Title: The Quest for Solving Quantum Chromodynamics: Status and Challenges

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Abstract: <p>The strong interaction of quarks and gluons is described theoretically within the framework of Quantum Chromodynamics (QCD). The most promising way to evaluate QCD for all energy ranges is to formulate the theory on a 4-dimensional Euclidean space-time grid, which allows for numerical simulations on state of the art supercomputers. We will review the status of lattice QCD calculations providing examples such as the hadron spectrum and the inner structure of nucleons. We will then point to problems that cannot be solved by conventional Monte Carlo simulation techniques, i.e. non-zero baryon density, the matter-antimatter asymmetry and real time simulations. It will be demonstrated at the example of the 1+1 dimensional Schwinger model that tensor network techniques are able to overcome these problems showing that with this approach --and eventual quantum simulations-- a path for solving QCD is opening up.</p>

The Quest for Solving Quantum Chromodynamics: status and challenges

Karl Jansen

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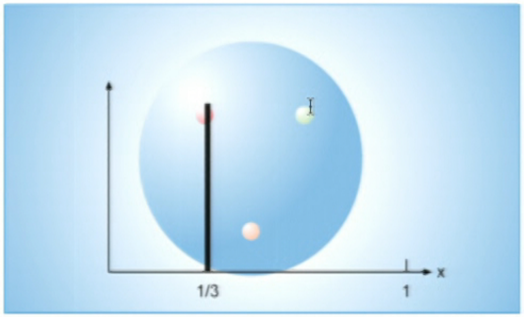
- **Status and difficulties of present lattice QCD calculations**
- **Hamiltonian approach to lattice gauge theory**
- **Matrix product states**
  - Spectrum
  - Chemical potential
- **A glimpse at quantum computing**
- **Conclusion**

Quarks are the fundamental constituents of nuclear matter



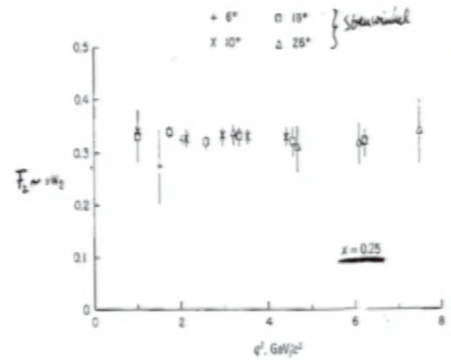


Fig. 7.17 νW_2 (or F_2) as a function of q^2 at $x = 0.25$. For this choice of x, there is practically no q^2-dependence, that is, exact "scaling". (After Friedman and Kendall 1972.)

Friedman and Kendall, 1972)

$f(x, Q^2)\big|_{x\approx 0.25, Q^2>10\mathrm{GeV}}$ independent of Q^2

(x momentum of quarks, Q^2 momentum transfer)

Interpretation (Feynman): scattering on single quarks in a hadron
→ (Bjorken) scaling

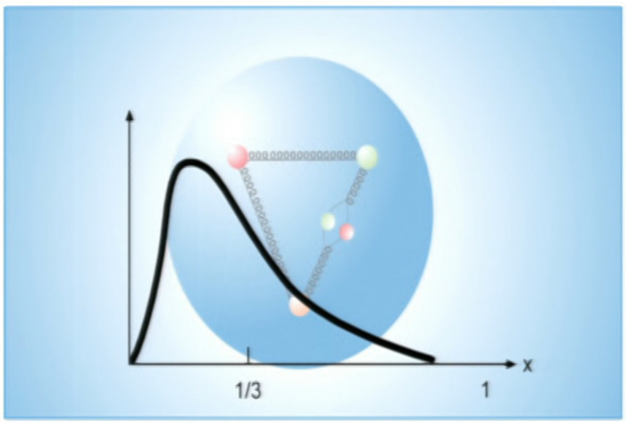
Quantum Fluctuations and the Quark Picture

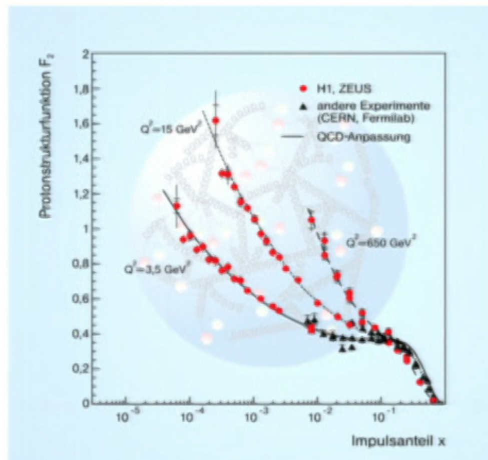
analysis in perturbation theory

$$\int_0^1 dx\, f(x,Q^2) = 3\left[1 - \frac{\alpha_s(Q^2)}{\pi} - a(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^2 - b(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^3\right]$$

