Diagrammatic Monte-Carlo algorithms for large-N quantum field theories from Schwinger-Dyson equations

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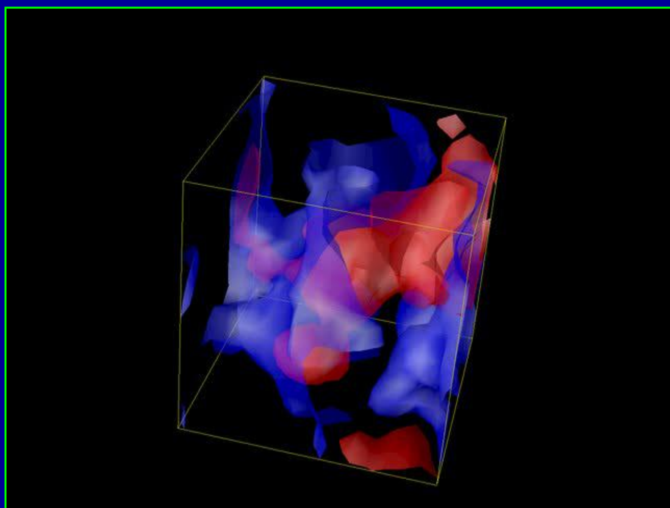
Motivation: Diagrammatic Monte-Carlo Quantum field theory:

Sum over fields



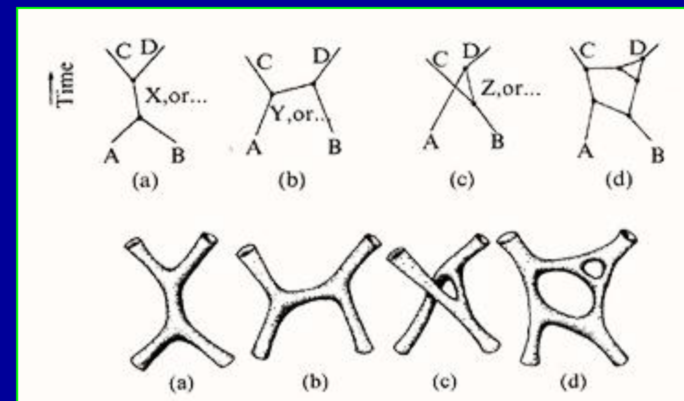
$$\mathcal{Z} = \mathrm{Tr}\, e^{-\hat{\mathcal{H}}/kT} =$$
$$= \int \mathcal{D}\phi\left(x^{\mu}\right) \exp\left(-S_E\left[\phi\left(x^{\mu}\right)\right]\right)$$

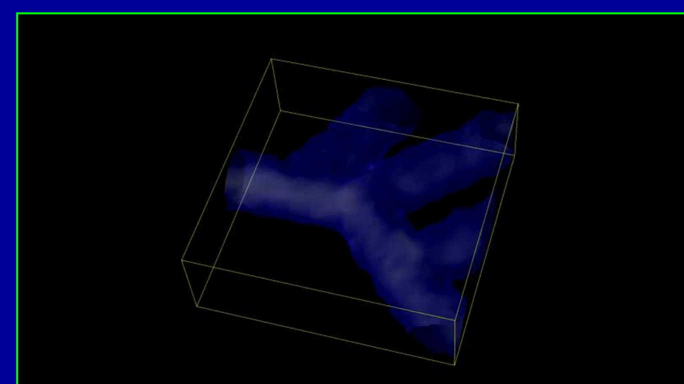
Euclidean action:

$$S_E = \int d^D x \left(\frac{1}{2}\,\partial_{\mu}\phi\partial_{\mu}\phi + \frac{m^2}{2}\,\phi^2 + V\left(\phi\right)\right)$$

Perturbative expansions

Sum over interacting paths





$$\mathcal{Z} = \sum_k \frac{\lambda^k}{k!} \exp\left(-L\left(\text{Paths connecting } k \text{ vertices}\right)\right)$$

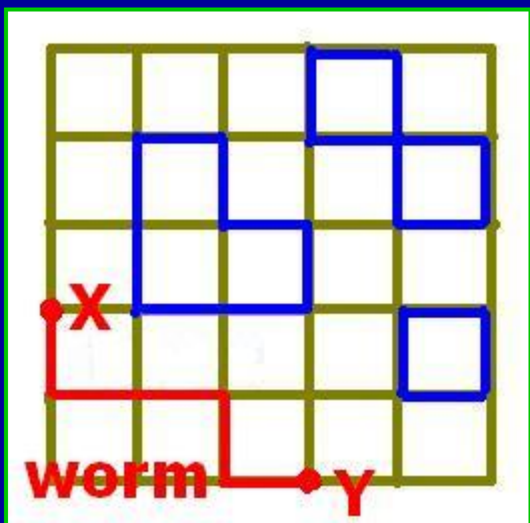
Motivation: QCD side

- Recent attempts to apply DiagMC to lattice QCD at finite density and reduce sign problem
- DiagMC relies on Abelian "Duality transformations"
- BUT: no convenient duality transformations for non-Abelian fields Weak-coupling expansions are also cumbersome and difficult to re-sum

- DiagMC in the non-Abelian case?
- Avoid manual duality transformations?
- How to avoid Borel resummations?

Worm Algorithm [Prokof'ev, Svistunov]

- Monte-Carlo sampling of closed vacuum diagrams:
  nonlocal updates, closure constraint
- Worm Algorithm: sample closed diagrams + open diagram
- Local updates: open graphs $\longleftrightarrow$ closed graphs
- Direct sampling of field correlators (dedicated simulations)



x, y – head and tail of the worm

$$\langle \sigma_x \sigma_y \rangle \sim p(x,y)$$

Correlator = probability distribution of head and tail

- Applications: systems with "simple" and convergent perturbative expansions (Ising, Hubbard, 2d fermions …)
- Very fast and efficient algorithm!!!

