From Tensor Networks to Quantum Computing

Karl Jansen

- **Supercomputers in high energy physics**
- **Hamiltonian approach to lattice gauge theory**
- **Matrix product states**
  - Spectrum
  - Chemical potential
- **Conclusion**

Large activity of theoretical lattice simulations of the standard model of particle interaction

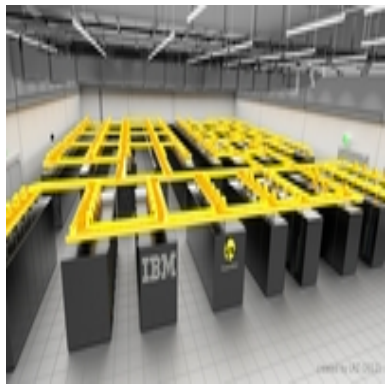
- discretize space and time
- use euclidean metric
- Feynman path integral $\rightarrow$ statistical mechanical system
- Lattice simulations of QCD, Higgs-Yukawa sector, Supersymmetry via **Markov Chain Monte Carlo Methods**

German Supercomputer Infrastructure

- JUQUEEN (IBM BG/Q)
  at Supercompter center Jülich
  5 Petaflops → 12 Petaflops (JUWEL)

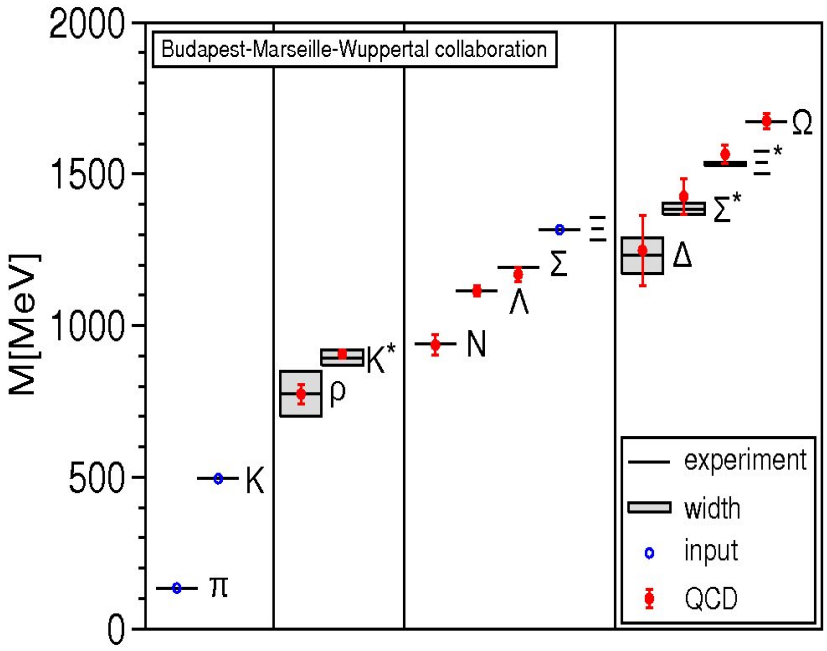
- HLRN (Hannover-Berlin)
  Gottfried and Konrad
  (CRAY XC30)
  2.6 Petaflops

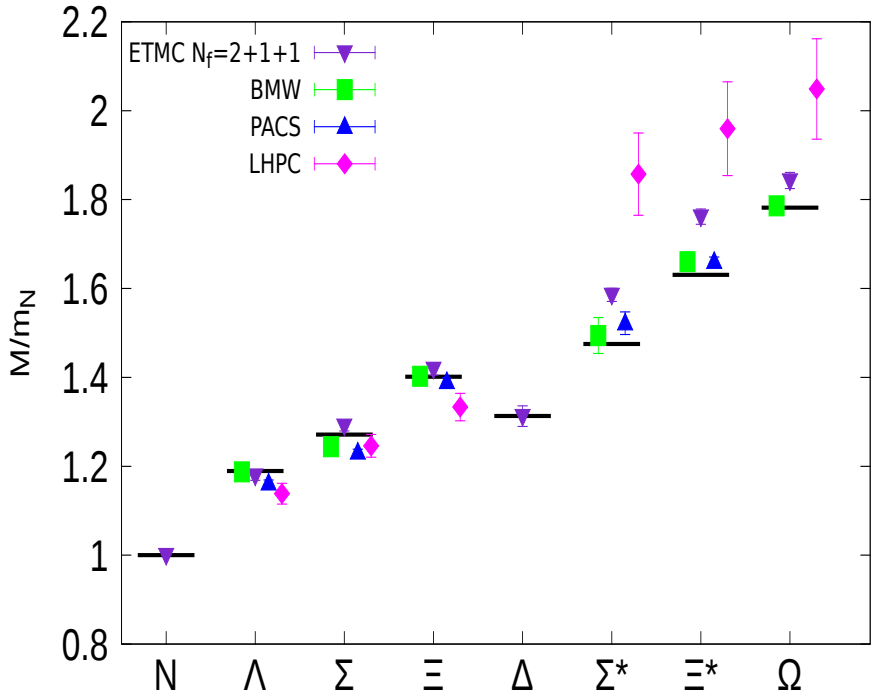
- Leibniz Supercomputer center Munich
  combined IBM/Intel system SuperMUC
  3 Petaflops



