Towards overcoming the Monte Carlo sign problem with tensor networks – the case of the two-flavour Schwinger model with chemical potential

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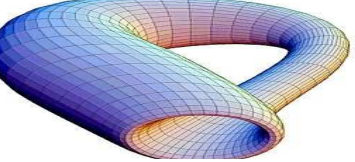
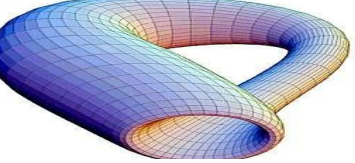


Seminar outline

1. Introduction and the method
   - Motivation – Lattice QCD
   - Tensor Network approach
2. The Schwinger model
   - Short reminder
   - Hamiltonian approach
3. Results
   - Chiral condensate $(T = 0)$
   - Chiral condensate $(T > 0)$
   - **Finite density** $(T = 0)$
4. Prospects

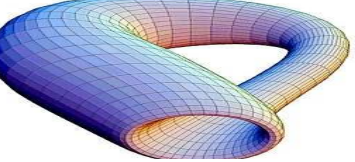
Based on:

- M. C. Bañuls, K. Cichy, K. Jansen and J. I. Cirac, "The mass spectrum of the Schwinger model with Matrix Product States," JHEP **1311** (2013) 158, [arXiv:1305.3765 [hep-lat]]
- M. C. Bañuls, K. Cichy, J. I. Cirac, K. Jansen and H. Saito, "Thermal evolution of the Schwinger model with Matrix Product Operators," Phys. Rev. **D92** (2015) 034519, [arXiv:1505.00279 [hep-lat]]
- M. C. Bañuls, K. Cichy, K. Jansen and H. Saito, "Chiral condensate in the Schwinger model with Matrix Product Operators," Phys. Rev. **D93** (2016) 094512, [arXiv:1603.05002 [hep-lat]]
- M. C. Bañuls, K. Cichy, J. I. Cirac, K. Jansen, S. Kühn and H. Saito, "The multi-flavor Schwinger model – Overcoming the sign problem with matrix product states," in preparation



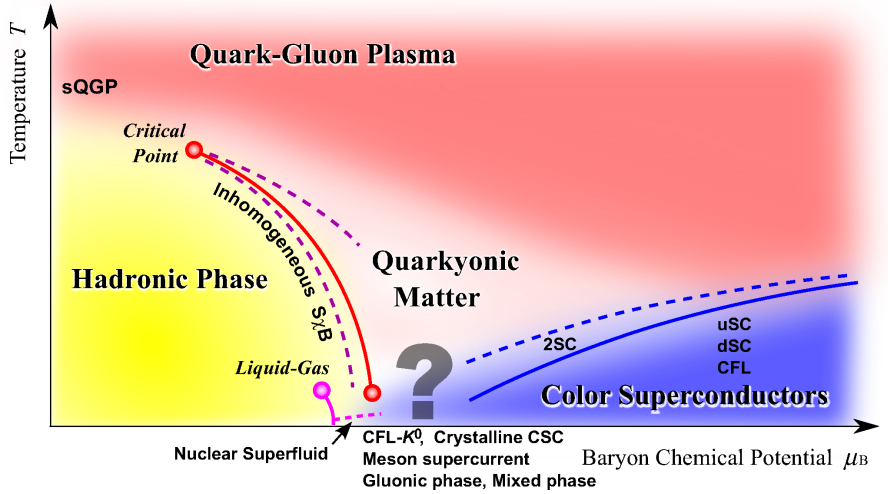
Lattice QCD

- The most common approach to Lattice QCD simulations consists in sampling the QCD path integral numerically via the Monte Carlo method.
- The QCD path integral: $Z = \int D\bar{\psi} D\psi DU \; e^{-S_{gauge}[U] - S_{ferm}[\psi,\bar{\psi},U]}$.
- The fermionic degrees of freedom can be integrated out:
  $Z = \int DU \; e^{-S_{gauge}[U]} \prod_{f=1}^{N_f} \det(\hat{D}_f[U])$,
  where $\det(\hat{D}_f[U])$ is the determinant of the Dirac operator matrix for fermion flavour f.
- The fermionic determinant $\det(\hat{D}_f[U])$ is by far the highest cost in a MC simulation. But, due to γ_5-Hermiticity ($\gamma_5 \hat{D}_f \gamma_5 = \hat{D}_f^\dagger$) it is real, so MC simulations are possible:
  $$\det\left(\gamma_5(\hat{D}_f + m)\gamma_5\right) = \det\left(\hat{D}_f^\dagger + m\right) = \det\left(\hat{D}_f + m\right)^\dagger.$$
- First approximation $\Rightarrow$ neglect the determinant ("quenched approximation") – commonly used until early 2000s.
- Dynamical simulations $\Rightarrow$ take the determinant into account.



Problems of Lattice QCD

LQCD simulations led to spectacular successes. However, there are some areas where progress is hard to achieve:

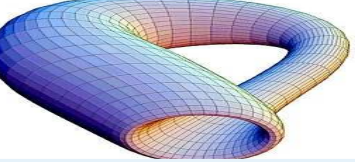


[K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74 (2011) 14001]

- non-vanishing chemical potential μ – if $\mu \neq 0$, the determinant becomes complex:
  $$\det\left(\gamma_5(\hat{D}_f + m + \mu\gamma_0)\gamma_5\right) = \det\left(\hat{D}_f^\dagger + m - \mu\gamma_0\right) =$$
  $$= \det\left(\hat{D}_f + m - \mu^*\gamma_0\right)^\dagger,$$
  determinant real only if μ taken to be purely imaginary.
  Ways to tackle the problem: reweighting, Taylor expansion, analytic continuation from imaginary μ.
- LQCD works in Euclidean space, related to Minkowski space by analytic continuation – hence time is imaginary. Hence, it is not possible to simulate real-time phenomena, i.e. non-equilibrium dynamics.

Alternative approaches wanted for these classes of problems!

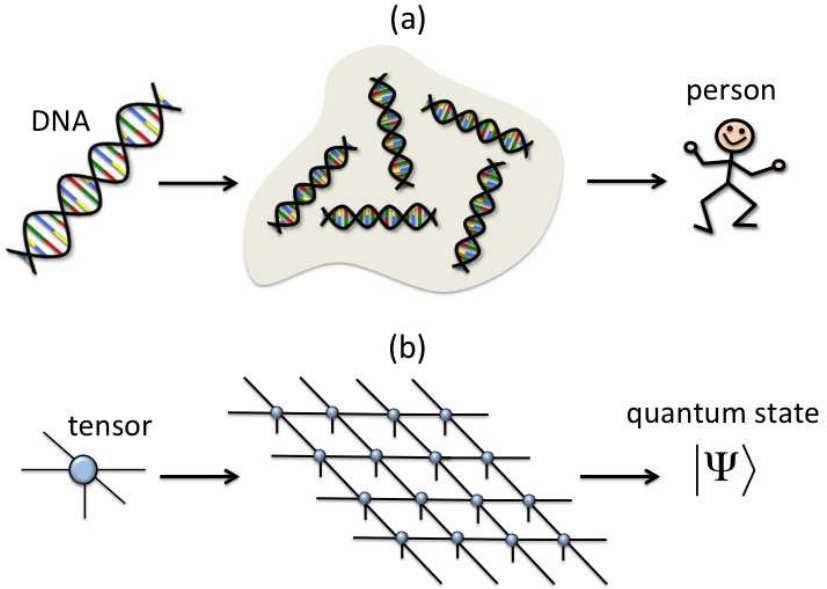
Tensor Networks?



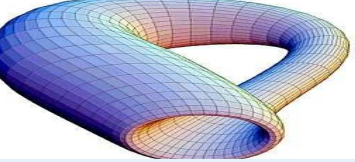
Tensor Network States

The name *Tensor Network* comes from the description of the wave function of a system in terms of a network of interconnected tensors. Poetic analogies:

- like decomposition in terms of LEGO pieces, where entanglement plays the role of glue connecting the pieces
- tensor as DNA of wave function

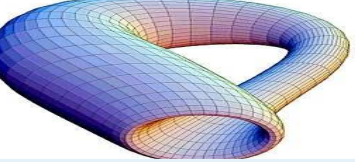


R. Orus, *A Practical Introduction to Tensor Networks*, Annals of Physics 349 (2014) 117-158, arXiv:1306.2164 [cond-mat.str-el]



Tensor Network States

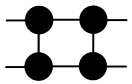
- An arbitrary state from a Hilbert space of an N-body interacting system needs in general an exponential number of coefficients – thus computational complexity increases very fast and prohibits exact diagonalization of systems larger than e.g.:
  - $\star$ $\mathcal{O}(20)$ Heisenberg spins (with a naive approach) or
  - $\star$ $\mathcal{O}(40)$ Heisenberg spins (using symmetries etc.).
- However, physical states (ground states, thermal states) of most systems are far from arbitrary.
- In many cases, they can be described by Tensor Network states that have only a polynomial number of parameters.
- In other words, only a small "corner" of the Hilbert space is physically relevant.

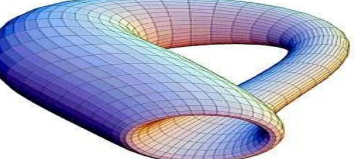


Graphical notation

Type	symbol	graphical symbol
scalar	A	
vector	A_α	
tensor of rank-2	$A_{\alpha\beta}$	
tensor of rank-3	$A_{\alpha\beta\gamma}$	

Some contractions:

Result	symbol	graphical symbol
scalar	$A_\alpha B_\alpha$	
tensor of rank-2	$A_{\alpha\beta} B_{\beta\gamma}$	
tensor of rank-4	$A_{\alpha\beta\gamma} B_{\gamma\delta\epsilon} C_{\zeta\delta\eta} D_{\eta\beta\theta}$	

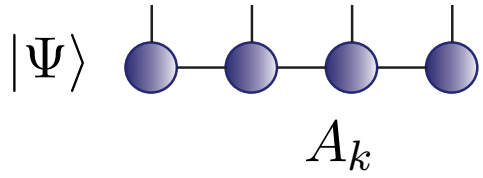


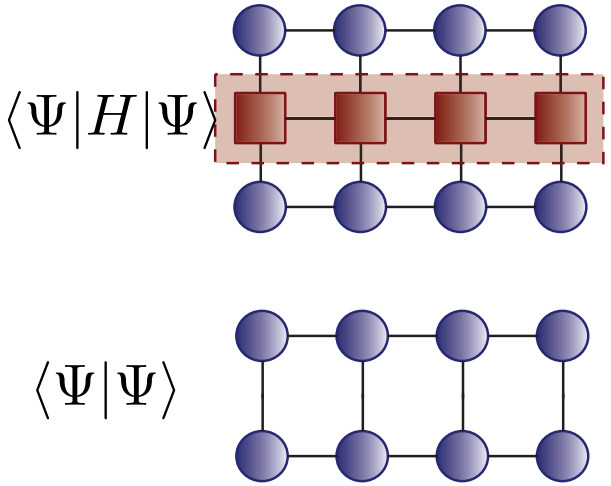
Matrix Product States

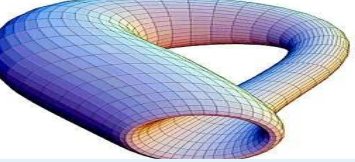
- A particularly successful and efficient family of Tensor Network states is called Matrix Product States (MPS).
- The MPS ansatz for some state $|\Psi\rangle$ has the following form:

$$|\Psi\rangle = \sum_{i_0 \ldots i_{N-1}=1}^{d} \mathrm{tr}\left(A_0^{i_0} \ldots A_{N-1}^{i_{N-1}}\right) |i_0 \ldots i_{N-1}\rangle,$$

where:
$|i_k\rangle$ are individual basis states for each site ($k = 0, \ldots, d-1$),
d – dimension of one-site Hilbert space,
each A_j^i is a D-dimensional matrix
and D is called the bond dimension.





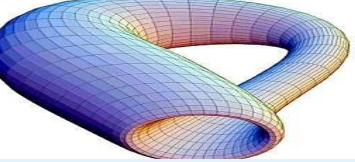


Counting of coefficients

- The description of a general state requires d^N numbers – exponential growth with system size.

- MPS representation with bond dimension D has only NdD^2 coefficients – polynomial growth with system size.

- Still, contraction of the MPS gives d^N coefficients for all d^N basis states. However, they are not independent – they have an underlying tensor structure.



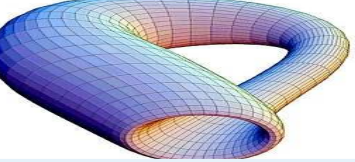
Why can MPS be useful?

- **Every** state has an MPS representation – with bond dimension of at most $D = d^{N/2}$, the number of numbers that characterizes an MPS becomes d^N.
- In this sense, MPS is just a representation that might or might not give some practical advantages.
- However, one typically refers to the name MPS when there exists some MPS representation with a relatively small D, which in particular does not grow with the system size.

Practical usefulness of MPS results from the facts:

1. Many of states in quantum 1D systems have a small D representation or are well-approximated by one.
2. One can efficiently obtain such approximating MPS.

[D. Perez-Garcia, F. Verstraete, M.M. Wolf, J.I. Cirac, *Matrix Product State Representations*, Quantum Inf. Comput. 7, 401 (2007), arXiv:quant-ph/0608197]



Why should MPS work?