General structure of SD equations

(everywhere we assume lattice discretization)

$$\int \mathcal{D}\phi \frac{\partial}{\partial\phi(X)} \left(O_1[\phi] \ldots O_n[\phi] \exp\left(-S[\phi]\right)\right) = 0$$

$$\sum_{A=1}^{n} \langle O_1[\phi] \ldots \frac{\partial O_A[\phi]}{\partial\phi(x)} \ldots O_n[\phi] \rangle =$$
$$= \langle O_1[\phi] \ldots O_n[\phi] \; \frac{\partial S[\phi]}{\partial\phi(x)} \rangle$$

Choose some closed set of observables *φ(X)*

***X* is a collection of all labels, e.g. for scalar field theory**

$$\phi(X) = \langle \phi(x_1) \ldots \phi(x_n) \rangle, \quad X = \{x_1, \ldots, x_n\}$$

SD equations (with disconnected correlators) are linear:

$$\phi(X) = \sum_{Y} A(X|Y)\,\phi(Y) + b(X)$$

A(X | Y): infinite-dimensional, but sparse linear operator

b(X): source term, typically only 1-2 elements nonzero

Stochastic solution of linear equations

Assume: *A(X|Y), b(X)* are positive, |eigenvalues| < 1

$$\phi = A\phi + b \Rightarrow \phi = (1-A)^{-1} b = \sum_{m=0}^{+\infty} A^m b$$

$$\phi(X) = \sum_{n=0}^{+\infty} \sum_{X_0} \ldots \sum_{X_n} \delta(X, X_n) A(X_n|X_{n-1}) \ldots A(X_1|X_0) b(X_0)$$

Solution using the Metropolis algorithm:

Sample sequences *{X_n, ..., X_0}* with the weight

$$w(X_n, \ldots, X_0) = \mathcal{N}_w^{-1} A(X_n|X_{n-1}) \ldots A(X_1|X_0) b(X_0)$$

Two basic transitions:

- **Add new index X_{n+1},**

$$\{X_{n+1}, X_n, \ldots, X_0\} \to \{X_n, \ldots, X_0\}$$

$$\pi(X_{n+1}|X_n) = \frac{A(X_{n+1}|X_n)}{\mathcal{N}(X_n)}$$

- **Remove index**

$$\{X_n, X_{n-1}, \ldots, X_0\} \to \{X_{n-1}, \ldots, X_0\}$$

- **Restart**

$$\{X_0\} \to \{X_0'\} \qquad \pi(X_0') = b(X_0') / \mathcal{N}_b$$

$$\mathcal{N}(Y) = \sum_X A(X|Y), \quad \mathcal{N}_b = \sum_X b(X)$$

Stochastic solution of linear equations

- With probability p_+: Add index step
- With probability $(1-p_+)$: Remove index/Restart

Ergodicity: any sequence can be reached
(unless A(X|Y) has some block-diagonal structure)

Acceptance probabilities (no detailed balance, Metropolis-Hastings)

$$\alpha\left(\mathcal{S} \to \mathcal{S}'\right) = \min\left(1, \frac{w\left(\mathcal{S}'\right)\pi\left(\mathcal{S}' \to \mathcal{S}\right)}{w\left(\mathcal{S}\right)\pi\left(\mathcal{S} \to \mathcal{S}'\right)}\right)$$

$$\alpha_{add} = \frac{\mathcal{N}(X_n)(1-p_+)}{p_+}, \quad \alpha_{remove} = \frac{p_+}{\mathcal{N}(X_{n-1})(1-p_+)}, \quad \alpha_{restart} = 1.$$

- Parameter p_+ can be tuned to reach optimal acceptance
- Probability distribution of $N(X)$ is crucial to asses convergence

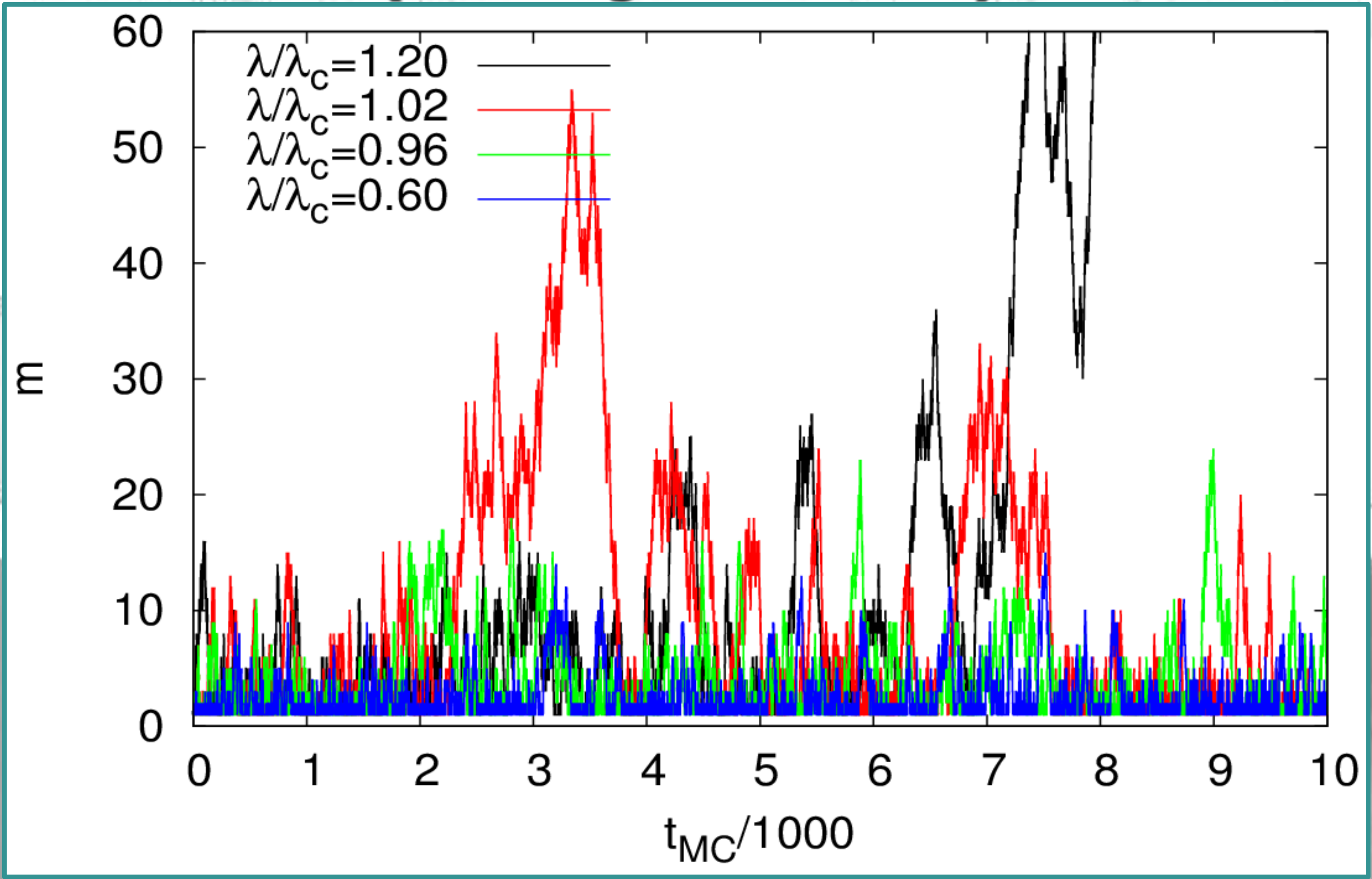
Finally: make histogram of the last element X_n in the sequence