The lattice QCD benchmark calculation: the spectrum

spectrum for $N_f = 2 + 1$ and $2 + 1 + 1$ flavours





first spectrum calculation BMW

repeated by other collaborations

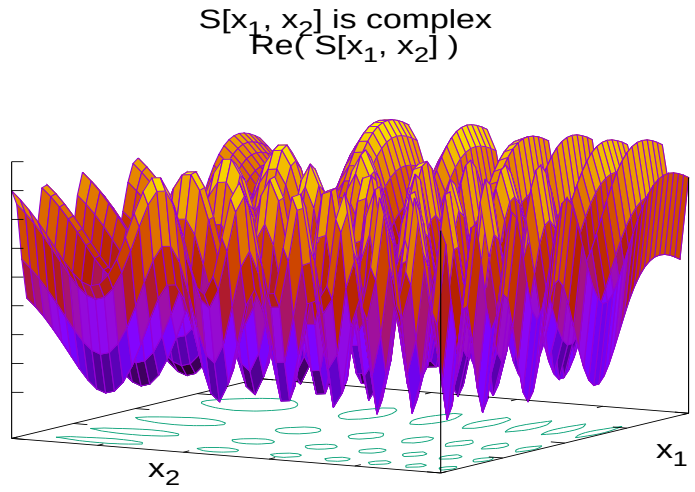
(ETMC: C. Alexandrou, M. Constantinou, V. Drach, G. Koutsou, K.J.)

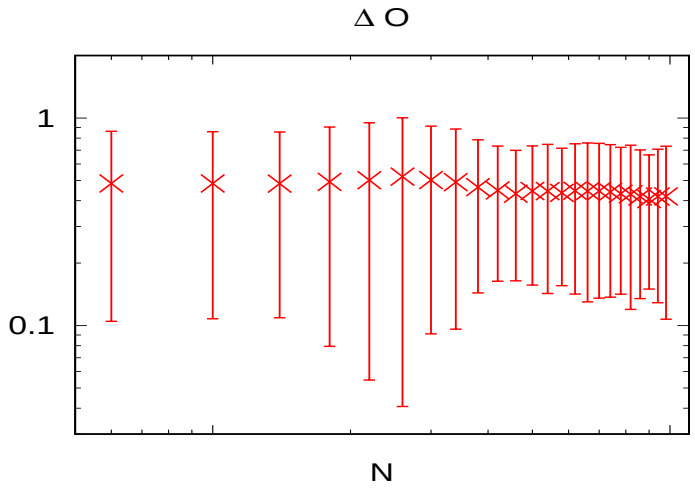
- spectrum for $N_f = 2$, $N_f = 2 + 1$ and $N_f = 2 + 1 + 1$ flavours
  $\rightarrow$ no flavour effects for light baryon spectrum

Markov Chain Monte Carlo (MCMC) Method

$$\langle \mathcal{O} \rangle = \int \mathcal{D}_{\text{Fields}} \mathcal{O} e^{-S} / \int \mathcal{D}_{\text{Fields}} e^{-S}$$

- needs real and positive probability density measure $\mathcal{D}_{\text{Fields}} e^{-S}$
- complex action not accessible to standard MCMC
  - chemical potential $i\mu\bar{\Psi}\Psi$
  - θ-term $i\theta\epsilon_{\mu\nu\rho\delta}F_{\mu\nu}F_{\rho\delta}$ (CP violation)
- constant error $O(1)$ as function of sample size N



