# Taylor expansion in chemical potential for 2 flavour QCD with $a = 1/4T$

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1. The conjectured phase diagram, the sign problem and recent solutions. Comparing different methods for doing Gaussian integrals.
2. The QCD Taylor series expansion— semi-automatic methods for large order expansions and their efficient computation.
3. The series for pressure and its breakdown, radii of convergence and the QCD phase diagram.
4. Summary

A conjectured phase diagram
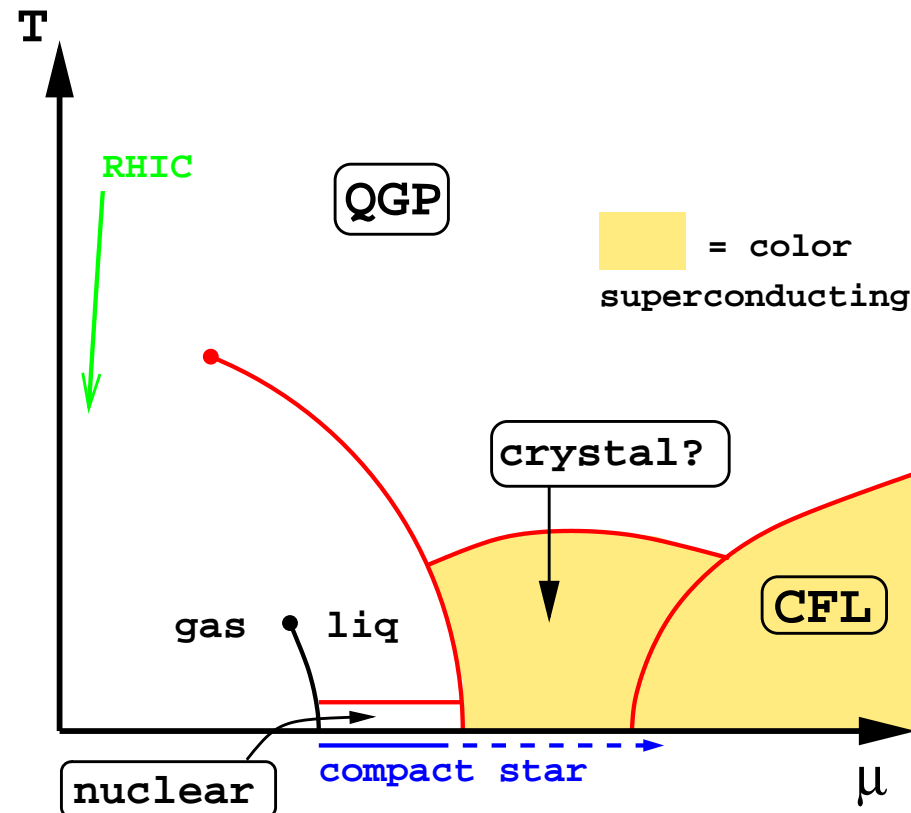
Flavour symmetry: one μ for every independent conserved charge.

M. G. Alford, K. Rajagopal, F. Wilczek, *Phys. Lett.*, B 422 (1998) 247,

R. Rapp, T. Schäfer, E. V. Shuryak, M. Velkovsky, *Phys. Rev. Lett.*, 81 (1998) 53.

The problem?

$$Z = \mathrm{e}^{-F/T} = \int DU\ \mathrm{e}^{-S}\ \prod_f \det M(U, m_f, \mu_f) = \int DU\ \mathrm{e}^{-\mathcal{S}(T,\mu)}$$

where the Dirac operator is the staggered quark discretisation of $M = m + \partial_\mu \gamma_\mu$.

- If there is a Q such that $M^\dagger = Q^\dagger M Q$, then clearly $\det M$ is real.

- $Q = \gamma_5$ for $\mu = 0$. Nothing for $\mu \neq 0$.

- Monte Carlo simulations of Z fail.

- Under CP symmetry $\{U\} \to \{U'\}$ such that $\det M(U) = [\det M(U')]^*$.

- Z remains real and non-negative— thermodynamics is safe.

Recent solutions

- Two parameter reweighting: Z. Fodor and S. D. Katz, *J. H. E. P.*, 03 (2002) 014. Simulate at (T, μ), reweight to (T', μ') by the factor $\exp[\Delta \mathcal{S}]$, where $\Delta \mathcal{S} = \mathcal{S}(T, \mu) - \mathcal{S}(T', \mu')$.

- Simulate imaginary μ (positive $\det M$) and do analytic continuation: M. D'Elia and M.-P. Lombardo, hep-lat/0209146, P. De Forcrand and O. Philipsen, *Nucl. Phys.*, B642 (2002) 290 Special care needed; find Yang-Lee zeroes directly: S, Gupta, hep-lat/0307007.

- Perform a Taylor series expansion of the free energy: C. R. Allton *et al.*, *Phys. Rev.*, D 66 (2002) 074507; R. V. Gavai and S. Gupta, *Phys. Rev.* D 68 (2003) 034506; C. R. Allton *et al.*, *Phys. Rev.*, D 68 (2003) 014507

Why Taylor series expansions?

- Reweighting and Taylor expansion methods have different systematics (example follows).

- Since the reweighting factor, $\exp[\Delta \mathcal{S}]$, is extensive, taking the continuum and/or thermodynamic limits, while keeping the relative error fixed, is an exponentially difficult problem.

- The continuum Dirac operator specifies effects of an infinitesimal time translation. On the lattice we deal with finite translations (by lattice spacing a). This gives a lattice ambiguity. Reweighting gives no indication of how large the lattice artifacts are. With explicit Taylor expansion one can take the continuum limit with relative ease.

- At present no analysis of the systematic errors in the determination of the critical end-point determined by reweighting are available.

Example: Gaussian integrals

$$Z(s) \equiv \exp[-F(s)] = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-(x-s)^2/2} = 1$$

$$\overline{x}(s) = s, \quad \text{and} \quad V(s) = 1,$$

where V denotes the variance of x. The Taylor coefficients of $F(s)$, $\overline{x}(s)$ and $V(s)$, in expansions around $s = 0$, can be read off from here.

The Monte Carlo procedure for $s = 0$ is well-known. Draw two random deviates from an uniform distribution $0 \leq r_1, r_2 \leq 1$. These give two Gaussian random numbers

$$x_1 = \sqrt{-2\ln r_1}\cos(2\pi r_2) \quad \text{and} \quad x_2 = \sqrt{-2\ln r_1}\sin(2\pi r_2).$$

Perform this Monte Carlo. Values of x in the range X and $X + dX$ are then obtained with frequency proportional to the unit Gaussian.

Example: Reweighting and Taylor expansion

In reweighting each point sampled by Monte Carlo is given an extra weight

$$w(x, s) = \mathrm{e}^{-(s^2 - 2xs)/2}$$

The statistical estimates of any quantity one wishes to evaluate are made using this weight for each sampled value of x. Taylor expand w and average.
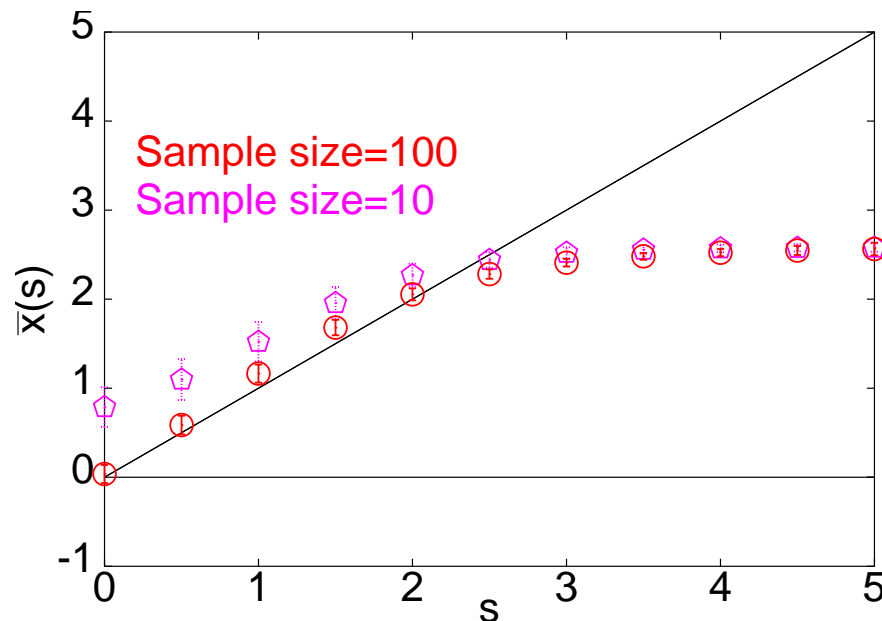
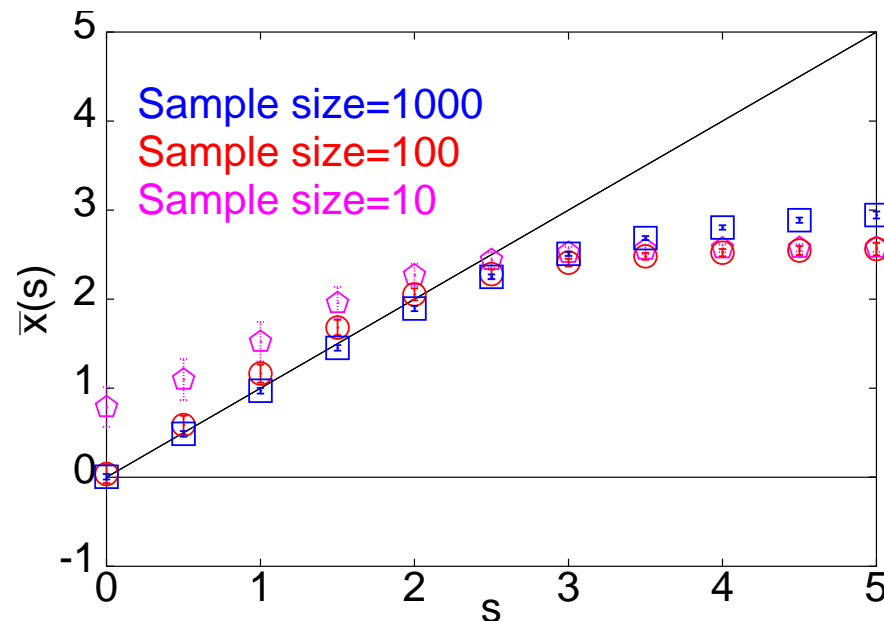# Example: Reweighting and Taylor expansion