Solution $\varphi(X)$, normalization factor

$$\mathcal{N}_w = \frac{\mathcal{N}_b}{1-\langle\mathcal{N}(X_n)\rangle} \Rightarrow \langle\mathcal{N}(X)\rangle < 1$$

Illustration: ϕ^4 matrix model

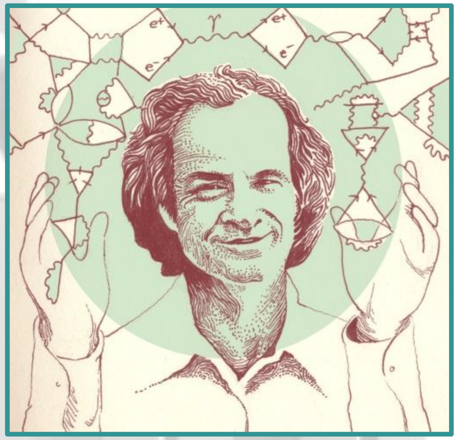
(Running a bit ahead)



Large autocorrelation time and large fluctuations near the phase transition

Practical implementation

- **Keeping the whole sequence $\{X_n, \ldots, X_0\}$ in memory is not practical (size of X can be quite large)**
- **Use the sparseness of $A(X \mid Y)$, remember the sequence of transitions $X_n \rightarrow X_{n+1}$**
- **Every transition is a summand in a symbolic representation of SD equations**
- **Every transition is a "drawing" of some element of diagrammatic expansion (either weak- or strong-coupling one)**



Save:

- **current diagram**
- **history of drawing**

Need DO and UNDO operations for every diagram element

Construction of algorithms is almost automatic and can be nicely combined with symbolic calculus software (e.g. Mathematica)

Sign problem and reweighting

- Now lift the assumptions *A(X | Y) > 0*, *b(X)>0*
- Use the absolute value of weight for the Metropolis sampling

$$w\left(X_n, \ldots, X_0\right) = \mathcal{N}_w^{-1} \left|A\left(X_n|X_{n-1}\right)\right| \ldots \left|A\left(X_1|X_0\right)\right| \left|b\left(X_0\right)\right|$$

- Sign of each configuration:

$$S\left(X_n, \ldots, X_0\right) = \operatorname{sign} A\left(X_n|X_{n-1}\right) \ldots \operatorname{sign} A\left(X_1|X_0\right) \operatorname{sign} b\left(X_0\right)$$

- Define $\tilde{A}\left(X|Y\right) = \left|A\left(X|Y\right)\right|$ $\tilde{b}\left(X\right) = \left|b\left(X\right)\right|$
- Effectively, we solve the system $\tilde{\phi} = \tilde{A}\tilde{\phi} + \tilde{b}$
- The expansion $\tilde{\phi} = \sum_{m=0}^{+\infty} \tilde{A}^m \tilde{b}$ has smaller radius of convergence
- Reweighting fails if the system $\tilde{\phi} = \tilde{A}\tilde{\phi} + \tilde{b}$ approaches the critical point (one of eigenvalues approach 1)

One can only be saved by a suitable reformulation of equations which makes the sign problem milder

Resummation/Rescaling

Growth of field correlators $\langle \phi(x_n) \ldots \phi(x_0) \rangle$ with n/ order:

- Exponential in the large-N limit
- Factorial at finite N, ϕ = A ϕ + b has no perturbative solution

How to interprete $\langle \phi(x_n) \ldots \phi(x_0) \rangle$ as a probability distribution?

Large N limit

Exponential growth? Introduce "renormalization constants" :

$$\langle \phi(x_n) \ldots \phi(x_0) \rangle = \mathcal{N} c^n w(x_n, \ldots, x_0)$$

$$\sum_{n=1}^{+\infty} \sum_{x_n \ldots x_0} w(x_n, \ldots, x_0)$$

is now finite ,

can be interpreted as probability

In the Metropolis algorithm: all the transition weights should be finite, otherwise unstable behavior

How to deal with factorial growth? ➡ Borel resummation

Borel resummation

- **Probability of "split" action grows as**

$$\sum_{A=1}^{m} \sum_{a=1}^{n_A+1} (n_A + 2 - a)$$

Obviously, cannot be removed by rescaling of the form *$N c^n$*

Introduce rescaling factors which depend on

number of vertices OR genus

$$G(n_1, \ldots, n_m) = \sum_{g=0}^{+\infty} \frac{1}{N^{2g}} G_g(n_1, \ldots, n_m)$$