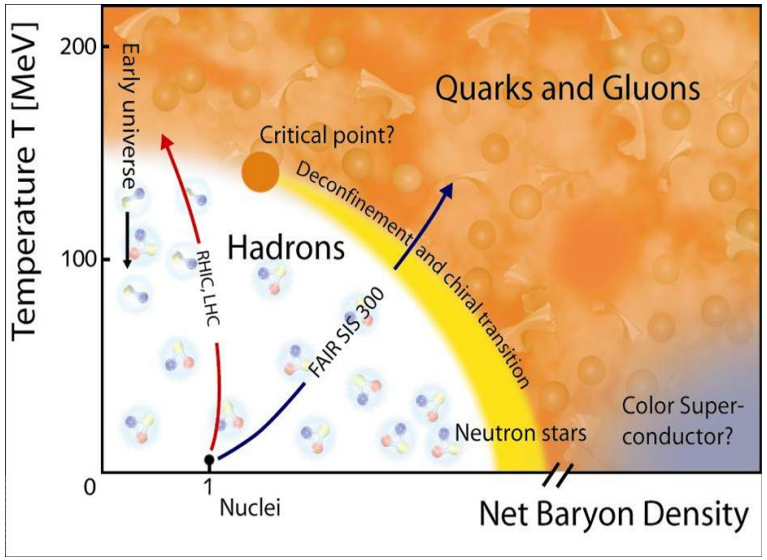


Understanding QCD phase diagram

- only zero baryon density accessible

→ understanding of phase transitions?
  - early universe
  - heavy ion experiments
  - exotic regions of PD

- do not understand origin of todays universe



Real time evolution

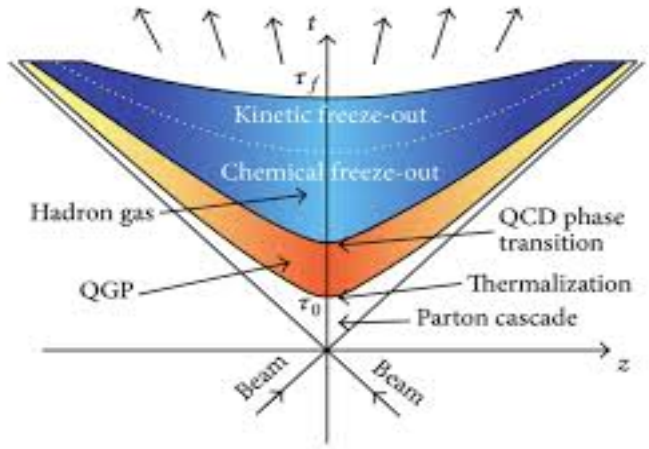
- only thermal equilibrium accessible

$\rightarrow$ no real time simulation

- understand real time processes in heavy ion collisions
  $\rightarrow$ complicated sequence of transitions

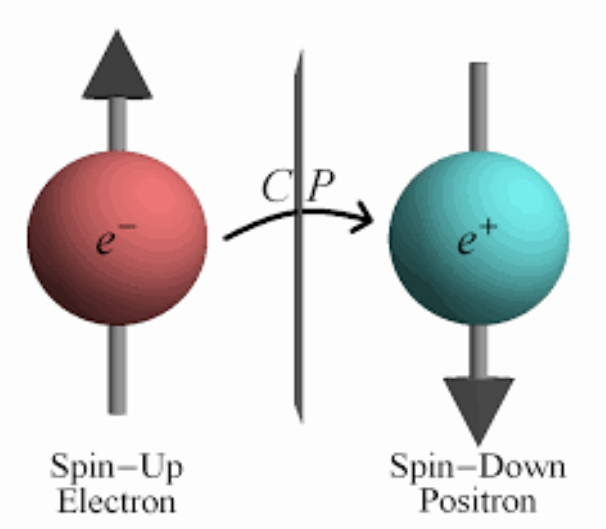
- standard way: linearize equations
  plus small fluctuations

- do we really understand
  the involved transitions?



CP violation

- in nature, we observe violation of charge and parity symmetry
  - induces difference between particles and anti-particles
  - asymmetry of matter and anti-matter
  - allows that there are more baryons than anti-baryons



- leads to our sheer existence

CP violation from strong interaction?

- CP-violation can originate from
  electroweak and strong sector of standard model

- do not understand amount of CP violation observed
  estimtated matter anti-matter asymmetry: $\eta = O(10^{-11})$
  electroweak interaction: $\eta = O(10^{-24})$

- Lagrangian of strong interaction
  invariant under CP
  $\rightarrow$ complex "theta"-term: $i\theta\epsilon_{\mu\nu\rho\delta}F_{\mu\nu}F_{\rho\delta}$

- can it explain the missing CP violation?
  (and therefore the matter anti-matter asymmetry)

- MCMC unable to answer this question

A solution to the sign problem: The Hamiltonian

- Hamiltonian approach has been much discussed in early stage of lattice field theory (Kogut and Susskind, Wilson, Lüscher, ...)