- Low D description is possible when the system has little entanglement.
- General result about entanglement in quantum systems: *The entanglement between a subsystem and the rest grows with the boundary of the subsystem.* (**area law**)
- For 1D non-critical systems with correlation length ξ, the entanglement entropy S of a subchain scales like:

$$S \propto \log(\xi).$$

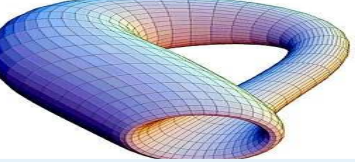
- For 1D critical systems, ξ has to be replaced with an extensive scale like the length of the subsystem L:

$$S \propto \log(L).$$

- But this is still exponentially better than the entanglement present in a random state:

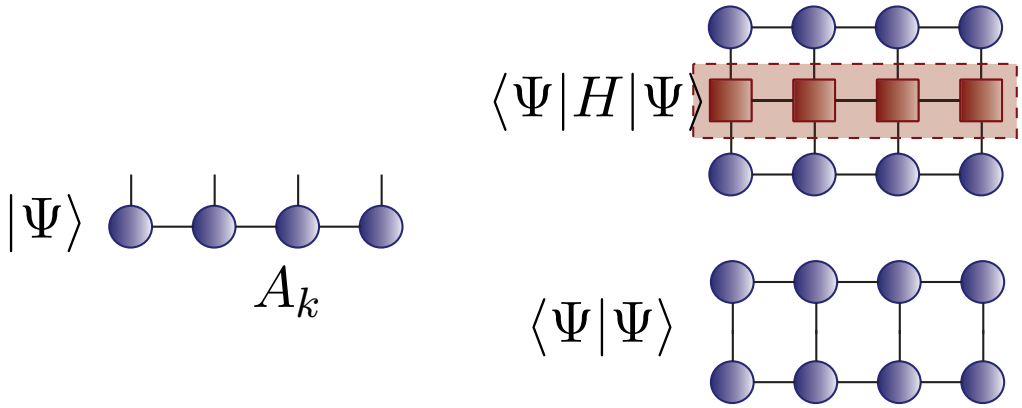
$$S \propto L.$$

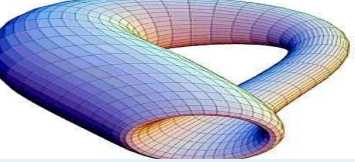
[D. Perez-Garcia, F. Verstraete, M.M. Wolf, J.I. Cirac, *Matrix Product State Representations*, Quantum Inf. Comput. 7, 401 (2007), arXiv:quant-ph/0608197]



Ground state and excited states

- The ground state can be found variationally by successively minimizing the energy $\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ with respect to each tensor A_j until convergence is achieved.
- The minimization is performed by varying one tensor at a time, and sweeping back and forth over the chain until convergence.
- Having the ground state, one can find ground state expectation values of any operator of interest.
- After having found the ground state of the system, we can also project it out and then look for the ground state of the projected system, thus obtaining excitations of the system.





Thermal properties

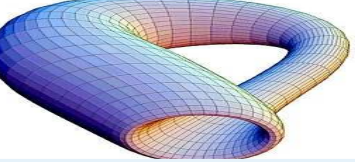
- The thermal expectation value of any operator $\mathcal{O}$ is given by:

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\left[\mathcal{O}\rho(\beta)\right]}{\mathrm{Tr}\left[\rho(\beta)\right]}$$

  where $\rho(\beta)$ – thermal equilibrium density operator at inverse temperature β.

- The approximation to the thermal state, $\rho(\beta) \propto e^{-\beta H}$, can be computed using imaginary time evolution acting on the identity matrix, which corresponds (up to normalization) to the exact thermal state at infinite temperature.

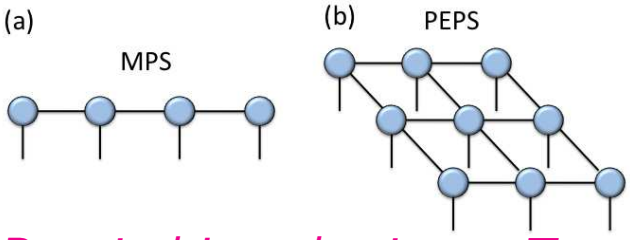
[F. Verstraete, J. J. García-Ripoll and J. I. Cirac, *Matrix product density operators: Simulation of finite-temperature and dissipative systems*, Phys. Rev. Lett. **93**, 207204 (2004)]



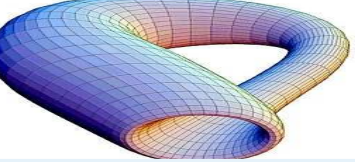
Higher dimensions?

- Although MPS is universal, it is not well-suited to describe an area law for 2D (or higher) as the required D would grow exponentially with the system size.
- A natural generalization to higher dimensions is Projected Entangled Pair States (PEPS).

  [F. Verstraete and J. Cirac, *Renormalization algorithms for quantum-many body systems in two and higher dimensions*, arXiv: cond-mat/0407066.
- Properties of PEPS are quite different from those of MPS.
- They have built-in the area law for general dimension: entanglement entropy of a subsystem scales with the size of its boundary.



Picture from: R. Orus, *A Practical Introduction to Tensor Networks*, Annals of Physics 349 (2014) 117-158, arXiv:1306.2164 [cond-mat.str-el]



Road map to QCD with Tensor Networks

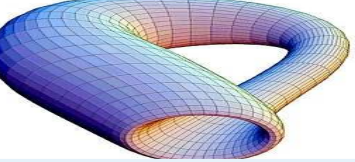
The way to apply TNS to QCD is a long one.

- START: Schwinger model, i.e. an Abelian gauge theory with U(1) gauge group, 1+1 dimensions

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi}(i \not{\partial} - g \not{A} - m)\psi$$

- NATURAL NEXT STEP: non-Abelian gauge theories (SU(2), SU(3)) in 1+1 dimensions
- AND ALSO: go to 2+1 dimensions
- FINALLY: go to 3+1 dimensions, non-Abelian gauge group SU(3) for QCD

All these next steps non-trivial and challenging.



The Schwinger model

The Schwinger model is QED in 1+1 dimensions:

[J. S. Schwinger, "Gauge Invariance and Mass. 2.," Phys. Rev. **128** (1962) 2425.]

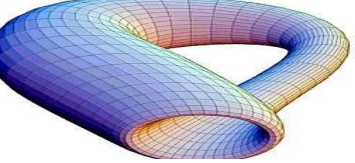
$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi}(i \not{\partial} - g \not{A} - m)\psi$$

where ψ is a 2-component spinor field.

- Simplest gauge theory, but physics still surprisingly rich,
- in several aspects resembles much more complex theories (QCD):
  - ⋆ confinement,
  - ⋆ chiral symmetry breaking (via anomaly, not spontaneous),
- standard toy model for testing lattice techniques.

Most prominent feature of the Schwinger model: non-perturbative generation of mass gap!

The mass gap can be calculated analytically: $\frac{M_V}{g} = \frac{1}{\sqrt{\pi}} \approx 0.564189584.$



Multi-flavour Schwinger model as a spin model

HOPPING TERM

$$H = -xi^{N_f-1} \sum_{f=0}^{N_f-1} \sum_{n=0}^{N-2} \Big[\sigma^+_{N_f n+f} \sigma^z_{N_f n+f+1} \cdots \sigma^z_{N_f n+N_f+f-1} \sigma^-_{N_f n+N_f+f} +$$

HOPPING TERM H.c.

$$(-1)^{N_f-1} \sigma^-_{N_f n+f} \sigma^z_{N_f n+f+1} \cdots \sigma^z_{N_f n+N_f+f-1} \sigma^+_{N_f n+N_f+f} \Big] +$$

$$+ \sum_{k=0}^{N_f N-1} \alpha_1(k) 1 + \sum_{k=0}^{N_f N-1} \alpha(k) \sigma^z_k + \sum_{k=0}^{N_f N-1} \sum_{k'=k+1}^{N_f N-1} \beta'(k') \sigma^z_k \sigma^z_{k'},$$

INHOMOGENEOUS OFFSET — INHOMOGENEOUS MAGNETIC FIELD — GAUGE TERM

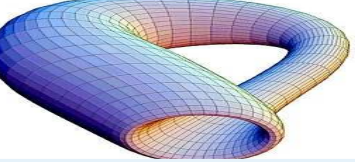
long-distance interaction!

with:

$$\alpha_1(k) = \frac{l_0^2}{N_f} \left(1 - \delta_{k/F, N-1}\right) + l_0 \left(1 - (k/N_f)\%2\right) + \frac{1}{2} M_{k\%N_f} + \frac{1}{8}(N + N_f - 1) + \xi,$$

$$\alpha(k) = l_0(N - k/N_f - 1) + \frac{\widetilde{\mu}_{k\%N_f}}{2} + \frac{1}{2} M_{k\%N_f} (-1)^{k/N_f} + \frac{N_f}{4} \left(N - k/N_f - (k/N_f)\%2\right),$$

$$\beta'(k) = \frac{1}{2} \left(N - k/N_f - 1 + 2\xi\right),$$



Our aims

We wanted to find:

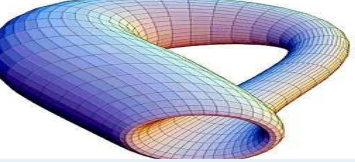
- ground state energy (1-flavour)
- vector and scalar mass gap (1-flavour)
- chiral condensate (1,2-flavours)
- particle number differences (2-flavours)

for selected values of the fermion mass $m/g = 0,\ 0.125,\ \ldots$.

Simulate with finite D (bond dimension), N (system size), $x \equiv \frac{1}{a^2 g^2}$ (inverse coupling, commonly denoted by β in LGT literature).

We need:

- large enough D – check $D \in [40, 200]$,
- infinite volume limit: $N \to \infty$ – choose $N \in [50, 850]$ (note that $N \propto \sqrt{x}$),
- continuum limit: $x \to \infty$ – choose $x \in [9, 1000]$.



Chiral condensate $T = 0$ $(N_f = 1)$

- The Schwinger model posesses a $U(1)_A$ chiral symmetry, which is broken by the chiral anomaly.
- This symmetry breaking is signaled by a non-zero value of the chiral condensate:

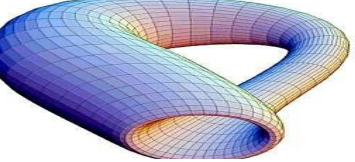
$$\Sigma = \frac{\sqrt{x}}{N} \sum_n (-1)^n \frac{1 + \sigma_n^z}{2}$$

$\longrightarrow$ compute GS expectation value of Σ.

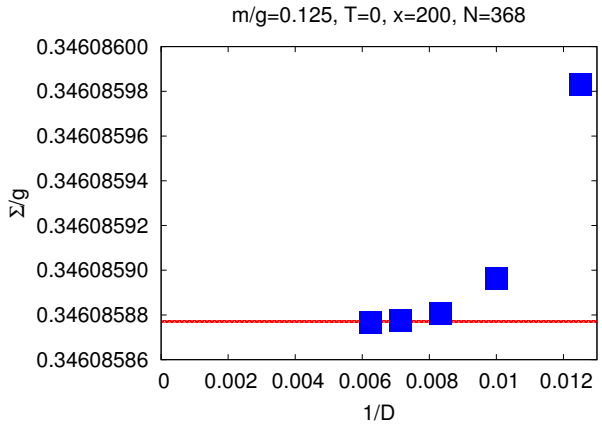
- The naively computed condensate has a logarithmic divergence $\propto \frac{m}{g} \log ag$. This divergence can be subtracted off by subtracting the free theory contribution (in the infinite volume limit):

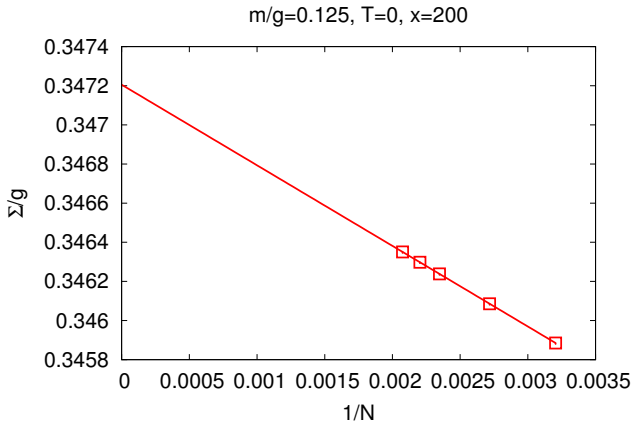
$$\Sigma_{\text{free}}^{(\text{bulk})}(m/g, x) = \frac{m}{\pi g} \frac{1}{\sqrt{1 + \frac{m^2}{g^2 x}}} \mathrm{K}\left(\frac{1}{1 + \frac{m^2}{g^2 x}} \right),$$

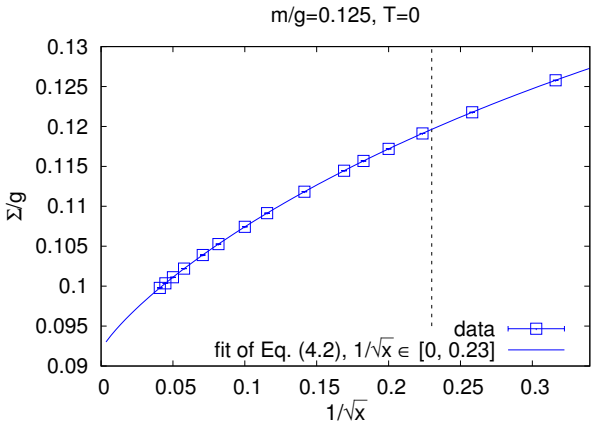
where $\mathrm{K}(u)$ is the complete elliptic integral of the first kind.