– $a(n_f), b(n_f)$ calculable coefficients

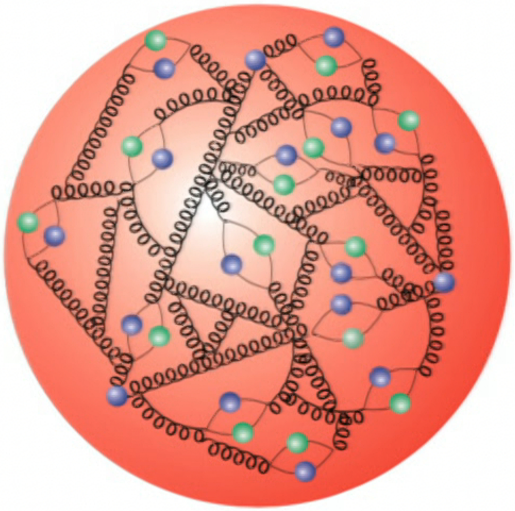
deviations from scaling → determination of strong coupling





Why we need lattice QCD

- situation becomes incredibly complicated



- value of the coupling (expansion parameter) $\alpha_{\text{strong}}(1\text{fm}) \approx 1$

$\Rightarrow$ need different ("exact") method

$\Rightarrow$ has to be non-perturbative
  $\rightarrow$ more than all Feynman graphs

- Wilson's Proposal: Lattice Quantum Chromodynamics

Lattice Gauge Theory had to be invented

$\rightarrow$ QuantumChromoDynamics

asymptotic freedom	confinement
distances $\ll 1\mathrm{fm}$	distances $\gtrsim 1\mathrm{fm}$
world of quarks and gluons	world of hadrons and glue balls
perturbative description	non-perturbative methods

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976

Schwinger model: 2-dimensional Quantum Electrodynamics

(Schwinger 1962)

Quantization via Feynman path integral (in Euclidean time)

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{\text{gauge}} - S_{\text{ferm}}}$$

Fermion action

$$S_{\text{ferm}} = \int d^2x \bar{\Psi}(x) \left[D_\mu + m\right] \Psi(x)$$

gauge covriant derivative

$$D_\mu \Psi(x) \equiv (\partial_\mu - ig_0 A_\mu(x))\Psi(x)$$

with A_μ gauge potential, g_0 bare coupling

$$S_{\text{gauge}} = \int d^2x F_{\mu\nu} F_{\mu\nu} \ , \ F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$$

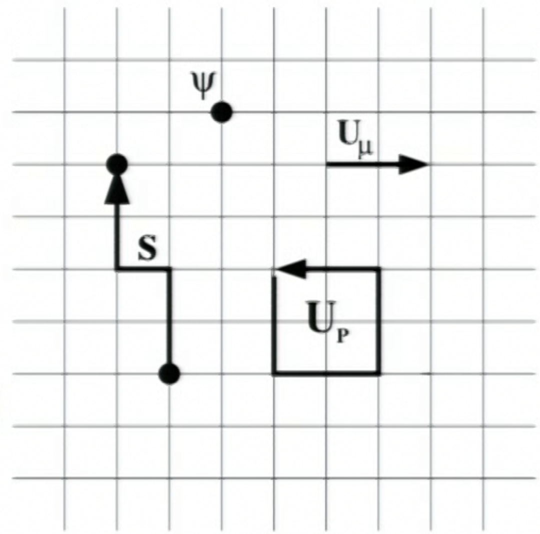
equations of motion: obtain classical Maxwell equations

Schwinger model: properties

- confinement of charges
- bound states
- chiral symmetry breaking
- super-renormalizable
- exactly solvable in massless case

Lattice Schwinger model

introduce a 2-dimensional lattice with lattice spacing a



fields $\Psi(x)$, $\bar{\Psi}(x)$ on the lattice sites

$x = (t, \mathbf{x})$ integers

discretized fermion action

$$S \rightarrow a^2 \sum_x \bar{\Psi}\left[\gamma_\mu \partial_\mu - r \underbrace{\partial_\mu^2}_{\nabla_\mu^* \nabla_\mu} + m\right] \Psi(x)$$

$$\partial_\mu = \frac{1}{2}\left[\nabla_\mu^* + \nabla_\mu\right]$$

discrete derivatives

$$\nabla_\mu \Psi(x) = \frac{1}{a}\left[\Psi(x + a\hat{\mu}) - \Psi(x)\right] , \quad \nabla_\mu^* \Psi(x) = \frac{1}{a}\left[\Psi(x) - \Psi(x - a\hat{\mu})\right]$$