- Hamiltonian H spin-1/2 system

  wavefunction $|\Psi>$

$$|\Psi>=\sum_{i_1,i_2,\cdots,i_N} C_{i_1,i_2,\cdots,i_N}|i_1 i_2 \cdots i_N>$$

  $C_{i_1,i_2,\cdots,i_N}$ coefficient matrix with 2^N entries

  $\Rightarrow$ becomes impossible ... very fast

  $\Rightarrow$ no practical solution to sign problem

- ≈ 1980 Creutz performs Markov Chain Monte Carlo
  $\rightarrow$ start of success story

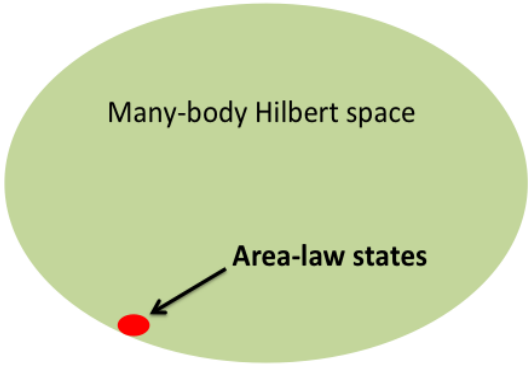
Relevant part of Hilbert space is very small

- (surface) area law:
  the entanglement between a subsystem and the rest
  grows with the boundary of the subsystem (area in 3 dimensions)

- entanglement entropy in one diemsion:
  - mass gap $1/\xi$: $S \propto \log(\xi)$
  - critical system of size L: $S \propto \log(L)$
  - exponential improvement
    compared to $S \propto L$

- for dimension $d > 1$: $S \propto L^{d-1}$
  $\rightarrow$ area law

- how can we use this property?



Matrix product states

A particular ansatz: matrix product state

$$|\Psi>=\sum_{i_1,i_2,\cdots i_N=1}^{d} \mathrm{Tr} A_1^{i_1} A_2^{i_2} \cdots A_N^{i_N} |i_1 i_2 \cdots i_N>$$

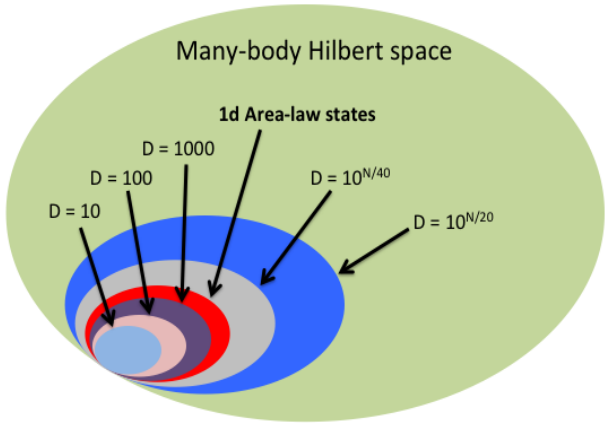
- A_i is $D \otimes D$ matrix $\rightarrow$ D *bond dimension*
- i_i physical index (e.g. spin $\pm 1/2$ for $d=2$)

Bond dimension for ground state

- approximation of ground state $|\Psi_0>$ with accuracy ϵ_0/L
- minimal bond dimension $D_{\min}$ to reach ϵ_0/L

$$D_{\min} \geq const.\frac{L^{\alpha}}{\epsilon_0}$$

- $\Rightarrow D$ scales polynomially
- Hasting's theorem: for a gapped system there is an exponential fast convergence in the bond dimension D (at least for ground state properties)
- **controlled** and **fast** convergence to solution



Schwinger Hamiltonian from Jordan-Wigner transformation

discretizing and reformulation in a spin language

$$H = x \sum_{n=0}^{N-2} \left[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+\right] + \frac{\mu}{2} \sum_{n=0}^{N-1} \left[1 + (-1)^n \sigma_n^z\right] + \sum_{n=0}^{N-2} \left(L_n + \alpha\right)^2$$

- $x = \frac{1}{g^2 a^2}$

Gauss-law: $L_n - L_{n-1} = \frac{1}{2}\left[\sigma_n^z + (-1)^n\right]$

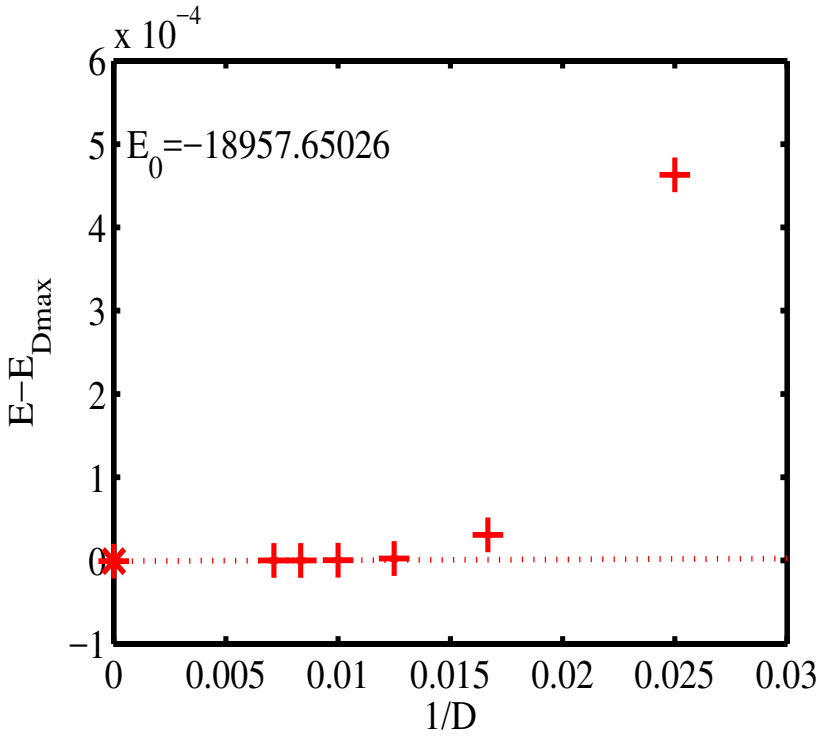
$\Rightarrow$ eliminate gauge degrees of freedom $\rightarrow$ pure spin formulation