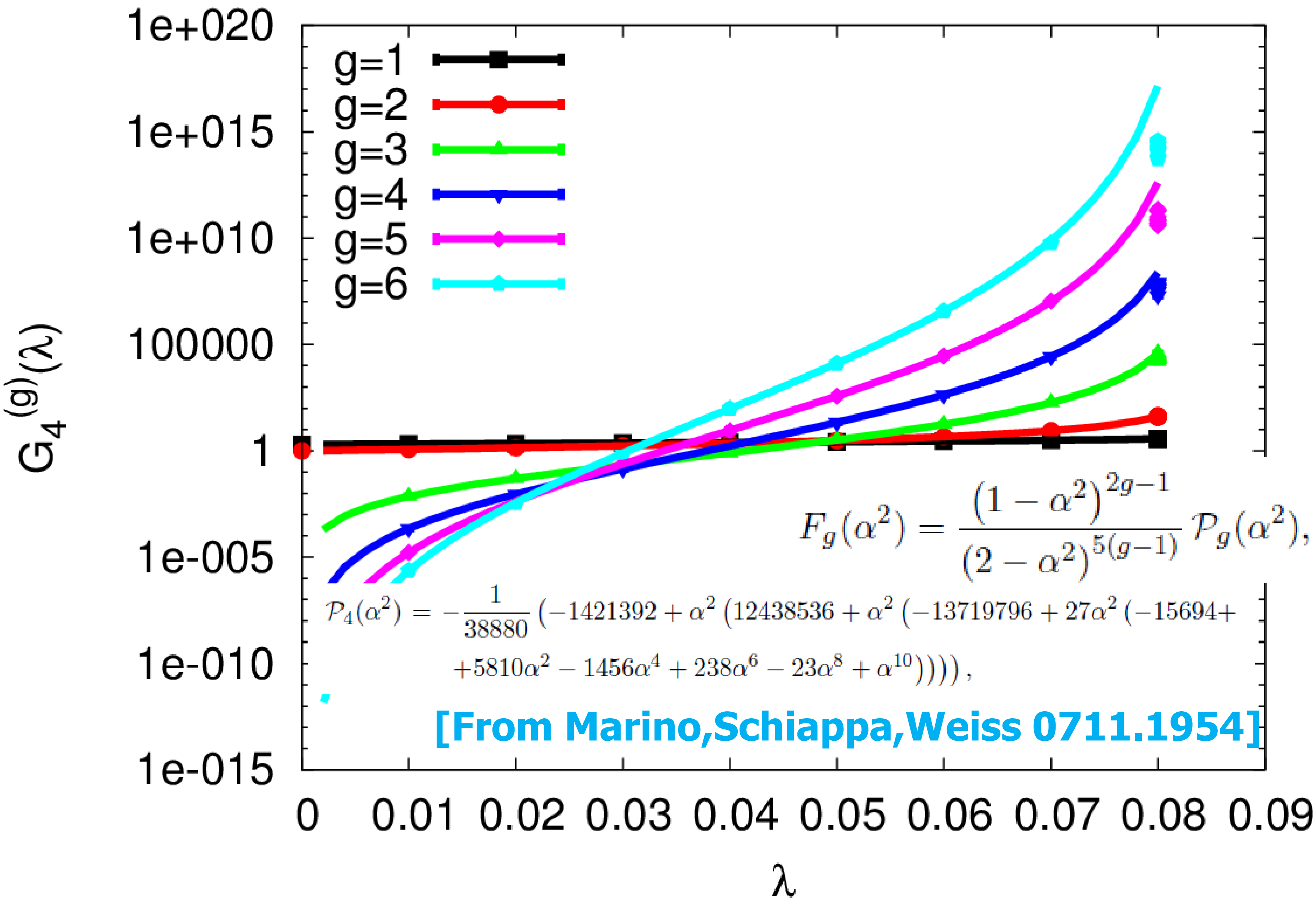
$$G_g(n_1, \ldots, n_m) = f(g, n, m) w_g(n_1, \ldots, n_m)$$

$$f(g, n, m) = f_g N_g^m c_g^n$$

$$f_g \sim \Gamma(2\nu g), \ \nu > 1$$

$$\frac{c_g}{c_{g+1}} = \left(1 + \frac{A}{g^\nu}\right)^{-1}$$

Genus expansion: ϕ^4 matrix model

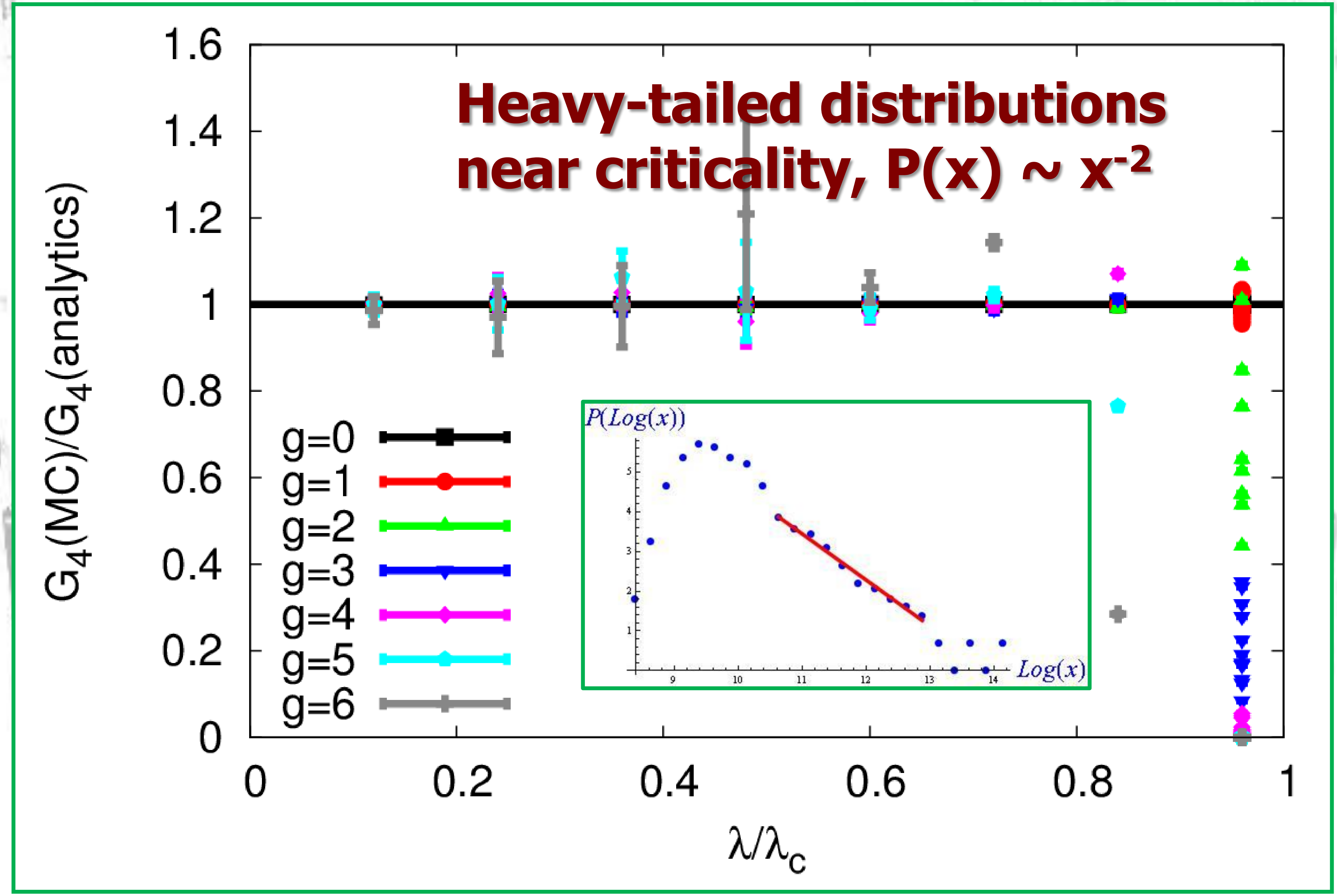


$$F_g(\alpha^2) = \frac{(1-\alpha^2)^{2g-1}}{(2-\alpha^2)^{5(g-1)}}\mathcal{P}_g(\alpha^2),$$

