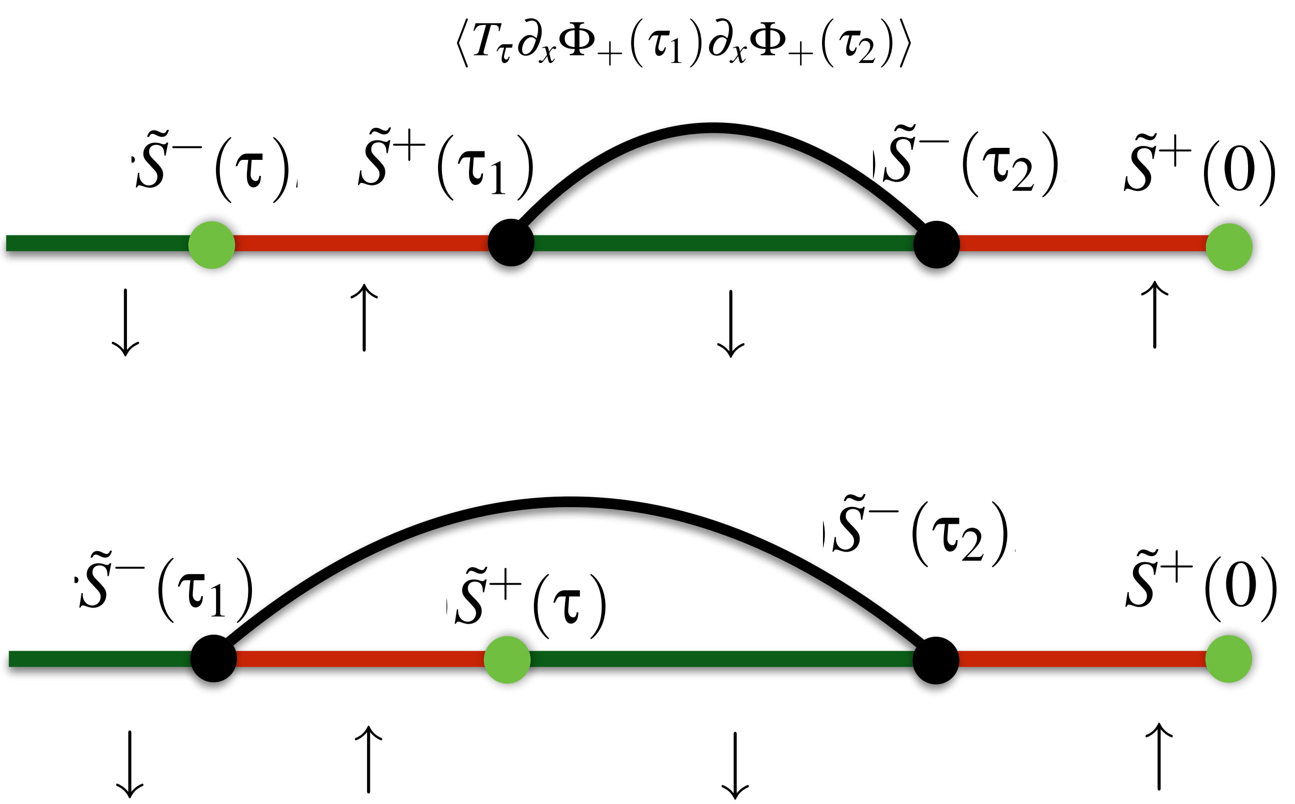
Perturbations from decoupled FP

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

change quantization axis

$$\delta\lambda_F = \lambda_F - g v_{\cdot}$$

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



$\sim \tau^{-2}$

$\sim \tau^{-2}$

$$\delta\chi_{zz}^{\mathrm{dFP}}(\tau) \simeq \frac{a^2\delta\lambda_F^2}{16 g v^2 \lambda_B^2}\frac{1}{\tau^2}$$

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

Notations

$$2\sqrt{\pi}\phi_{\text{Maciejko}} = \phi_L - \phi_R \qquad \frac{J_{\perp,\text{Maciejko}} a_{\text{Maciejko}}}{2\pi\xi} = \frac{\lambda_B}{a}$$

$$\begin{aligned} 2\sqrt{\pi}\Pi_{\text{Maciejko}} &= \partial_x(\phi_L + \phi_R) \\ &\to \sqrt{\frac{2}{g}}\partial_x \Phi_+(0) \quad (x \to 0) \end{aligned}$$

$$S^{\pm}_{\text{Maciejko}} = S^{\mp}, S^z_{\text{Maciejko}} = -S^z \qquad \rho_{\text{Maciejko}} J^{\text{dFP}}_{z,\text{Maciejko}} = 2K = \frac{2\lambda_F}{v}$$