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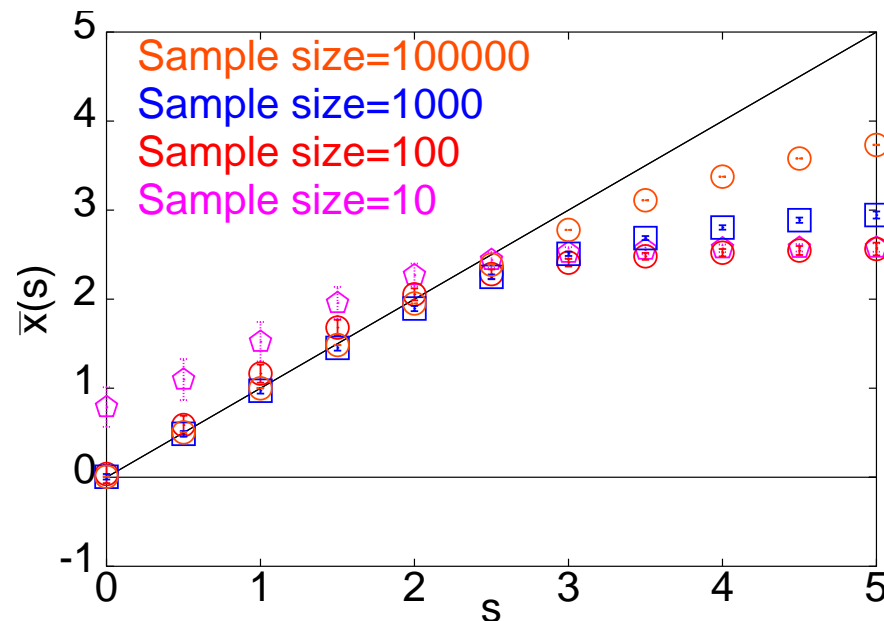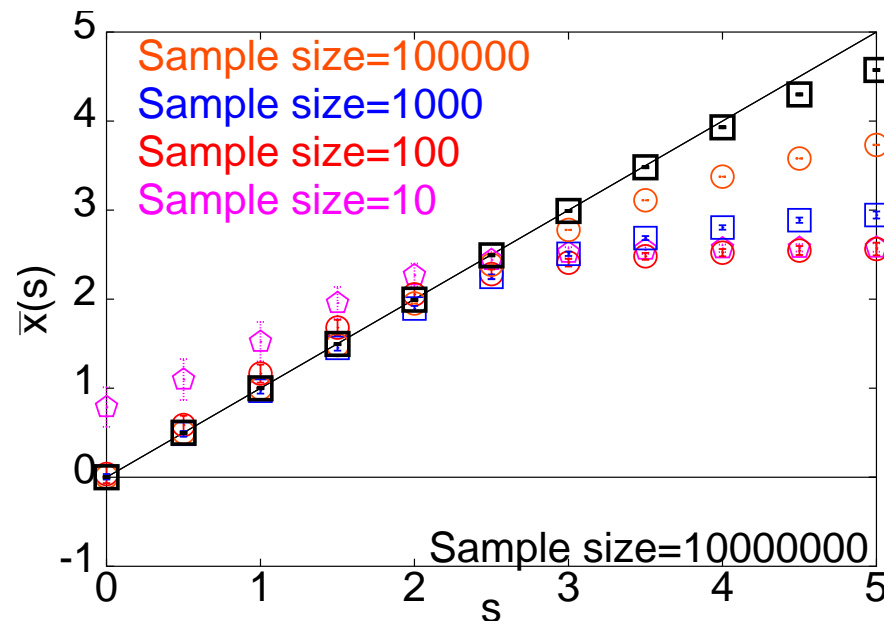
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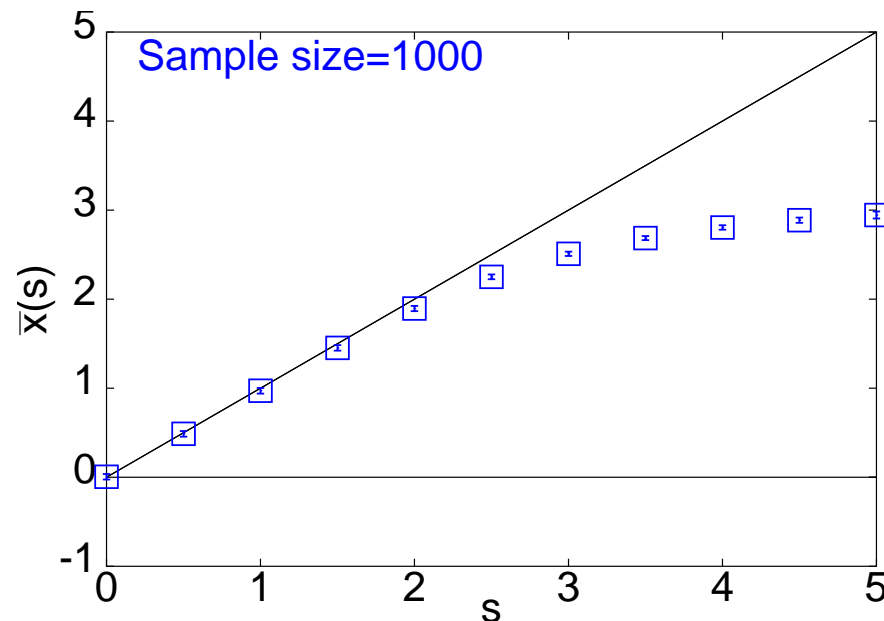
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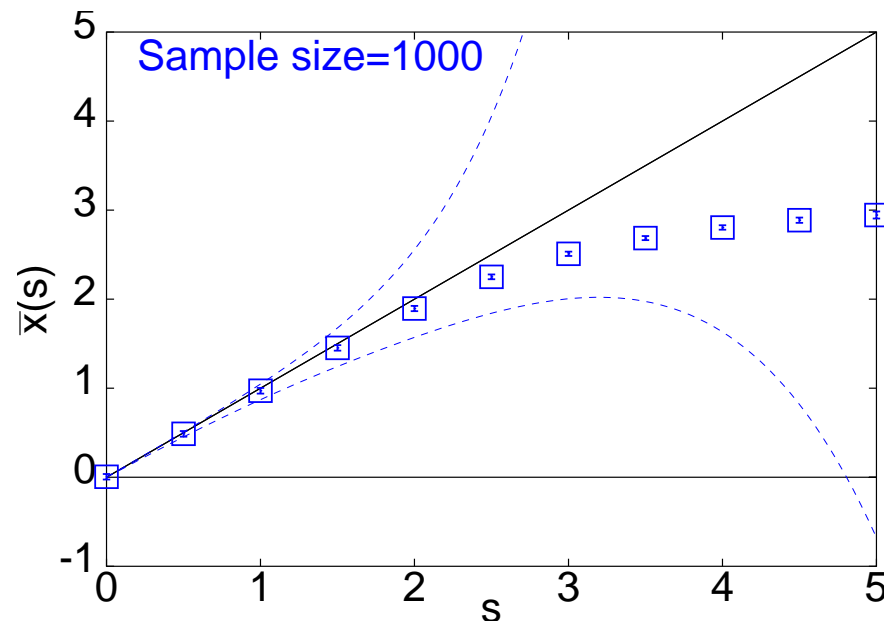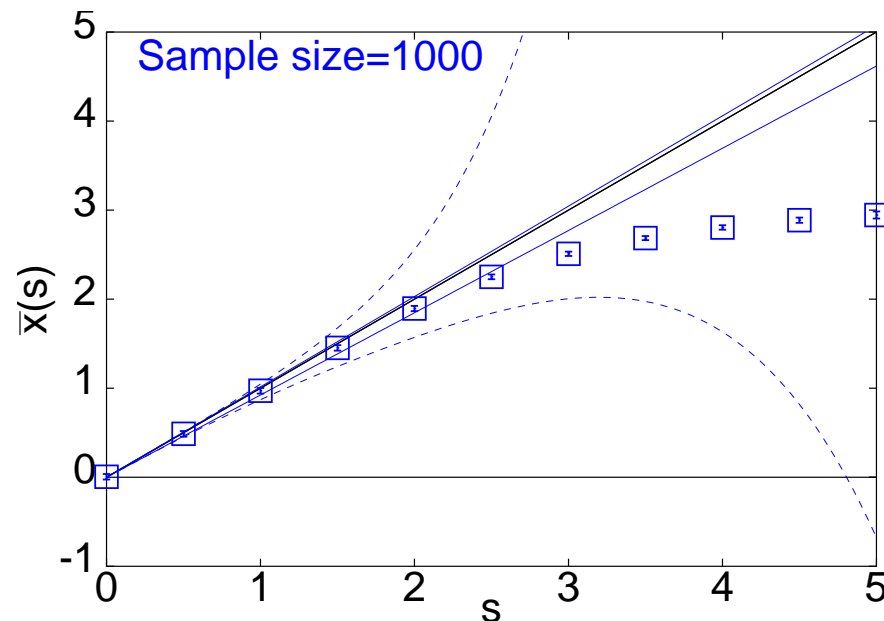# Example: Reweighting and Taylor expansion