$$\mathcal{P}_4(\alpha^2) = -\frac{1}{38880}\left(-1421392 + \alpha^2\left(12438536 + \alpha^2\left(-13719796 + 27\alpha^2\left(-15694+ +5810\alpha^2 - 1456\alpha^4 + 238\alpha^6 - 23\alpha^8 + \alpha^{10}\right)\right)\right)\right),$$

[From Marino,Schiappa,Weiss 0711.1954]

Genus expansion: ϕ^4 matrix model



Lessons from SU(N) sigma-model

Nontrivial playground similar to QCD!!!

Action:

$$\mathcal{Z} = \int\limits_{SU(N)} \mathcal{D}g_x \, \exp\left(-\frac{N}{\lambda} \sum_{x,y} D_{xy} \mathrm{tr}\, g_x g_y^\dagger \right)$$

Observables:

$$\mathcal{G}\left(x_1, y_1, \ldots, x_n, y_n\right) = \\ = \frac{1}{N} \left\langle \mathrm{tr}\, \left(g_{x_1} g_{y_1}^\dagger \ldots g_{x_n} g_{y_n}^\dagger \right) \right\rangle$$

Schwinger-Dyson equations:

$$\begin{aligned}
&\mathcal{G}\left(x_1, y_1, \ldots, x_n, y_n\right) = \sum_{A=2}^{n-1} \delta_{x_1, y_A} \mathcal{G}\left(x_A, y_1, \ldots, x_{A-1}, y_{A-1}\right) \mathcal{G}\left(x_{A+1}, y_{A+1}, \ldots, x_n, y_n\right) + \\
&+ \delta_{x_1, y_1} \mathcal{G}\left(x_2, y_2, \ldots, x_n, y_n\right) + \delta_{x_1, y_n} \mathcal{G}\left(x_n, y_1, \ldots, x_{n-1}, y_{n-1}\right) - \\
&- \sum_{A=2}^{n} \delta_{x_1, x_A} \mathcal{G}\left(x_1, y_1, \ldots, x_{A-1}, y_{A-1}\right) \mathcal{G}\left(x_A, y_A, \ldots, x_n, y_n\right) - \\
&- \frac{1}{\lambda} D_{x_1 x} \mathcal{G}\left(x, y_1, \ldots, x_n, y_n\right) + \frac{1}{\lambda} D_{x_1 x} \mathcal{G}\left(x_1, x, x_1, y_1, \ldots, x_n, y_n\right)
\end{aligned}$$

Stochastic solution naturally leads to strong-coupling series!

Alternating sign already @ leading order

Lessons from SU(N) sigma-model

SD equations in momentum space:

$$\mathcal{G}\left(p_1, q_1, \ldots, p_n, q_n\right) = \frac{1}{V^{2n}} \sum_{x_1, y_1} \cdots \sum_{x_n, y_n} \exp\left(i \sum_A p_A x_A + i \sum_A q_A y_A\right) \mathcal{G}\left(x_1, y_1, \ldots, x_n, y_n\right)$$

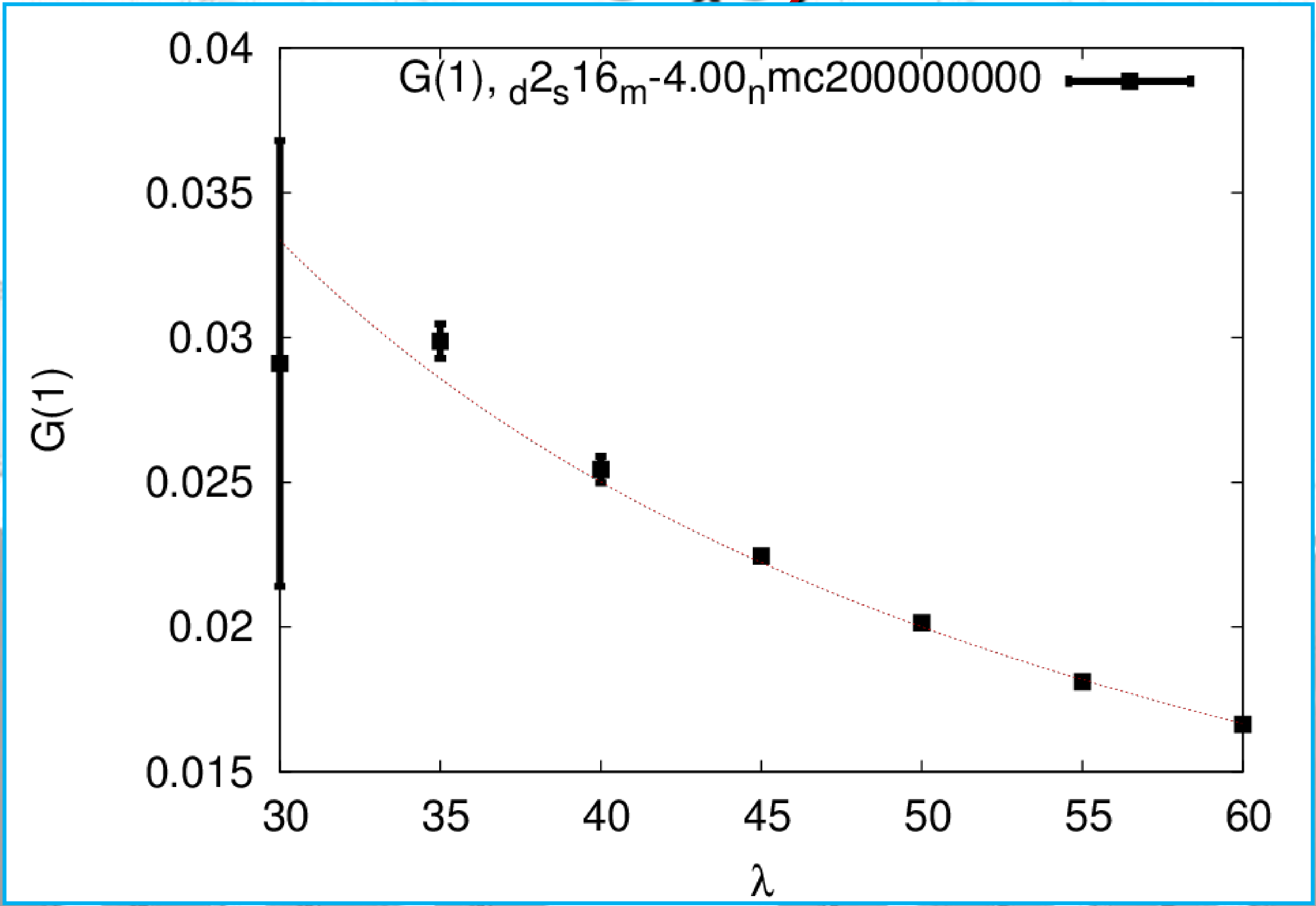
$$\mathcal{G}_0\left(p\right) = \left(\lambda + D\left(p\right)\right)^{-1}$$