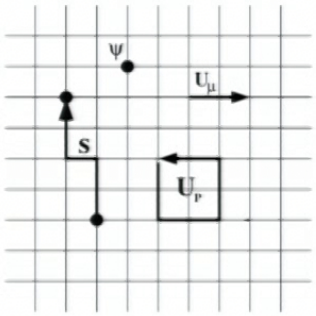
second order derivative $\rightarrow$ remove doubler $\leftarrow$ break chiral symmetry

Implementing gauge invariance

Wilson's fundamental observation: introduce parallel transporter connecting the points x and $y = x + a\hat{\mu}$:

$$U(x,\mu) = e^{iaA_\mu(x)} \in U(1)$$

$\Rightarrow$ lattice derivative: $\nabla_\mu \Psi(x) = \frac{1}{a}\left[U(x,\mu)\Psi(x+\mu) - \Psi(x)\right]$



$$U_p = U(x,\mu)U(x+\mu,\nu)U^\dagger(x+\nu,\mu)U^\dagger(x,\nu)$$

$$\rightarrow F_{\mu\nu}F^{\mu\nu}(x) \quad \text{for} \quad a \rightarrow 0$$

$$S = a^2 \sum_x \left\{ \beta(= \tfrac{1}{g_0^2}) \left[1 - \mathrm{Re}(U_{(x,p)})\right] + \bar{\psi}\left[m + \tfrac{1}{2}\{\gamma_\mu(\nabla_\mu + \nabla^\star_\mu) - a\nabla^\star_\mu \nabla_\mu\}\right]\psi \right\}$$

partition functions (path integral) with Boltzmann weight (action) S

$$\mathcal{Z} = \int_{\text{fields}} e^{-S}$$

Physical Observables

expectation value of physical observables $\mathcal{O}$

$$\underbrace{\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int_{\text{fields}} \mathcal{O} e^{-S}}$$

$\downarrow$ lattice discretization

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$\downarrow$

From the Schwinger model to quantum chromodynamics

- system becomes 4-dimensional:
  $[50 \cdot 50] \to [50 \cdot 50] \cdot 2500$

- gauge field $U(x,\mu) \in U(1) \to U(x,\mu) \in SU(3)$

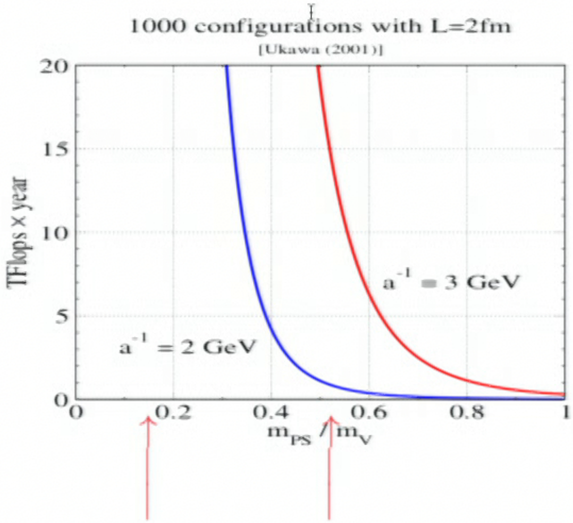
- quarks receive 4 Dirac and 3 color components:
  $[50 \cdot 50] \to [50 \cdot 50] \cdot 30000$

- Schwinger model simulation $O(1\text{day})$
  QCD: $\to$ need massive parallelization

- theory needs *non-perturbative* renormalization

The graph that wrote history: the "Berlin Wall"

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

$$z_\pi = 6, \;\; z_L = 5, \;\; z_a = 7$$

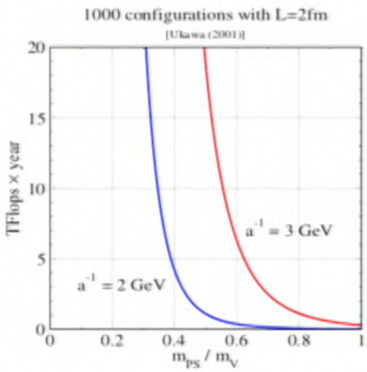
"both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place." (Wilson, 1989)