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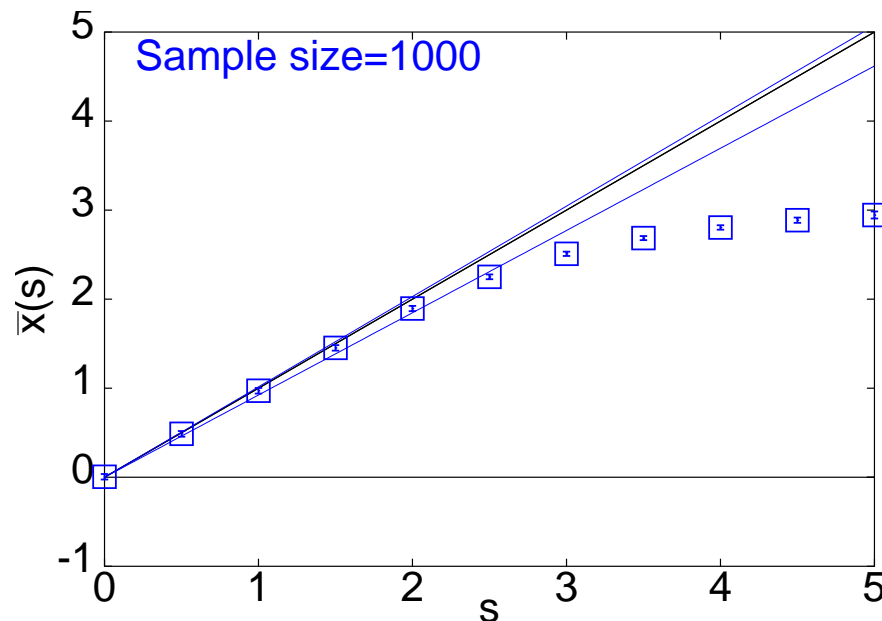

Sample size=1000

Example: Reweighting and Taylor expansion

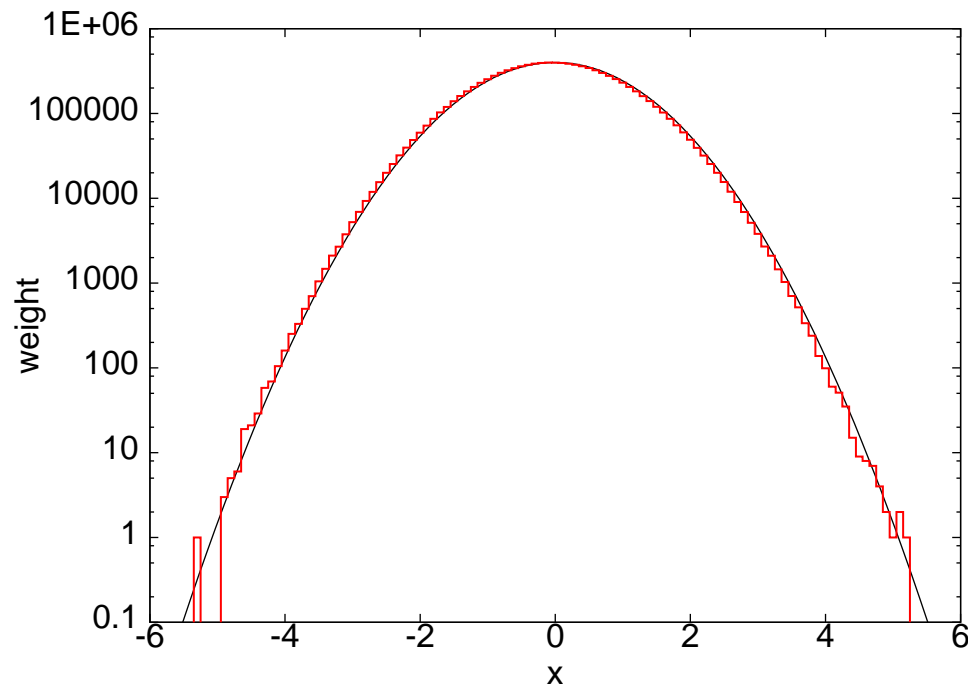In reweighting each point sampled by Monte Carlo is given an extra weight