consistent with ours

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

$$J_{z,\text{Maciejko}} a_{\text{Maciejko}} = 2\pi\lambda_F$$

$$\rho_{\text{Maciejko}} J^{*,\pm}_{z,\text{Maciejko}} = 2(K \pm \sqrt{K}) = 2\pi\lambda_F \rho / a = \frac{2\lambda_F}{v}$$

$$\lambda_F^{*,\pm}/v = (g \pm \sqrt{g})$$

Details of G's

$$
\begin{aligned}
\mathscr{G}^{(2n)}_{i>j} &= -\langle T_\tau F_L(\tau_i)V_{-\lambda}(\tau_i)F^\dagger(\tau_j)V_\lambda(\tau_j)\hat{P}_{2n}\rangle/\delta Z_{2n} \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+\langle F^\dagger_* F_{\bar{*}}(\tau_1)\cdots F_L(\tau_i)\cdots F^\dagger_L(\tau_j)\cdots F^\dagger_* F_{\bar{*}}(\tau_{2n})\rangle}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+\langle F^\dagger_* F_{\bar{*}}(\tau_1)\cdots\cdots F^\dagger_* F_{\bar{*}}(\tau_{2n})\rangle}. \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+\langle F_L(\tau_i)F^\dagger_L(\tau_j)F^\dagger_* F_{\bar{*}}(\tau_1)\cdots\cdots F^\dagger_* F_{\bar{*}}(\tau_{2n})\rangle(-1)^{P_{ij}}}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+\langle F^\dagger_* F_{\bar{*}}(\tau_1)\cdots\cdots F^\dagger_* F_{\bar{*}}(\tau_{2n})\rangle}
\end{aligned}
$$

