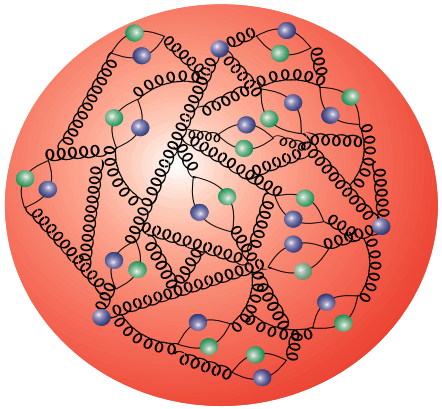
Introduction to Lattice QCD

Karl Jansen

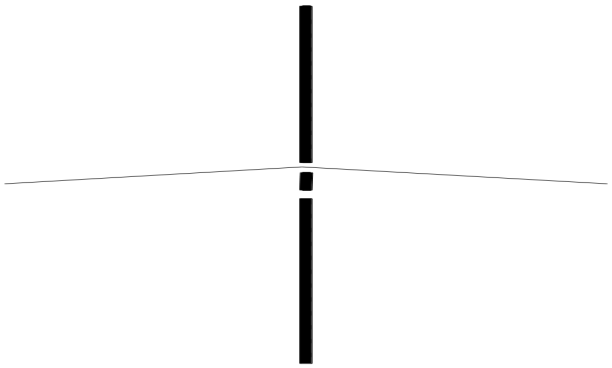
- **Task: compute the proton mass**
  - need an action
  - need an algorithm
  - need an observable
  - need a supercomputer ...
  - ... and then we get ...



- **Going further: from tensor networks to quantum simulations**

Feynman's alternative formulation of quantum mechanics

the double slit experiment



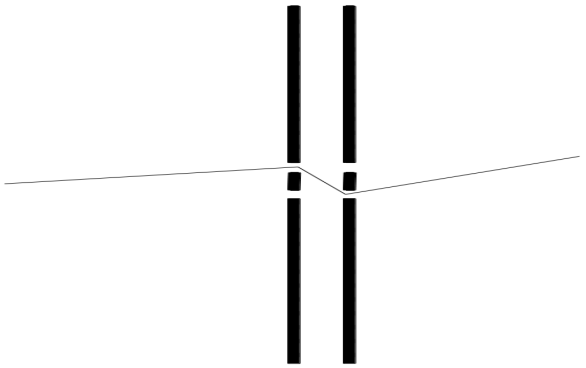
superposition principle

$\rightarrow$ interference pattern

$\rightarrow$ probability $P = |\Phi_1 + \Phi_2|^2$

Φ_i quantum mechanical amplitude

Adding slits

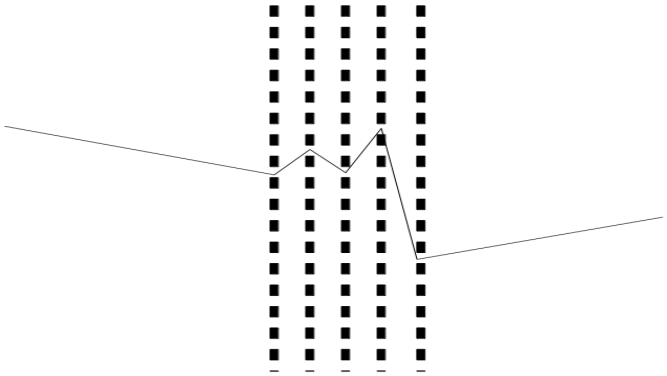


four possible paths

$\rightarrow$ probability $P = |\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4|^2$

Φ_i quantum mechanical amplitude

Even more ...



$\rightarrow$ probability $P = |\sum_i \Phi_i|^2 \equiv |\sum_{\text{paths}} \Phi_{\text{path}}|^2$

Feynman $\Phi_{\text{path}} = e^{\frac{i}{\hbar} S_{\text{cl}}(\text{path})}$

$S_{\text{cl}}(\text{path})$ *classical action of path*

Quantum mechanical oscillator in Euclidean time

Feynman path integral in quantum mechanics

$$\boxed{\mathcal{Z} = \int \mathcal{D}x e^{\frac{i}{\hbar} S_{\rm cl}}}$$

- $S_{\rm cl}$ *classical* action, e.g. quantum mechanical oscillator

$$S_{\rm cl} = \int dt \left[\tfrac{1}{2}\dot{x}^2(t) - V(x(t))\right]$$

- $x(t)$ are *classical* paths

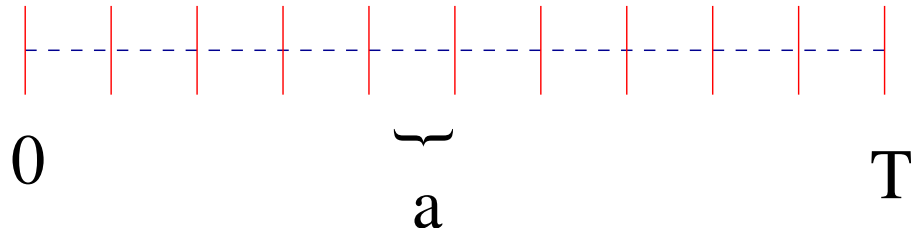
perform analytical continuation to imaginary (Euclidean) time τ

$$t \to -i\tau \qquad f(t) \to f(\tau)$$

$$\boxed{\mathcal{Z} = \int \mathcal{D}x e^{-\frac{1}{\hbar} S_{\rm E}},\ S_E = \int d\tau \left[\tfrac{1}{2}\dot{x}^2 + V(x)\right]}$$

Discretizing

"time lattice" with $N = T/a$ lattice points



$x(\tau) \to x(n)$ boundary condition: $x(N+1) = x(0)$

standard lattice derivative

$$\dot{x} \to [x(n+a) - x(n)]/a$$

$$= \tfrac{1}{a}\left[x(n) + \dot{x}a + \tfrac{1}{2}\dot{x}^2a^2 + \cdots - x(n)\right] = \dot{x} + O(a)$$

$\Rightarrow$ linear discretization effects

A generalized discretizing of the quantum mechanical oscillator

(Verstegen, 1983)

$$S_{\mathrm{E}} = \int dt \left[\dot{x}^2(t) + \tfrac{1}{2}mx^2(t)\right]$$

$$S_{\mathrm{E}}^{\mathrm{discr}} = a\sum_n \left(\tfrac{1}{a}\left[\tfrac{1}{2}(1+\beta)x(n+a) - \beta x(n) - \tfrac{1}{2}(1-\beta)x(n-a)\right]\right)^2 + \tfrac{m}{2}x^2(n)$$

$\beta = 1$:

$$\tfrac{[x(n+a)-x(n)]}{a} = \tfrac{1}{a}\left[x(n) + ax' + \tfrac{1}{2}x''a^2 + \cdots - x(n)\right] = \dot{x} + O(a)$$

$\beta = 0$:

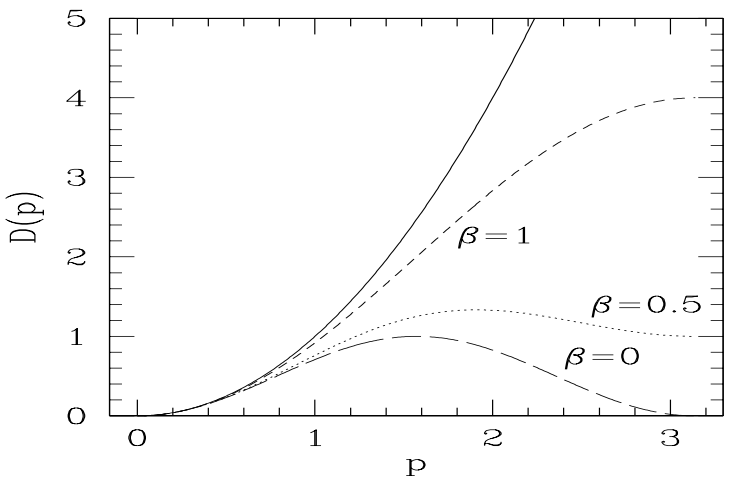
$$\tfrac{[x(n+a)-x(n-a)]}{2a} = \tfrac{1}{2a}\left[x(n) + ax' + \tfrac{1}{2}x''a^2 + \cdots - x(n) + x'a - \tfrac{1}{2}x''a^2\right] = \dot{x} + O(a^2)$$

Effects of different Discretizations

with $x(n) = \frac{1}{\sqrt{2}} \sum_p e^{ipna} \hat{x}(p)$, $p = j\pi/aN$, $j = 0, 1, 2, \cdots, N-1$

$$S_{\mathrm{E}}^{\mathrm{discr}} = \frac{1}{2a} \sum_p \hat{q}^*(p) D(p) \hat{q}(p)$$

$$D(p) = 4 \sin^2(\tfrac{1}{2}pa) + 4(\beta^2 - 1) \sin^4(\tfrac{1}{2}pa) + a^2 m$$



- different β : obtain continuum p^2 *with different rate*
- $\beta = 0$: obtain continuum p^2 behaviour for $p \to 0$ and $p \to \pi$

Lattice version of quantum mechanical oscillator

- discretization provides well defined path integral

$$\mathcal{Z} = \underbrace{\int \prod_{n=1}^{N} dx_n}_{\int \mathcal{D}x} e^{-a \sum_{n=1}^{N} \left[\frac{(x(n+a)-x(n))^2}{a^2} + V(x(n)) \right]}$$