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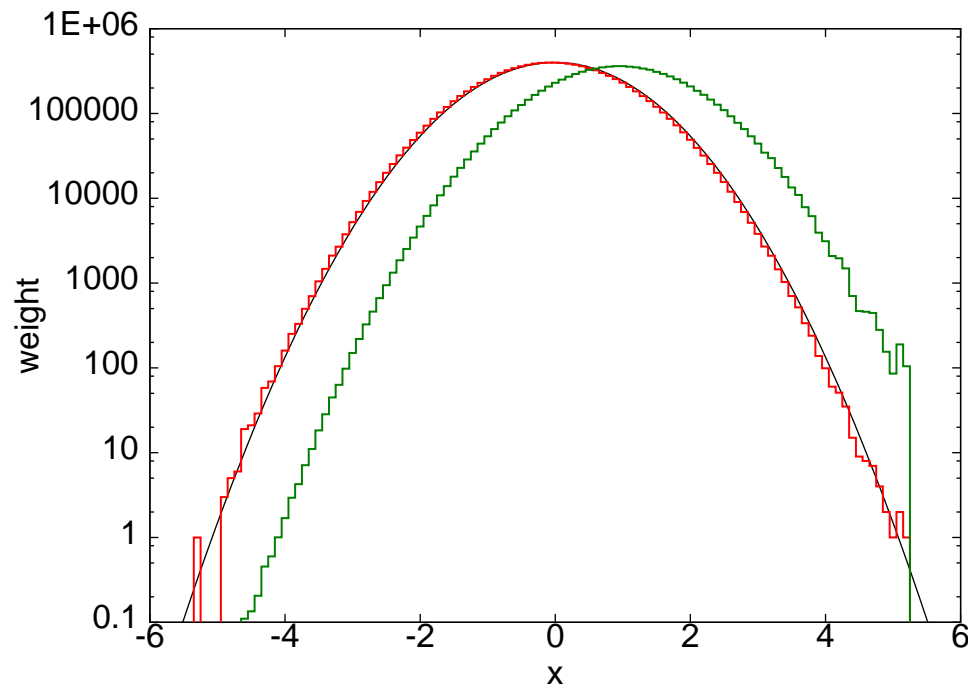
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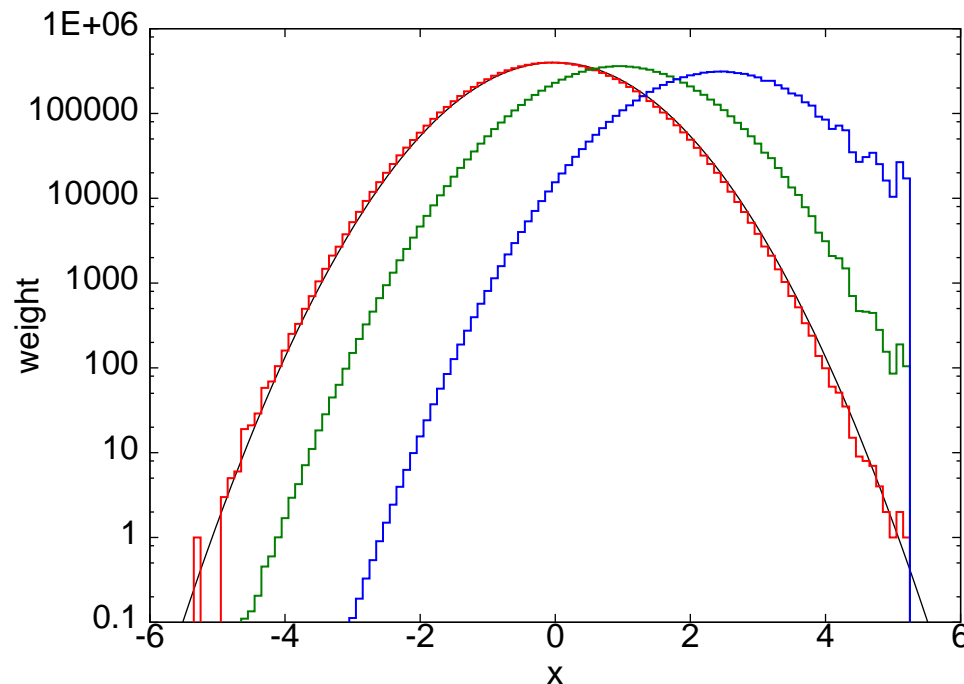
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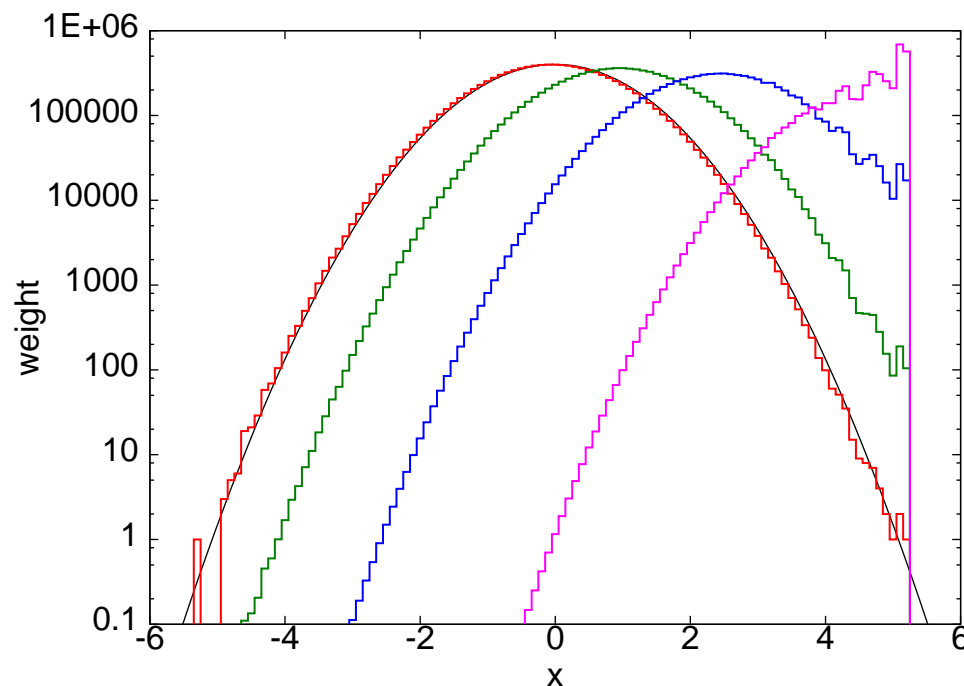
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Example: Why the Taylor expansion remains sane

The Taylor expansion can be rearranged in terms of cumulants—

$$
\begin{aligned}
1!t_1 &= \langle x^2 \rangle \equiv \left[x^2 \right], \\
2!t_2 &= \langle x(x^2 - 1) \rangle \equiv 0, \\
3!t_3 &= \langle x^2(x^2 - 3) \rangle \equiv \left[x^4 \right] + 3 \left[x^2 \right] \left(\left[x^2 \right] - 1 \right), \\
4!t_4 &= \langle x(3 - 6x^2 + x^4) \rangle \equiv 0, \\
5!t_5 &= \langle x^2(15 - 10x^2 + x^4) \rangle \equiv \left[x^6 \right] + \left[x^4 \right] \left(15 \left[x^2 \right] - 10 \right) + 15 \left[x^2 \right] \left(\left[x^2 \right] - 1 \right)^2 .
\end{aligned}
$$

The symmetries of the Gaussian for $s = 0$ imply that alternate coefficients vanish. Only the second cumulant, $\left[x^2 \right]$, is non-vanishing. As a result, for a Gaussian of unit variance, only the first Taylor coefficient is non-vanishing. A variance reduction of the Taylor expansion follows from this.

The Taylor Expansion for QCD

Since $PV = -F = T \log Z$, the Taylor expansion of P is the same as of F!

$$P(T, \mu_u, \mu_d) = P(T, 0, 0) + \sum_f n_f \mu_f + \frac{1}{2!} \sum_{fg} \chi_{fg} \mu_f \mu_g + \cdots$$

where the quark number densities and susceptibilities are—

$$n_f = \left. \frac{T}{V} \frac{\partial \log Z}{\partial \mu_f} \right|_{\mu_f = 0}$$

$$\chi_{fg} = \left. \frac{T}{V} \frac{\partial^2 \log Z}{\partial \mu_f \partial \mu_g} \right|_{\mu_f = \mu_g = 0}$$

$$\chi_{fgh\cdots} = \left. \frac{T}{V} \frac{\partial^n \log Z}{\partial \mu_f \partial \mu_g \partial \mu_h \cdots} \right|_{\mu_f = \mu_g = \cdots = 0}$$

Differential calculus by machine: 1

There are mechanical and (almost) fully programmable methods to take the derivatives involved in a high-order Taylor series expansion of the partition function with fermions and finding the most efficient way of programming the Taylor coefficients.

Step 1

Relate the derivatives of $\log Z$ to the derivatives of Z. Trivially accomplished by, *e.g.*, the simple Mathematica program

$$\mathtt{chi[n\_, m\_]} := \mathtt{D[\ Log[Z[u, d]],\ \{u, n\},\ \{d, m\}]},$$

or its generalization to a larger number of flavours. Notation used is

$$\chi_{nm} = \chi \underbrace{uu\cdots}_{n\,times}\ \underbrace{dd\cdots}_{m\,times}$$

Differential calculus by machine: 2

Relate the derivatives Z to fermion traces. As long as we work with equal mass flavours, the fermion traces are flavour independent. Introduce the notation

$$Z_{10} = Z\langle\mathcal{O}_1\rangle, \qquad \mathcal{O}'_n = \mathcal{O}_{n+1}.$$

Use the rule $[\det M]' = [\exp \mathrm{Tr}\ \log M]' = \mathrm{Tr}\ M'M^{-1}\det M$, to write
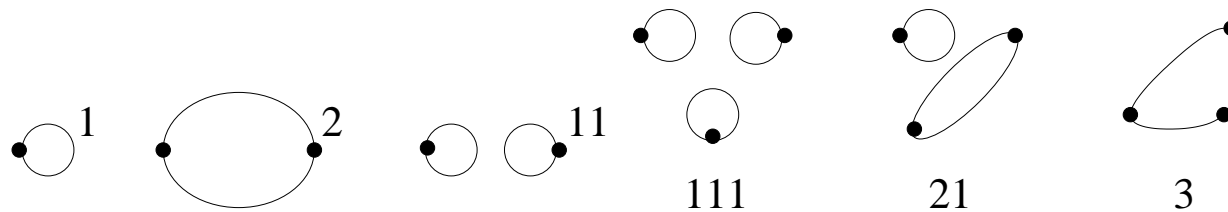
$$Z_{10} = Z_{01} = \frac{\partial Z}{\partial \mu_f} = \int DU \mathrm{e}^{-\mathcal{S}}\ \mathrm{Tr}\ M_f^{-1}M'_f.$$

Note: $M' = \gamma_0$ and $M^{-1} = \psi\overline{\psi}$, so $\mathrm{Tr}\ M^{-1}M' = \psi^\dagger\psi$. S. Gottlieb *et al.*, *Phys. Rev. Lett.*, 59 (1987) 2247

Differential calculus by machine: 3

Use the chain rule to write down higher order derivatives in terms of the $\mathcal{O}_n$ and their products. A diagrammatic representation of these quantities is possible, and can be used to check the results.

