Strong coupling expansion Monte Carlo

Ulli Wolff

Humboldt University, Berlin

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Capri 1989, Ulli Wolff

Critical Slowing Down

- The Problem

Alleviations and cures:

- Over-Relaxation
- Multi-Grid
- Percolation-Methods (Swendsen, Wang)

Left out:
small stepsize methods
→ try talks on dynamical fermions

Further reading:
A. Sokal, Lecture Notes
"Cours de 3ème Cycle de la Physice en Suisse Romande" 1989

Related recent plenaries in this conference series:

- Shailesh Chandrasekharan, Williamsburg 2008
- watched by $\mu_{\text{chem}} \neq 0$ community: Philippe de Forcrand, Beijing 2009, Sourendu Gupta, here 2010

Aliases:

- World-line formalism
- Loop (gas) representation
- Simulated all-order strong coupling/hopping parameter expansion

Disclaimers:

- not 'just' a new algorithm, but...
- simulation of a reformulated system, which...
- is not the dual model (despite similarities)

Basic idea, exemplified for good old Ising

Two point function (torus, any D)

$$\langle \sigma(u)\sigma(v)\rangle = \frac{Z_2(u,v)}{Z_0} = \frac{\sum_{\{\sigma(x)=\pm 1\}} \mathrm{e}^{-S[\sigma]}\sigma(u)\sigma(v)}{\sum_{\{\sigma(x)=\pm 1\}} \mathrm{e}^{-S[\sigma]}}$$

with

$$-S[\sigma] = \beta \sum_{l=\langle xy\rangle} \sigma(x)\sigma(y)$$

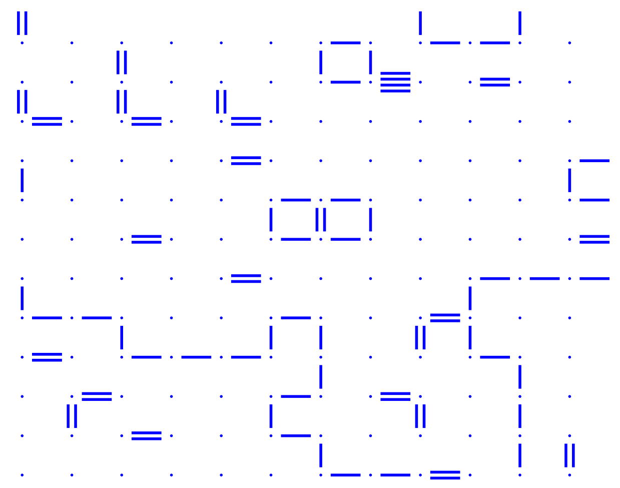
- $Z_0, Z_2\,(, Z_4 \ldots)$ have expansions in β
- convergent for all β in a finite volume
- this includes $\beta \approx \beta_c, \xi \gg 1$
- but: contributions $\sim \beta^{\mathrm{volume}}$ will be important!
- [normal (truncated) s.c.: $V \to \infty$ term by term in Z_2/Z_0]

$$
\mathrm{e}^{\beta\sigma(x)\sigma(y)} = \sum_{k=0}^{\infty} \frac{\beta^k}{k!}\,\sigma(x)^k \sigma(y)^k
$$