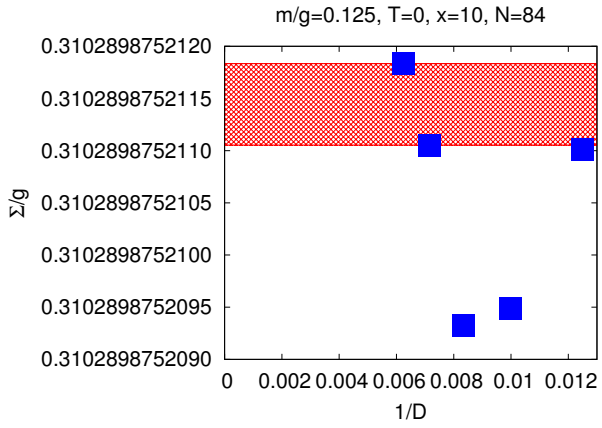


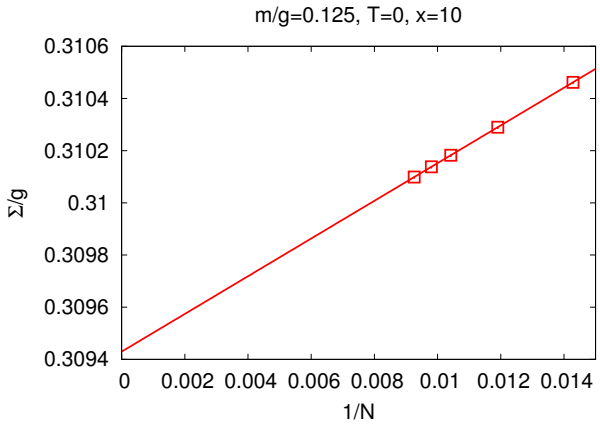
Results for the chiral condensate $T = 0$ ($N_f = 1$)

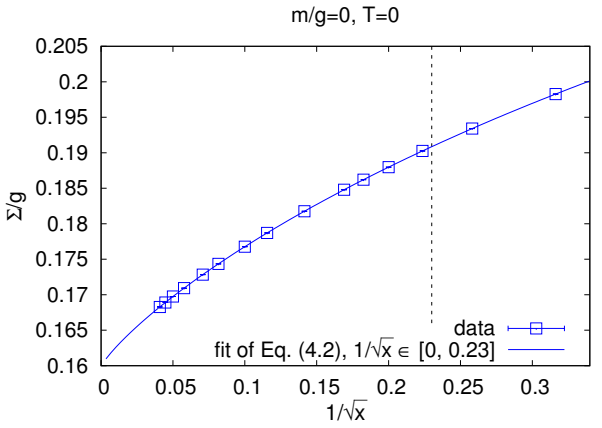








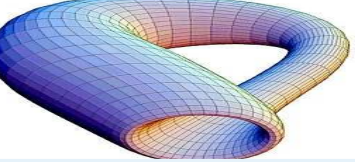




Truncation

Finite size scaling (linear in $1/N$)

Continuum extrapolation (quadratic in lat.spac., + log.-corrections)



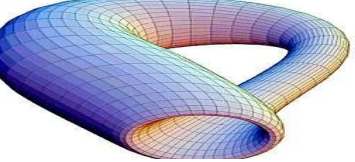
Results for the chiral condensate $T = 0$ $(N_f = 1)$

	Subtracted condensate		
m/g	Our result MPS	Buyens et al. MPS	Exact $(m = 0)$ or Hosotani $(m > 0)$
0	0.159929(7)	0.159929(1)	0.159929
0.0625	0.1139657(8)	–	0.1314
0.125	0.0920205(5)	0.092019(2)	0.1088
0.25	0.0666457(3)	0.066647(4)	0.0775
0.5	0.0423492(20)	0.042349(2)	0.0464
1.0	0.0238535(28)	0.023851(8)	0.0247

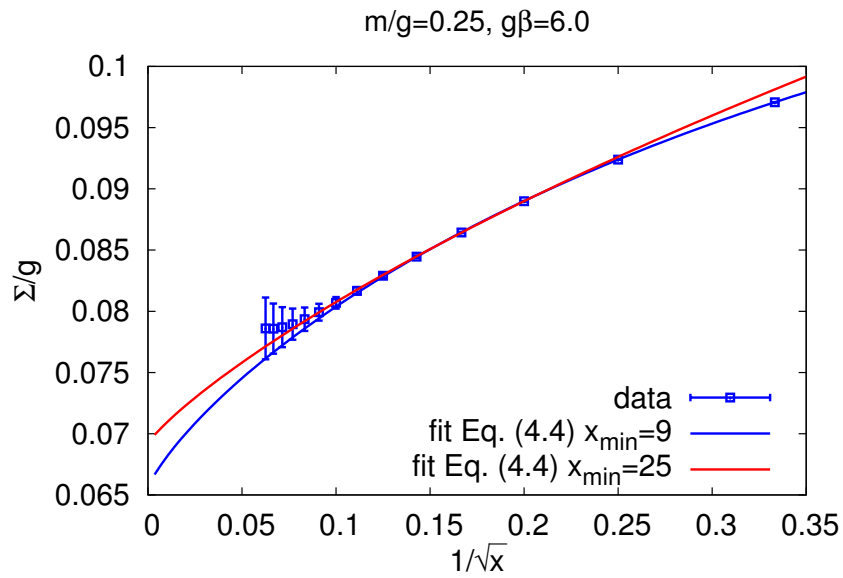
Exact result (massless case): $\frac{\Sigma}{g} = \frac{1}{2\pi^{3/2}} e^{\gamma_E} \approx 0.1599288$.

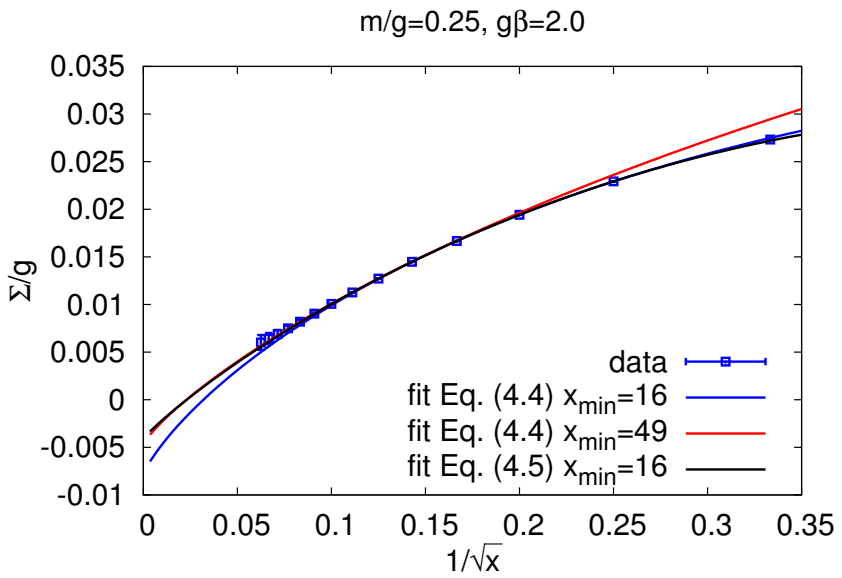
[K. Van Acoleyen, B. Buyens, J. Haegeman and F. Verstraete, "Matrix product states for Hamiltonian lattice gauge theories," PoS LATTICE **2014** (2014) 308]

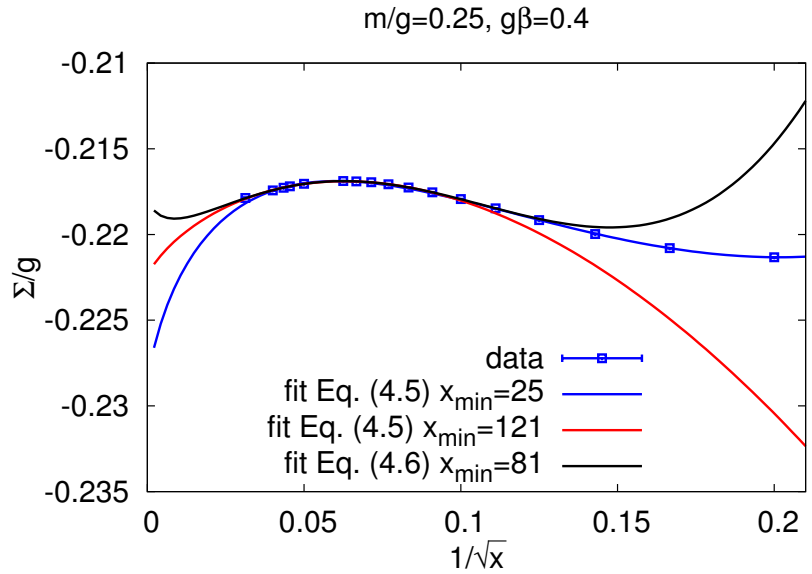
[Y. Hosotani, "Chiral dynamics in weak, intermediate, and strong coupling QED in two-dimensions," In: Nagoya 1996, Perspectives of strong coupling gauge theories, 390-397 [hep-th/9703153].]

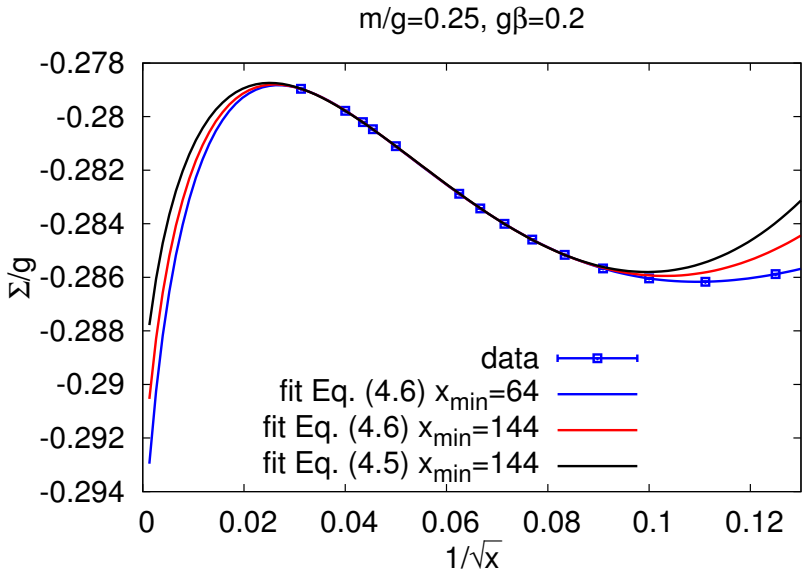


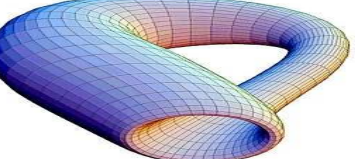
Thermal case – continuum extrapolation ($N_f = 1$)







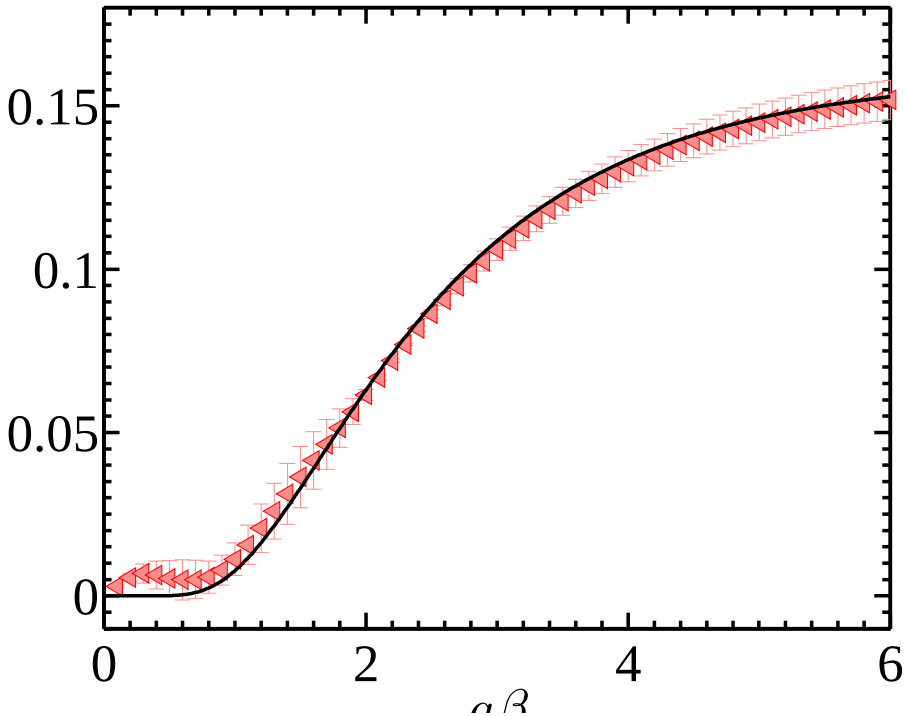




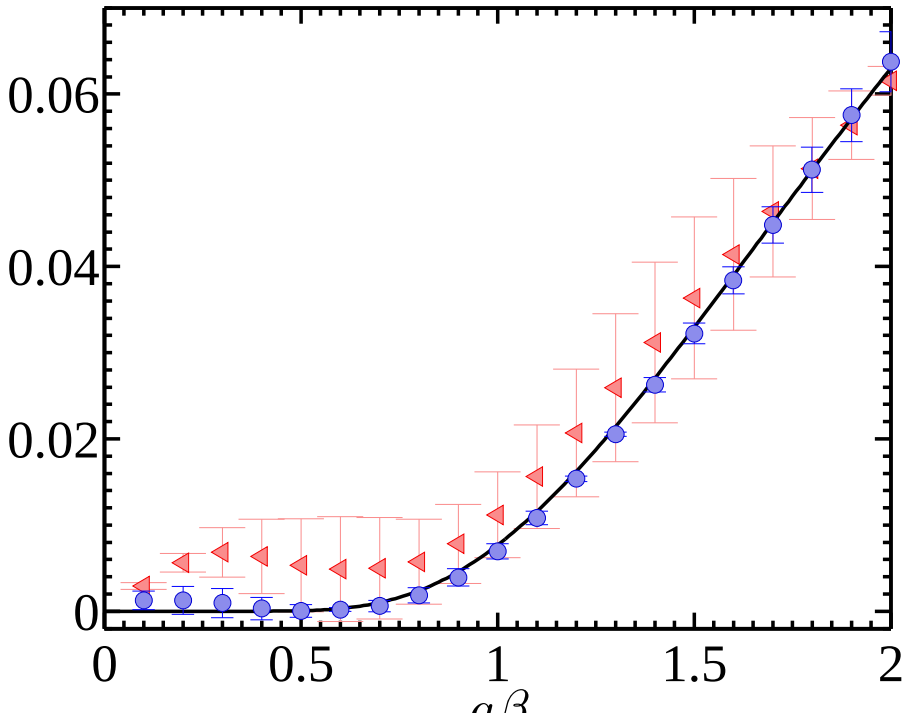
Temperature dependence ($N_f = 1$)