- measuring observables
  - average position $\langle x \rangle = \int \prod_{n=1}^{N} dx_n x e^{-S} / \mathcal{Z}$
  - average position square $\langle x^2 \rangle = \int \prod_{n=1}^{N} dx_n x^2 e^{-S} / \mathcal{Z}$

The Transfer Matrix

Restricting ourselves to the choice $\dot{q} \to \frac{q_{n+1}-q_n}{a}$ (T=Na)

$$\mathcal{Z} = \prod_n \int dq_n e^{-\frac{a}{\hbar}\sum_n \left\{ \frac{1}{2}\left(\frac{q_{n+1}-q_n}{a}\right)^2 + V(q) \right\}}$$

we obtain he continuum expression by sending $\mathrm{N} \to \infty$
while keeping T fixed $\Rightarrow a \to 0$

relation to canonical quantization:

$$a\tfrac{1}{2}\dot{q}_n^2 + V(q_n) \to a\tfrac{1}{2}\left(\tfrac{q'-q}{a}\right)^2 + V(q)a$$

introduce coordinate and momentum operators:

$$\boxed{\hat{p}|p\rangle = p|p\rangle;\;\; \hat{q}|q\rangle = q|q\rangle \;\; \hat{p} = \dot{\hat{q}} = (\hat{q}' - \hat{q})/a}$$

matrix element

$$\langle q'|e^{a\frac{1}{2}\left(\frac{\hat{q}'-\hat{q}}{a}\right)^2 + V(\hat{q})a}|q\rangle$$

$$= \int dp \langle q'|e^{-\hat{p}^2 a}|p\rangle\langle p|e^{-V(\hat{q})a}|q\rangle$$

$$= \int dp \underbrace{\langle q'|p\rangle\langle p|q\rangle}_{e^{ip(q-q')}} e^{-p^2 a} e^{-V(q)a}$$

using the Baker-Hausdorff formula

$$e^{\mathbf{A}}e^{\mathbf{B}} = e^{\mathbf{A}+\mathbf{B}+\frac{1}{2}[\mathbf{A},\mathbf{B}]+\ldots}$$

we obtain for an infinitesimal change from $q(t) \to q'(t+a)$

$$\langle q'|e^{-\hat{p}^2 a}e^{-V(\hat{q})a}|q\rangle + \mathrm{O}(a^2) = \langle q'|e^{-a\mathbf{H}}|q\rangle$$

with **Hamilton operator $\mathbf{H}$**

$$\mathbf{H} = \tfrac{1}{2}\hat{p}^2 + V(\hat{q})$$

the operator $\mathbf{T} = e^{-\frac{1}{\hbar}\mathbf{H}a}$

is called the transfer matrix and describes infinitesimal time steps of the system

the matrix elements of the transfer operator are

$$\langle q_{i+1}|e^{-\frac{1}{\hbar}\mathbf{H}a}|q_i\rangle$$

with $q_{\mathrm{N}} = q_0 \equiv q$

$$\mathcal{Z} = \mathrm{Tr}\mathbf{T}^{\mathrm{N}}$$

$\rightarrow$ partition function in statistical mechanics

inserting an energy eigenbasis

$$\begin{aligned}\langle q_{i+1}|e^{-\frac{1}{\hbar}\mathbf{H}a}|q_i\rangle &= \sum_{\mathrm{E}}\langle q_{i+1}|e^{-\frac{1}{\hbar}\mathbf{H}a}|\mathrm{E}\rangle\langle \mathrm{E}|q_i\rangle \\ &= \sum_{\mathrm{E}}\langle q_{i+1}|\mathrm{E}\rangle\langle \mathrm{E}|q_i\rangle e^{-\frac{1}{\hbar}\mathrm{E}a}\end{aligned}$$

$\rightarrow$ Hamilton operator

$$\boxed{\mathbf{H} = -\tfrac{\hbar}{a}\ln \mathbf{T}}$$

$\Rightarrow$ transfer matrix has to be positive definite

- positivity of $\mathbf{T}$ is sufficient to guarantee that all n-point functions can be rotated back to Minkowski space (reconstruction theorem)
- positivity of $\mathbf{T} \Leftrightarrow$ Osterwalder-Schrader reflection positivity

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

$$D_\mu \Psi(x) \equiv (\partial_\mu - i g_0 A_\mu(x)) \Psi(x)$$

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

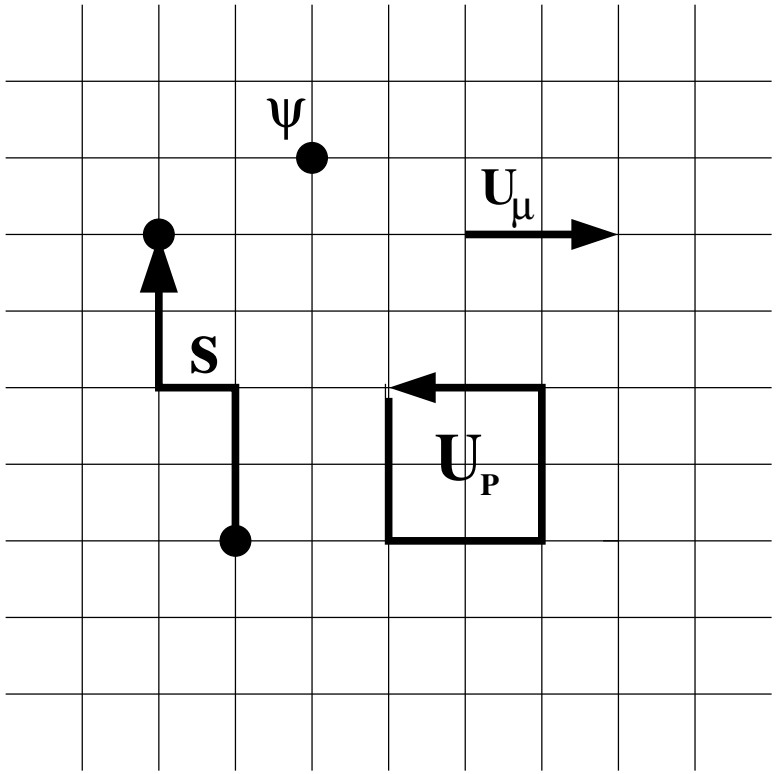
The Schwinger model

- Quantum electrodynamics in 1+1 dimensions
- U(1) gauge fields coupled to fermionic matter
- confinement of charges
- bound states
- chiral symmetry breaking
- super-renormalizable
- exactly solvable in massless case

$\Rightarrow$ testbench for new methods and algorithms

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

$S \to a^2 \sum_x \bar{\Psi} \left[\gamma_\mu \partial_\mu + m\right] \Psi(x)$

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

discrete derivatives

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

a first look at the continuum limit

we introduce external sources η, $\bar{\eta}$ and write the action as $S = \bar{\Psi} K \Psi$

$$\mathcal{Z}(\eta, \bar{\eta}) = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi e^{-\bar{\psi}D\Psi + \bar{\psi}\eta + \bar{\eta}\Psi}$$

the 2-point function (Green's function) G is obatined by

$$G = \frac{1}{\mathcal{Z}(0,0)} \frac{\partial}{\partial\eta}\frac{\partial}{\partial\bar{\eta}}\mathcal{Z}(\eta, \bar{\eta})\Big|_{\eta=\bar{\eta}=0}$$

we have

$$\mathcal{Z}(\eta, \bar{\eta}) = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi e^{-(\bar{\Psi} - \bar{\eta}D^{-1})D(\Psi - D^{-1}\eta) + \bar{\eta}D^{-1}\eta} = \det(D) e^{\bar{\eta}D^{-1}\eta}$$

and obtain

$$G = D^{-1} = \left(\tfrac{1}{2}\gamma_\mu \left[\nabla^*_\mu + \nabla_\mu\right] + m\right)^{-1}$$

we evaluate the 2-point function in momentum space

impose periodic boundary conditions

$$\Psi(x + L_\mu) = \Psi(x)$$

This means that

- the momenta at restricted $-\pi/a < p_\mu \leq \pi/a$ (the first Brillouin zone)
- the momenta are quantized $(\Leftarrow e^{ip(x+L)} = e^{ipx})$
  $p_\mu = 2n\pi/L_\mu, \;\; n = 0, 1, \ldots, L_\mu - 1$

and we have

$$\Psi(x) = \tfrac{1}{V} \textstyle\sum_p \tilde{\Psi}_p e^{ipx}$$

with $V = L^2$ the lattice volume assuming $L_\mu \equiv L$ for each μ

Analysis in Fourier space

$$\left\{\tfrac{1}{2}\gamma_\mu\left[\nabla^*_\mu+\nabla_\mu\right]+m\right\}\tilde{\Psi}_p e^{ipx}=\tfrac{1}{2a}\gamma_\mu\underbrace{\left[e^{ip(x+a\mu)}-e^{ip(x-a\mu)}\right]}_{e^{ipx}\left(e^{ipa\mu}-e^{-iap\mu}\right)}\tilde{\Psi}_p+m\tilde{\Psi}_p e^{ipx}$$

$$\tilde{G}=\left[\tfrac{1}{a}\left(i\gamma_\mu\sin p_\mu a\right)+m\right]^{-1}\equiv\tfrac{i}{a}\left(\hat{p}_\mu\gamma_\mu+m\right)^{-1}=\frac{-\frac{i}{a}\gamma_\mu\sin p_\mu a+m}{\hat{p}^2+m^2}$$

continuum limit $a\to 0$

$$-\tfrac{i}{a}\gamma_\mu\sin p_\mu a\to\gamma_\mu p_\mu$$

and we obtain

$$\lim_{a\to 0}\tilde{G}=\frac{-ip_\mu\gamma_\mu+m}{p^2+m^2}$$

this is exactly the free continuum propagator!