$$
Z_0 = \textstyle\sum_{g\in\mathcal{G}_0} \ \beta^{\sum_l k(l)} W[k]
$$

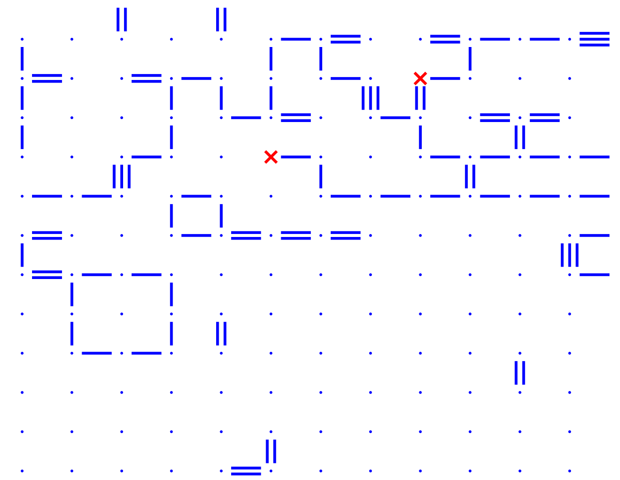
- graphs g with $k(l) = 0, \ldots, \infty$
- $(\mathrm{div}\, k)(x) \equiv \text{even}$
- $W[k] = \prod_l \frac{1}{k(l)!}$

$\Rightarrow \beta\langle\sigma\sigma\rangle_{n.n.} = \langle k(l)\rangle_{g\in\mathcal{G}_0} = \mathrm{O}(1)$



$$
Z_2 = \textstyle\sum_{g\in\mathcal{G}_{2|u,v}} \ \beta^{\sum_l k(l)} W[k]
$$

- $(\mathrm{div}\, k)(x) \equiv \text{even} + \delta_{x,u} + \delta_{x,v}$
- ‘defects’ at u and v
- $\mathcal{G}_{2|u,u} = \mathcal{G}_0$



The break-through of Prokof'ev and Svistunov

- Z_0 has been simulated as $\sum_{g \in \mathcal{G}_0} \ldots$ in ancient history [Berg & Förster, 1981]
  - $k(l) \to k(l) \pm 1$ on 4 l around plaquettes (constraint!)
  - additional steps
  - not efficient, critical slowing down

P&S: enlarge the ensemble

$$\mathcal{Z} = \sum_{g \in \mathcal{G}_2} \beta^{\sum_l k(l)} W[k] = \sum_{u,v} Z_2(u,v) \qquad \mathcal{G}_2 = \cup_{u,v} \mathcal{G}_{2|_{u,v}}$$

- PS 'worm' algorithm works on $\mathcal{G}_2$:
  - $k(l) \to k(l) \pm 1$ on single $l = \langle ux \rangle$ with $u \to x$
  - defect moves, constraint preserved
  - (practically) no critical slowing down

- easier to move $\mathcal{G}_0 \ni g \to g' \in \mathcal{G}_0$ by cutting through $\mathcal{G}_2$
- the intermediate configurations are extremely useful:

$$\langle \sigma(x)\sigma(0)\rangle = \frac{\langle \delta_{x,u-v}\rangle_g}{\langle \delta_{u,v}\rangle_g}, \qquad \langle \delta_{u,v}\rangle_g = \chi^{-1}, \quad \langle \cdot \rangle_g \equiv \langle \cdot \rangle_{g\in\mathcal{G}_2}$$