MASSLESS CASE

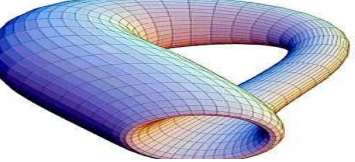
without flux truncation



without/with flux truncation



Analytical result from: [I. Sachs, A. Wipf, "Finite Temperature Schwinger Model," Helv. Phys. Acta 65, 652 (1992), arXiv:1005.1822 [hep-th]]



Temperature dependence ($N_f = 1$)

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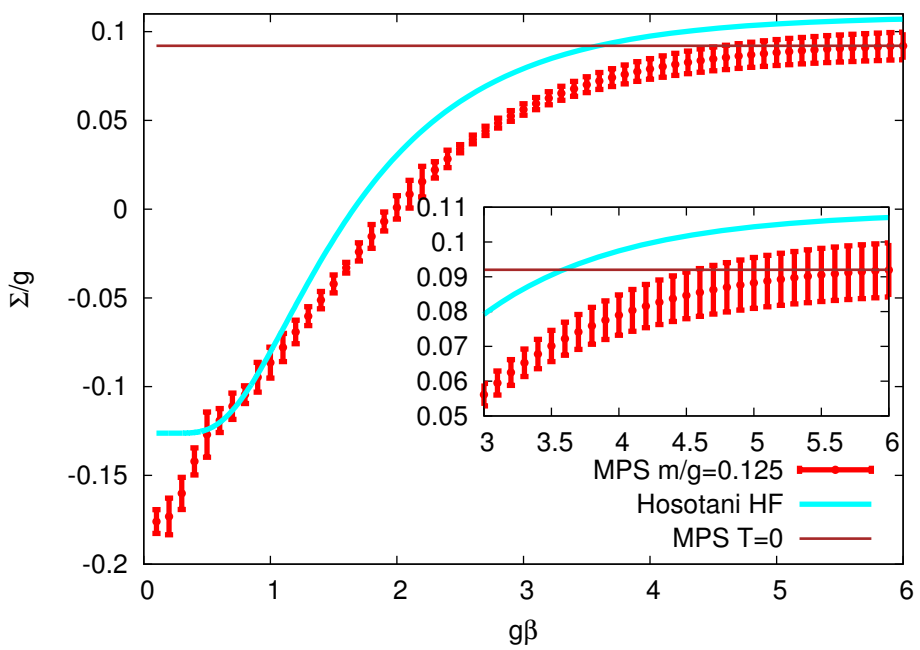
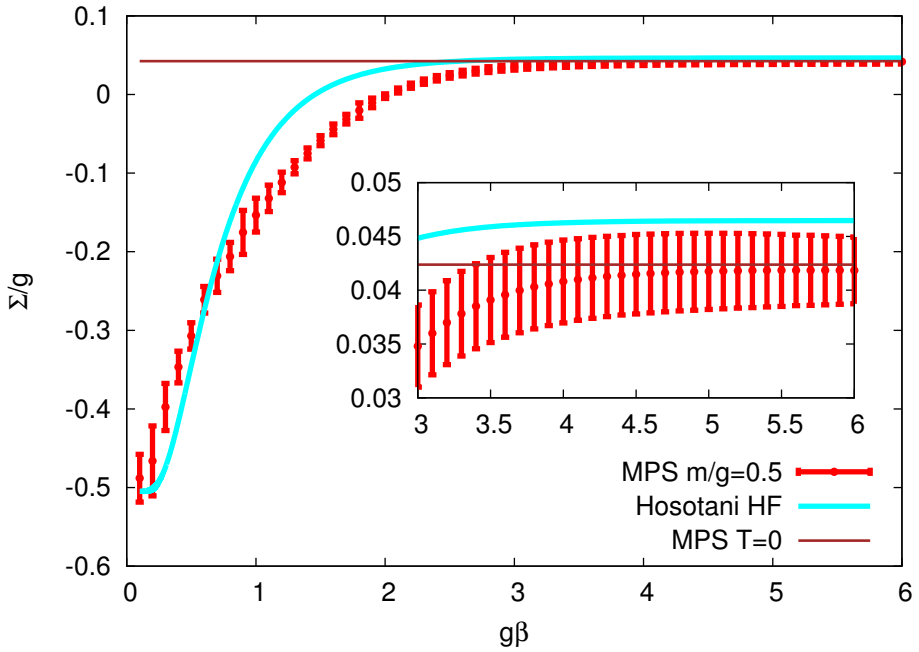
MASSIVE CASE

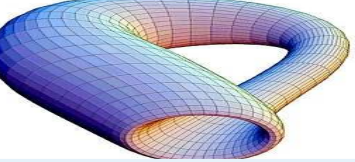
$m/g = 0.125$



$m/g = 0.5$



Reference curve (generalized Hartree-Fock approximation): [Y. Hosotani and R. Rodriguez, "Bosonized massive N flavor Schwinger model," J. Phys. A **31** (1998) 9925]



Two flavours with chemical potential

Recently, we analyzed the first case for which a MC simulation would encounter the sign problem :

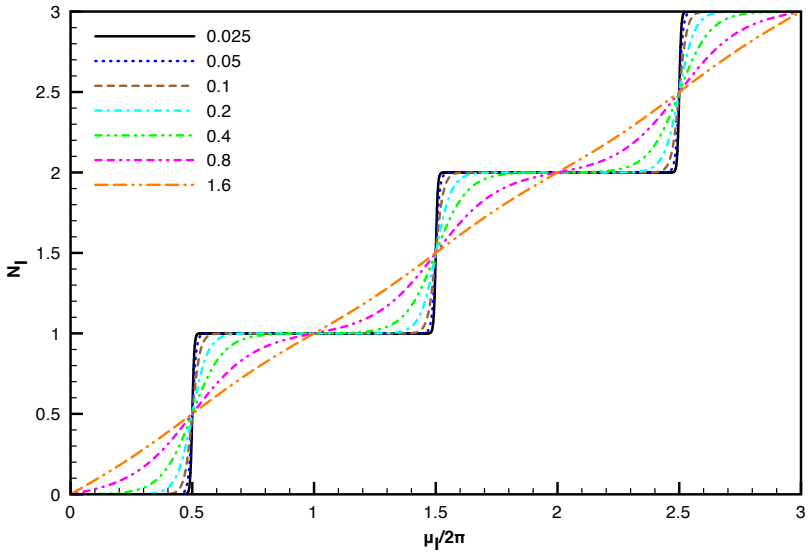
the 2-flavour Schwinger model with a chemical potential.

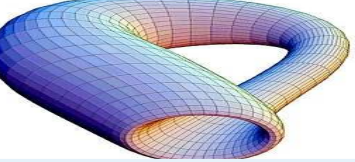
Quantity of interest:

the difference in particle numbers $N_1 - N_2$ vs. $\mu_I/2\pi \propto \mu_1 - \mu_2$.

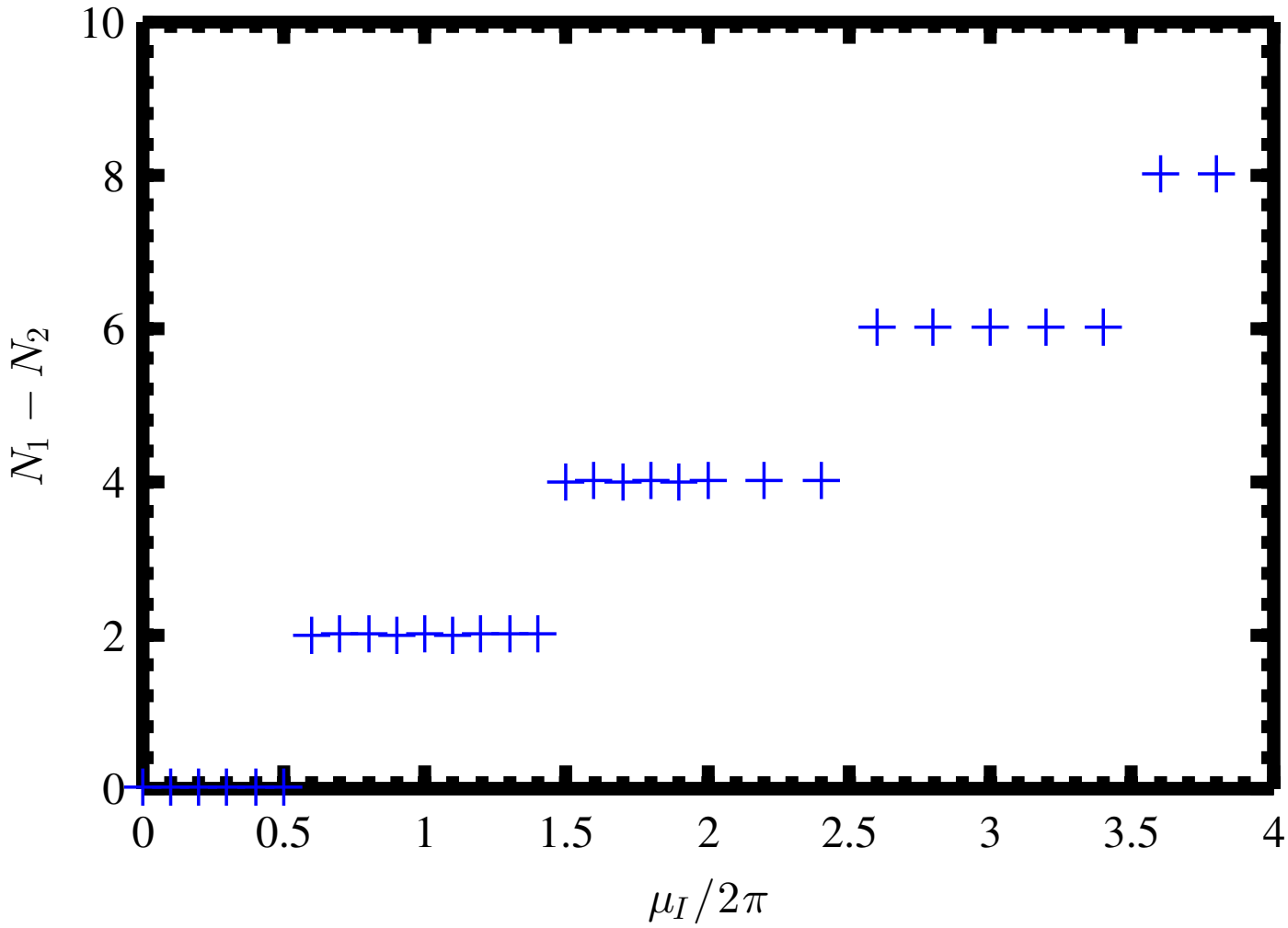
Analytical computation ($m = 0$):

[R. Narayanan, "Two flavor massless Schwinger model on a torus at a finite chemical potential," Phys. Rev. D **86** (2012) 125008]

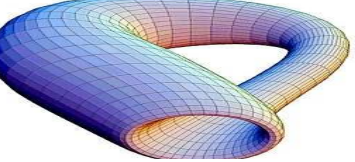




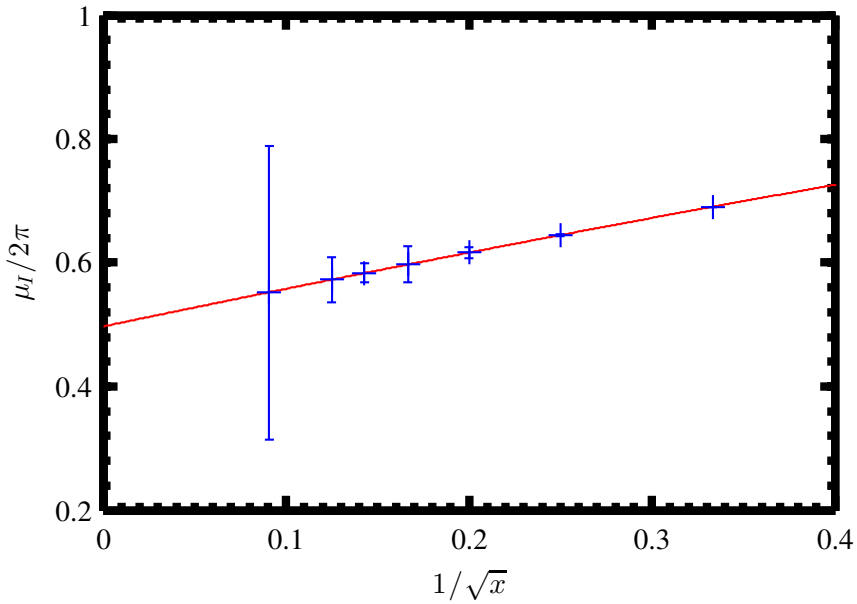
Example ($N_f = 2$)