- perfect formulation for matrix product states

- accessible for quantum simulators
  (C. Muschik, M. Heyl, E. Martinez, T. Monz, P. Schindler,
  B. Vogell, M. Dalmonte, P. Hauke, R. Blatt, P. Zoller, New J.Phys. 19 (2017) no.10, 103020)

Controlling systematic errors: bond dimension

- rapid convergence to infinite bond dimension



- linear extrapolation in $1/D$

- error: difference between extrapolated and largest bond dimension value

Calculating the mass spectrum in the Schwinger model

(M.C. Banuls, K. Cichy, I. Cirac, K.J.)

- reach values of $x = 600 \rightarrow$ MC-MC: $x \approx 20$

	Vector binding energy		
m/g	MPS with OBC	DMRG result	exact
0	0.56421(9)	0.5642(2)	0.5641895
0.125	0.53953(5)	0.53950(7)	-
0.25	0.51922(5)	0.51918(5)	-
0.5	0.48749(3)	0.48747(2)	-

- vector case: agreement with and comparable accuracy to DMRG

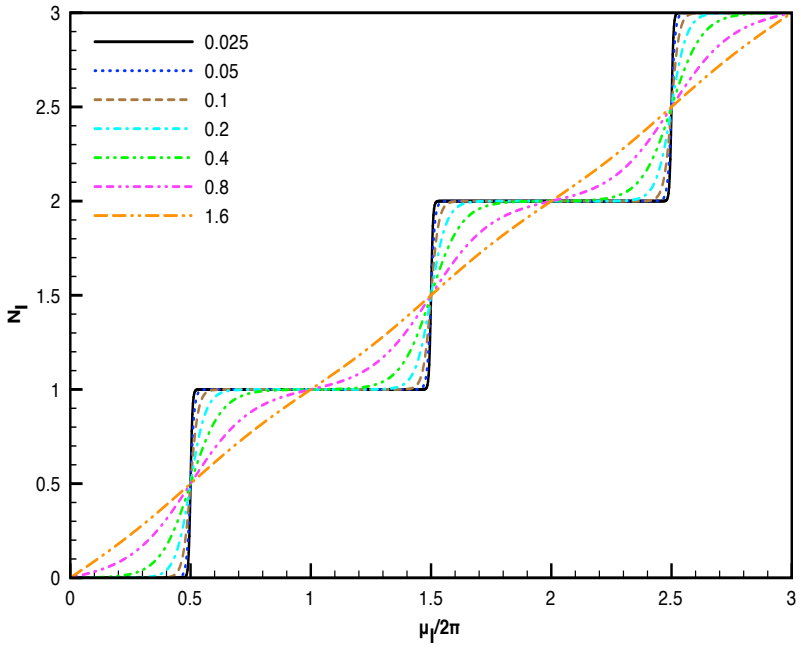
	Scalar binding energy		
m/g	MPS with OBC	SCE result	exact
0	1.1279(12)	1.11(3)	1.12838
0.125	1.2155(28)	1.22(2)	-
0.25	1.2239(22)	1.24(3)	-
0.5	1.1998(17)	1.20(3)	-

- scalar case: accurate determination of energy
- MPS approach works for gauge theories!

Sign problem in multi-flavour Schwinger model

(M.C. Banuls, K. Cichy, I. Cirac, S. Kühn, H. Saito, K.J.)