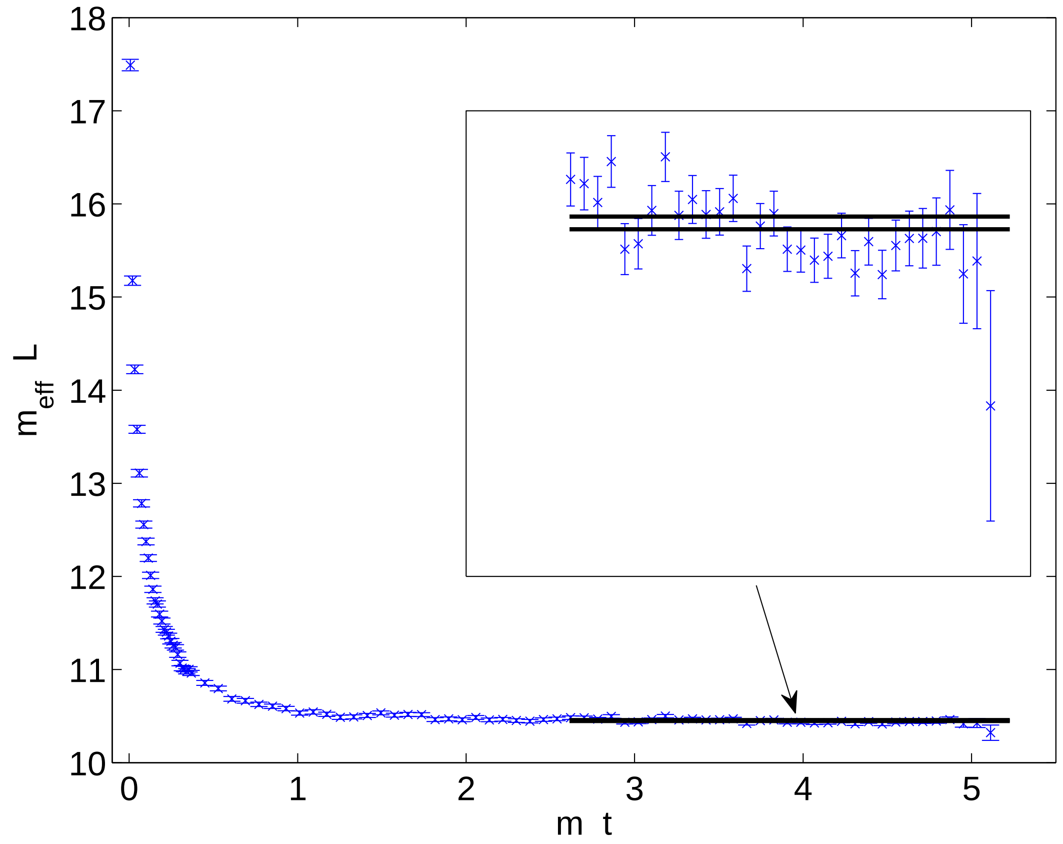
- all-x 2-point function = histogram $u-v$ of graphs

A very simple generalization:

$$\mathcal{Z} = \sum_{g\in\mathcal{G}_2} \beta^{\sum_l k(l)} W[k] \times \rho^{-1}(u-v) \qquad [\rho > 0]$$

$$\langle \sigma(x)\sigma(0)\rangle = \frac{\langle \delta_{x,u-v}\rangle_g}{\langle \delta_{u,v}\rangle_g} \times \rho(x)$$

- use a guess $\rho(x) \approx \langle \sigma(x)\sigma(0) \rangle$
- then $\langle \delta_{x,u-v} \rangle_g$: guess $\rightarrow$ exact answer
- $\langle \delta_{x,u-v} \rangle_g \approx$ const $\Rightarrow$ all bins $u-v$ get $\approx$ same statistics $\Rightarrow$ signal/noise x-independent!



$\leftarrow$ CP(3) model

$L \times L = 780 \times 780$

$m_{\rm eff}$ vs. $t = x_0$ from time slices

$\xi = 74.619(32)$

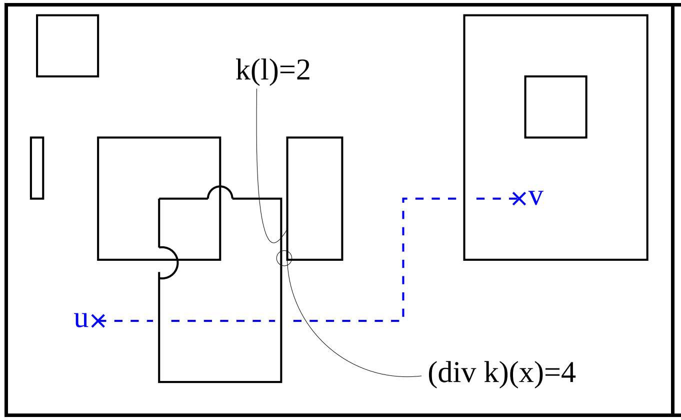
$\mathbf{O}(\boldsymbol{N})$ sigma model