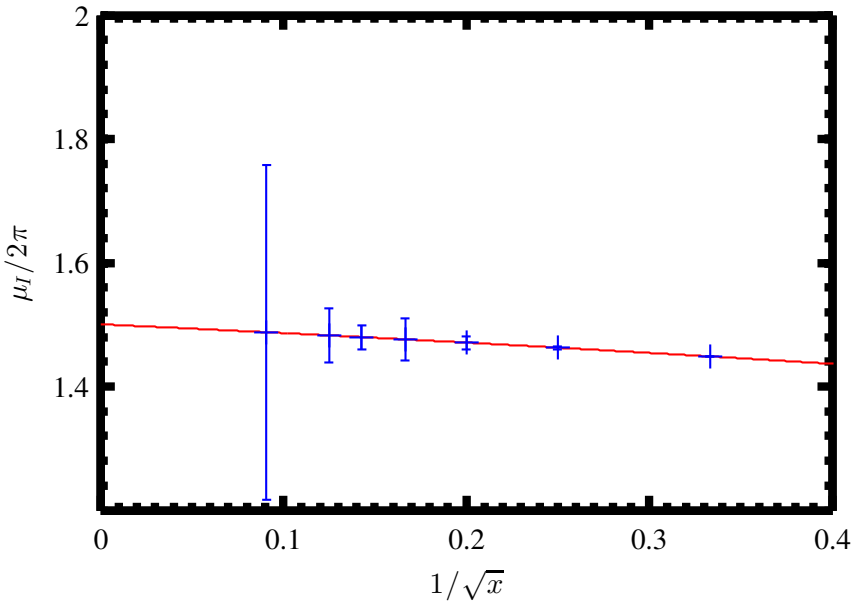


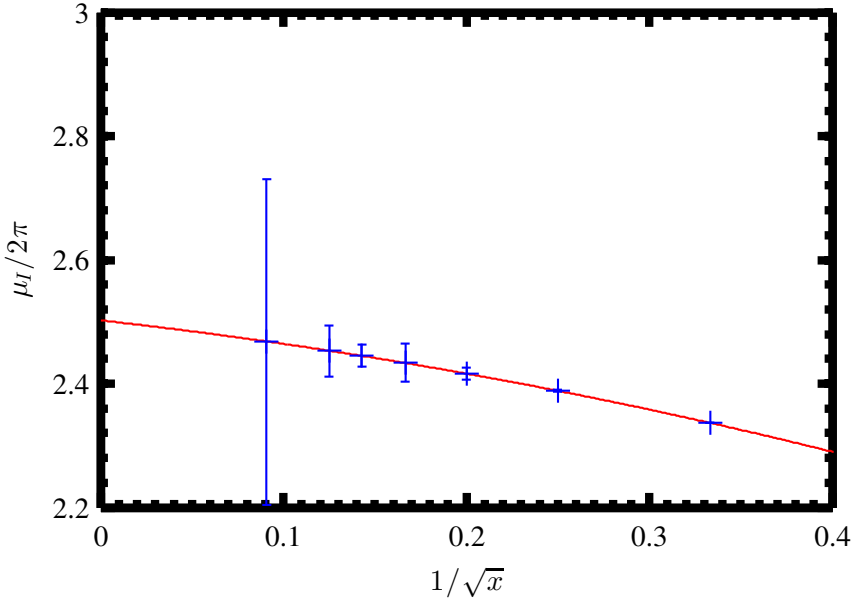
$x = 121,\ N = 88$

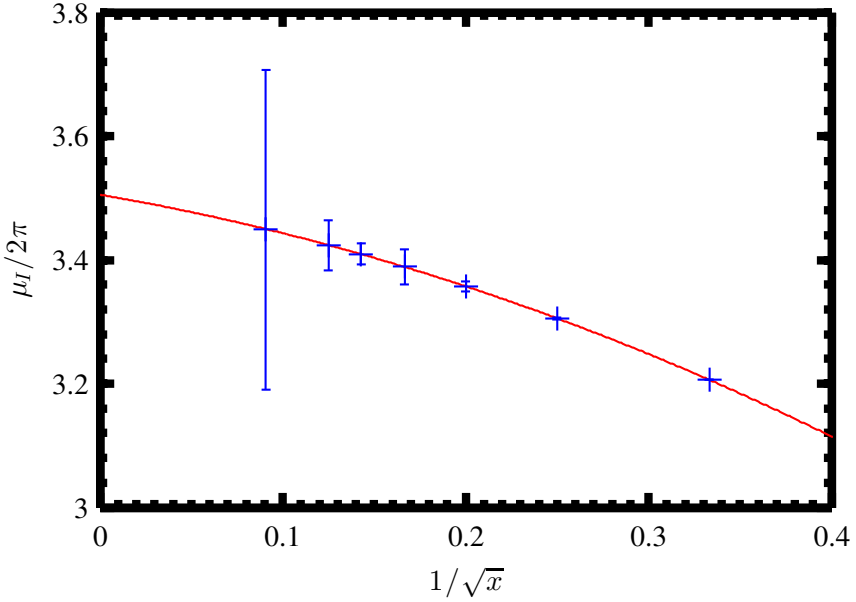


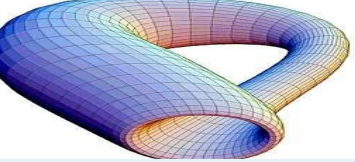
Continuum extrapolation of jumps



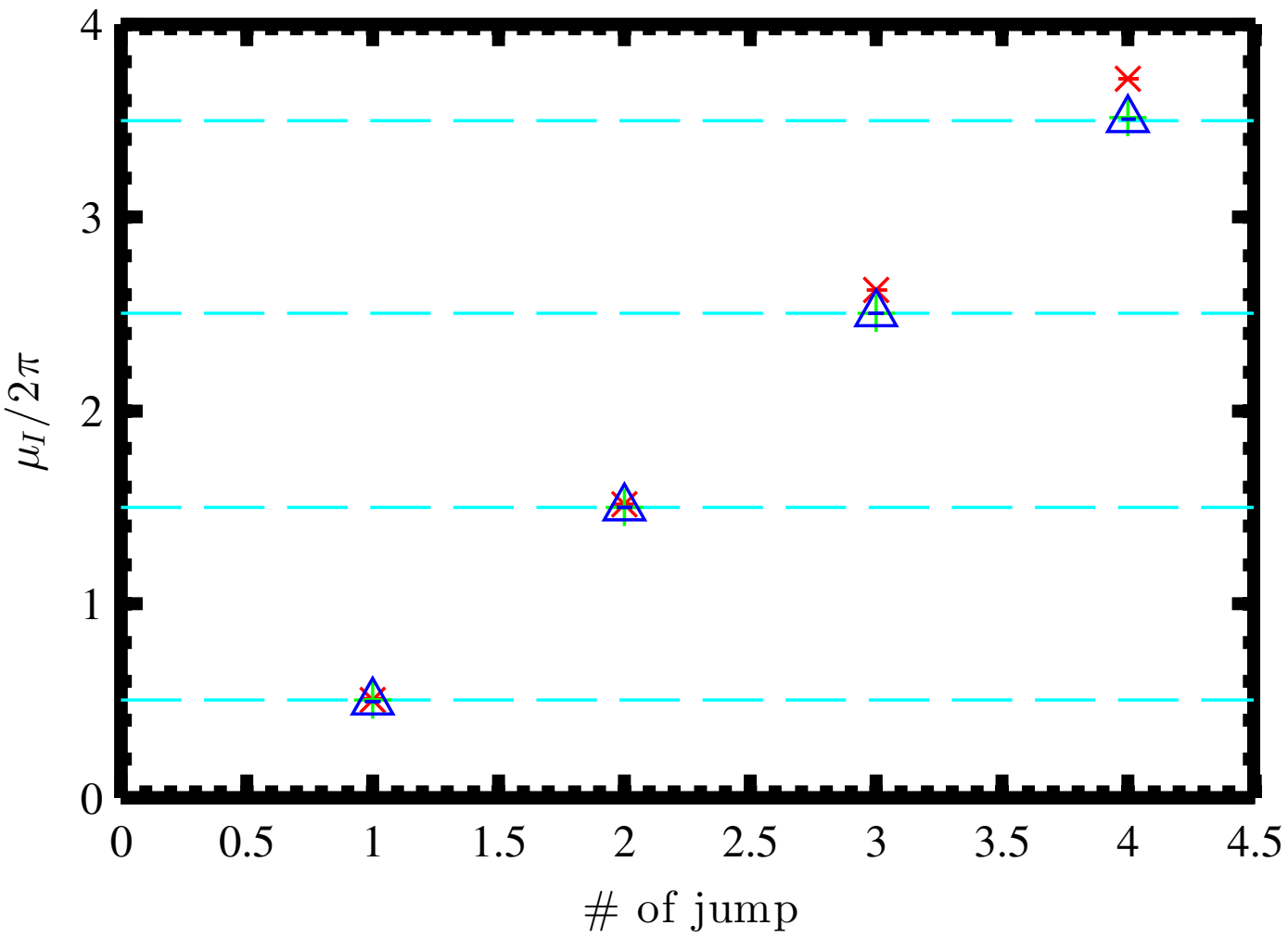






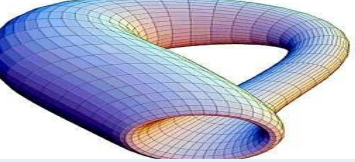


FVE and final result ($N_f = 2$)



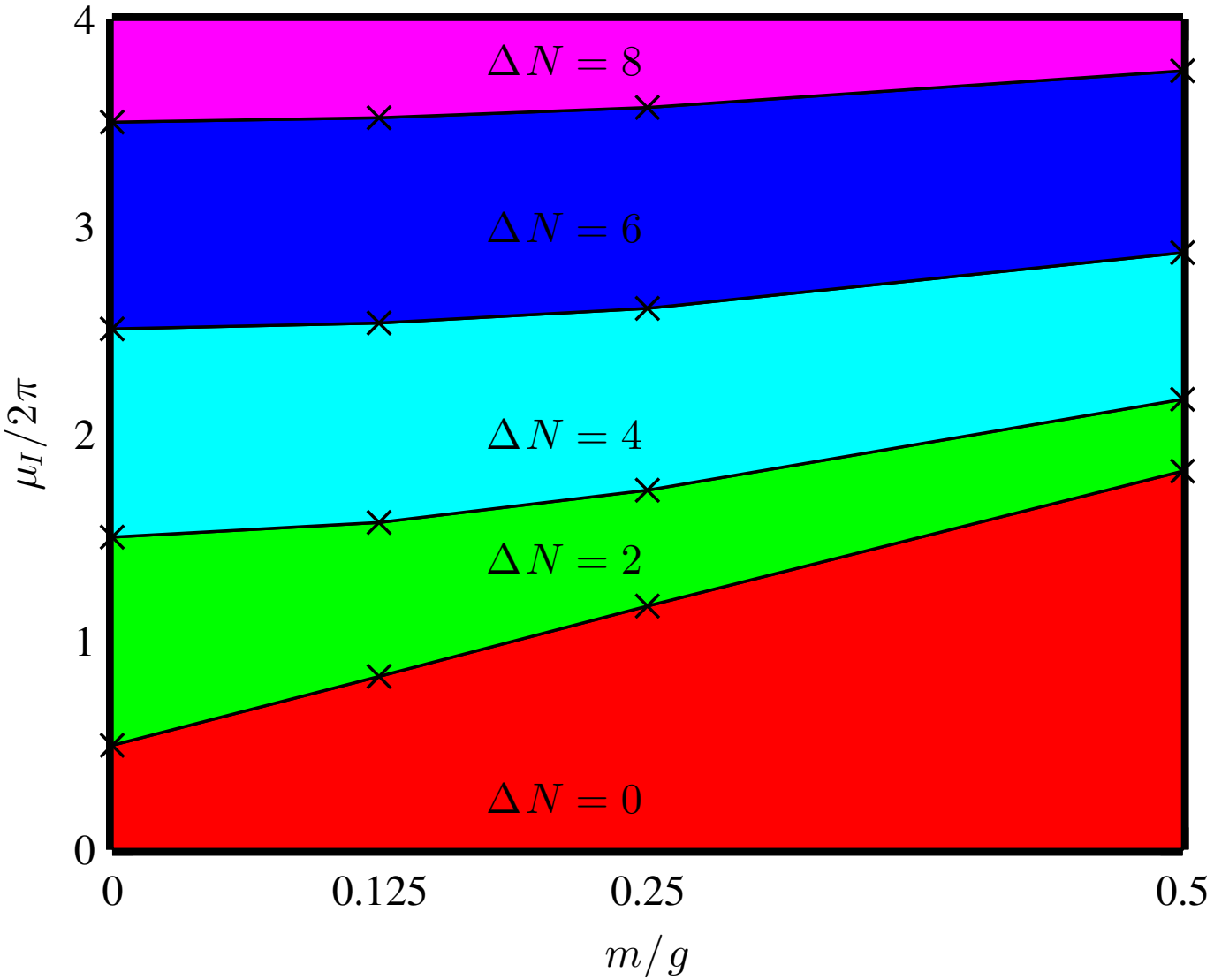
FVE negligible when going from $N/\sqrt{x} = 6$ to $N/\sqrt{x} = 8$

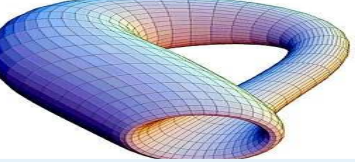
($\Rightarrow N/\sqrt{x} = 8$ is FINAL RESULT)



Phase diagram ($N_f = 2$)

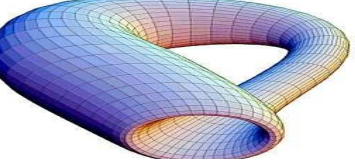
PRELIMINARY phase diagram $\mu_I/2\pi$ vs. m/g





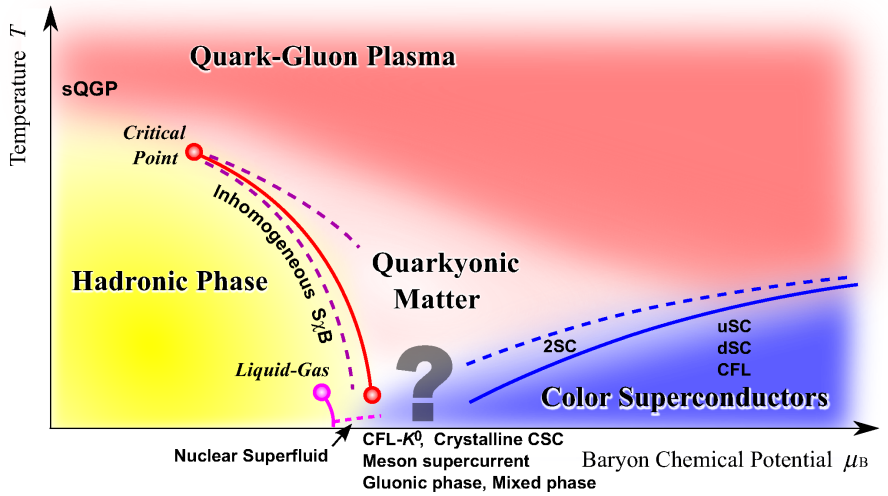
Conclusions

- Proof of concept – the MPS approach can be used to extract:
  - ⋆ mass spectrum (GS energy, masses of lightest particles of a theory),
  - ⋆ ground state expectation values (chiral condensate),
  - ⋆ thermal properties (chiral condensate),
  - ⋆ properties at finite density (jump locations).
- The latter is a demonstration that tensor networks can **overcome the sign problem**!
- Precision better or comparable to best results in the literature, in some cases better than 0.001%.