$\Rightarrow$ need of **Exaflops Computers**

A generic improvement for Wilson type fermions

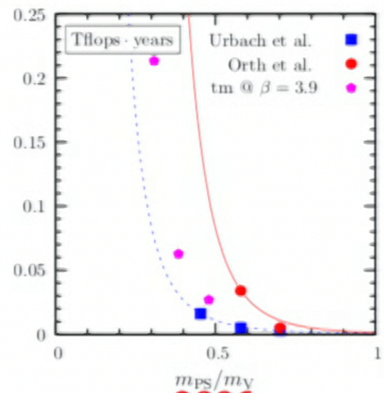
New variants of HMC algorithm
(here (Urbach, Shindler, Wenger, K.J.), see also RHMC, SAP)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps



2001

→



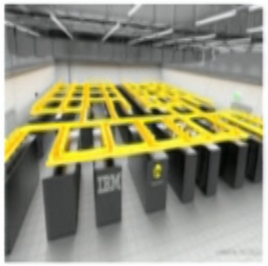
2006

German Supercomputer Infrastructure

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

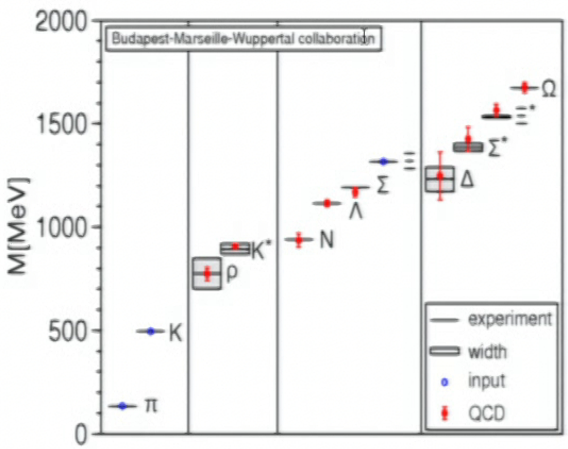
- HLRN (Hannover-Berlin)
  Gottfried and Konrad
  (CRAY XC30)
  2.6 Petaflops

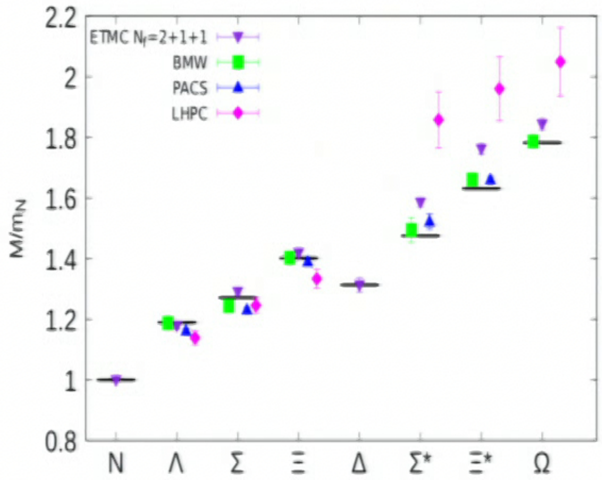
- Leibniz Supercomputer center Munich
  combined IBM/Intel system SuperMUC
  3 Petaflops