S. Gupta, *Acta Phys. Pol.*, B 33 (2002) 4259

Example: Z_{60} contains $\mathcal{O}_{1122}$ with coefficient equal to the number of ways of partitioning 6 objects into groups of 2 ones and 2 twos, *i.e.*,

$$\left\{ \frac{1}{2} \binom{6}{1} \binom{5}{1} \right\} \times \left\{ \frac{1}{2} \binom{4}{2} \right\} = 45.$$

Differential calculus by machine: 4

Step 4

The diagrams still have to be related to fermion traces. In the continuum this is trivial because only $M' = \gamma_0 \neq 0$. On the lattice there are several more steps, since arbitrary derivatives, $M^{(p)}$, exist. Introduce further notation

$$\lfloor n_1 \cdot p_1 \oplus n_2 \cdot p_2 \oplus \cdots \rceil = \mathrm{Tr} \, \left[\left(M^{-1} M^{(p_1)} \right)^{n_1} \left(M^{-1} M^{(p_2)} \right)^{n_2} \cdots \right].$$

Then derivatives are given by the rule—

$$\lfloor n \cdot p \rceil' = -n \lfloor 1 \oplus n \cdot p \rceil + n \lfloor (n - 1) \cdot p \oplus (p + 1) \rceil.$$

The chain rule is equivalent to making the derivative linear over $\oplus$.

Example: $\lfloor 1 \rceil = \mathrm{Tr} \, M^{-1} M'$, and $\lfloor 1 \rceil' = -\lfloor 2 \cdot 1 \rceil + \lfloor 2 \rceil$.

Differential calculus by machine: 5

Step 5

Numerical estimates of traces are made by the usual noisy method, which involves the identity $I = \overline{|r\rangle \langle r|}$, where r is a vector of complex Gaussian random numbers. We choose to use 100 vectors in the averaging.
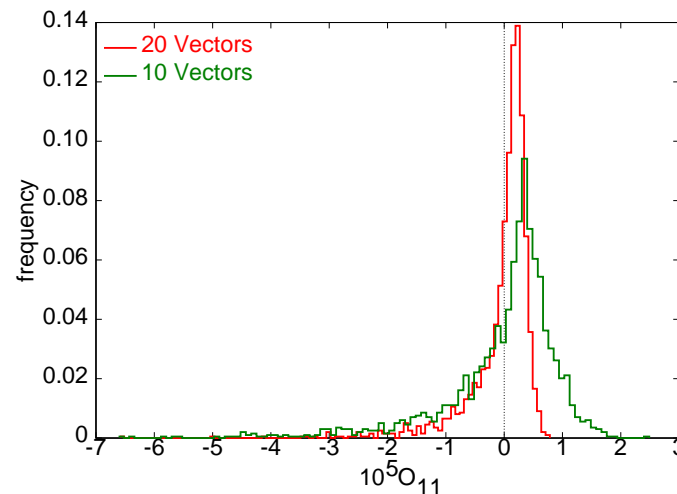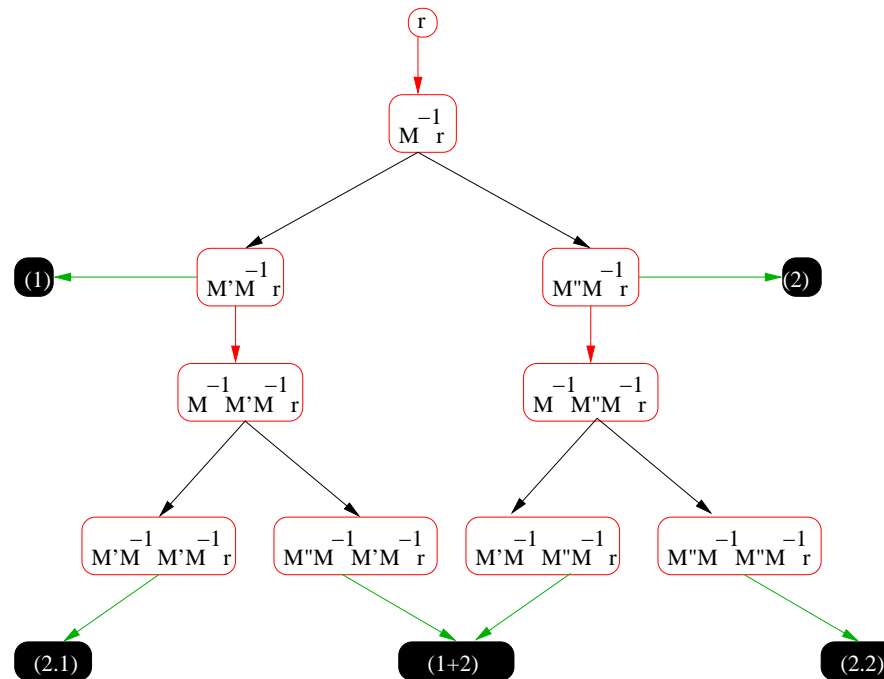

The histogram of O_{11} where $\chi_{ud} = \langle O_{11} \rangle$. In the limit of infinite number of vectors the histogram should be skew, a tail to the left and vanishing abruptly at zero.

Differential calculus by machine: 6

Optimisation of the computation of multiple traces reduces to a problem called the Steiner problem. Need 20 matrix inversions to perform a single measurement of upto 8th order susceptibilities.
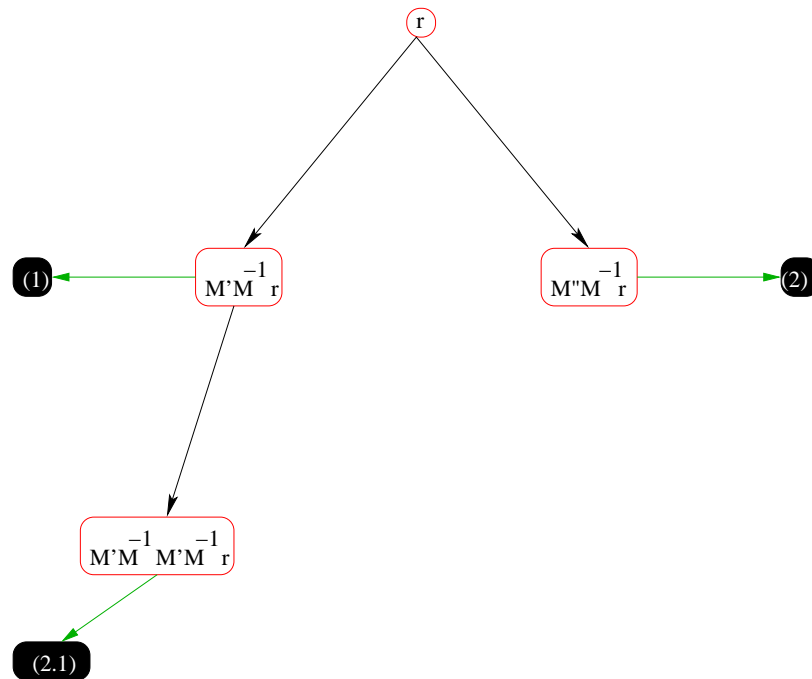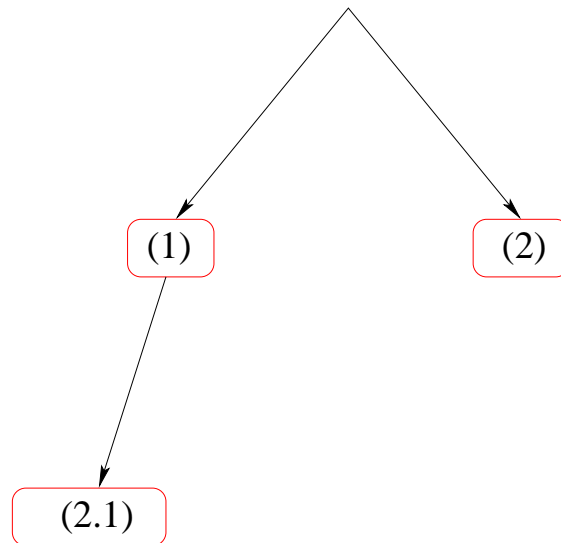
Differential calculus by machine: 6

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r

$M'M^{-1}r$ → (1) $M''M^{-1}r$ → (2)