The Unwanted

what if $p_\mu \approx \pi$? (remember our quantum mechanical example)

with $p_\mu = k_\mu + \pi/a$: $\quad \sin p_\mu a = \sin(k_\mu + \pi) = -\sin k_\mu$

which means that for $a \to 0$ we obtain

$$\tilde{G} \to -\frac{-ik_\mu\gamma_\mu + m}{k^2 + m^2}$$

$\Rightarrow$ again we obtain the continuum 2-point function!

the opposite sign can be interpreted such that this continuum fermion at $p \approx \pi/a$ has the opposite chirality from the one at $p \approx 0$

$\to$ find proliferation of fermions

Brillouin zones $\left.\begin{matrix}(0,0)\\(\pi,0)\\(0,\pi)\\(\pi,\pi)\end{matrix}\right\}$ 4 fermions

The Wilson-Dirac Operator

can we repair this?

Wilson suggested to add a second derivative term

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

$$\to \tilde{G} = \left[\frac{1}{a} \left(i \gamma_\mu \sin p_\mu a \right) + \frac{r}{a} \sum_\mu (1 - \cos p_\mu a) + m \right]^{-1}$$

now, for $a \to 0$, $p_\mu \ll \pi/a$

$$\tilde{G} \to \frac{-i p_\mu \gamma_\mu + m}{p^2 + m^2} \quad \text{Good!}$$

analysis at Brillouin corners $p_\mu = k_\mu + \pi/a$, $k_\mu \ll 1$

$$\frac{r}{a}(1 - \cos\left[k_\mu + \pi/a\right] a) = \frac{r}{a}(1 + \cos k_\mu a) \to \frac{r}{a}$$

$$\tilde{G} \to \frac{r}{a}(1 + \cos k_\mu a)$$

fermions become infinitely heavy $\to$ they decouple in the continuum limit

Gauge Invariance

under a gauge transformation

$$A_\mu(x) \to A_\mu(x) + \partial_\mu \Lambda(x)$$

the parallel transporter $U^z(x,y) = e^{i\int_x^y dz_\mu A_\mu(z)}$ transforms as

$$U^z(x,y) \to e^{i\Lambda(x)} U^z(x,y) e^{-i\Lambda(y)}$$

and hence for

$$\Psi(x) \to e^{i\Lambda(x)}\,, \quad \bar{\Psi}(x) \to e^{-i\Lambda(x)}\bar{\Psi}(x)$$

the expression

$$\bar{\Psi}(x) U^z(x,y) \Psi(y)$$

is gauge invariant

Lattice gauge covariant derivative

on the lattice, z_μ is just a line element, a so-called *link* that connects the points x and $y = x + a\hat{\mu}$:

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

this suggest to take the lattice derivatives

$$\begin{aligned} \nabla_\mu \Psi(x) &= \tfrac{1}{a}\left[U(x,\mu)\Psi(x+\mu) - \Psi(x)\right] \\ \nabla^*_\mu \Psi(x) &= \tfrac{1}{a}\left[\Psi(x) - U^{-1}(x-\mu,\mu)\Psi(x-\mu)\right] \end{aligned}$$

then we obtain the gauge invariant expression

$$\bar{\Psi}(x)\left[m_q + \gamma_\mu(\nabla_\mu + \nabla^*_\mu) - r\nabla^*_\mu\nabla_\mu\right]\Psi(x) \equiv \bar{\Psi}(x) D_{\text{Wilson}}\Psi(x)$$

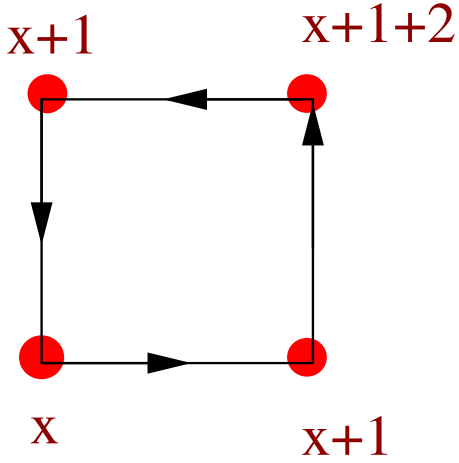
The Gauge Field Action

gauge invariant correspondence to the field strength tensor with parallel transporter

the link variables transform as

$$U(x,\mu) \to g(x)U(x,\mu)g^{-1}(x+\mu)$$

gauge invariant self-interaction: need to parallel transport around a closed loop



$$U(x,\mu)U(x+\mu,\nu)U^{-1}(x+\nu,\mu)U^{-1}(x,\nu)$$

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

Exercise: check gauge invariance; continuum limit

change from **Lie algebra valued** vector potential A_μ to **group valued** $U(x,\mu)$
(Wilson's fundamental observation)

Nota bene: need to take trace for non-abelian gauge group

From the action to physical observables

- the Schwinger model action

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

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

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

- the programme

$$0101110001110001111001 1$$

- the supercomputer

From the Schwinger model to quantum chromodynamics

- system becomes 4-dimensional:
  $[50 \cdot 50] \rightarrow [50 \cdot 50] \cdot 2500$
- gauge field $U(x, \mu) \in U(1) \rightarrow U(x, \mu) \in SU(3)$
- quarks receive 4 Dirac and 3 color components:
  $[50 \cdot 50] \rightarrow [50 \cdot 50] \cdot 30000$
- Schwinger model simulation $O(1\text{day})$
  QCD: $\rightarrow$ need massive parallelization
- theory needs *non-perturbative* renormalization
  $\rightarrow$ see lecture by R. Sommer

The Continuum Action for Quantum Chromodynamics

$$S = S_{\rm Ferm} + S_{\rm gauge} = \int d^4x \bar{\Psi}(x) \left[\gamma_\mu D_\mu + m\right] \Psi(x) + \int d^4x {\rm Tr} F_{\mu\nu} F_{\mu\nu}$$

Holy Principles of Quantum Chromodynamics

- Gauge Invariance $\leftrightarrow$ renormalizability
- Local Theory $\leftrightarrow$ (micro) causality
- Lorentz Invariance $\leftrightarrow$ relativistic theory
- Chrial Invariance $\leftrightarrow$ spontaneous symmetry breaking $\leftrightarrow$ spectrum of light mesons
  massless limit:
  action invariant under chiral transformations ($\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3$, α real)

$$\Psi \to e^{i\alpha\gamma_5}\Psi \ , \quad \bar{\Psi} \to e^{-i\alpha\gamma_5}\bar{\Psi} = \bar{\Psi}e^{i\alpha\gamma_5}$$

  equivalent condition: $\gamma_5 D(m=0) + D(m=0)\gamma_5 = 0$

  $\Leftarrow$ very important physical consequences for the low energy behaviour of QCD

Chiral Symmetry

free Wilson fermion action

$$S = a^4 \sum_p \bar{\Psi}(p) \left[m_q + i\gamma_\mu \sin p_\mu a + \frac{r}{a} \sum_\mu (1 - \cos p_\mu a) \right]$$

- Locality: *okay*
- continuum limit: *okay*
- Lorentz Invariance: *replaced by hypercubic group*
- Chiral invariance for $m_q = 0$, : $\Psi \to e^{i\alpha\gamma_5}\Psi$, $\bar{\Psi} \to e^{-i\alpha\gamma_5}\bar{\Psi}$
  broken by mass-like term $\frac{r}{a}$
  chiral symmetry only recovered in continuum limit
  (Bochicchio, Maiani, Martinelli, Rossi, Testa)

clash between *chiral symmetry* and *fermion proliferation*

$\rightarrow$ Nielsen-Ninomiya theorem:

For any lattice Dirac operator D the conditions

- D is local (bounded by $Ce^{-\gamma/a|x|}$)
- $\tilde{D}(p) = i\gamma_\mu p_\mu + \mathrm{O}(ap^2)$ for $p \ll \pi/a$
- $\tilde{D}(p)$ is invertible for all $p \neq 0$
- $\gamma_5 D + D\gamma_5 = 0$

can not be simultaneously fulfilled

Chiral fermions

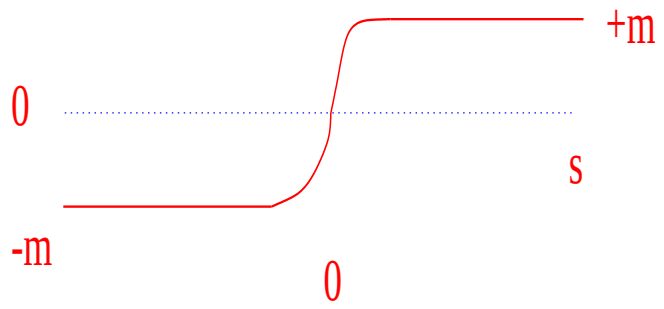
→ lecture by D. Kaplan

also, let us start with *continuum field theory*

we consider a 5-dimensional theory (free fermions for the moment)
mass defect in extra dimension s

$$D_5 = \partial_\mu \gamma_\mu + m_0 + \gamma_5 \partial_s + m(s)$$

$$m(s) = \begin{cases} -m; & s \to -\infty \\ +m; & s \to +\infty \end{cases}$$



let us try to solve the massless Dirac equation

$$D_5(m_0 = 0)\psi = 0$$

this can be solved by the ansatz

$$\begin{aligned} \psi_\pm &= e^{ipx}\Phi_\pm(s)u_\pm \\ \Phi_\pm(s) &= \exp\left\{\pm\int_0^s m(s')ds'\right\} \\ \gamma_5 u_\pm &= \pm u_\pm \end{aligned}$$

only Φ_- *normalizable* $\Rightarrow$ only one solution

- massless fermion travelling along the domain wall
- it has a definite chirality
- bound to the domain wall with exponential fall-off with a rate $|m|$ when going to $|s| \gg 1$