The lattice QCD benchmark calculation: the spectrum

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





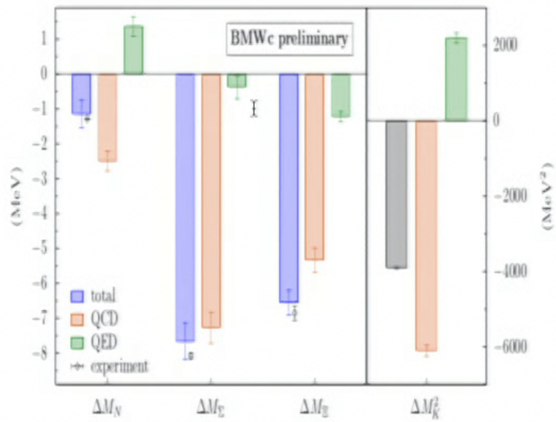
first spectrum calculation BMW

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

Even isospin and electromagnetic mass splitting

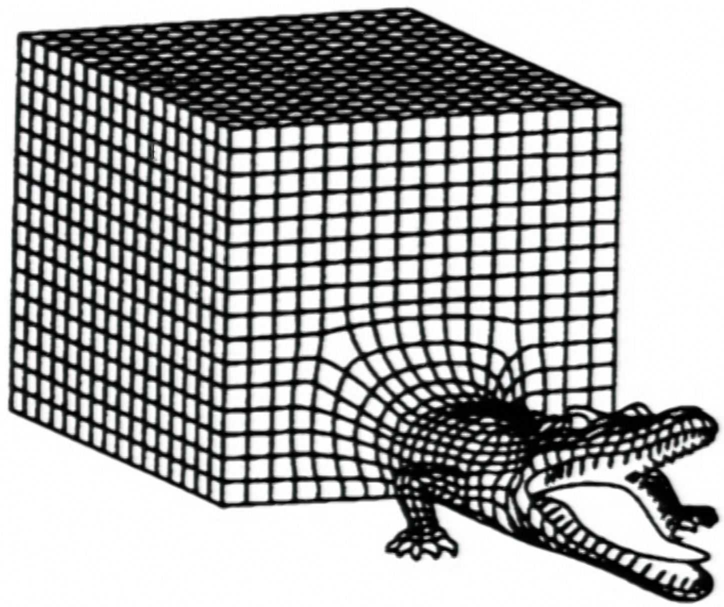
(BMW collaboration)



baryon spectrum with mass splitting

- nucleon: isospin and electromagnetic effects with opposite signs
- nevertheless physical splitting reproduced

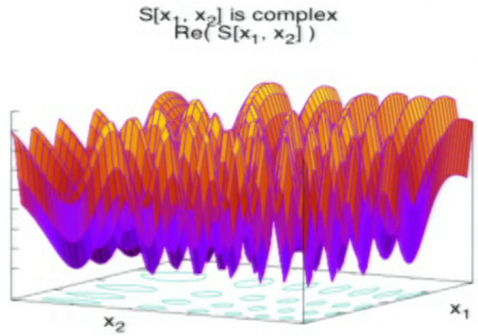
There are dangerous lattice animals



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



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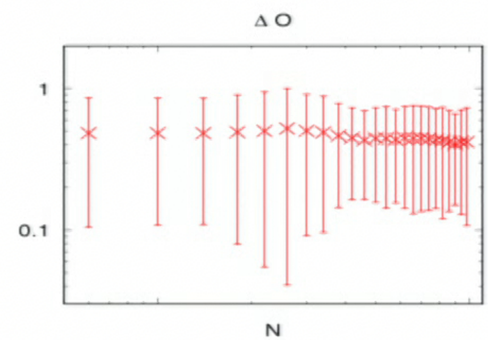
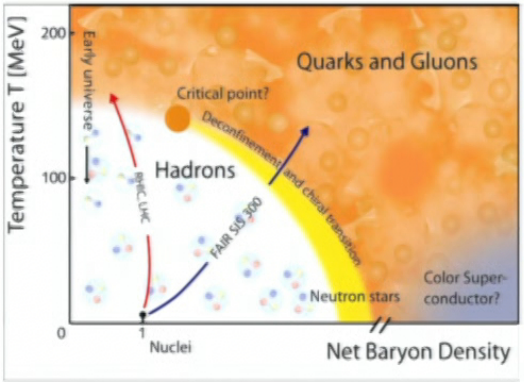


Understanding QCD phase diagram

- 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

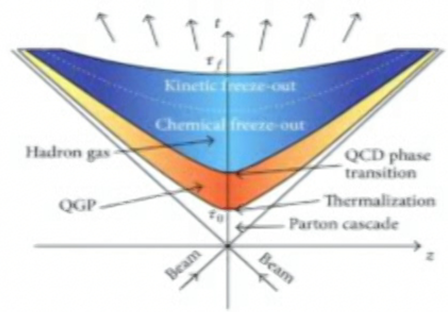
- only thermal equilibrium accessible

→ no real time simulation

- understand real time processes in heavy ion collisions
  → complicated sequence of transitions

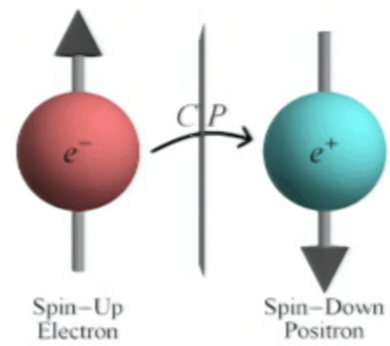
- standard way: linearize equations
  plus small fluctuations

- 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

We want too much

consider system with mass gap $\Delta(L) \rightarrow$ assume FSE polynomially in $1/L$

local density operator, e.g. $\rho_i = \Phi_i^\dagger \Phi_{i+1}$

If $\|\rho_{\mathrm{exact}} - \rho_{\mathrm{approx}}\| \leq \delta$

then the wavefunction

$\| |\Psi_{\mathrm{exact}}> - |\Psi_{\mathrm{approx}}> \| \leq \frac{L\delta}{\Delta(L)}$

- sufficient accuracy of local properties
  provides accurate
  description of global properties

- δ scales polynomially

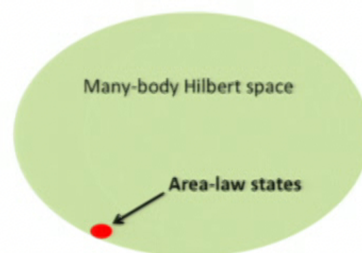
Relevant part of Hilbert space is very small

- (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

(S. White, M. Hastings, I. Cirac, G. Vidal (+his group), ...)