$$\mathcal{G}\left(p_1, q_1\right) = \lambda \frac{\mathcal{G}_0(p_1) \delta(p_1 + q_1)}{V} + \mathcal{G}_0\left(p_1\right) \sum_{\tilde{p}_1, \tilde{q}_1, \tilde{p}_2} \delta\left(p_1, \tilde{p}_1 + \tilde{q}_1 + \tilde{p}_2\right) D\left(\tilde{q}_1\right) \mathcal{G}\left(\tilde{p}_1, \tilde{q}_1, \tilde{p}_2, q_1\right)$$

$$\begin{aligned}
&\mathcal{G}\left(p_1, q_1, \ldots, p_n, q_n\right) = \\
&= \sum_{A=2}^{n-1} \lambda \frac{\mathcal{G}_0(p_1)\, \delta(p_1 + q_A)}{V} \mathcal{G}\left(p_A, q_1, \ldots, p_{A-1}, q_{A-1}\right) \mathcal{G}\left(p_{A+1}, q_{A+1}, \ldots, p_n, q_n\right) + \\
&+ \lambda \frac{\mathcal{G}_0(p_1)\, \delta(p_1 + q_1)}{V} \mathcal{G}\left(p_2, q_2, \ldots, p_n, q_n\right) + \\
&+ \lambda \frac{\mathcal{G}_0(p_1)\, \delta(p_1 + q_n)}{V} \mathcal{G}\left(p_n, q_1, p_2, q_2, \ldots, p_{n-1}, q_{n-1}\right) - \\
&- \lambda \frac{\mathcal{G}_0(p_1)}{V} \sum_{A=2}^{n} \sum_{\tilde{p}_1 \tilde{p}_A} \delta\left(p_1 + p_A, \tilde{p}_1 + \tilde{p}_A\right) \mathcal{G}\left(\tilde{p}_1, q_1, p_2, q_2, \ldots, p_{A-1}, q_{A-1}\right) \mathcal{G}\left(\tilde{p}_A, q_A, \ldots, p_n, q_n\right) + \\
&+ \mathcal{G}_0\left(p_1\right) \sum_{\tilde{p}_1, \tilde{q}_1, \tilde{p}_2} \delta\left(p_1, \tilde{p}_1 + \tilde{q}_1 + \tilde{p}_2\right) D\left(\tilde{q}_1\right) \mathcal{G}\left(\tilde{p}_1, \tilde{q}_1, \tilde{p}_2, q_1, p_2, q_2, \ldots, p_n, q_n\right)
\end{aligned}$$

Lessons from SU(N) sigma-model

$\langle 1/N \, \mathrm{tr} \, g^{+}_{x} \, g_{y} \rangle$ vs λ



Deep in the SC regime, only few orders relevant…

Lessons from SU(N) sigma-model

Matrix Lagrange Multiplier

$$\mathcal{Z} = \int dg_x \int d\xi_x \exp\left(-\frac{N}{\lambda} \sum_{x \neq y} D_{xy} \mathrm{tr}\,\left(g_x^\dagger g_y\right) - \frac{iN}{\lambda} \sum_x \mathrm{tr}\,\left(\xi_x g_x^\dagger g_x - \xi_x\right)\right) =$$

$$= \int d\xi_x \exp\left(N \mathrm{tr}\,\ln\left(D_{xy} + i\xi_x \delta_{xy}\right) + \frac{iN}{\lambda} \sum_x \mathrm{tr}\,\xi_x \right)$$