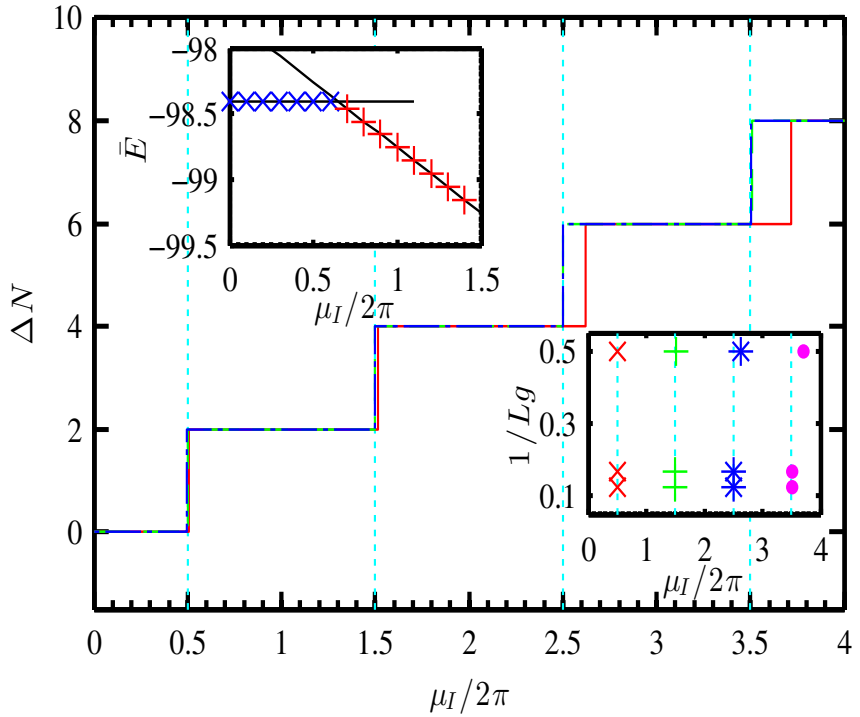
- The goal: **solve sign problem**
- Analytical prediction for phase diagram (Narayanan)



- chemical potential μ_I
- continuum calculation in finite volume
- prediction of first order phase transitions at $T = 0$ for isospin chemical potential $\mu_I = 0.5, 1.5, \cdots$
- smooth behaviour for $T > 0$

Location of phase transitions in massless case

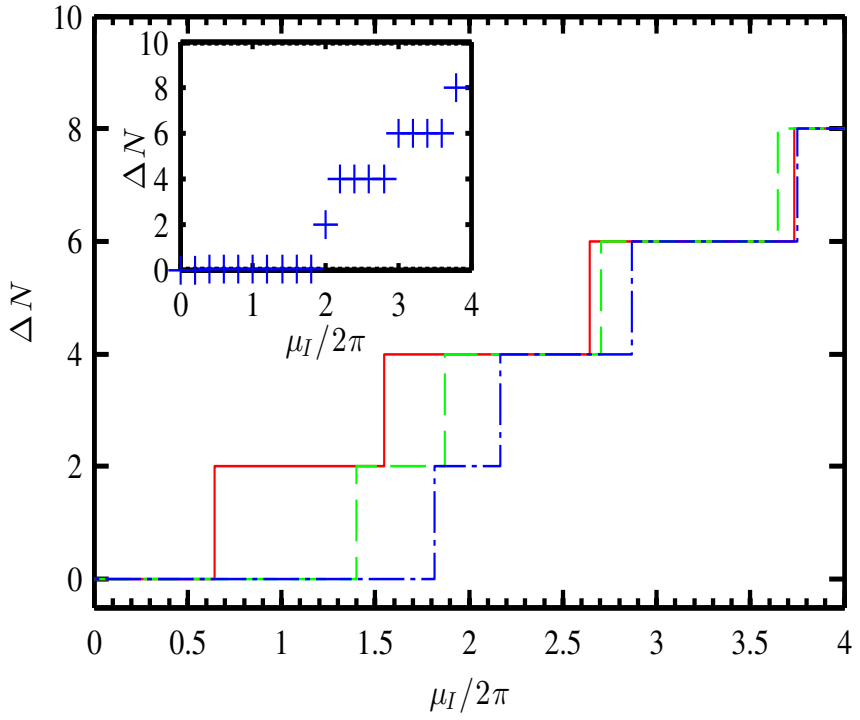
- change in particle number ΔN
- energy in given phase $E \propto \frac{\Delta N}{2} \mu_I / 2\pi$
  $\Rightarrow$ slope of E changes as function of μ_I
- analytical prediction: no finite volume effect
- as usual: $D \to \infty, N \to \infty, x \to 0$