A particular ansatz: matrix product state

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

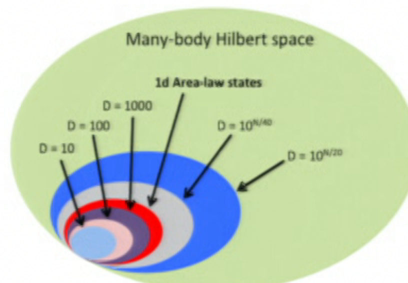
- A_i is $D \otimes D$ matrix $\rightarrow$ D *bond dimension*
- i_i physical index (e.g. spin $\pm 1/2$ for $d = 2$)

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 model Hamiltonian

- $1+1$(space+time) dimensional

Hamiltonian formulation: $\mathcal{H} = \pi^\mu \dot{A}_\mu - \mathcal{L}$, $\pi^\mu = \frac{\partial \mathcal{L}}{\partial \dot{A}_\mu} = -F^{0\mu}$

$$\mathcal{H} = -i\bar{\Psi}\sigma^1(\partial_1 - igA_1)\Psi + m\bar{\Psi}\Psi + \frac{1}{2}E^2$$

E: electric field, σ_i: Pauli matrices

Gauss-law: $\partial_1 E = g\bar{\Psi}\sigma^0\Psi$, g coupling

Kogut-Susskind (staggered fermion) formulation

$$H = -\frac{i}{2a}\sum_n \left(\phi_n^\dagger e^{i\theta_n}\phi_{n+1} - \text{h.c.}\right) + m\sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2}\sum_n L_n^2,$$

ϕ_n single component fermion field

$\theta_n = iaA_1(n)$ gauge variables

$L_n = gE_n$ electric field (conjugate variable, $[\theta_n, L_m] = i\delta_{n,m}$)

Schwinger Hamiltonian from Jordan-Wigner transformation

discretizing and reformulation in a spin language

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

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

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)

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!

The CP(N-1) model

continuum action

$$S = \frac{1}{2g^2} \int dx^2 \partial_\nu \mathbf{n} \partial_\nu \mathbf{n}$$

– $\mathbf{n}$ N-component vector, $\mathbf{n}^2 = 1$

– $1/g^2 \equiv \beta$ coupling

- asymptotic freedom
- non-perturbative generated mass scale
- topological properties
- can be coupled to chemical potential
  $\Rightarrow$ not accessible to standard Markov chain Monte Carlo

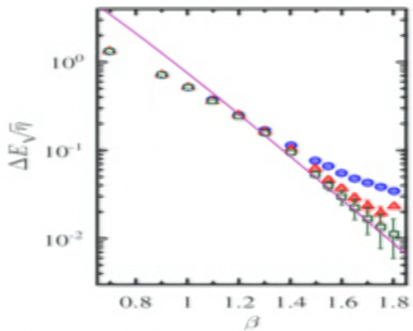
Results for the special case of O(3) model

(Falk Bruckmann, Stefan Kühn, K.J.)

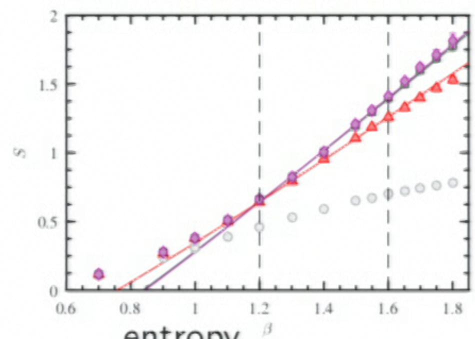
- lattice Hamiltonian

$$H = \frac{1}{2\beta}\sum_{k=1}^{N} L_k^2 - a\mu\sum_{k=1}^{N} L_k^z - \beta\sum_{k=1}^{N} \mathbf{n}_k \mathbf{n}_{k+1}$$