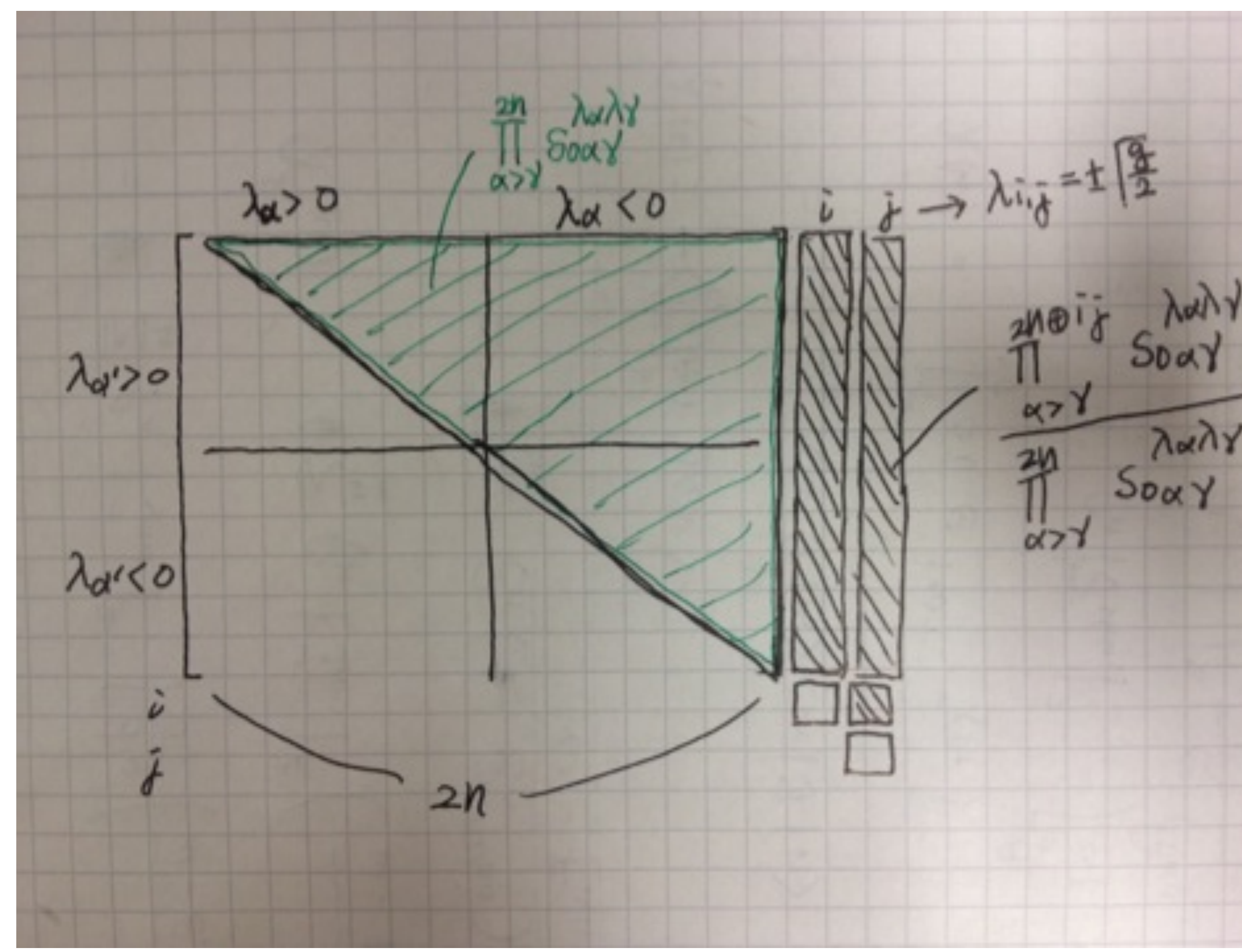
$$\lambda = \sqrt{\frac{g}{2}}$$

$$\lambda_1,\cdots,\lambda_{2n} = \pm\sqrt{2g}$$

Details of G's

$$
\begin{aligned}
\mathcal{G}^{(2n)}_{i>j} &= -\langle T_\tau F_L(\tau_i) V_{-\lambda}(\tau_i) F^\dagger(\tau_j) V_\lambda(\tau_j) \hat{P}_{2n}\rangle / \delta Z_{2n} \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots F_L(\tau_i)\cdots F_L^\dagger(\tau_j)\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}. \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_L(\tau_i) F_L^\dagger(\tau_j) F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle (-1)^{P_{ij}}}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{G}^{(2n)}_{i>j} &= -(-1)^{P_{ij}} \frac{\prod_{\alpha>\gamma}^{2n\oplus ij} s_{0\alpha\gamma}^{\lambda_\alpha\lambda_\gamma}}{\prod_{\alpha'>\gamma'}^{2n} s_{0\alpha'\gamma'}^{\lambda_{\alpha'}\lambda_{\gamma'}}}, \\
&= -(-1)^{P_{ij}} s_{0ij}^{-\lambda^2} \prod_{\gamma}^{2n} s_{0i\gamma}^{-\lambda\lambda_\gamma} \prod_{\alpha}^{2n} s_{0\alpha j}^{\lambda\lambda_\alpha}
\end{aligned}
$$



Details of G's

$$\begin{aligned}
\mathscr{G}^{(2n)}_{i>j} &= -\langle T_\tau F_L(\tau_i) V_{-\lambda}(\tau_i) F^\dagger(\tau_j) V_\lambda(\tau_j) \hat{P}_{2n}\rangle / \delta Z_{2n} \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots F_L(\tau_i)\cdots F_L^\dagger(\tau_j)\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}. \\
&= -\frac{\langle V_{\lambda_1}(\tau_1)\cdots V_{-\lambda}(\tau_i)\cdots V_\lambda(\tau_j)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_L(\tau_i) F_L^\dagger(\tau_j) F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle (-1)^{P_{ij}}}{\langle V_{\lambda_1}(\tau_1)\cdots V_{\lambda_{2n}}(\tau_{2n})\rangle_+ \langle F_*^\dagger F_{\bar{*}}(\tau_1)\cdots\cdots F_*^\dagger F_{\bar{*}}(\tau_{2n})\rangle}
\end{aligned}$$

$$\begin{aligned}
\mathscr{G}^{(2n)}_{i>j} &= -(-1)^{P_{ij}} \frac{\prod_{\alpha>\gamma}^{2n\oplus ij} s_{0\alpha\gamma}^{\lambda_\alpha\lambda_\gamma}}{\prod_{\alpha'>\gamma'}^{2n} s_{0\alpha'\gamma'}^{\lambda_{\alpha'}\lambda_{\gamma'}}}, \\
&= -(-1)^{P_{ij}} s_{0ij}^{-\lambda^2} \prod_{\gamma}^{2n} s_{0i\gamma}^{-\lambda\lambda_\gamma} \prod_{\alpha}^{2n} s_{0\alpha j}^{\lambda\lambda_\alpha} \\
&= -(-1)^{P_{ij}} s_{0ij}^{\frac{g}{2}} \left(\frac{\prod_{\alpha>\gamma}^{2n\oplus ij} s_{0\alpha\gamma}^{w_\alpha w_\gamma}}{\prod_{\alpha>\gamma}^{2n} s_{0\alpha\gamma}^{w_\alpha w_\gamma}} \right)^g \quad \text{with } w_\alpha, w_\gamma = \mathrm{sgn}(\lambda_\alpha),\ \mathrm{sgn}(\lambda_\gamma) \\
&= -(-1)^{P_{ij}} s_{0ij}^{\frac{g}{2}} \left| \frac{\det \hat{S}_{n\oplus ij}}{\det \hat{S}_n} \right|^g .
\end{aligned}$$