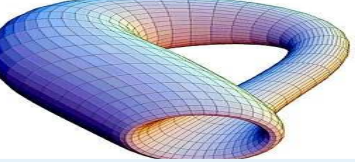
Prospects

- We want to look into aspects of lattice gauge theories where the standard methods have problems:
  - ⋆ thermodynamics at non-zero chemical potential,
  - ⋆ non-equilibrium properties.

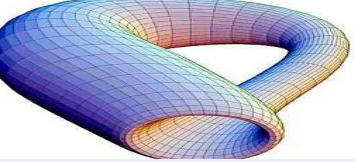


[K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74 (2011) 14001]

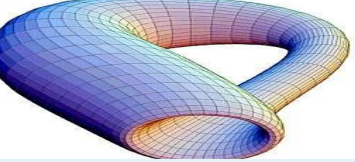
- Already underway: chemical potential and non-Abelian SU(2) case.
- But still 1+1 dimensions...
- Ultimate aim: full QCD, i.e.:
  - ⋆ a non-Abelian theory with SU(3) gauge group,
  - ⋆ in **3+1** dimensions.
- **Needs a lot of work of the Tensor Network + lattice gauge theory community...**



Thank you for your attention!

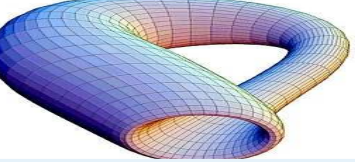


Backup slides

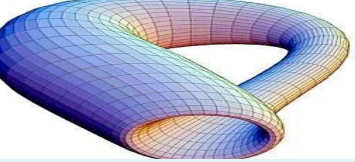


MPS properties

- Gapped 1D systems are well described by MPS with a relatively small bond dimension D, independent of the system size.
- The precise mathematical statement is for gapped local Hamiltonians, about the ground state only, and says that MPS approximate the ground state exponentially well (with increasing D, the error decreases exponentially).
- For non-gapped systems, D can grow with the system size, but only logarithmically $\Rightarrow$ so it is still effective in practice.
- MPS are especially effective in 1D, because they have built in area law for 1D $\Rightarrow$ other tensor network methods exist for higher dimensions (see later)
- Still, MPS can be used in 2D and actually the best results for certain 2D Hamiltonians are from MPS (e.g. frustrated Heisenberg spin model on a kagome lattice).



- The MPS description is not unique.
- However, there exists a unique description in terms of the *canonical MPS form*.
- MPS satisfy 1D area law.
- Expectation value can always be done efficiently:
  - ⋆ $\mathrm{O}(NdD^3)$ time for open boundary conditions (OBC),
  - ⋆ $\mathrm{O}(NdD^5)$ time for periodic boundary conditions (PBC).
- Note that a great deal of properties of MPS can be proved rigorously – hence the expectations that the approach works and that it works *efficiently* have good ground.

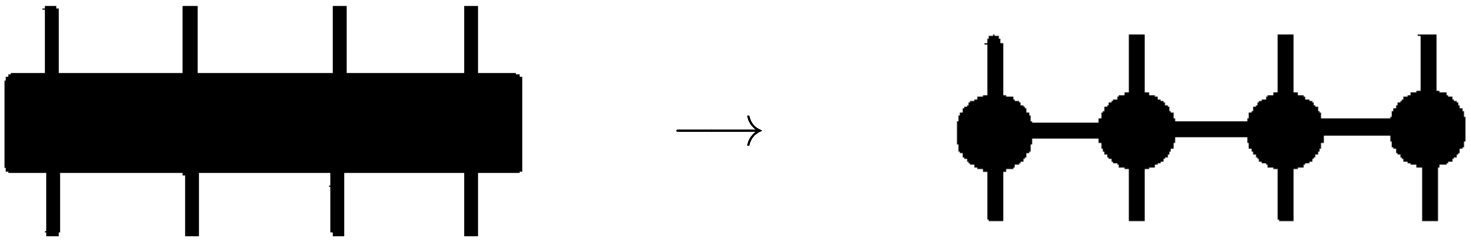


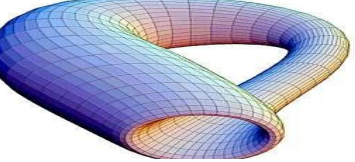
Matrix Product Operators

In analogy to the MPS description of quantum states, one can also represent operators as **Matrix Product Operators** (MPOs).

- introduced in: [F. Verstraete, J. J. García-Ripoll and J. I. Cirac, *Matrix product density operators: Simulation of finite-temperature and dissipative systems*, Phys. Rev. Lett. **93**, 207204 (2004)]
  M. Zwolak, G. Vidal, *Mixed-state dynamics in 1D quantum lattice systems: a time-dependent superoperator renormalization algorithm*, Phys. Rev. Lett. **93**, 207205 (2004)]
- important properties also discussed in:
  B. Pirvu, V. Murg, J.I. Cirac, F. Verstraete, *Matrix product operator representations*, New J. of Phys. **12** 025012 (2010)

Main idea:





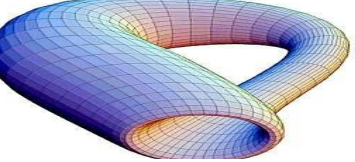
Excited states

- After having found the ground state of the system, $|\Psi_0\rangle$, we can construct the projector onto the orthogonal subspace, $\Pi_0 = 1 - |\Psi_0\rangle\langle\Psi_0|$.
- The projected Hamiltonian, $\Pi_0 H \Pi_0$, has $|\Psi_0\rangle$ as eigenstate with zero eigenvalue, and the first excited state as eigenstate with energy E_1.
- Given that $E_1 < 0$, what we can always ensure by adding an appropriate constant to H, the first excitation corresponds then to the state that minimizes the energy of the projected Hamiltonian:

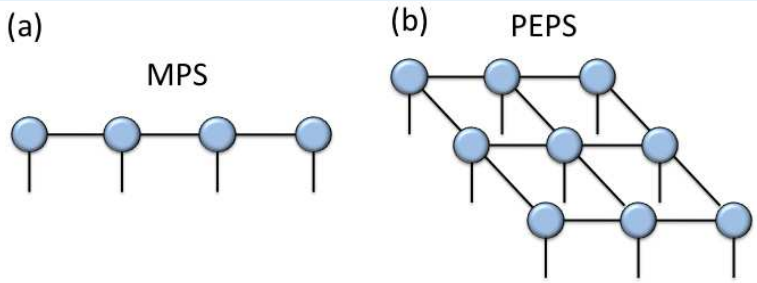
$$E_1 = \min_{|\Psi\rangle} \frac{\langle\Psi|\Pi_0 H \Pi_0|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|\left(H - E_0|\Psi_0\rangle\langle\Psi_0|\right)|\Psi\rangle}{\langle\Psi|\Psi\rangle}.$$

- This minimization corresponds to finding the ground state of the effective Hamiltonian $H_{\text{eff}}[1] = \Pi_0 H \Pi_0$.
- The procedure can be concatenated to find subsequent energy levels, so that, to find the M-th excited state, we will search for the ground state of the Hamiltonian:

$$H_{\text{eff}}[M] = \Pi_{M-1} \ldots \Pi_0 H \Pi_0 \ldots \Pi_{M-1} = H - \sum_{k=0}^{M-1} E_k |\Psi_k\rangle\langle\Psi_k|.$$



PEPS



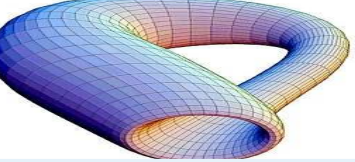
Picture from: R. Orus, *A Practical Introduction to Tensor Networks*, Annals of Physics 349 (2014) 117-158, arXiv:1306.2164 [cond-mat.str-el]

Main practical difference:

- exact contraction of two arbitrary PEPS (even one PEPS with itself) is an exponentially hard problem (complexity class #P-Hard, related to counting the number of solutions of NP-Complete problems).
- Hence, computing scalar products of PEPS is inefficient.
- However, clever numerical methods, e.g. cluster ideas, can be used to approximate exact contractions.

  M. Lubasch, J. I. Cirac, M.-C. Banuls, *Unifying Projected Entangled Pair States contractions*, New J. Phys. 16, 033014 (2014), arXiv:1311.6696 [quant-ph]

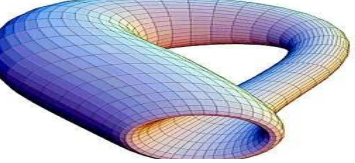
  M. Lubasch, J. I. Cirac, M.-C. Banuls, *Algorithms for finite Projected Entangled Pair States*, Phys. Rev. B 90, 064425 (2014), arXiv:1405.3259 [quant-ph]



Active area of research – methods

TN methods come under several acronyms:

- Density Matrix Renormalization Group (DMRG)
- Time-Evolving Block Decimation (TEBD)
- Projected Entangled Pair States (PEPS)
- Tensor Renormalization Group (TRG)
- Tensor-Entanglement Renormalization Group (TERG)
- Tensor Product Variational Approach (TPVA)
- Multi-scale Entanglement Renormalization Ansatz (MERA)
- Entanglement Renormalization (ER)
- Weighted Graph States (WGS)
- String-Bond States (SBS)
- Monte Carlo Matrix Product States (MCMPS)
- continuous Matrix Product States (cMPS)
- infinite Matrix Product States (iMPS)
- Time-Dependent Variational Principle (TDVP)
- Second Renormalization Group (SRG)
- Higher Order Tensor Renormalization Group (HOTRG)
- **. . . and much more**



Hamiltonian approach

The Hamiltonian of the Schwinger model in the staggered discretization:

$$H = \frac{x}{2} \sum_{n=0}^{N-1} \Big(\sigma^+(n) e^{i\theta(n)} \sigma^-(n+1) + \sigma^+(n+1) e^{-i\theta(n)} \sigma^-(n) \Big) + \\ + \frac{m}{ag^2} \sum_{n=0}^{N-1} \big(1 + (-1)^n \sigma^3(n) \big) + \sum_{n=0}^{N-1} L^2(n),$$

where: $x = 1/a^2 g^2$.

- Natural choice of basis: direct product of Ising basis $\{|i\rangle\}$, acted upon by Pauli spin operators, and the ladder space of states $\{|l\rangle\}$:

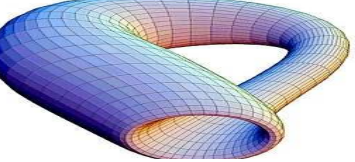
$$|i_0 i_1 \dots i_{N-2} i_{N-1}\rangle \otimes |l_{0,1} l_{1,2} \dots l_{N-2,N-1} l_{N-1,0}\rangle,$$

- The gauge degrees of freedom $l_{i,i+1}$ can be eliminated using the Gauss law:

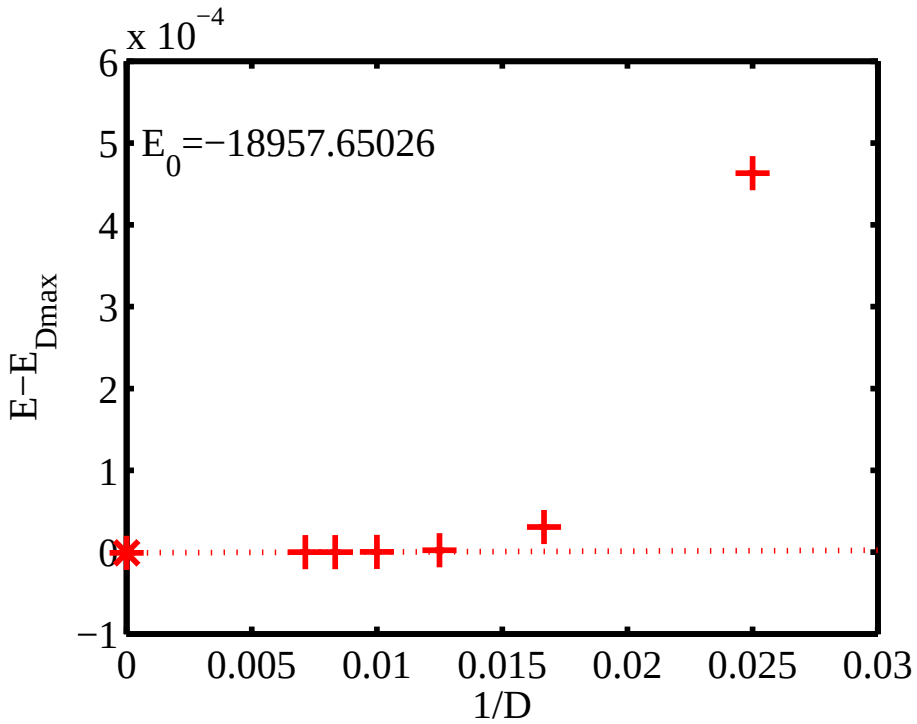
$$L_n - L_{n-1} = \frac{1}{2} \left(\sigma_n^z + (-1)^n \right),$$

leaving the basis states as:

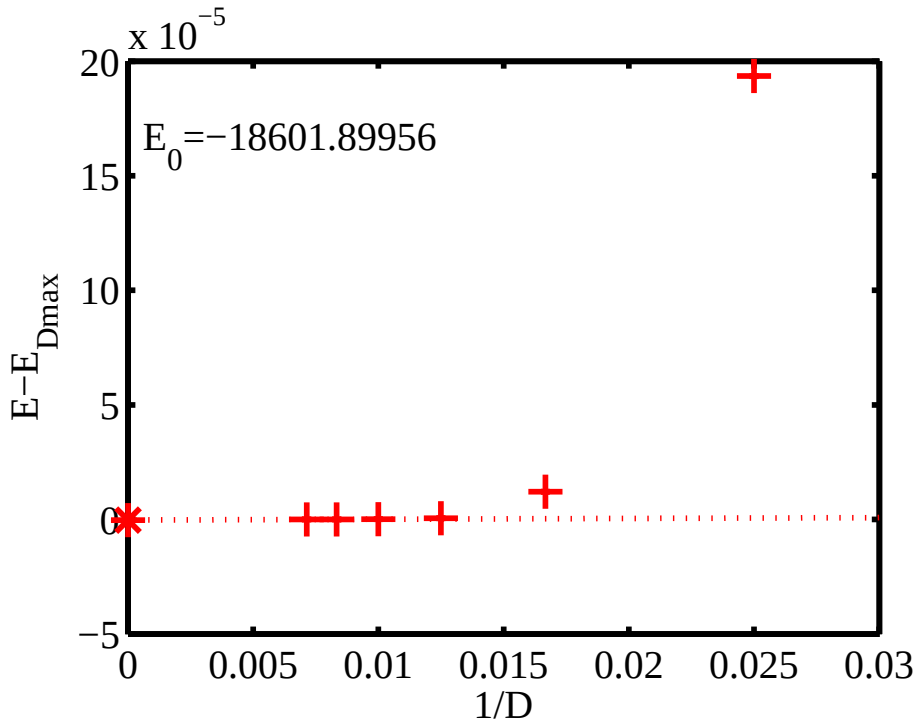
$$|i_0 i_1 \dots i_{M-2} i_{M-1}\rangle \otimes |l\rangle,$$



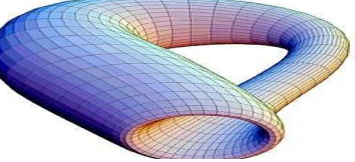
GS energy. Bond dimension



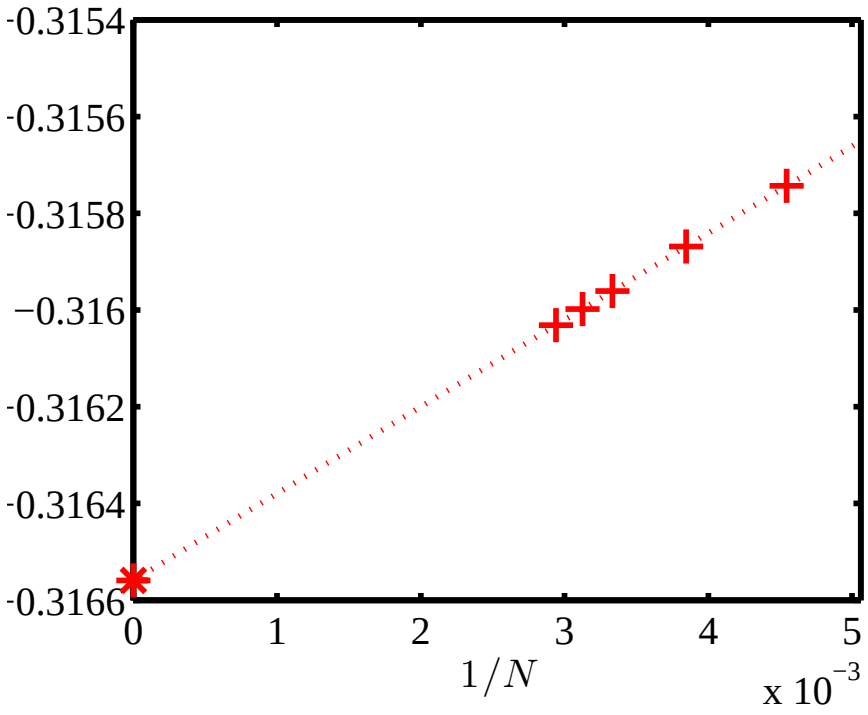
$m/g = 0,\ x = 100,\ N = 300$



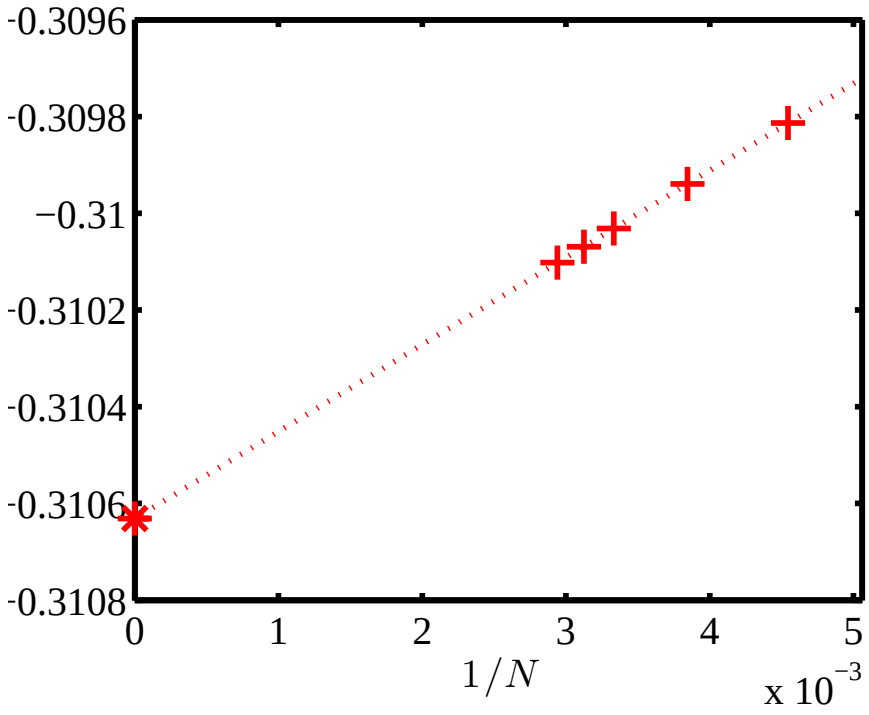
$m/g = 0.125,\ x = 100,\ N = 300$



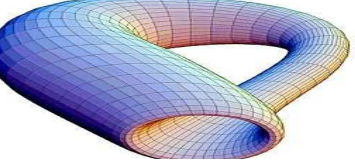
GS energy. Finite size scaling



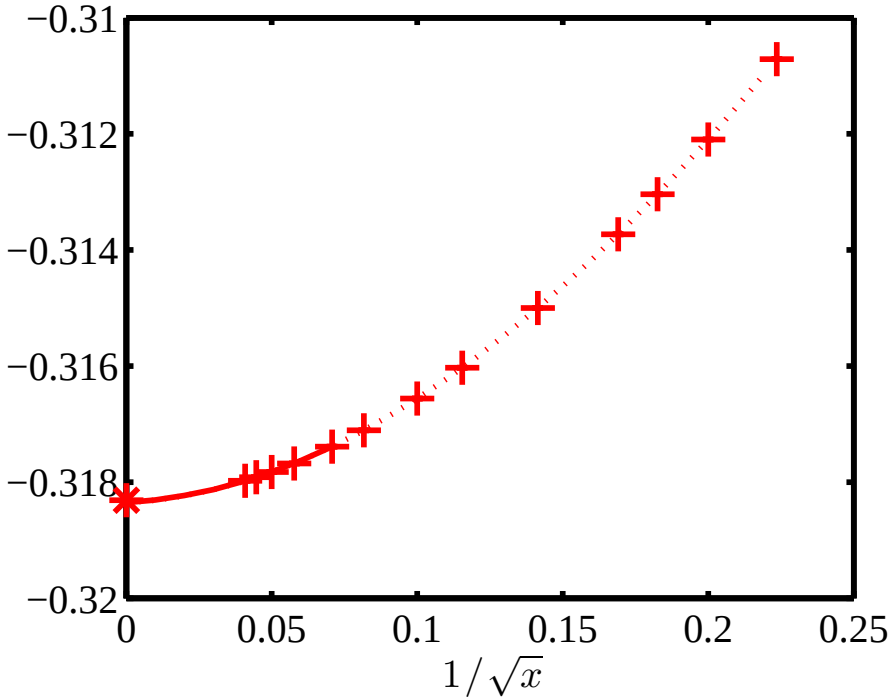
$m/g = 0,\ x = 100$



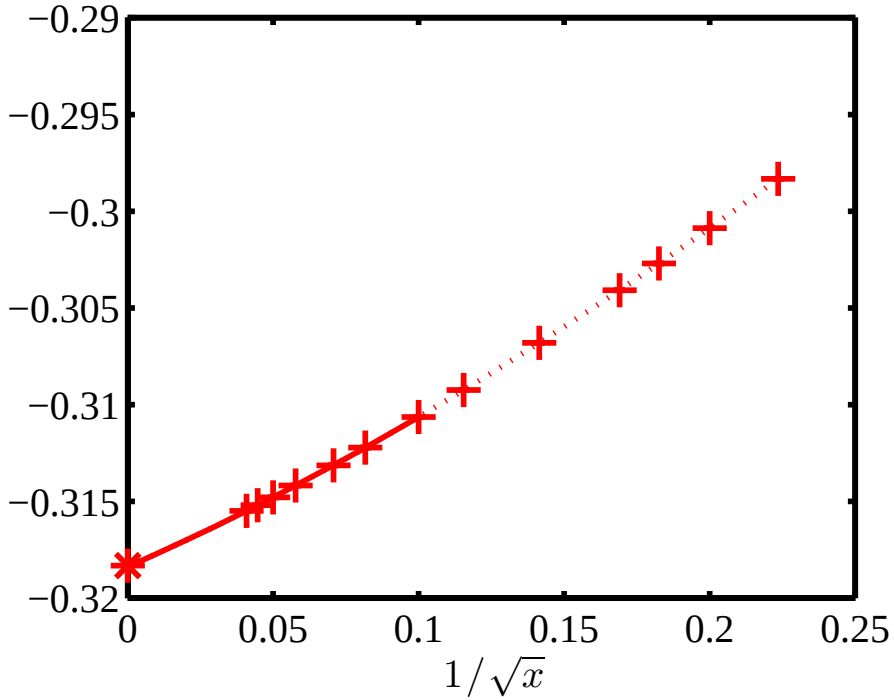
$m/g = 0.125,\ x = 100$



GS energy. Continuum extrapolation



$m/g = 0$

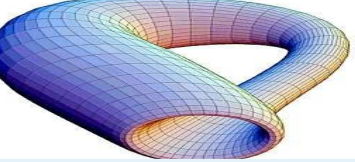


$m/g = 0.125$

continuum result:

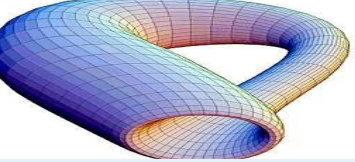
$-0.318338(22)_{D,N,x\,\text{extrapol.}}(24)_{\text{fitansatz}}$ $-0.318343(96)_{D,N,x\,\text{extrapol.}}(25)_{\text{fit ansatz}}$

exact result: $1/\pi \approx -0.318310$

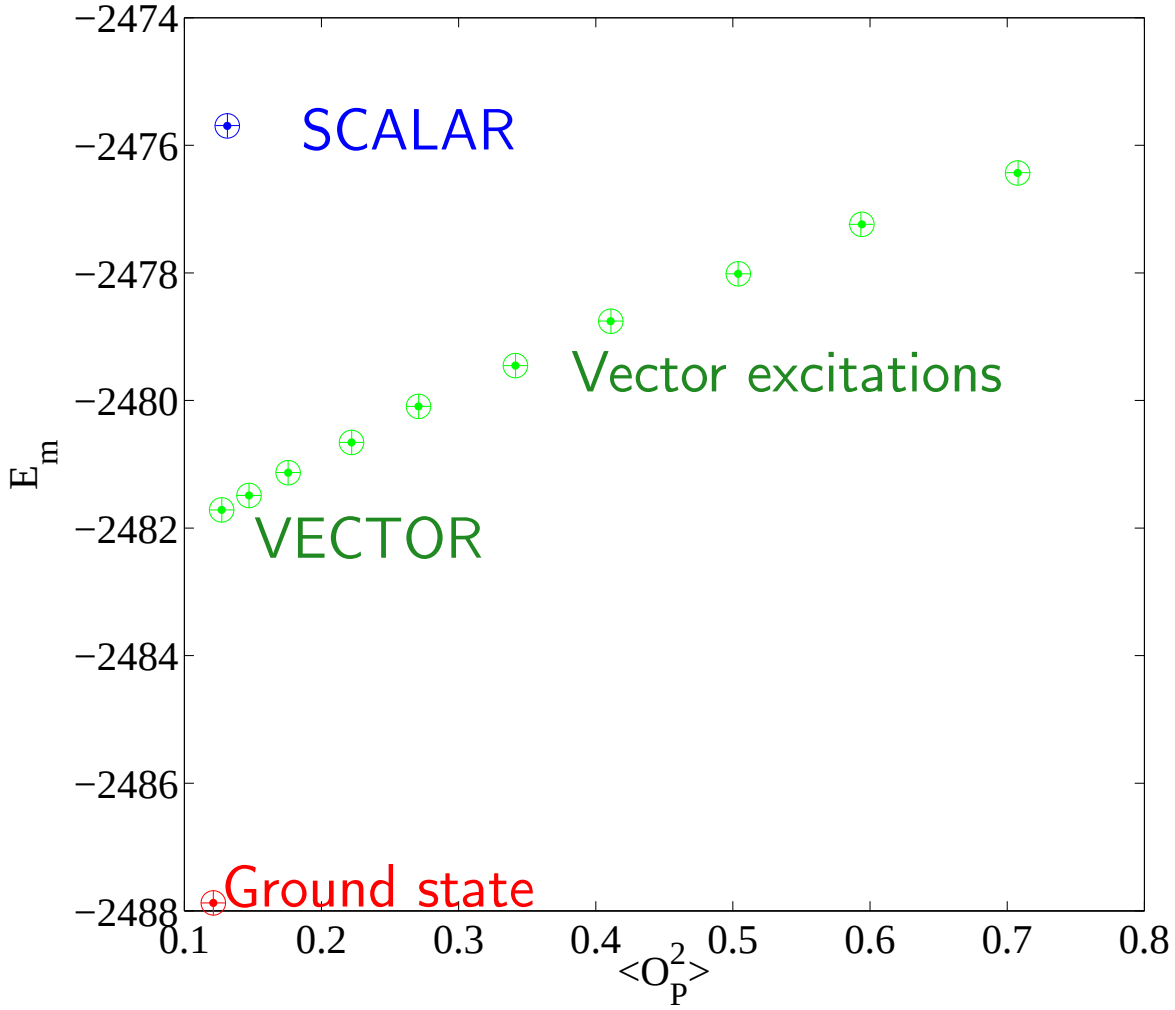


Computing the mass gap

- After having computed the GS energy, we want to compute the masses of the two lightest bound states ("mesons") of the theory:
  - ⋆ vector meson,
  - ⋆ scalar meson.
- Important: we have to recognize the vector and scalar states – use the charge conjugation transformation:
  - ⋆ PBC – $C = -1 \Rightarrow$ vector state, $C = +1 \Rightarrow$ scalar state,
  - ⋆ OBC – C no longer an exact symmetry, but "enough" to differentiate vector vs. scalar.
- Note: with OBC translational symmetry is lost – hence we also have momentum excitations of the vector meson *before* we reach the scalar.