- perform matrix product state calculation



mass gap



entropy

$$am = 128\pi\beta\exp(-2\pi\beta)$$

$$S_{\mathrm{ent}} = c/6(2\pi/\beta - \log(\beta) + \mathrm{const.}$$

$l_{\max}$	c
3	2.0140 ± 0.1183
4	2.0423 ± 0.1428

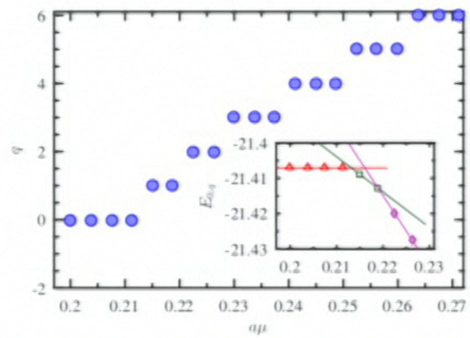
Coupling a chemical potential: the phase structure

$$aH = -a\mu Q + aW$$

energy in charge sector q

$$aE_{0,q}(\mu) = -\mu q + E_0(W|_q)$$

$\Rightarrow$ changing $q \Leftrightarrow$ intersection of energy $E_0(W|_q)$

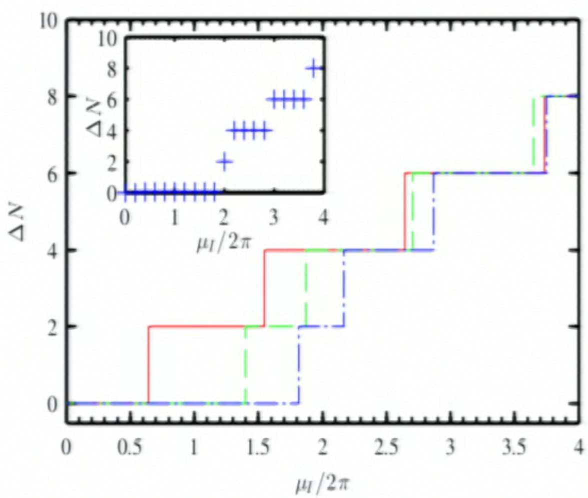


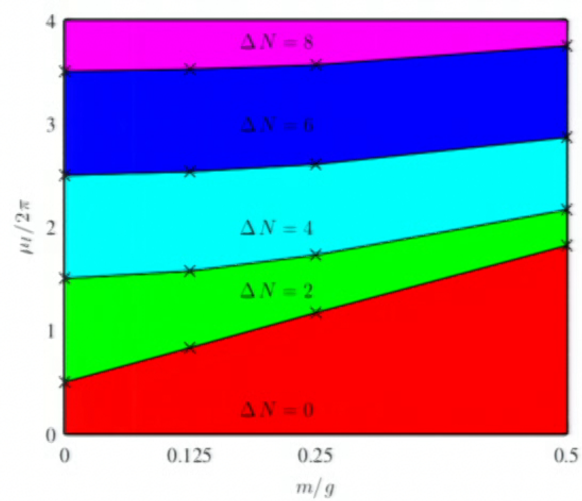
- find first order jumps
  - $\rightarrow$ explore phase structure at non-zero chemical potential
  - $\rightarrow$ MPS solves sign problem

Phase structure in the Schwinger model at non-zero density

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

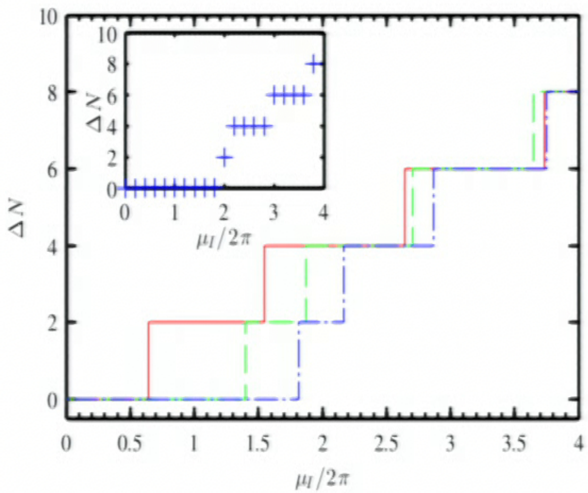
- no analytical solution available
- prediction of phase diagram in $\mu - m$ plane