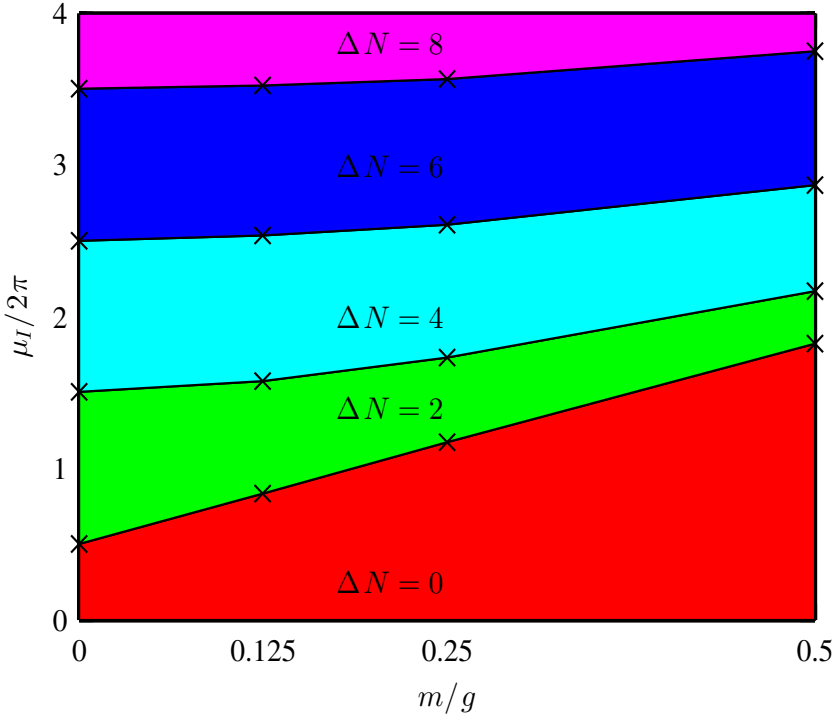


- intersection point:
  $\to$ location of jump
- no noticeable fse
- reproduce phase diagram
- no sign of sign problem

Location of phase transitions in massive case

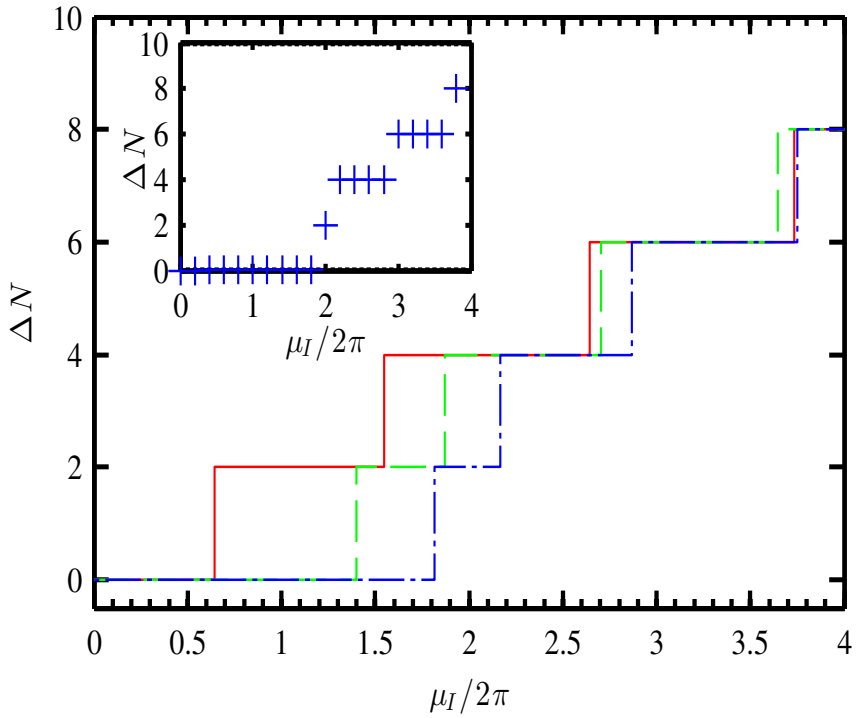
- use again $E \propto \frac{\Delta N}{2} \mu_I / 2\pi$
- no analytical solution available
- observe finite size effects
- prediction of phase diagram in $\mu_I - m$ plane