$$Z(u,v)=\left[\prod_x \int d^N s\,\delta(s^2-1)\right] \mathrm{e}^{\beta\sum_l s(x)\cdot s(y)} s(u)\cdot s(v)$$

to generate graphs we need:

$$\int d^N s\,\delta(s^2-1)\,\mathrm{e}^{j\cdot s}=\sum_{n=0}^{\infty} c[n;N]\,(j\cdot j)^n \longrightarrow c[n;N]\,\text{known}$$

$$\mathcal{Z}=\sum_{g\in\mathcal{G}_2} \beta^{\sum_l k(l)} W[k;N]\,\frac{N^{|g|}}{\mathcal{S}[g]}\times\rho^{-1}(u-v)$$



- lines now paired around sites
- $c[.,.]$ enter into W
- $|g| = \#$ of closed loops
- $\mathcal{S}[g]$ symmetry factor of g

yes, we can .... ergodically sample such graphs:

- g stored and updated as (multiply) linked list
- size a priori unknown, no problem: $\sum_l k(l) = \mathrm{O}(V) \pm \mathrm{O}(\sqrt{V})$
- also $|g| = \mathrm{O}(V)$
- beside updates $\Delta k(l) = \pm 1$ (with u hopping), we make
- line re-connect-steps at u and v
- 1 iteration := V steps at u, v ~ 1 'sweep'
- (practically) no slowing down in units 'iterations'
- N may be treated stochastically (I-algo) or exactly (R-algo)
- I: cost/it $\propto L^D$, integer N only
- R: cost/it $\propto L^{D+z}$, real N, $z_{\mathrm{eff}} \sim 0.3$ $(D=2, N=3, \xi=7...65)$

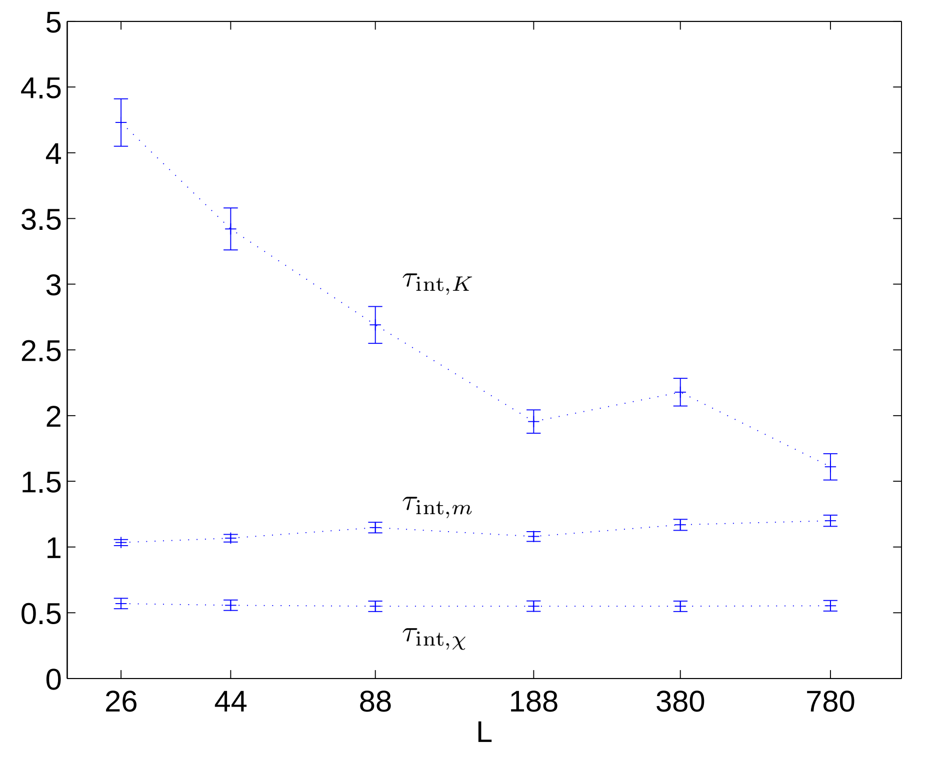
$\mathbf{CP}(\boldsymbol{N}-\mathbf{1})$