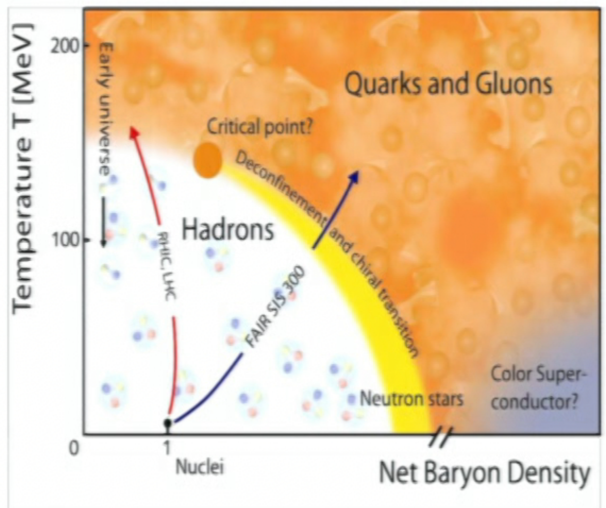




Phase structure in the Schwinger model at non-zero density

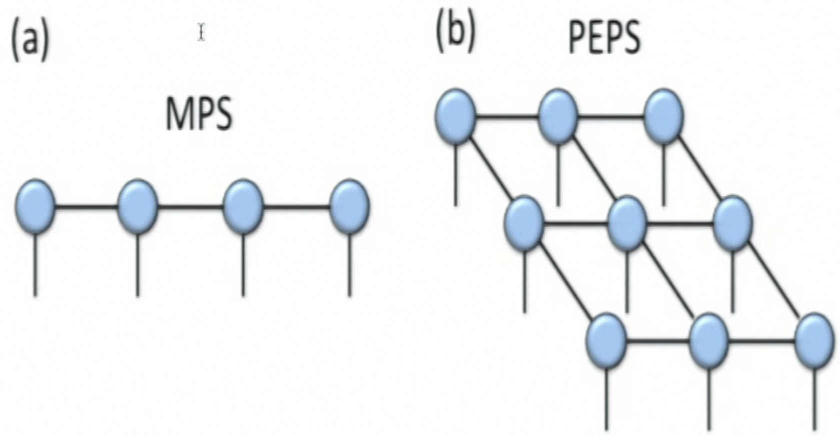
- no analytical solution available
- prediction of phase diagram in $\mu - m$ plane





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

Zeta-regularizing Feynman's path integral

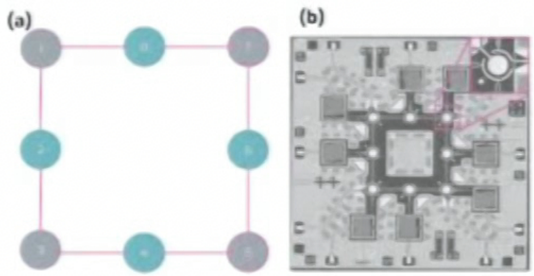
- *Quantum computing of zeta-regularized vacuum expectation values* (Tobias Hartung, Karl Jansen, arXiv:1808.06784)
- Prime goal: give mathematical meaning to Feynman's trace formula

$$\langle O \rangle = \mathrm{Tr} O e^{iHT} / \mathrm{Tr} e^{iHT}$$

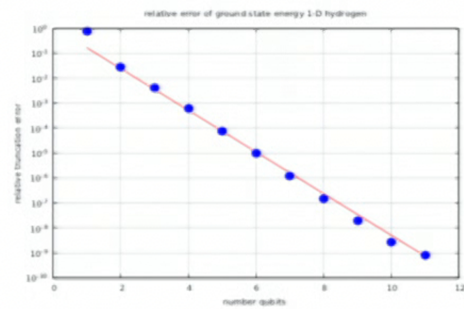
- provide proof that $\langle O \rangle$ *is physical vacuum expectation value*
- advantage of ζ-regularization
  - defined in the continuum (although lattice setup included)
  - comprises Minkowski space
- $\Rightarrow$ solves sign problem:
  chemical potential, topological term, real time, ...
- how to apply this in practice?

Qubit scaling for groundstate calculation

- Our solution: perform quantum computer calculation
- Practical example: compute ground state energy of 1-dimensional hydrogen atom on Rigetti's 8-qubit Agave chip
  - performed variational quantum simulation
  - continuum MPS also possible?



Agave chip



Scaling (simulator, no noise)

- simulator: find exponentially fast convergence
- reality on hardware
  - gate fidelity $F_{1Q} = 0.982$, readout fidelity $F_{RO} = 0.94$
  - ground state energy with 4.9% error
  - more qubits: no significant result

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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 CP(N-1) and Schwinger models
  - spectrum
  - chemical potential
  - entropy
- MPS: much larger systems than MC-MC $\Rightarrow$ closer to continuum
- overcomes sign problem
- challenge: higher dimensions
  $\rightarrow$ quantum simulations
- tensor networks still important tool to check quantum simulations