Going to the lattice

- remove doublers in extra dimension: add Wilson term

$$D_5 = \partial_\mu \gamma_\mu + m_0 + \gamma_5 \partial_s + m(s) - \nabla^*_\mu \nabla_\mu - \nabla^*_s \nabla_s$$

- the limit of infinite extra dimension

$$aD \equiv \lim_{N_s \to \infty} aD_5 = 1 - \frac{A}{\sqrt{A^\dagger A}}$$

$$A = 1 - \left(\nabla_\mu \gamma_\mu - \nabla^*_\mu \nabla_\mu \right)$$

massless Wilson-Dirac operator

D is a (practical !) example of an operator that satisfies the celebrated
Ginsparg-Wilson relation

$$\boxed{\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D}$$

$$\Rightarrow D^{-1}_{xy}\gamma_5 + \gamma_5 D^{-1}_{xy} = 2a\gamma_5\delta_{x,y}$$

D^{-1} anti-commutes with γ_5 at all non-zero distances

$\rightarrow$ only mild (i.e. local) violation of chiral symmetry

Ginsparg and Wilson arrived at this expression already
in the early days of lattice gauge theories from a completely different path
$\Leftarrow$ block spinning from the continuum

local (Hernandez, K.J., Lüscher) solution: overlap operator $D_{\rm ov}$ (Neuberger)

$$\boxed{D_{\rm ov} = \left[1 - A(A^\dagger A)^{-1/2}\right]}$$

with $A = 1 + s - D_{\rm w}$ s a tunable parameter, $0 < s < 1$

Moreover: Ginsparg-Wilson relation implies an
exact lattice chiral symmetry (Lüscher):

for any operator D which satisfies the Ginsparg-Wilson relation, the action

$$S = \bar{\psi} D \psi$$

is invariant under the transformations

$$\boxed{\begin{aligned} \delta\psi &= \gamma_5 (1 - \tfrac{1}{2} a D)\psi \\ \delta\bar{\psi} &= \bar{\psi}(1 - \tfrac{1}{2} a D)\gamma_5 \end{aligned}}$$

$\Rightarrow$ have a notion of chiral symmetry on the lattice

$$\gamma_5 \to \gamma_5 (1 - \tfrac{1}{2} a D)$$

the *lattice* operator D enjoys many properties of
the *continuum* operator:
$Z_A = Z_V = 1$, anomaly, index theorem, ...

Decide for an action

ACTION	ADVANTAGES	DISADVANTAGES
clover improved Wilson	computationally fast	breaks chiral symmetry needs operator improvement
twisted mass fermions	computationally fast automatic improvement	breaks chiral symmetry violation of isospin
staggered	computationally fast	fourth root problem complicated contraction
domain wall	improved chiral symmetry	computationally demanding needs tuning
overlap fermions	exact chiral symmetry	computationally expensive

For all actions: $O(a)$-improvement

$\Rightarrow \langle O^{\text{latt}}_{\text{phys}} \rangle = \langle O^{\text{latt}}_{\text{cont}} \rangle + O(a^2)$

Monte Carlo Method

$$\langle f(x)\rangle = \int dx f(x) e^{-x^2} / \int dx e^{-x^2}$$

$\rightarrow$ solve numerically:

- generate succesively Gaussian random numbers x_i
- do this N-times

$$\Rightarrow \langle f(x)\rangle \approx \frac{1}{N}\sum_i f(x_i) \pm O(1/\sqrt{N})$$

- but, what if I have a distribution $e^{-S(\phi)}$?
  (Φ representing generic degrees of freedom)

need a transition probality $W(\phi, \phi')$:
$\rightarrow$ field configuration $\{\phi\} \rightarrow \{\phi'\}$
$\rightarrow$ satisfies

- $W(\phi, \phi') > 0$ strong ergodicity ($W \geq 0$ is weak ergodicity)
- $\int d\phi' W(\phi, \phi') = 1$
- $W(\phi, \phi') = \int d\phi'' W(\phi, \phi'') W(\phi'', \phi')$ (Markov chain)
- $W(\phi, \phi')$ is measure preserving, $d\phi' = d\phi$

under these conditions, we are guaranteed

– convergence to a unique equilibrium distribution P^{eq}
  $\rightarrow$ Boltzmann distribution e^{-S}
– independence from the initial conditions

$\rightarrow$ proof: (Creutz and Freedman; Lüscher, Cargese lectures)

Detailled balance

- Markov chain condition

$$W(\phi, \phi') = \int d\phi'' W(\phi, \phi'') W(\phi'', \phi')$$

- alternative form

$$P(\phi') = \int d\phi W(\phi', \phi) P(\phi)$$

sufficient (not neccessary): detailled balance condition

$$\frac{W(\phi,\phi')}{W(\phi',\phi)} = \frac{P(\phi')}{P(\phi)}$$

- find

$$\begin{aligned} \int d\phi P(\phi) W(\phi, \phi') &= \int d\phi P(\phi) \frac{P(\phi')}{P(\phi)} W(\phi', \phi) \\ &= \int d\phi P(\phi') W(\phi', \phi) = P(\phi') \end{aligned}$$

- many possible choices for W

Metropolis Algorithms

$W_{\mathrm{Metro}}(\Phi, \Phi') = \exp\left(-\Delta S(\Phi', \Phi)\right) \Theta(S(\Phi'(x)) - S(\Phi(x)))$

$\Delta S(\Phi'(x), \Phi(x)) = S(\Phi'(x) - S(\Phi(x))$, $\Theta()$ Heavyside function

How this works:

$i)$ generate uniformly distributed $\Phi'(x)$ in a neighbourhood of $\Phi(x)$

- discretized quantum mechanics: $x_i' \in [x_i - \Omega, x_i + \Omega]$
- $SU(N)$: $U'_{n,\mu} = RU_{n,\mu}$, elements of R "close to" $U_{n,\mu}$

$ii)$ if $\Delta S(\Phi'(x), \Phi(x)) \leq 0)$ accept $\Phi'(x)$

$iii)$ if $\Delta S(\Phi'(x), \Phi(x)) > 0)$ accept with probability $\exp(-\Delta S(\Phi'(x), \Phi(x))$

- steps $i) - iii)$ are repeated N-times
- step $iii)$ can be realized by uniformly choosing randon number $r \in [0, 1]$ and accept, if $\exp(-\Delta S) > r$

Metropolis Algorithms

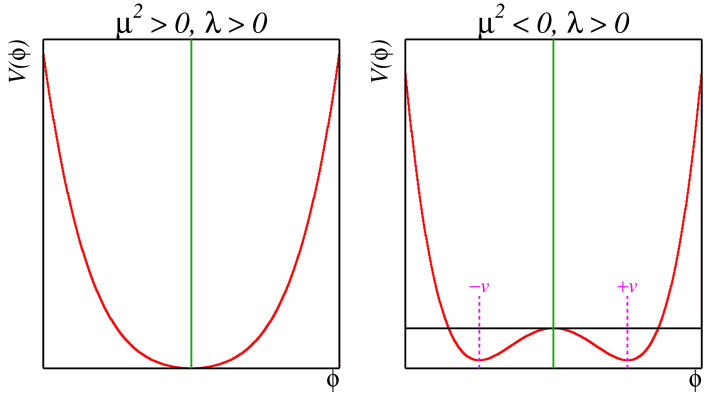
- very general algorithm, can be used for many physical systems
- shows, however, often very long autocorrelation times
- much too costly for fermionic systems (why?)

Action to be programmed

$$S = a \sum_{i=1}^{N} \frac{1}{2} M_0 \frac{(x_{i+1} - x_i)^2}{a^2} + \frac{1}{2}\mu^2 x_i^2 + \lambda x_i^4$$

periodic boundary condition: $x_{N+1} = x_1 \ , \ x_0 = x_N$

- potential $V(x)$
  - $\mu^2 > 0, \lambda > 0$: harmonic potential $\langle x \rangle = 0$
  - $\mu^2 < 0, \lambda > 0$: anharmonic potential $\langle x \rangle = \pm v \neq 0$



Observables

- average position

$$\langle x \rangle = \frac{1}{\text{MCsteps}} \sum_{\text{MCsteps}} \left[\frac{1}{N} \sum_{i=1}^{N} x_i \right] ,$$

- average position squared
  $\rightarrow$ theoretical value known for $a > 0$ and $\mu^2 > 0$

$$\langle x^2 \rangle = \frac{1}{\text{MCsteps}} \sum_{\text{MCsteps}} \left[\frac{1}{N} \sum_{i=1}^{N} x_i^2 \right]$$

- acceptance rate, should be $\approx 50\%$
- error for observable O

$$\Delta O = \sqrt{\frac{1}{(\text{MCsteps})(\text{MCsteps}-1)} \sum_{\text{MCsteps}} [\langle O^2 \rangle - \langle O \rangle^2]}$$