- field: $\varphi(x) \in \mathbb{C}^N, |\varphi(x)| = 1$
- invariant: $\varphi(x) \to \varphi(x) \mathrm{e}^{i\alpha(x)}$ and global $\mathrm{SU}(N)$
- lattice actions: quartic in φ or explicit $\mathrm{U}(1)$ gauge field expected (and seen): same universality class
- $\mathrm{SU}(N)$ adjoint correlations of $j^a(x) = \varphi^\dagger(x) \lambda^a \varphi(x)$

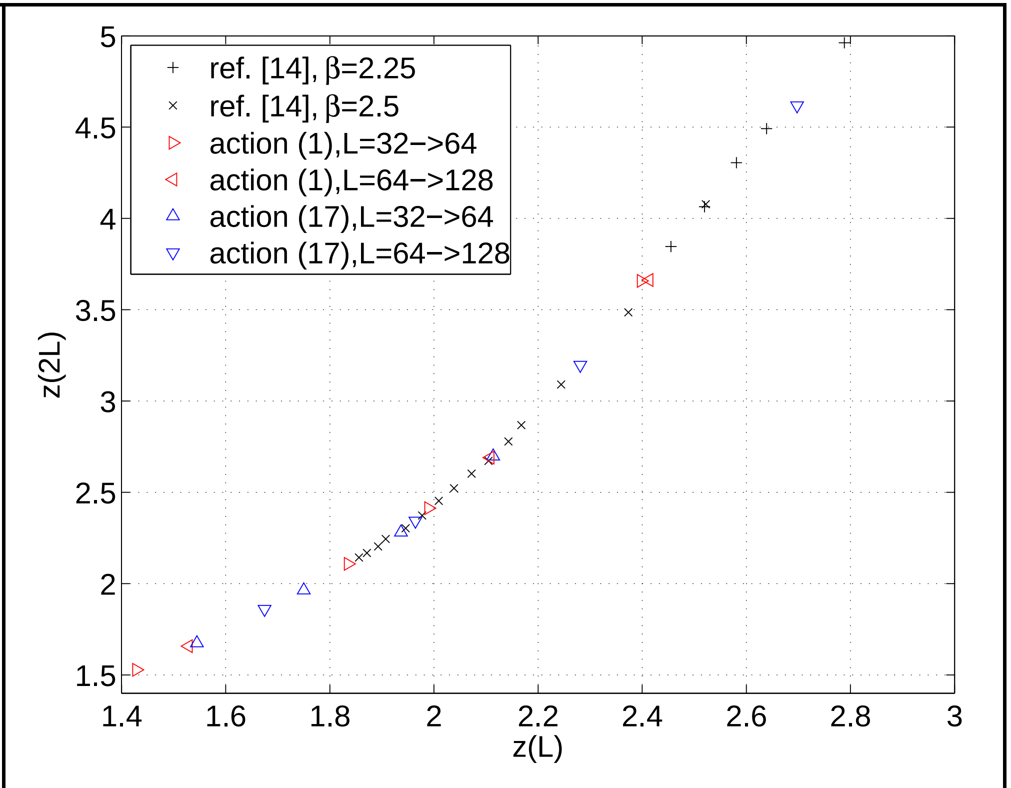
$$\langle j^a(u) j^a(v) \rangle = \frac{Z_2(u,v)}{Z_0} \qquad \ldots\ldots \longrightarrow \ldots\ldots$$

$$\mathcal{Z} = \sum_{g \in \mathcal{G}_2} \beta^{\sum_l k(l)} W[k; N] \frac{N^{|g|}}{\mathcal{S}[g]} \times \rho^{-1}(u-v)$$

- different $\mathcal{G}_2$ now (compared to $\mathrm{O}(N)$):
  - oriented lines and loops, but
  - flux zero through each link