$$\lambda = \sqrt{\frac{g}{2}}$$

$$\lambda_1, \cdots, \lambda_{2n} = \pm\sqrt{2g}$$

Basic algorithm of CTQMC

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

"Non-interacting" part:

$$H_0 = H_c + H_f$$

$$H_c = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

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

"perturbation" part:

$$H_1 = \sum_\sigma H_{1\sigma}, \quad H_{1\sigma} = v c^\dagger_\sigma f_\sigma + \mathrm{h.c.} \qquad c_\sigma = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}$$

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

$$\begin{aligned}(-)^{2k}\langle H_1(\tau_1)\cdots\rangle &= \pm v^{2k}\langle c^\dagger_\uparrow(\tau_1)c_\uparrow(\tau_2)c^\dagger_\uparrow(\tau_3)\cdots c_\uparrow(\tau_{n_\uparrow})\rangle_{\uparrow,c}\langle c^\dagger_\downarrow(\tau'_1)c_\downarrow(\tau'_2)c^\dagger_\downarrow(\tau'_3)\cdots c_\downarrow(\tau'_{n_\downarrow})\rangle_{\downarrow,c} \\ &\quad\times\langle f_\uparrow(\tau_1)f^\dagger_\uparrow(\tau_2)f_\downarrow(\tau'_1)\cdots\rangle_f \\ &= \pm v^{2k}\det\hat{G}_{c\uparrow}\det\hat{G}_{c\downarrow}\langle f_\uparrow(\tau_1)f^\dagger_\uparrow(\tau_2)f_\downarrow(\tau'_1)\cdots\rangle_f \equiv W\end{aligned}$$

$\because$ Wick's theorem

"weight" for the config.

with $n_\uparrow + n_\downarrow = 2k$

Some details

Green's function matrix:

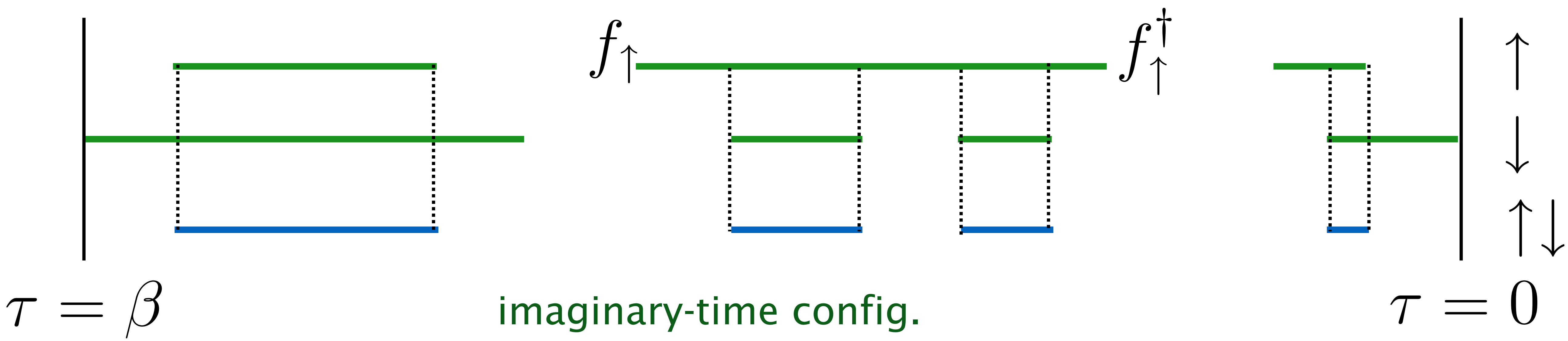
$$\left[\hat{G}_{c\uparrow}\right]_{ij} = \langle c^\dagger_\uparrow(\tau_{2i-1}) c_\uparrow(\tau_{2j}) \rangle = G^0_{c\uparrow}(\tau_{2j} - \tau_{2i-1})$$: free electron Green's function

Matrix products for local degrees of freedom:

$$\langle f_\uparrow(\tau_1) f^\dagger_\uparrow(\tau_2) f_\downarrow(\tau'_1) \cdots \rangle_f = \exp\{-\epsilon_f(l_\uparrow + l_\downarrow) - U l_{\text{doublon}}\}/Z_f$$

$$Z_f = 1 + 2e^{-\beta\varepsilon_f} + e^{-\beta(2\varepsilon_f + U)}$$

"Segment" representation:



imaginary-time config.