Observables considered

Cumulants

$\langle x^2 \rangle = \langle \frac{1}{d} \sum_i x_i^2 \rangle$

$\langle x^4 \rangle = \langle \frac{1}{d} \sum_i x_i^4 \rangle$

Correlator

$\langle x_k x_{k+t} \rangle = \langle \frac{1}{d} \sum_i x_i x_{i+t} \rangle \propto e^{-(E_1 - E_0)t}$

Energies

ground state energy: $E_0 = 3\lambda \langle x^4 \rangle + \mu^2 \langle x^2 \rangle + \frac{\omega^4}{16}$

energy gap $E_1 - E_0$

Exercise

- programme action of quantum mechanical oscillator
- evaluate path integral by Metropolis algorithm
- compute observables $\langle x \rangle$, $\langle x^2 \rangle$ with error
- compare $\langle x^2 \rangle$ to theoretically known value

Hybrid Monte Carlo Algorithm

- expectation values

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi O e^{-S}}{\int \mathcal{D}\Phi e^{-S}}$$

- add field independeint terms

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi \int \mathcal{D}\pi O e^{-\frac{1}{2}\pi^2 - S}}{\int \mathcal{D}\Phi \int \mathcal{D}\pi e^{-\frac{1}{2}\pi^2 - S}}$$

field configurations are generated in a fictitious (computer) time τ

take π's Gaussian distributed, satisfying

$$< \pi(\tau) >= 0, \;\; < \pi(\tau)\pi(\tau') >= \delta(\tau - \tau')$$

- 4-dimensional Hamiltonian

$$H = \frac{1}{2}\pi^2 + S$$

HMC in practise

- quantum mechanical action: $S = \sum_n (x(n+a) - x(n))^2 + m^2 x^2(n)$
- ficititious time τ: evolve system with Hamilton's equations of motion

$$\frac{\partial}{\partial \tau}\pi(n) = -\frac{\partial}{\partial \mathbf{x(n)}} S \equiv \text{force}, \quad \frac{\partial}{\partial \tau}\mathbf{x(n)} = \pi(n)$$

$\Rightarrow$ conservation of energy

- numerical integration through leap frog algorithm
  $\rightarrow$ discretization such that $T = N\delta\tau$:

$$\begin{aligned}
\pi(\delta\tau/2) &= \pi(0) - \frac{\delta\tau}{2}\frac{\partial}{\partial \mathbf{x}} S\big|_{\mathbf{x}(0)} \\
\mathbf{x}(\delta\tau) &= \mathbf{x}(0) + \pi(\delta\tau/2)\delta\tau \\
\pi(3\delta\tau/2) &= \pi(\delta\tau/2) - \delta\tau\frac{\partial}{\partial \mathbf{x}} S\big|_{\mathbf{x}(\delta\tau)} \\
&\vdots \\
\pi(T) &= \pi(N\delta\tau/2) - \frac{\delta\tau}{2}\frac{\partial}{\partial \mathbf{x}} S\big|_{\mathbf{x}((N-1)\delta\tau)}
\end{aligned}$$

Adding a Metropolis test

leap-frog scheme has a *finite* step-size $\delta\tau \Rightarrow$ energy is no longer conserved

$$H(\mathbf{x}_{\text{ini}}, \pi_{\text{ini}}) \neq H(\mathbf{x}_{\text{end}}, \pi_{\text{end}})$$

introduce a Metropolis like accept/reject step

accept new field configuration $\{\mathbf{x}_{\text{end}}, \pi_{\text{end}}\}$ with a probability

$$P_{\text{acc}} = \min\left(1, e^{H(\mathbf{x}_{\text{ini}}, \pi_{\text{ini}}) - H(\mathbf{x}_{\text{end}}, \pi_{\text{end}})}\right)$$

- algorithm fulfills detailled balance condition
- needs measure conservation $\leftarrow$ reversibility violations

The case of Lattice QCD

- two flavors of fermions (mass degenerate up and down quark)

$$S = a^4 \sum_x \bar{\psi} M^\dagger M \psi$$

- path integral

$$\mathcal{Z} = \prod_x d\bar{\psi}(x) d\Psi(x) e^{-S} = \det[M^\dagger M] = \prod_x d\Phi^\dagger(x) d\Phi(x) e^{-\Phi^\dagger \left[M^\dagger M\right]^{-1} \Phi}$$

  $\rightarrow$ need to compute inverse fermion matrix $\left[M^\dagger M\right]^{-1}$ (?)

- simulate with Hybrid Monte Carlo algorithm

$$\begin{aligned} \frac{d}{d\tau}\pi &= -\frac{dS}{d\Phi^\dagger} = \left[M^\dagger M\right]^{-1} \Phi \equiv \text{force} \\ \frac{d}{d\tau}\Phi &= \pi \end{aligned}$$

- update of the momenta $\pi(x)$ independent of update of $\Phi(x)$
- How would a Metropolis algorithm work?

to update the momenta, have to compute the vector

$$X = \left[M^\dagger M\right]^{-1} \Phi$$

$\Rightarrow$ solve an equation

$$\left[M^\dagger M\right] X = \Phi$$

Exercise:

estimate the number of flops to apply the Wilson operator on a vector

assume you want to have 2000 thermalization and 5000 measurement steps on a $48^3 \cdot 96$ lattice

assume number of iterations to solve $\left[M^\dagger M\right] X = \Phi$ is 500

assume number of time steps in the HMC is 100

How long would the program run on your laptop?
(assume –unrealistic– efficiency of 50%)

If you save the 5000 configurations, would this fit on your laptop disk?

autocorrelation times

generating field configurations as a Markov process,
$\Rightarrow$ configurations are not independent from each other

free field theory $S = \int d^4x \Phi(x)[\nabla^*_\mu \nabla_\mu + m_0^2]\Phi(x)$ in Fourier space

$$S = \int d^4k \Phi(k)[k^2 + m_0^2]\Phi(k)$$

Langevin equation $\leftrightarrow$ HMC algorithm

$$\frac{d}{d\tau}\Phi(k,\tau) = -[k^2 + m_0^2]\Phi(k,\tau) + \eta(k,\tau)$$

$$< \eta(\tau) >= 0, \;\; < \eta(\tau)\eta(\tau') >= \delta(\tau - \tau')$$

then a solution may be written down

$$\Phi(k,\tau) = \int^\tau ds \exp\left\{-(\tau - s)[k^2 + m_0^2]\eta(k,s)\right\}$$

compute correlation of fields at $\tau = 0$ with fields at τ

consider the autocorrelation function

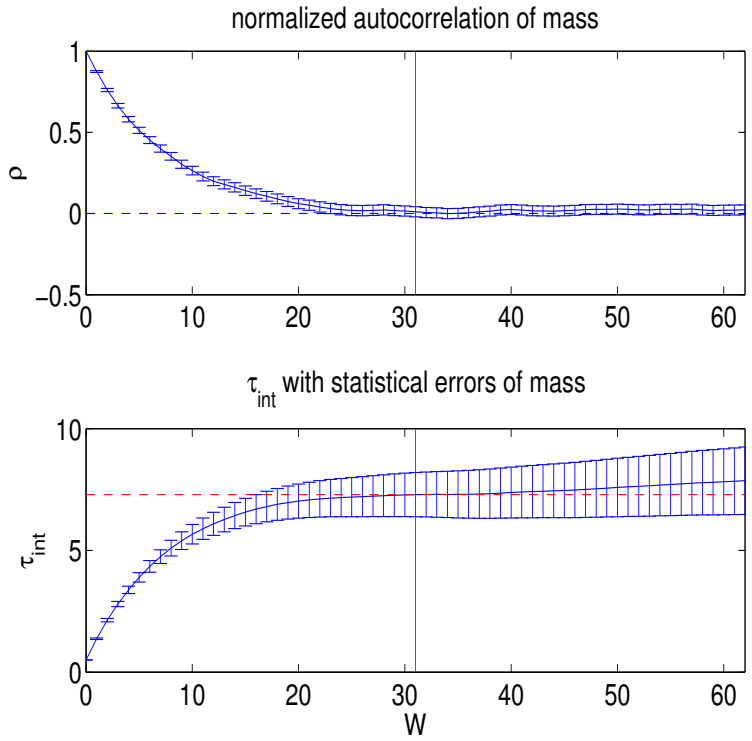
$$
\begin{aligned}
C(k,\tau) &= \Phi(k,0)\Phi(k,\tau) \\
&= \int ds_1 ds_2 \exp\left\{[k^2+m_0^2]s_1\left(-(\tau-s)[k^2+m_0^2]\right)\right. \\
&\qquad\qquad \left.\eta(k,s_1)\eta(k,s_2)\right\} \\
&\propto \frac{e^{-[k^2+m_0^2]\tau}}{k^2+m_0^2} \equiv \frac{e^{-\tau/\tau_0}}{k^2+m_0^2}
\end{aligned}
$$

- the autocorrelation function $C(k,\tau)$ decays exponentially
  autocorrelation time τ_0
- decay is lowest for the zero mode $k=0$
- $\tau \propto 1/m_0^2 \quad \Rightarrow$ the correlations become stronger closer to the critical point $m_0 = 0 \rightarrow$ *critical slowing down*
- scaling law $\tau_0 \propto 1/m^z$, $\quad z$ *the dynamical critical exponent*

How to deal with the autocorrelation?

measure it:

$$\Gamma(\tau) = \langle x(\tau) \cdot x(0) \rangle / \langle x(0) \rangle^2 \propto e^{-\tau/\tau_{\mathrm{int}}}$$