$M'M^{-1}M'M^{-1}r$ $M''M^{-1}M'M^{-1}r$ $M'M^{-1}M''M^{-1}r$ $M''M^{-1}M''M^{-1}r$

(2.1)   (1+2)   (2.2)

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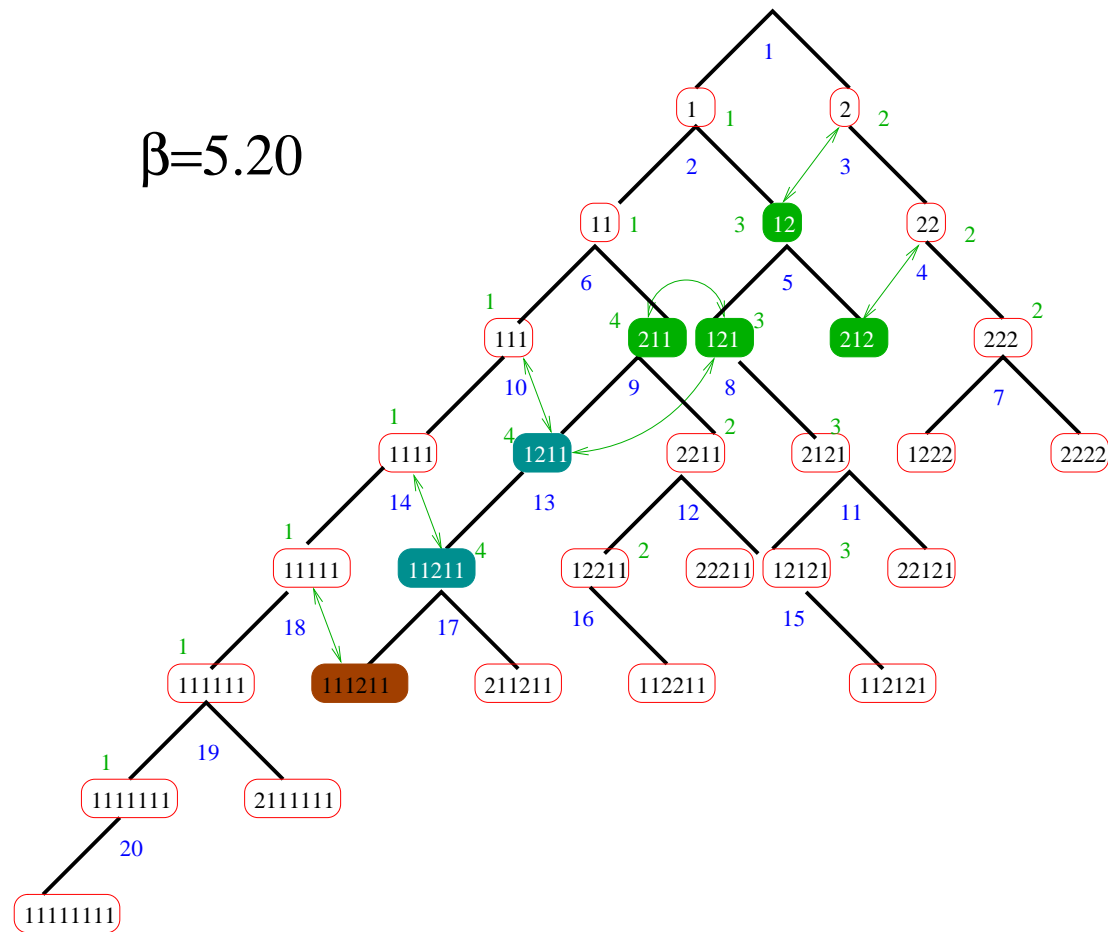
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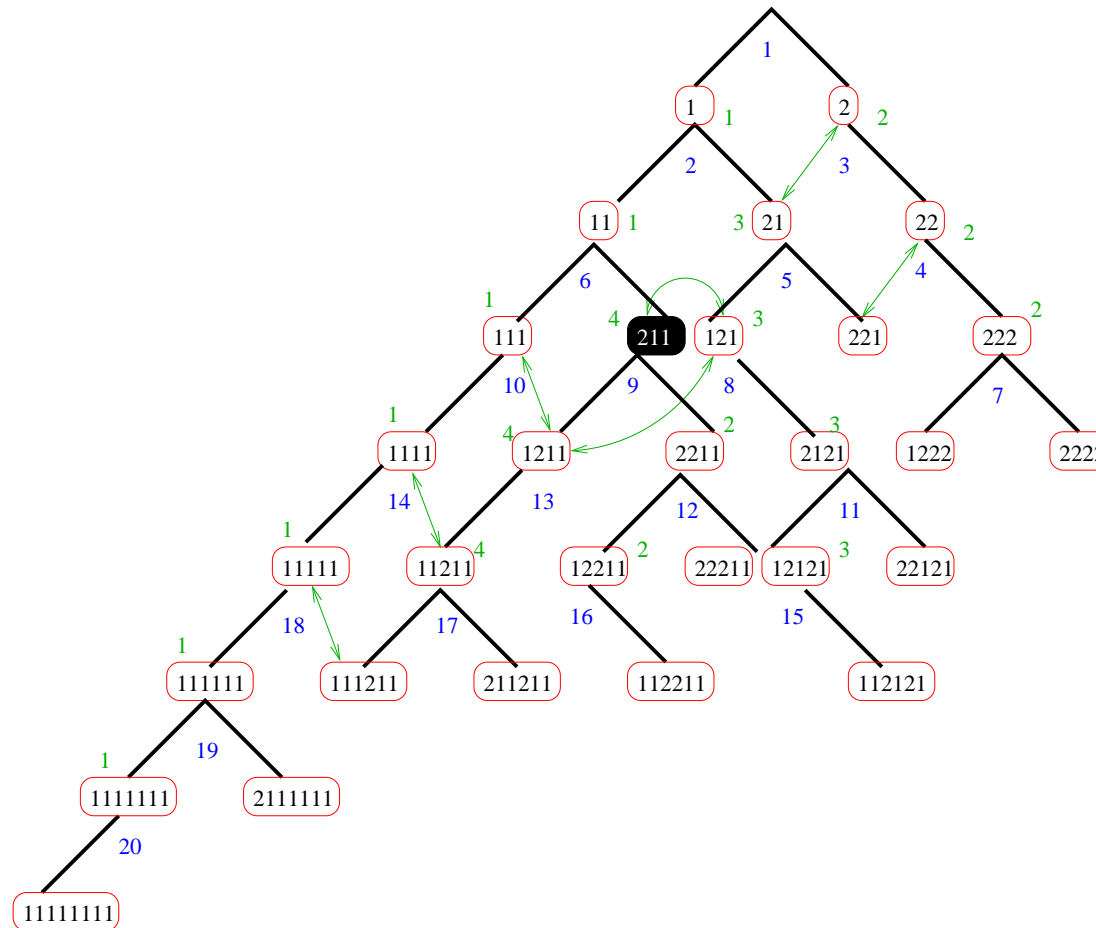
Note the accuracy checks built into the optimal computation.

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β=5.20

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Convergence of the series for the pressure

$$\Delta P(T,\mu) \quad \equiv \quad P(T,\mu) - P(T,0) = \chi_{20}(T)\mu^2 + \frac{1}{12}\chi_{40}(T)\mu^4 + \mathcal{O}\left(\mu^6\right)$$

$$= \quad \chi_{20}\mu^2 \left[1 + \left(\frac{\mu}{\mu_*^{(2)}}\right)^2 \left\{ 1 + \left(\frac{\mu}{\mu_*^{(4)}}\right)^2 \left(1 + \cdots\right) \right\} \right].$$

where $\quad \mu_*^{(2)} = \sqrt{\dfrac{12\chi_{20}}{\chi_{40}}} \qquad \mu_*^{(4)} = \sqrt{\dfrac{30\chi_{40}}{\chi_{60}}} \qquad etc.$