τ_{int}: [I-iterations]
$\mathrm{CP}(3), D=2, mL\approx 10,\ \xi=2.6\ldots 75$



step scaling, $z(L)=m(L)L$
$\mathrm{CP}(2)$, both actions + Pepe&Wiese data

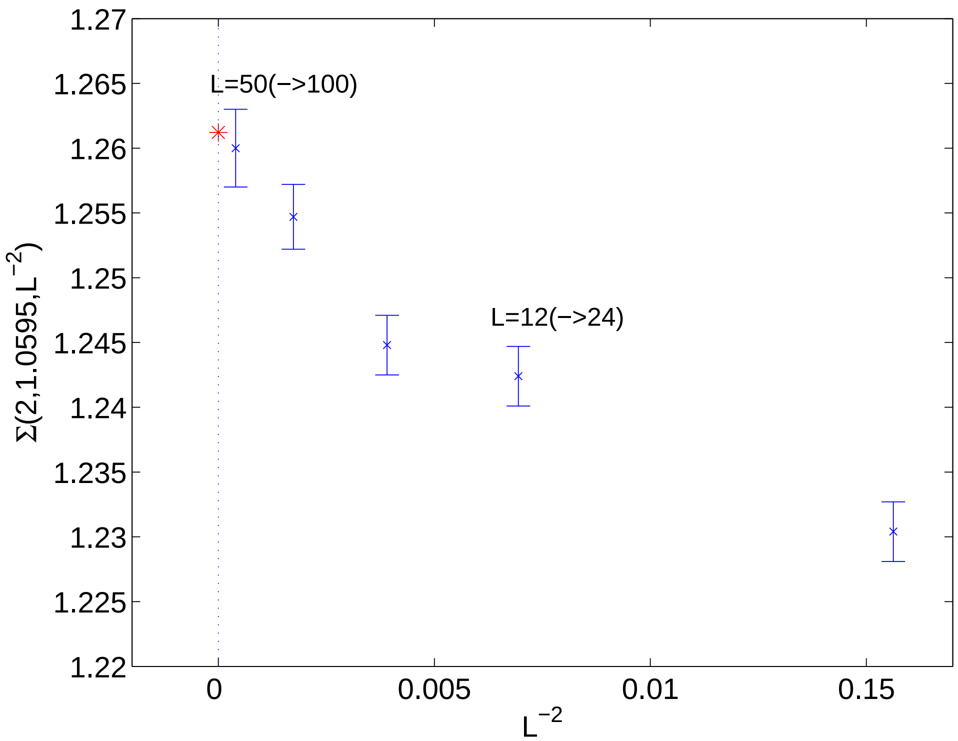
Nienhuis action in the O(3) model

- allow only $g \in \mathcal{G}_2$ with $k(l) = 0, 1$ on all links
- g-simulation: no problem
- equivalent to Nienhuis (first: Domany et al. 1981) action:

$$Z_0 = \left[\prod_x \int d^N s \delta(s^2 - 1) \right] \prod_{l = \langle x y \rangle} [1 + \beta s(x) \cdot s(y)]$$

- Nienhuis: exactly solved for $D = 2, N \leqslant 2$
  honeycomb lattice, $\beta \leqslant 1$
- sign problem for $\beta > 1$!