Comment: *integrated auto correlation time* τ_{int} observable dependent

A consequence from autocorrelations: Errors

measure average position of quantum mechanical particle $\bar{x}$ from N measurements

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

This has a variance

$$\sigma = \frac{1}{N-1} \left(\bar{x^2} - \bar{x}^2 \right)$$

and a standard deviation

$$\Delta_0 \equiv \sqrt{\sigma} \propto 1/\sqrt{N} \quad \text{for} \quad N \gg 1$$

If we have an autocorrelation time $\tau \Rightarrow$ statistics reduces to $n = N/\tau$

$\Rightarrow \Delta_{\text{true}} \propto 1/\sqrt{n} = \sqrt{\tau}/\sqrt{N} = \sqrt{\tau}\Delta_0$

Observables

- average position

$$\langle x \rangle = \frac{1}{\text{MCsteps}} \sum_{\text{MCsteps}} \left[\frac{1}{N} \sum_{i=1}^{N} x_i \right] ,$$

- average position squared
  $\rightarrow$ theoretical value known for $a > 0$ and $\mu^2 > 0$

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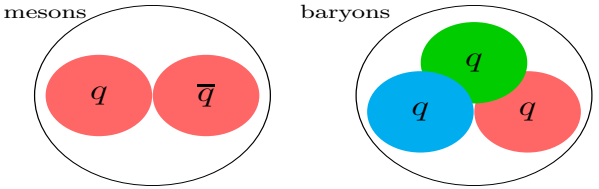
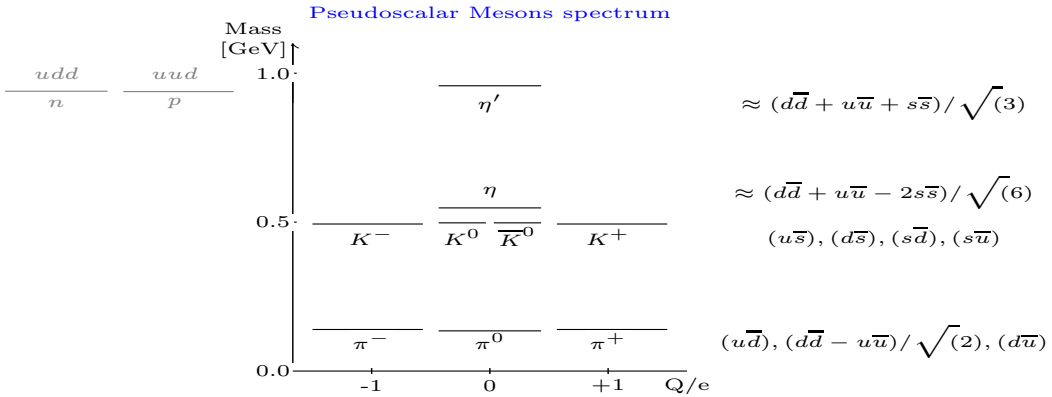
ground state energy: $E_0 = 3\lambda \langle x^4 \rangle + \mu^2 \langle x^2 \rangle + \frac{\omega^4}{16}$

energy gap $E_1 - E_0$

The observable

What we learn from mesons and baryons





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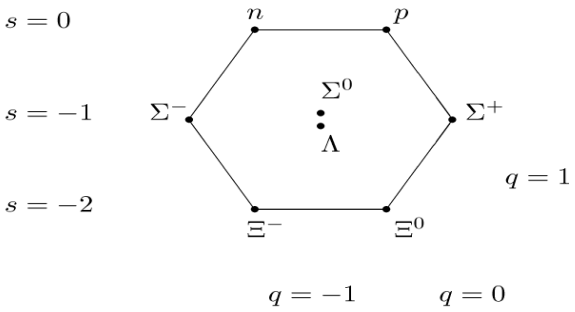
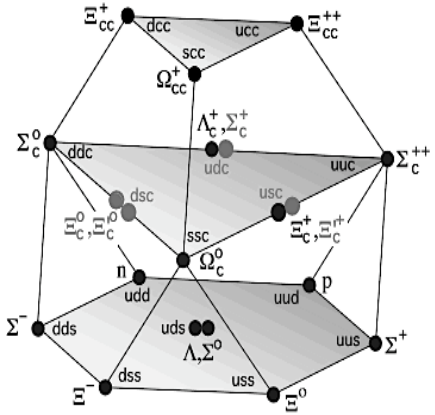
- confinement of quarks
- spontaneous chiral symmetry breaking
- topological effects of gluon field configurations

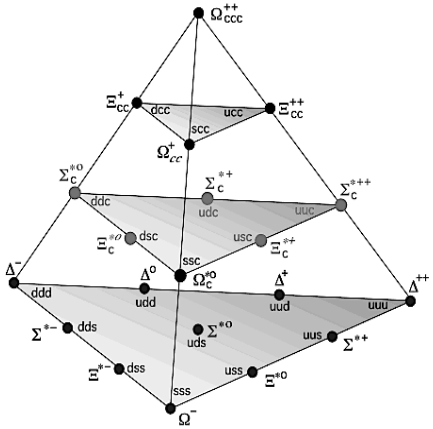
The complicated baryon spectrum



Octet



Decuplett



32-plet

QCD: the Mass Spectrum

goal: **non-perturbative computation of this rich bound state spectrum**

using QCD alone

$\rightarrow$ euclidean correlation functions
Reconstruction theorem relates this to Minkowski space

operator $O(\mathbf{x}, t)$ with quantum numbers of a given particle

correlation function decays exponentially: e^{-Et} , $E^2 = m^2 + \mathbf{p}^2$
$\Rightarrow$ mass obtained at zero momemtum

$$O(t) = \sum_{\mathbf{x}} O(\mathbf{x}, t)$$

correlation function

$$\begin{aligned} \langle O(0)O(t)\rangle &= \tfrac{1}{\mathcal{Z}} \sum_n \langle 0|O(0)e^{-\mathbf{H}t}|n\rangle\langle n|O(0)|0\rangle \\ &= \tfrac{1}{\mathcal{Z}} \sum_n |\langle 0|O(0)|n\rangle|^2 e^{-(E_n - E_0)t} \end{aligned}$$

connected correlation function

$$\lim_{t\to\infty}\left[\langle O(0)O(t)\rangle - |\langle O(0)\rangle|^2\right] \propto e^{-E_1 t}$$

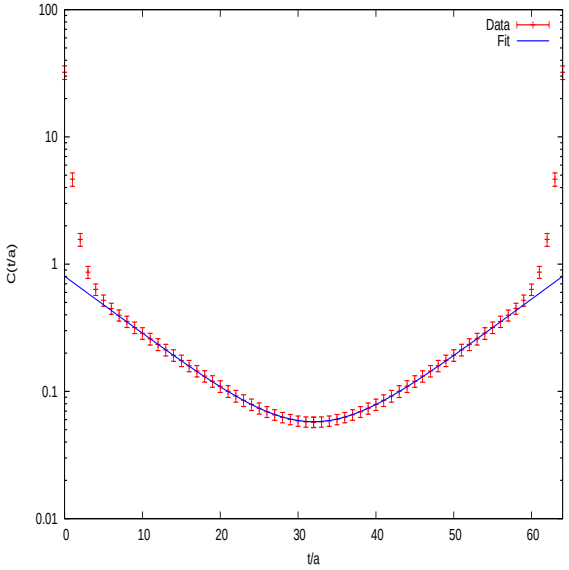
vanishing of connected correlation function at large times

$\rightarrow$ cluster property $\Rightarrow$ *locality of the theory*

periodic boundary conditions

$$\langle O(0)O(t)\rangle_c = \sum_n c_n \left[e^{-E_n t} + e^{-E_n(T-t)}\right]$$

$$1 \ll t \ll T: \quad \langle O(0)O(t)\rangle_c \propto e^{-mt} + e^{-m(T-t)}$$



Hadron Spectrum in QCD

hadrons are bound states in QCD

- mesons pion, kaon, eta, ...
- baryons neutron, proton, Delta, ..

for the computation of the hadon spectrum

- construct operators with the suitable quantum numbers
- compute the connected correlation function
- take the large time limit of the correlation function

Lorentz symmetry, parity and charge conjugation

rotational symmetry $\rightarrow$ hypercubic group: discrete rotations and reflections
classification of operators: irreducible representations R
(note hypercubic group is a subgroup of $SO(3)$)

parity	charge conjugation
$\Psi(\mathbf{x},t) \rightarrow \gamma_0 \Psi(-\mathbf{x},t)$	$\Psi(\mathbf{x},t) \rightarrow C\bar{\Psi}^T(\mathbf{x},t)$
$\bar{\Psi}(\mathbf{x},t) \rightarrow \bar{\Psi}(-\mathbf{x},t)\gamma_0$	$\bar{\Psi}(\mathbf{x},t) \rightarrow -\Psi^T(\mathbf{x},t)C^{-1}$

C charge conjugation matrix $C = \gamma_0\gamma_2$
C satisfies

$$C\gamma_\mu C^{-1} = -\gamma_\mu^T = -\gamma_\mu^*$$

The Proton

Nucleon: baryonic isospin-doublet, $I = \frac{1}{2}$:

proton (uud) $I_3 = +\frac{1}{2}$ and neutron (udd) $I_3 = -\frac{1}{2}$

local interpotating field of proton

$$P(x) = -\epsilon_{abc} \left[u_a^T(x) C \gamma_5 d_b(x) \right] u_c(x) \ , \quad [\ ] \, \text{spin trace}$$

u^C charged conjugate quark field

$$\psi^C(x) = C \bar{\psi}^T(x) \ , \quad \bar{\psi}^C = -\psi^T(x) C^{-1}$$

leading to

$$\Gamma_P(t) = \sum_{\vec{x}} \langle 0 | P(x) \bar{P}(0) | 0 \rangle$$

Exercise:

using the operator

$$P(x) = -\epsilon_{abc} \left[u_a^T(x) C\gamma_5 d_b(x) \right] u_c(x) \ , \quad [\ ]\,\text{spin trace}$$

will we really get the proton?