$$G_{xy} = \left(D_{xy} + i\xi_x \delta_{xy}\right)^{-1}$$

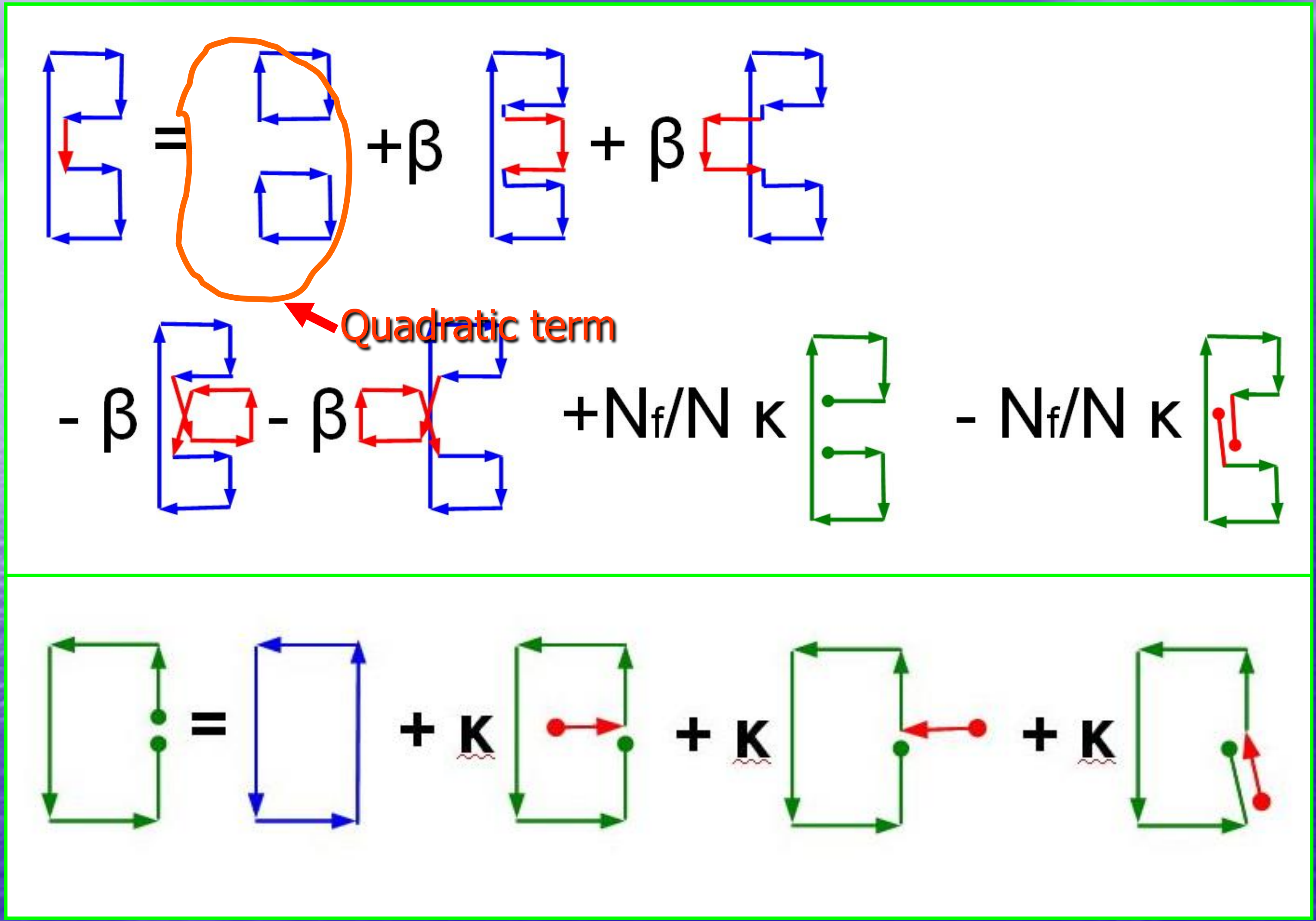
$$m^2 \equiv \lambda + 2D\left(1 - \langle\, \mathrm{tr}\, g_x^\dagger g_{x+\hat{0}} \,\rangle\right)$$

Nonperturbative improvement!!! [Vicari, Rossi,…]

$$\begin{aligned}
&\langle G_{p_1 q_1} \ldots G_{p_n q_n} \rangle = \frac{1}{V} \mathcal{G}\left(p_1\right) \delta\left(p_1 + q_1\right) \langle G_{p_2 q_2} \ldots G_{p_n q_n} \rangle + \\
&+ \frac{\lambda}{V} \mathcal{G}\left(p_1\right) \sum_{A=2}^{n} \sum_{\tilde{p}_1, \tilde{p}_A} \delta\left(p_1 + p_A - \tilde{p}_1 - \tilde{p}_A\right) \langle G_{\tilde{p}_1 q_1} \ldots G_{p_{A-1} q_{A-1}} \rangle \langle G_{\tilde{p}_A q_A} \ldots G_{p_n q_n} \rangle - \\
&- \lambda \mathcal{G}\left(p_1\right) \sum_{A=2}^{n} \sum_{\tilde{p}_1 \tilde{q}_A \tilde{p}_A} \delta\left(p_1 - \tilde{p}_1 - \tilde{q}_A - \tilde{p}_A\right) K^2\left(\tilde{q}_A\right) \langle G_{\tilde{p}_1 q_1} \ldots G_{p_A \tilde{q}_A} \rangle \langle G_{\tilde{p}_A q_A} \ldots G_{p_n q_n} \rangle + \\
&+ \lambda \mathcal{G}\left(p_1\right) \sum_{\tilde{p}_1, \tilde{p}_2, \tilde{q}_1} \delta\left(p_1 - \tilde{p}_1 - \tilde{p}_2 - \tilde{q}_1\right) K^2\left(\tilde{q}_1\right) \langle G_{\tilde{p}_1 \tilde{q}_1} G_{\tilde{p}_2 q_1} G_{p_2 q_2} \ldots G_{p_n q_n} \rangle
\end{aligned}$$

But: A in φ = A φ + b has unit eigenvalue…

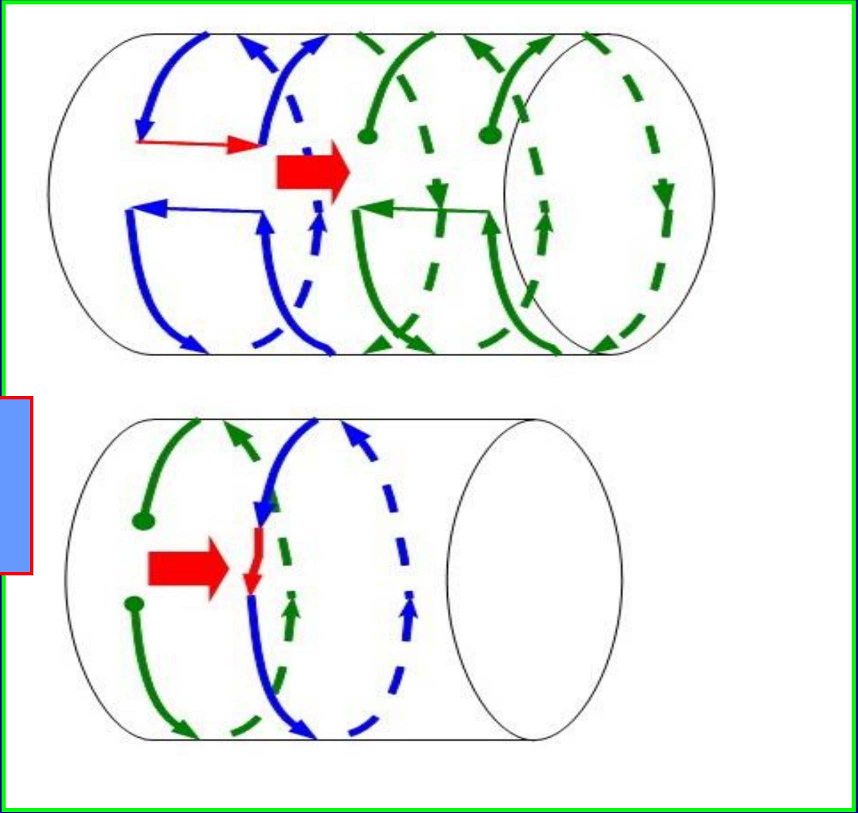
Large-N gauge theory, Veneziano limit



Migdal-Makeenko loop equations illustrated

Temperature and chemical potential

- Finite temperature: strings on cylinder R ~1/T
- Winding strings = Polyakov loops ~ quark free energy
- No way to create winding string in pure gauge theory at large-N → EK reduction