If $\mu_*^{(n)}$ increases without limit then the series is well behaved for all μ. Else, for $\mu < \mu_*$,

$$\Delta P(T,\mu) = \chi_{20}\mu^2 \sum_{n=0}^{\infty} \left(\frac{\mu}{\mu_*}\right)^{2n} \simeq \frac{\chi_{20}\mu^2}{1 - (\mu/\mu_*)^2}$$
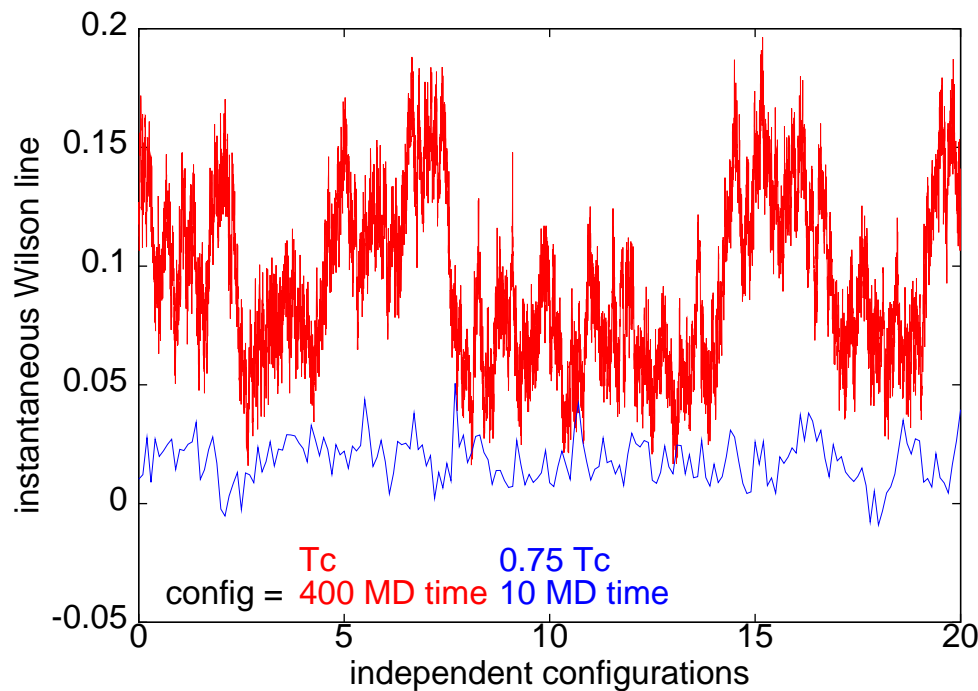
A related expansion is

$$\Delta P(T, \mu) = \sum_{n=1}^{\infty} \left(\frac{\mu}{\mu_*^{(2n)}} \right)^{2n} \qquad \text{where } \mu_*^{(n)} = \left(\frac{n!}{2\chi_{n0}} \right)^{1/n}.$$
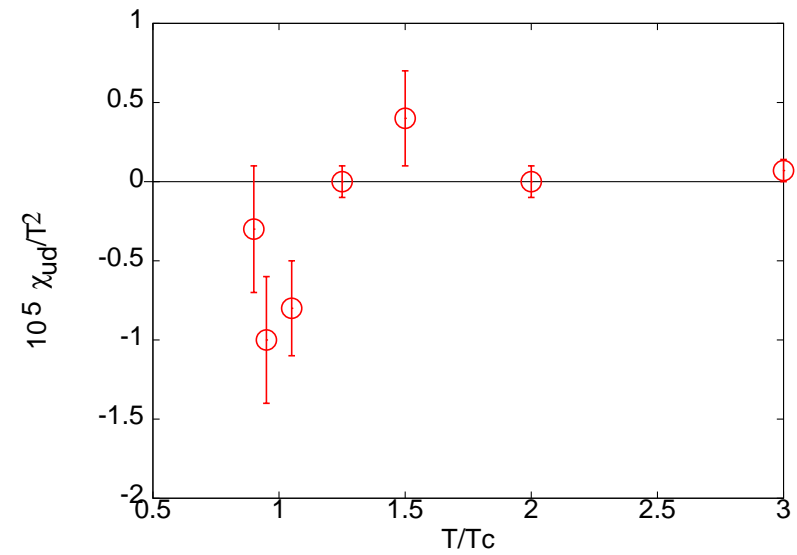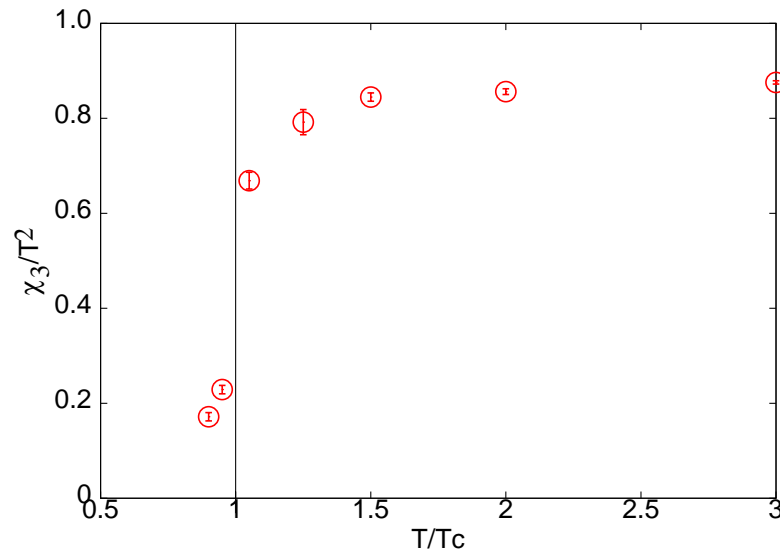
Again, for $\mu < \mu_*$,

$$\Delta P(T, \mu) \simeq \frac{\chi_{20} \mu^2}{1 - (\mu/\mu_*)^2}$$

Simulations

Simulations at constant $m/T_c = 0.1$, corresponding to $m_\pi/T_c \approx 1.6$. Lattice spacing $a = 1/4T$, *i.e.*, $N_t = 4$. Care needed to use roughly equal number of uncorrelated configurations at all T.
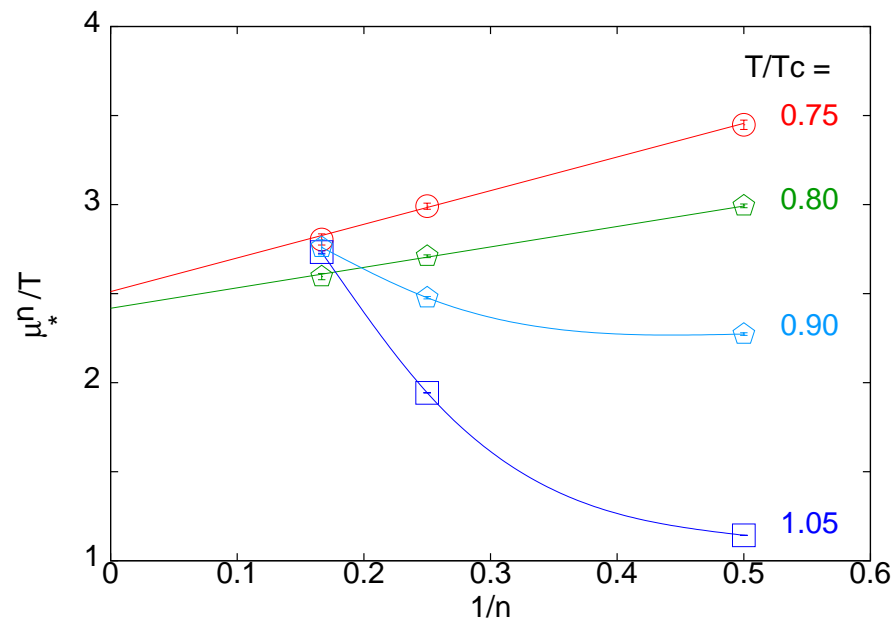
χ_{11} **and** χ_{20}

Radius of convergence

The series expansion breaks down when a phase transition line is encountered. Use estimates of the radius of convergence, $\mu_*^{(n)}$, to obtain an estimate of the position of the phase transition line.

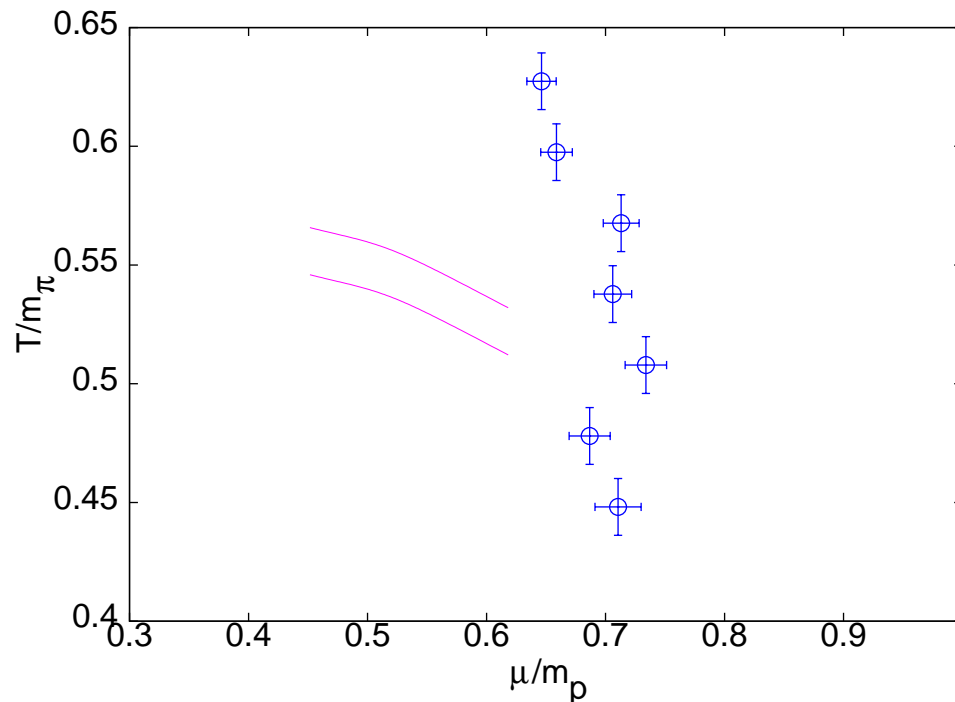Qualitative change in the range $0.8 < T/T_c < 0.9$ (for $m/T_c = 0.1$).