Dispersion relation

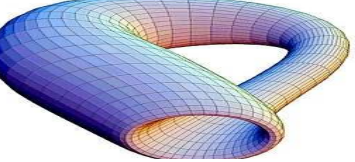


Continuum momentum operator

$$\hat{P} = \int dx \Psi^\dagger(x) i\partial_x \Psi(x)$$

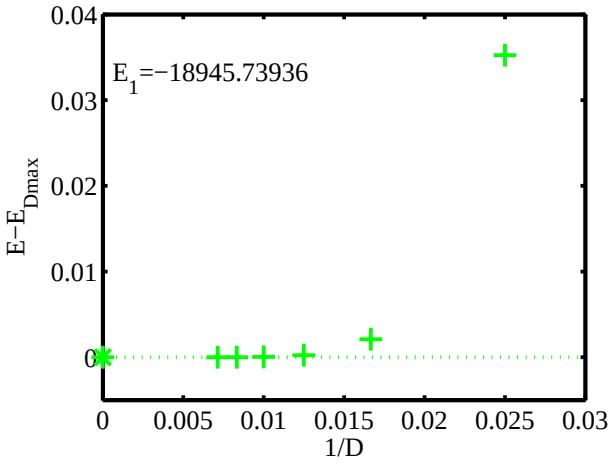
Lattice spin representation

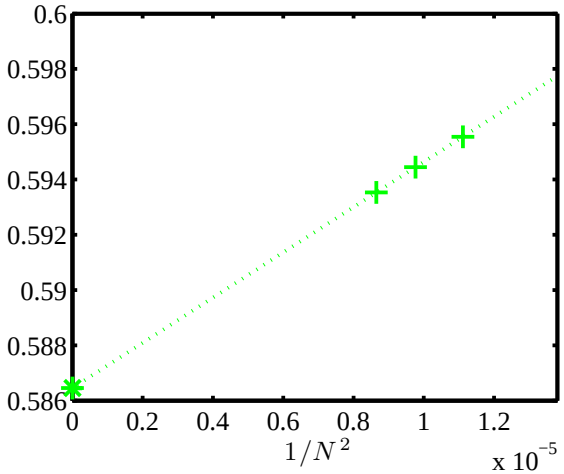
$$\hat{O}_P = -ix \sum_n \left(\sigma_n^- \sigma_{n+1}^z \sigma_{n+2}^+ - H.c.\right)$$

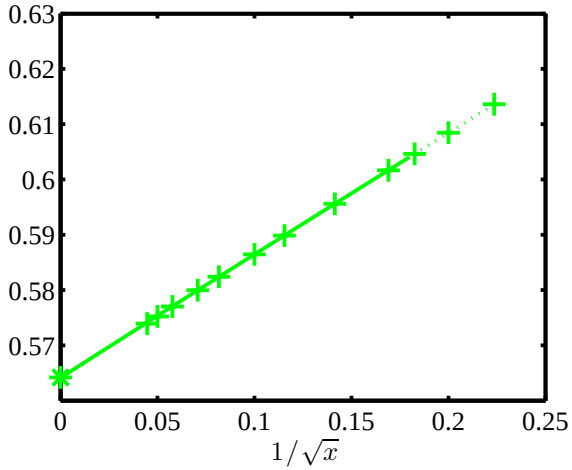


Results for the mass gaps, $m/g = 0$

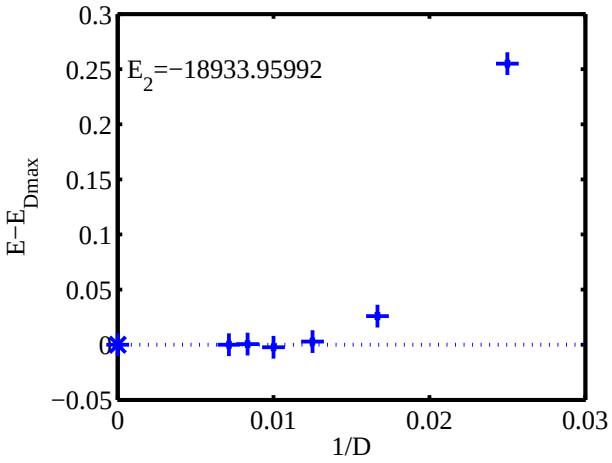
VECTOR

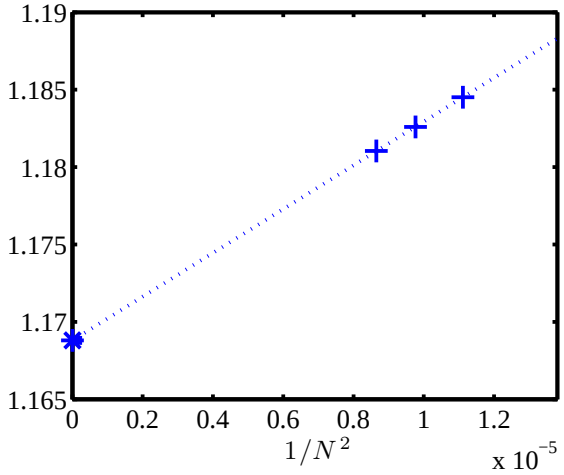


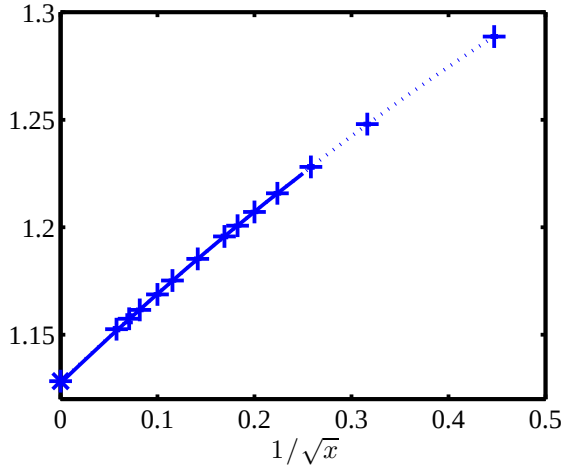




SCALAR







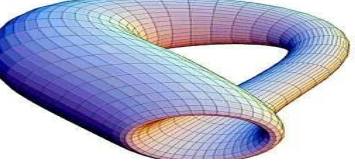
Truncation

$x = 100,\ N = 300$

Finite size scaling

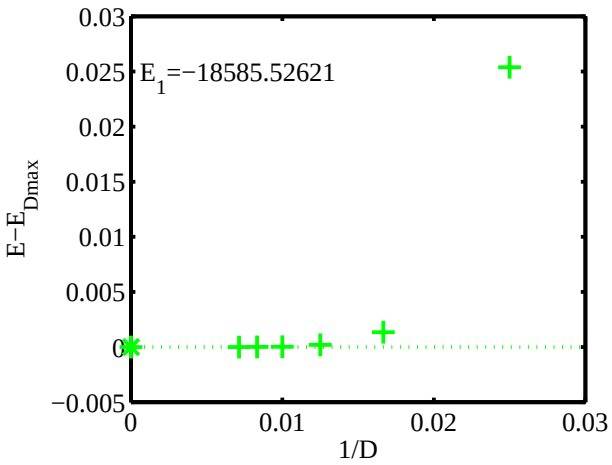
$x = 100$

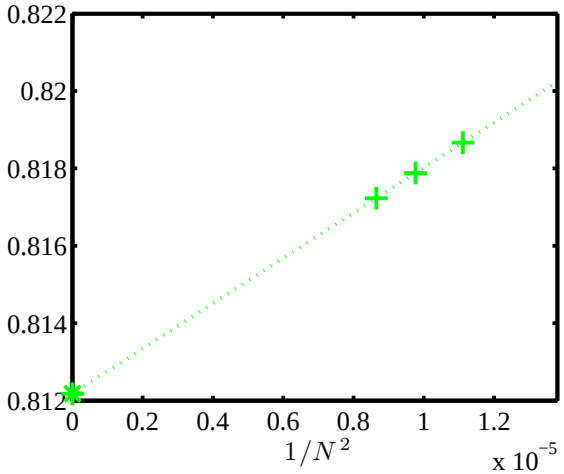
Continuum extrapolation

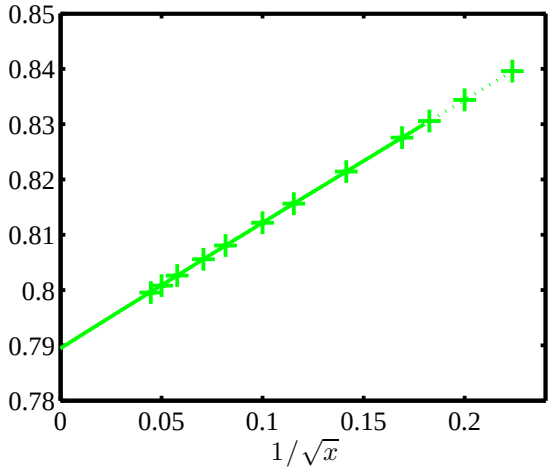


Results for the mass gaps, $m/g = 0.125$

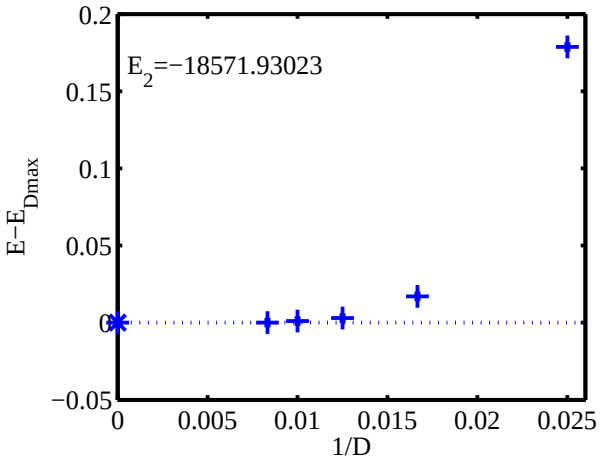
VECTOR

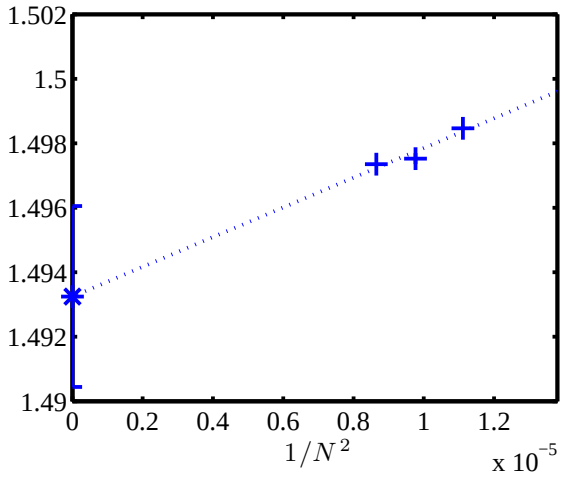


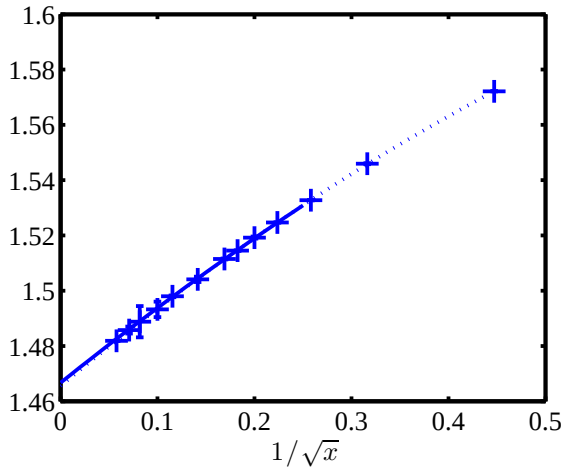




SCALAR



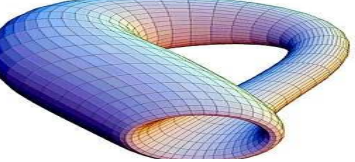




Truncation
$x = 100,\ N = 300$

Finite size scaling
$x = 100$

Continuum extrapolation



Results for the mass gaps

	Vector binding energy exact 0.5641895	
m/g	**MPS with OBC**	DMRG result
0	**0.56421(9)**	0.56419(4)
0.125	**0.53953(5)**	0.53950(7)
0.25	**0.51922(5)**	0.51918(5)
0.5	**0.48749(3)**	0.48747(2)

	Scalar binding energy exact 1.12838	
m/g	**MPS with OBC**	SCE result
0	**1.1279(12)**	1.11(3)
0.125	**1.2155(28)**	1.22(2)
0.25	**1.2239(22)**	1.24(3)
0.5	**1.1998(17)**	1.20(3)

DMRG result:

[T. Byrnes, P. Sriganesh, R. J. Bursill and C. J. Hamer, Phys. Rev. D **66** (2002) 013002]

SCE result:

[P. Sriganesh, R. Bursill and C. J. Hamer, Phys. Rev. D **62** (2000) 034508]