- Veneziano limit: open strings wrap and close
- Chemical potential:

κ -> κ exp(+/- μ)

No signs or phases!

- Strings oriented in the time direction are favoured

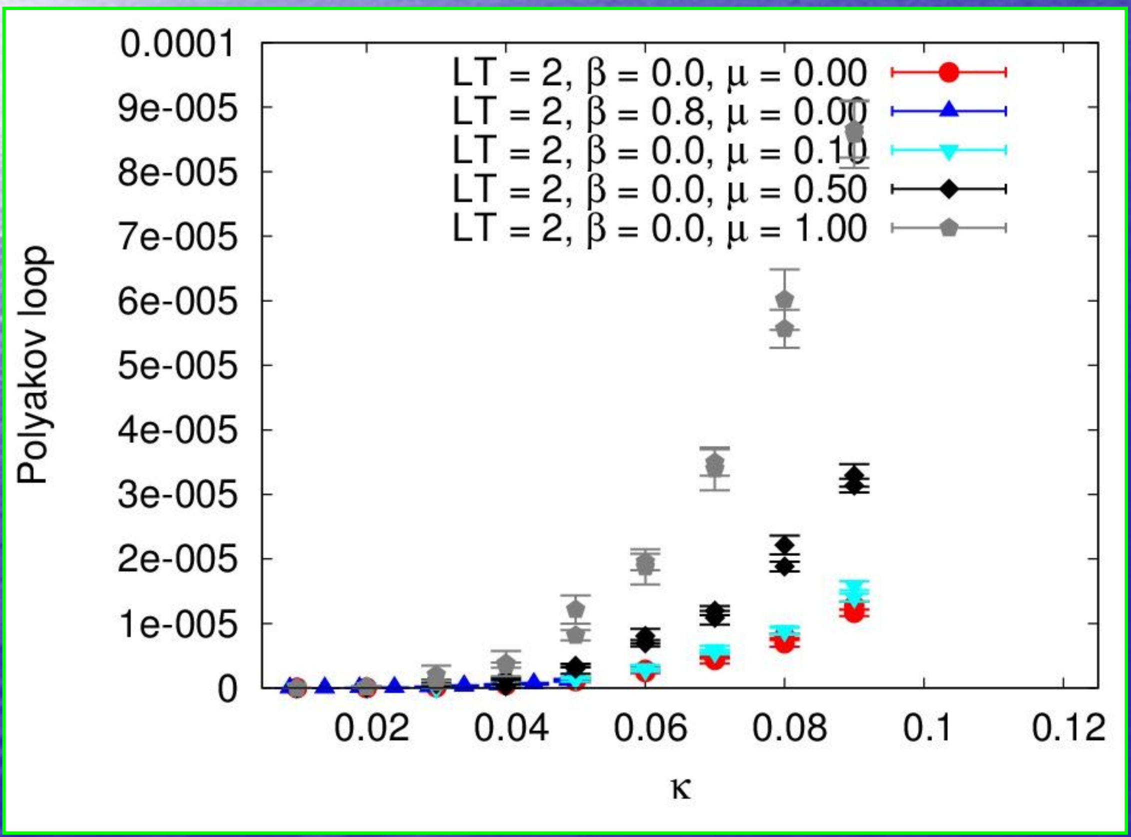
Phase diagram of the theory: a sketch

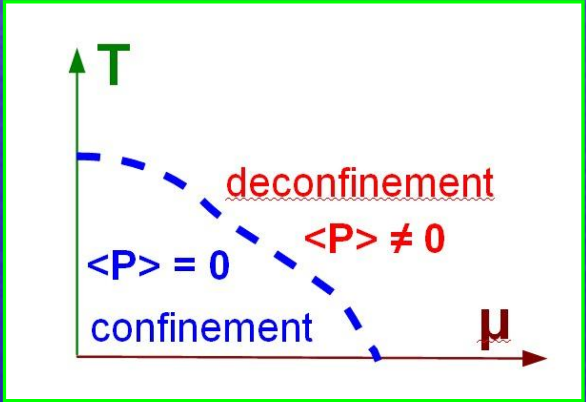
High temperature
(small cylinder radius)
OR
Large chemical potential

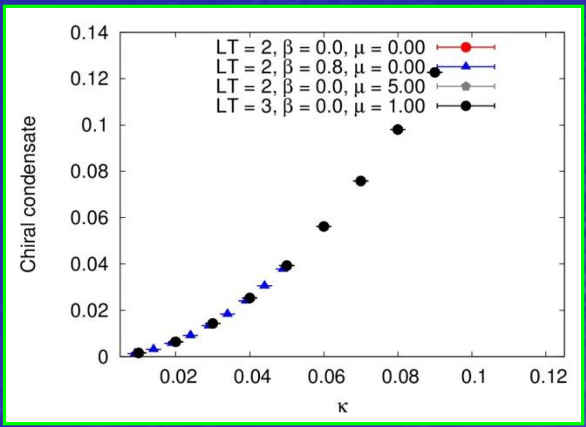
Numerous winding strings

Nonzero Polyakov loop

Deconfinement phase







Conclusions

- Schwinger-Dyson equations provide a convenient framework for constructing DiagMC algorithms
- 1/N expansion is quite natural (other algorithms cannot do it AUTOMATICALLY)
- Good news: it is easy to construct DiagMC algorithms for non-Abelian field theories
- Then, chemical potential does not introduce additional sign problem
- Bad news: sign problem already for higher-order terms of SC expansions
- Can be cured to some extent by choosing proper observables (e.g. momentum space)