$$\Sigma(2,u,a/L) = m(2L)2L|_{m(L)L=u} = \sigma(2,u) + \mathrm{O}(a^2)$$

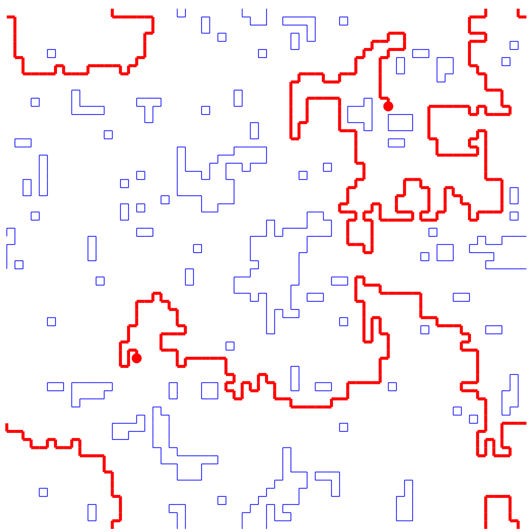
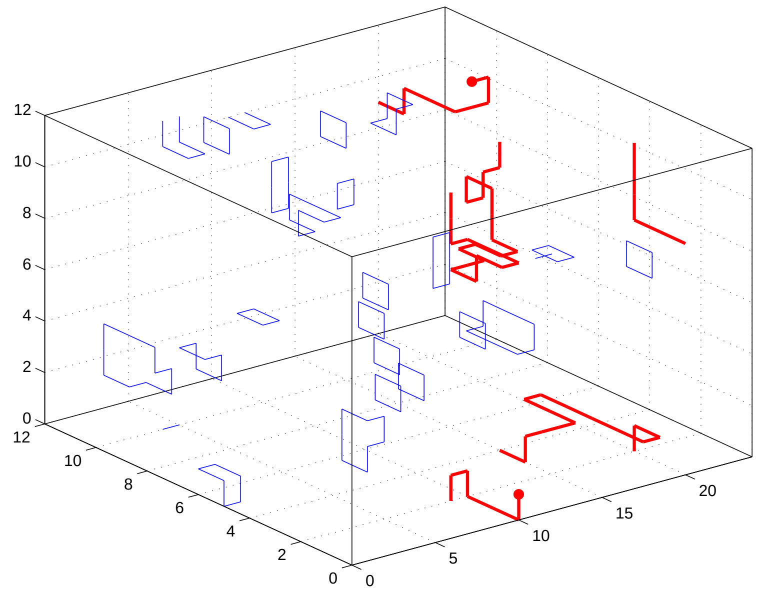


this plot: $\beta = 1.8 \ldots 3.1$

exact continuum result (Balog & Hegedus, 2004, Bethe Ansatz):