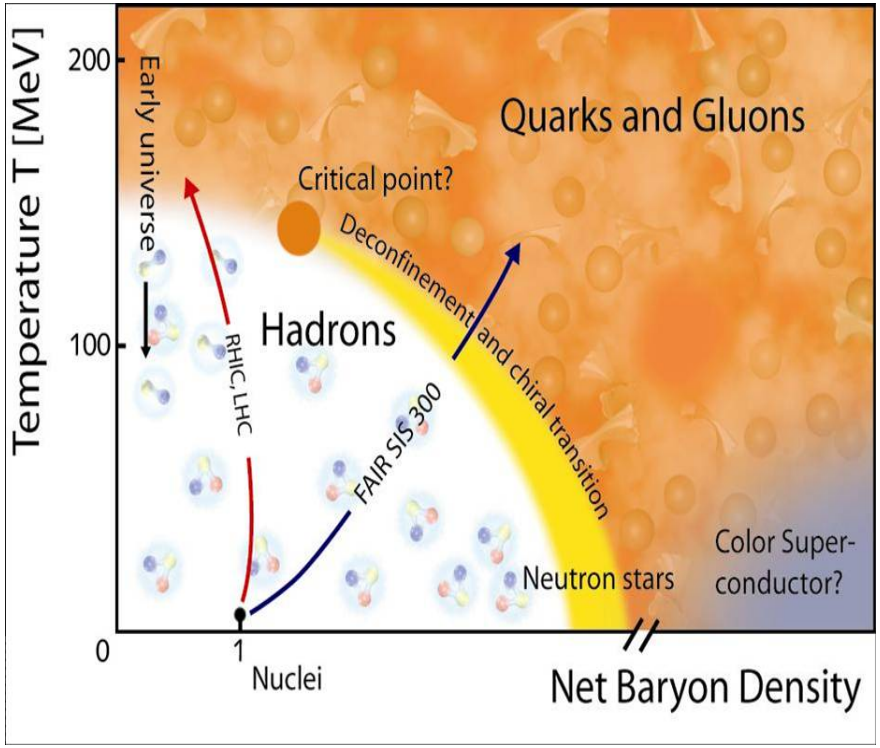




Location of phase transitions in massive case

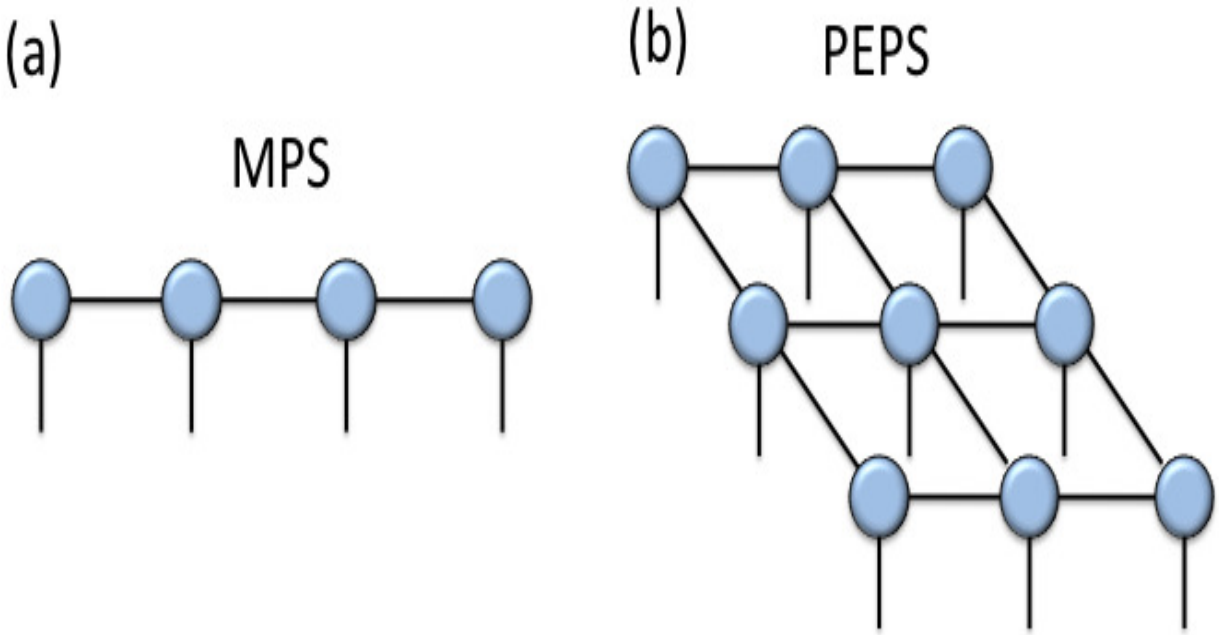
- use again $E \propto \frac{\Delta N}{2} \mu_I / 2\pi$
- no analytical solution available
- observe finite size effects
- prediction of phase diagram in $\mu_I - m$ plane





Higher dimensions

- Projected Entangled Pair States (PEPS)



- PEPS are tensor networks for 2-d systems
- used in solid state physics
- computational cost $\propto D^{10} \rightarrow$ need new ideas for tensor networs ...
- ... or quantum simulations

Summary

- lattice QCD calculations very much advanced
- outstanding challenges: chemical potential, CP violation, real time processes
- new ansatz: Matrix product states and matrix product operators
- testbench calculation: $1+1$-dimensional Schwinger model
  - spectrum
  - chemical potential
  - entropy
- overcomes sign problem
- challenge: higher dimensions
  $\rightarrow$ quantum simulations
  $\rightarrow$ talks by C. Muschik & M. Savage
- tensor networks still important tool to check quantum simulations