The phase diagram

The same information can be written as a phase diagram. Here is the phase
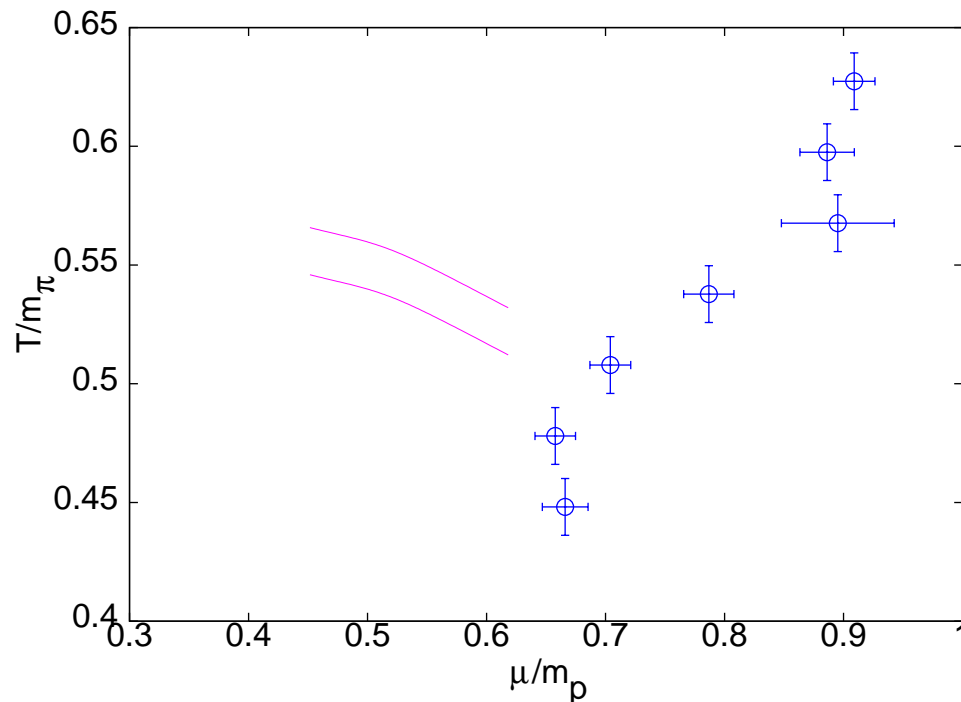diagram in a Taylor series at order 2.
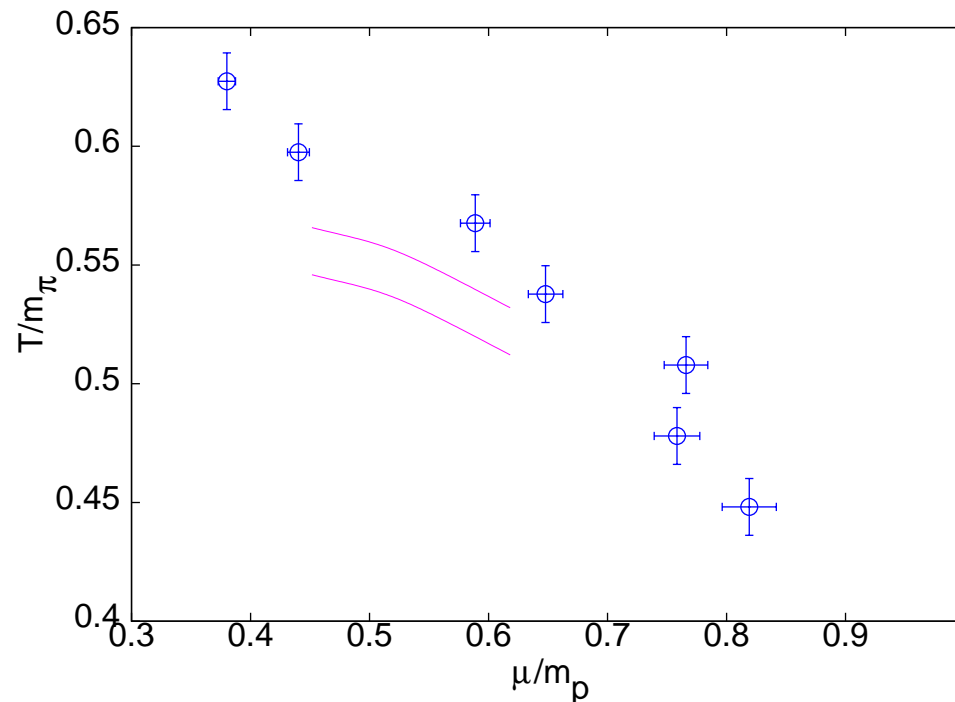
The phase diagram

The same information can be written as a phase diagram. Here is the phase diagram in a Taylor series at order 4.

The phase diagram

The same information can be written as a phase diagram. Here is the phase diagram in a Taylor series at order 6.

The phase diagram

The same information can be written as a phase diagram. Here is the phase diagram in a Taylor series extrapolated to all orders.
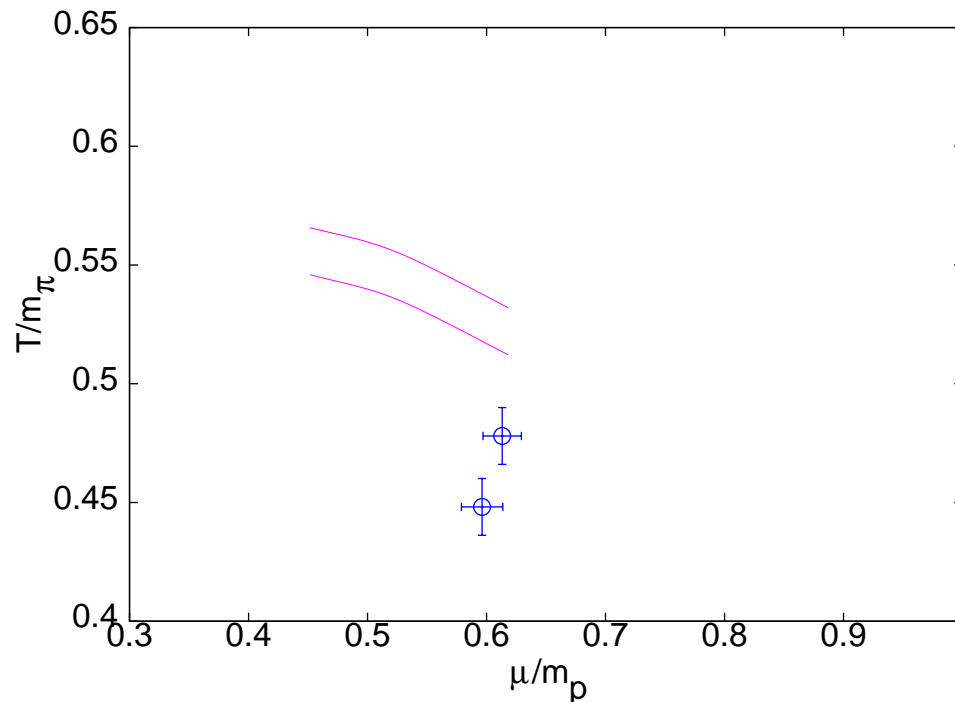
Summary

More than one method for computing physics at finite μ.

- The Taylor expansion is a systematic method which allows us to quantify uncertainties in the evaluation of the phase boundaries, and systematically improve them.

- There is a systematic method for generating high order susceptibilities and computing them efficiently. Algebraic methods are used for automatic generation of the terms, and combinatorial techniques have been developed to test their correctness. An algorithm exists for writing down the most efficient computation upto a given fixed order.

- Computation of several high order susceptibilities allows an estimation of the critical end point by series extrapolation methods.

- Phenomenological consequences will be discussed by Rajiv Gavai next week.