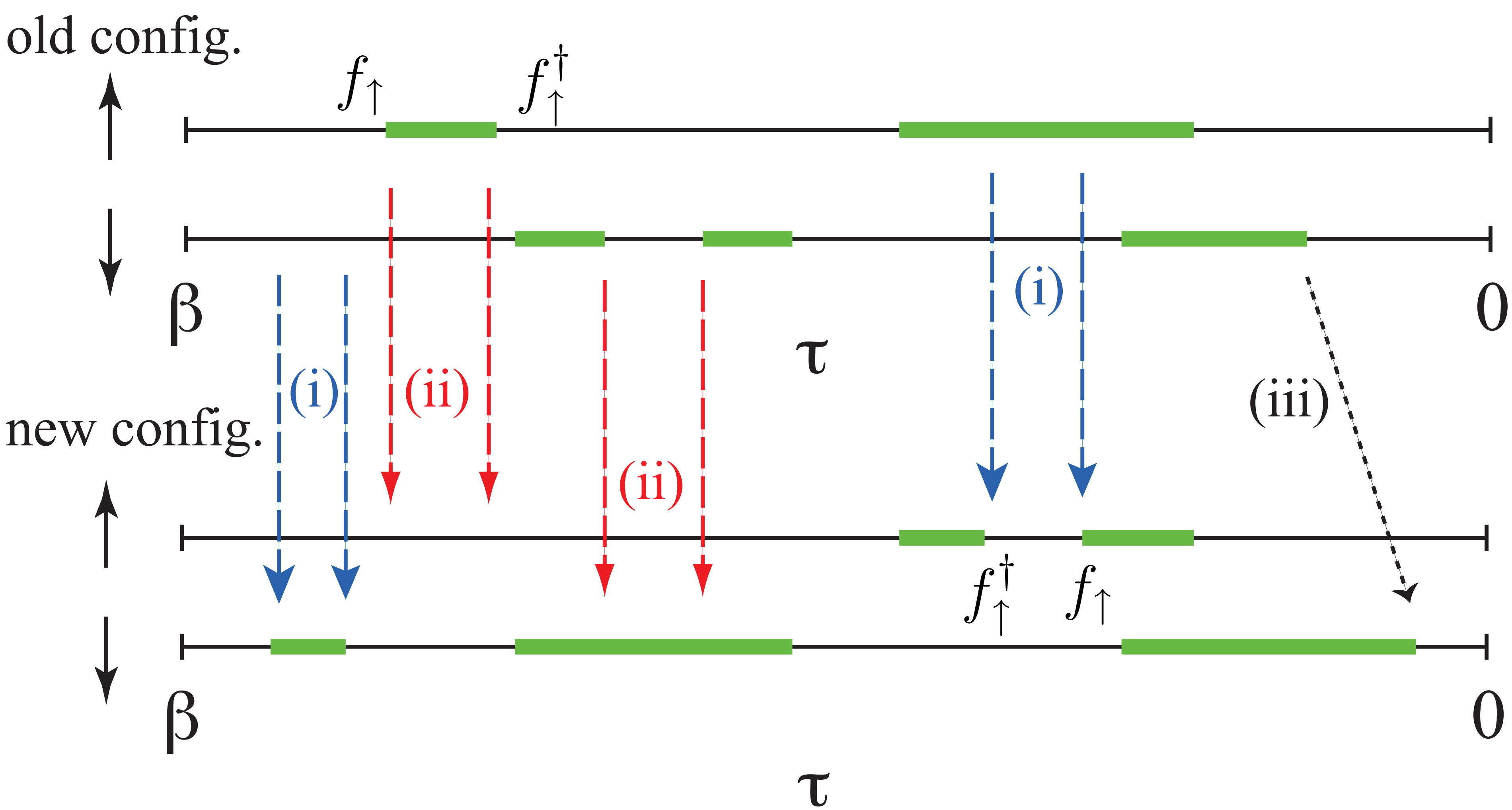
Update operations

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

calculate ratio: $R = \frac{W_{\mathrm{new}}}{W_{\mathrm{old}}} F$

accept if $\min(R, 1) > r, \quad 0 \le r \le 1$

deny otherwise (Metropolis)



F : config. dep. for (i) and (ii)

$F = 1$ for (iii)

R = empirically positive for Anderson model