$$\sigma(2, 1.0595) = 1.261210 \longleftrightarrow *$$

Fermions

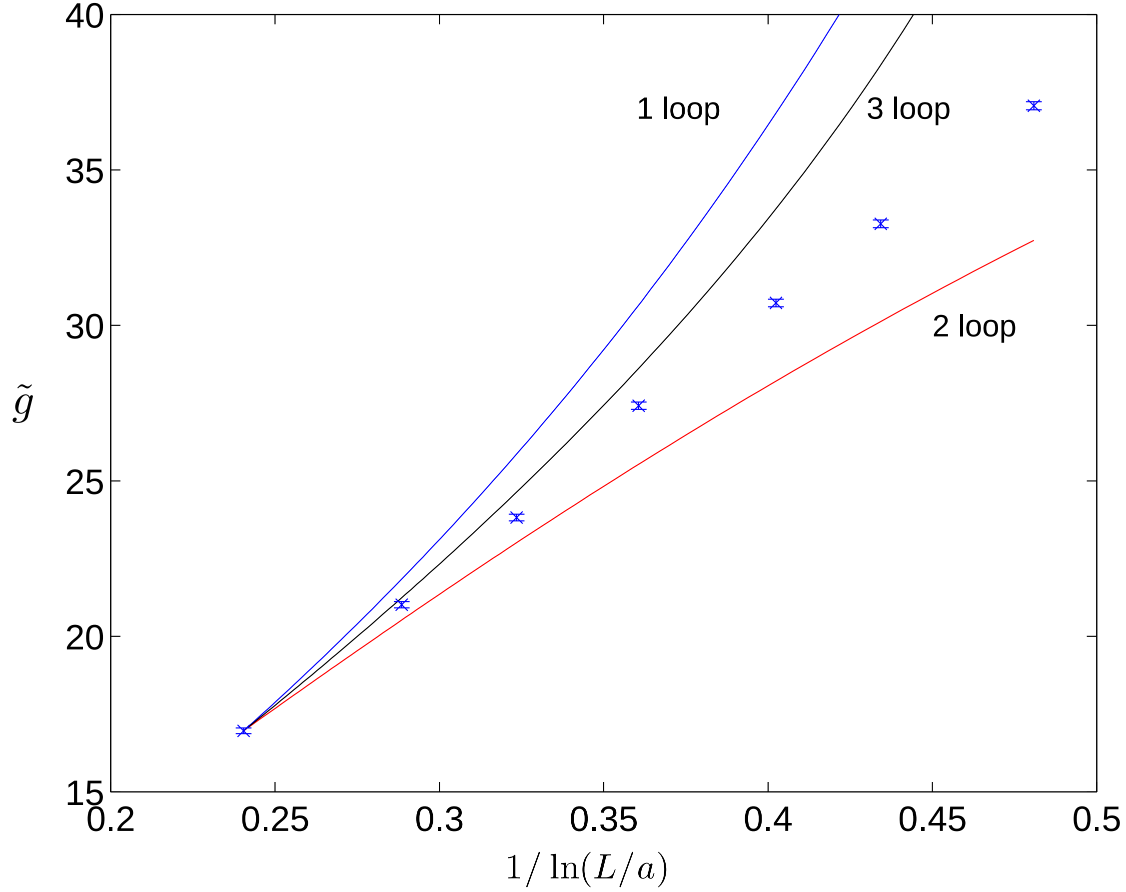
Wilson-Majorana $\leftrightarrow$ self-avoiding loops essentially positive for $D=2$: $(-)_{\mathrm{Fermi}} \times (-)_{2\pi\,\mathrm{spin-rot.}}$ below: typical graph g for $\langle \psi_\alpha(u)\overline{\psi}_\beta(v)\rangle$: Gross-Neveu possible to simulate	representation and algorithm also for $D=3$ spin-phase now in Z(8) [continuum $\rightarrow$ U(1)] for non-planar loops $\rightarrow$ sign problem $\rightarrow$ no small mass possible
	

Triviality of φ^4

- Aizenman's rigorous proofs (bounds) for $D > 4$ use
  - our $g \in \mathcal{G}_2$ representation for Ising
  - plus: replica and percolation ideas
- Translate into MC estimators for any D (incl. $D = 4$)
- Result

$$g_R = -\frac{\chi_4}{\chi^2}(m_R)^D = 2z^D \langle \mathcal{X} \rangle_{(g,g') \in \mathcal{G}_2 \times \mathcal{G}_2} \quad \mathcal{X} \in \{0, 1\}, z = m_R L$$

- no numerical cancellation for connected χ_4
- Lebowitz inequality manifest



$$D=4,\ m_R L=4,\ L/a=64,\ldots,8$$

Conclusions

- some lattice QFTs can be represented by their all-order $\beta(\kappa)$ expansion (without sign problem! In general?)
- MC sampling possible by locally deforming graphs
  - CSD seems a new question: generate large independent equilibrium graphs $\leftrightarrow$ long distance correlated configs
- new opportunities for certain observables (adapted ensemble)
- sign problem can be different for $\sum_{\text{conf}} \cdots$ vs. $\sum_{\text{graphs}} \cdots$ example: bosons with μ_{chem} [Endres; Banarjee, Chandrasekharan]
- gauge theory, defects: points $\rightarrow$ loops [$\rightarrow$ talk Tomasz Korzec]
- fermions in $D > 2$ (even free!)??

Other contributors (incomplete, 1002 apologies): O.Bär, D.Baumgärtner, Y.Deng, P.DeForcrand, T.M.Garoni, C.Gattringer, W.Janke, T.Korzec, V.Maillart, T.Neuhaus, F.Niedermayer, W.Rath, A.M.J.Schakel, A.D.Sokal, J.W.Cherrington, U.Wenger, U.J.Wiese