$\rightarrow$ check quantum numbers

Contraction

- 2-point-function calculation

$\mathcal{O}_\Gamma(x) = \bar{\psi}\Gamma\psi(0)$

$\langle \mathcal{O}_\Gamma(x)\mathcal{O}_\Gamma(0)\rangle = \bar{\psi}(x)\Gamma\bar{\psi}(0)\psi(x)\Gamma\psi(0) = tr[\Gamma S(x,0)\Gamma S(0,x)]$

$\rightarrow$ need propagator $S(0,x)$

in terms of eigenvalues and eigenvectors:

$$tr[\Gamma S(x,0)\Gamma S(0,x)] = \sum_{\lambda_i,\lambda_j} \frac{1}{\lambda_i\lambda_j} \sum_{\alpha\beta\gamma\delta} \left[(\phi_j^{\dagger\alpha}(x)\Gamma_{\alpha\beta}\phi_i^{\beta}(x))(\phi_i^{\dagger\gamma}(0)\Gamma_{\gamma\delta}\phi_j^{\delta}(0)) \right]$$

Example: pion operator $\rightarrow$ need pseudoscalar operator

$$O_{\mathrm{PS}}(\mathbf{x},t) = \bar{\Psi}(\mathbf{x},t)\gamma_5\Psi(\mathbf{x},t)$$

correlation function

$$\begin{aligned} f_{\mathrm{PS}}(t) \equiv \langle O_{\mathrm{PS}}(0)O_{\mathrm{PS}}(t)\rangle &= \sum_{\mathbf{x}} \left[\bar{\psi}(\mathbf{x},t)\gamma_5\Psi(\mathbf{x},t)\right]\left[\bar{\psi}(0,0)\gamma_5\Psi(0,0)\right] \\ &= \sum_{\mathbf{x}} \mathrm{Tr}\left[S_F(0,0;\mathbf{x},t)\gamma_5 S_F(\mathbf{x},t;0,0)\gamma_5\right] \end{aligned}$$

used Wick's theorem and $S_F = D^{-1}$ the fermion propagator

remark: formula simplifies using γ_5 hermiticity of D_{Wilson}

$\Rightarrow$ need to compute inverse (?) of the fermion matrix

$$a \ll t \ll T: \quad f_{\mathrm{PS}}(t) = \underbrace{\frac{|\langle 0|P|\mathrm{PS}\rangle|^2}{2m_{\mathrm{PS}}}}_{\equiv F_{\mathrm{PS}}^2/2m_{\mathrm{PS}}} \cdot \left(e^{-m_{\mathrm{PS}}t} + e^{-m_{\mathrm{PS}}(T-t)}\right)$$

F_{PS} pion decay constant

Obtaining the propagator

- we need the propgator D^{-1}
  - D large (nowadays $O(100^4)$)
  - D is sparse (only nearest neighbour interaction)

  $\Rightarrow$ can use sparse matrix algorithms, minimal residue, conjugate gradient

- task: solve linear equation

$$MX = \Phi$$

- point source $\Phi = \delta \underbrace{x, y}_{\text{points}} \delta \underbrace{a, b}_{\text{colour}} \delta \underbrace{\alpha, \beta}_{\text{dirac}}$

- solve for all colour and Dirac components (12 inversions)
  and one lattice point (translational invariance)
  $\rightarrow$ obtain point to all propagator

Minimal Residual

- basic gradient descent algorithm
- convergence not guaranteed

- general idea: minimize $\min_X \langle X|D|X\rangle - \Phi|X\rangle$

Require: lattice Dirac operator D, source vector Φ, tolerance ϵ
Ensure: residual sufficiently small
residual vector $R \leftarrow \Phi - D \cdot X$, X initial guess
$\delta = R^\dagger R$
while $\delta > \epsilon$ **do**
$Q \leftarrow D \cdot R$
$\alpha \leftarrow \frac{R^\dagger R}{R^\dagger Q}$
$R \leftarrow R - \alpha Q$
$\delta \leftarrow R^\dagger R$
end while

Conjugate Gradient Algorithm

- very stable
- guaranteed that residual is reduced in every step

Require: lattice Dirac operator D, source vector Φ, tolerance ϵ
Ensure: residual sufficiently small
residual vector $R \leftarrow \Phi - D \cdot X$, X initial guess
conjugate direction vector $S \leftarrow R$
$\delta_{\text{new}} = R^\dagger R$
while $\delta_{\text{new}} > \epsilon$ **do**
$Q \leftarrow D \cdot R$
$\alpha \leftarrow \frac{R^\dagger R}{R^\dagger Q}$
$X \leftarrow X + \alpha S$
$R \leftarrow R - \alpha Q$
$\delta_{\text{old}} \leftarrow \delta_{\text{new}}$
$\delta_{\text{new}} \leftarrow R^\dagger R$
$\beta \leftarrow \frac{\delta_{\text{new}}}{\delta_{\text{old}}}$
$S \leftarrow R + \beta S$
end while

Improvements

- preconditioning
  - even/odd preconditioning
  - low mode preconditioning
- better algorithms
  - Schwarz alternating procedure
  - Multigrid
- thinning
  - deflation
  - destillation

→ see lecture by G. Herdioza

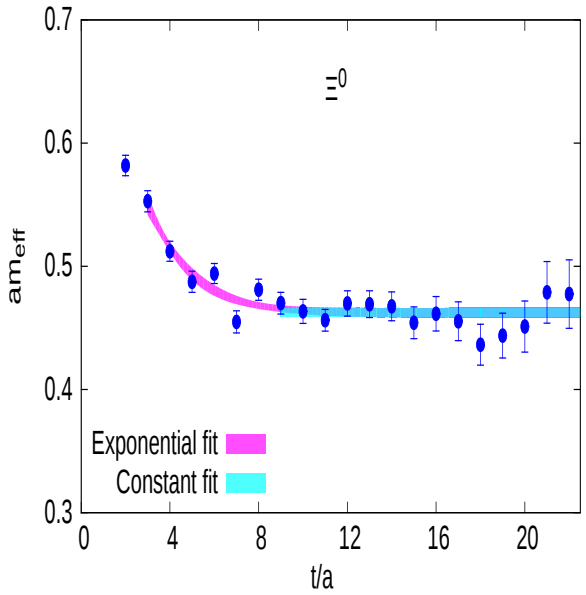
Effective Masses and exponential fits

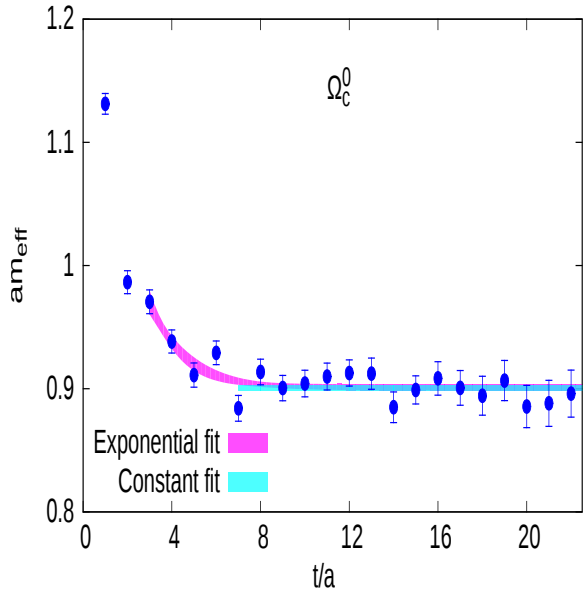
effective mass (neglecting boundary)

$$am^X_{\text{eff}}(t) = \log\left(\frac{C_X(t)}{C_X(t+1)}\right) = am_X + \log\left(\frac{1+\sum_{i=1}^{\infty} c_i e^{-\Delta_i t}}{1+\sum_{i=1}^{\infty} c_i e^{-\Delta_i (t+1)}}\right) \longrightarrow_{t\to\infty} am_X$$

$\Delta_i = m_i - m_X$ mass difference of the excited state i to the ground mass m_X

in practise: $am^X_{\text{eff}}(t) \approx am_X + \log\left(\frac{1+c_1 e^{-\Delta_1 t}}{1+c_1 e^{-\Delta_1 (t+1)}}\right)$

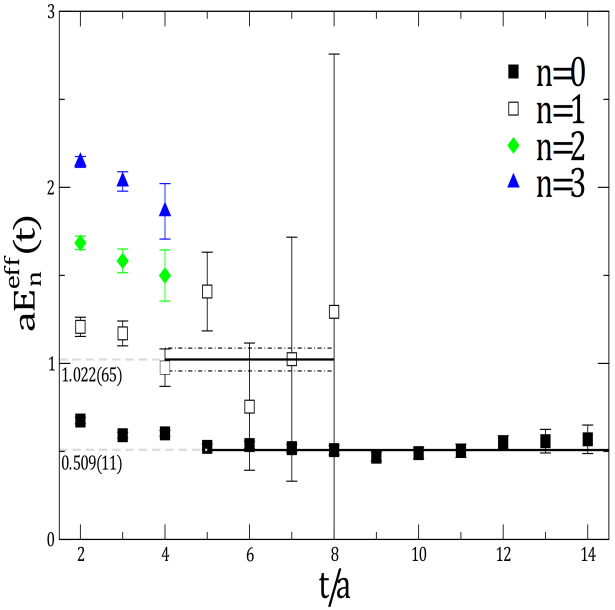




Identifying exicited states

$$am^X_{\text{eff}}(t) = \log\left(\frac{C_X(t)}{C_X(t+1)}\right) = am_X + \log\left(\frac{1+\sum_{i=1}^{\infty} c_i e^{-\Delta_i t}}{1+\sum_{i=1}^{\infty} c_i e^{-\Delta_i (t+1)}}\right) \longrightarrow_{t\to\infty} am_X$$

$\Delta_i = m_i - m_X$ mass difference of the excited state i to the ground mass m_X



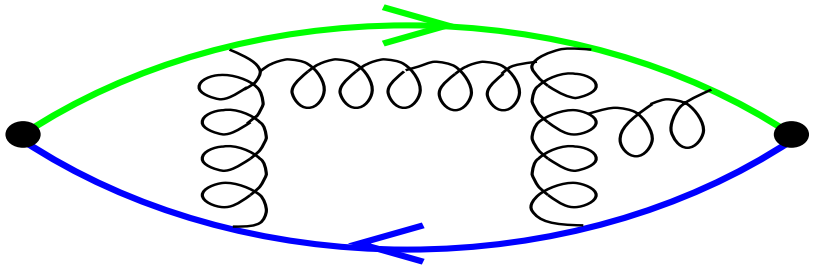
- large errors for excited states
- generalized eigenvalue approach
- need of large operator basis

Quenched approximation

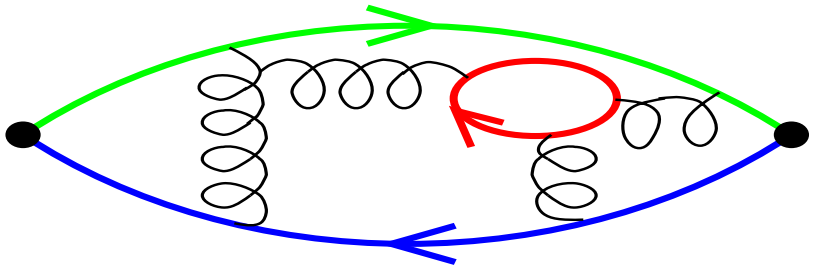
The Quenched Approximation

$\rightarrow$ neglect steady generation of quarks and antiquarks in physical quantum processes

$\Rightarrow$ *truncation*, works surprisingly well however



(A) Quenched QCD: no internal quark loops



(B) full QCD

A short history of proton mass computation

(take example of Japanese group)

1986 (Itoh, Iwasaki, Oyanagi and Yoshie)

quenched approximation, $12^3 \cdot 24$ lattice

$a \approx 0.15\text{fm}$, 30 configurations

Machine: HITAC S810/20 $\rightarrow$ 630 Mflops

$\Rightarrow$ only meson masses, conclusion:
time extent of $T = 24$ too small to extract baryon ground state

1988 (plenary talk by Iwasaki at Lattice symposium at FermiLab)

quenched approximation, $16^3 \cdot 48$ lattice

$a \approx 0.11\text{fm}$, 15 configurations

particle	lattice	experiment
Kaon	470(45)	494
Nucleon	866(108)	938
Ω	1697(89)	1672

The story goes on ...

1992 (Talk Yoshie at Lattice '92 in Amsterdam):

quenched approximation, $24^3 \cdot 54$ lattice

two lattice spacings: $a \approx 0.11\text{fm}$, $a \approx 0.10\text{fm}$, $O(200)$ configurations

Machine: QCDPAX 14 Gflops

$\Rightarrow$ worries about excited state effects

$\Rightarrow$ worries about finite size effects

1995 (paper by QCDPAX collaboration)

		stat.	sys.(fit-range)		sys.(fit-func.)		
$\beta = 6.00$	$m_N = 1.076$	± 0.060	$+0.047$	-0.020	$+0.0$	-0.017	GeV
$\beta = 6.00$	$m_\Delta = 1.407$	± 0.086	$+0.096$	-0.026	$+0.038$	-0.015	GeV

"Even when the systematic errors are included, the baryon masses at $\beta = 6.0$ do not agree with experiment. Our data are consistent with the GF11[1] data at finite lattice spacing, within statistical errors. In order to take the continuum limit of our results, we need data for a wider range of β with statistical and systematic errors much reduced."

[1] GF11 has been a 5.6Gflops machine developed by IBM research.

where the quenched story ends

2003 (Paper by CP-PACS collaboration):

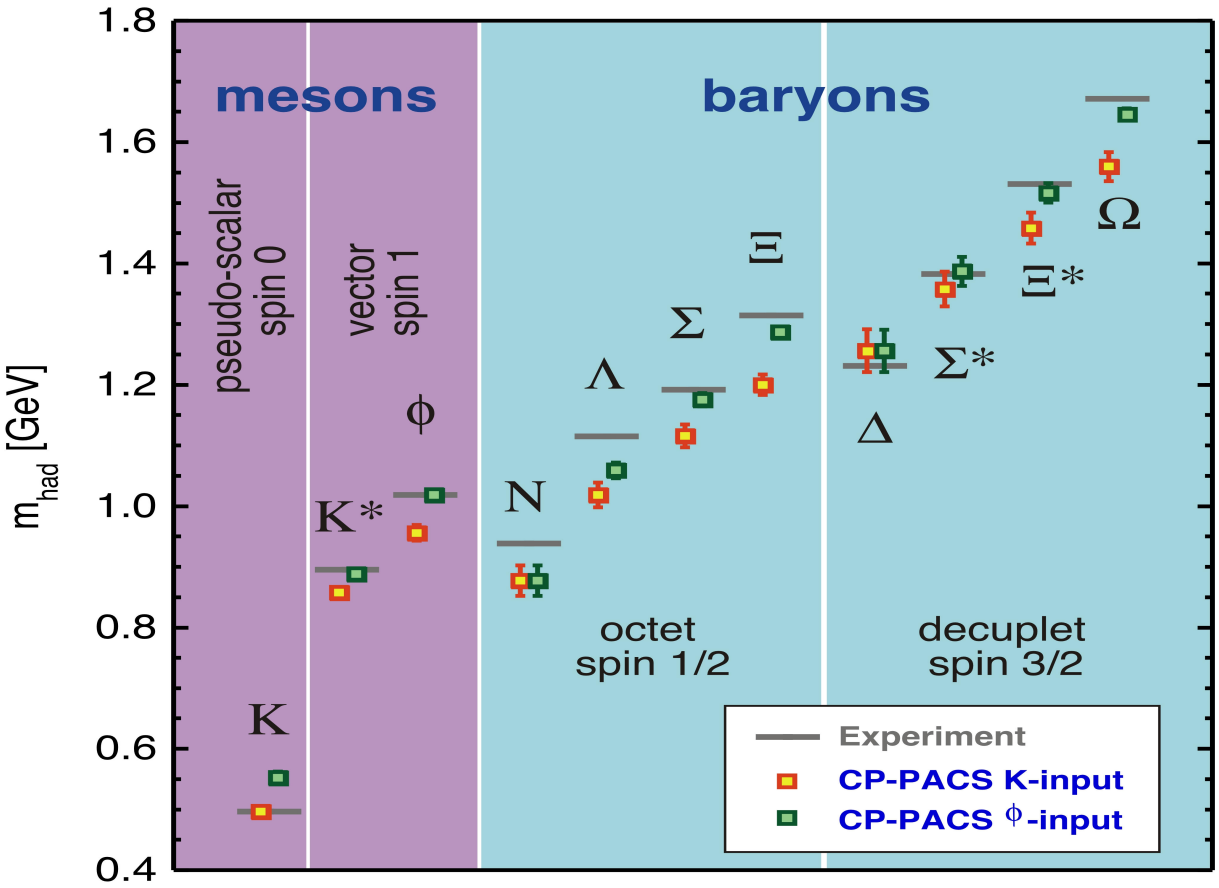
quenched approximation from $32^3 \cdot 56$ to $64^3 \cdot 112$ lattice

two lattice spacings: $a \approx 0.05\text{fm}$ $-$ $a \approx 0.10\text{fm}$, $O(150)$ – $O(800)$configurations

Machine: CP-PACS, massively parallel, 2048 processing nodes,
completed september 1996

$\rightarrow$ reached 614Gflops

- control of systematic errors
  - finite size effects
  - lattice spacing
  - chiral extrapolation
  - excited states



quenched

quenched

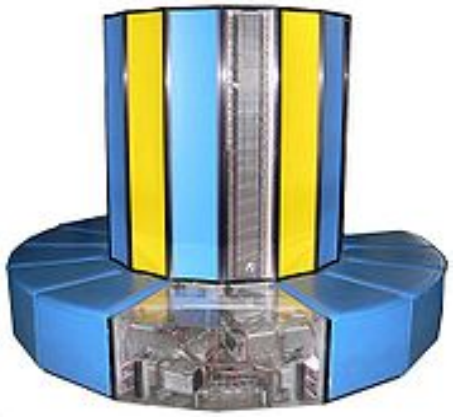
CP-PACS collaboration

Solution of QCD?

→ a number of systematic errors

start of dynamical (mass-degenerate up and down) quark simulations

1998 (Paper by UKQCD collaboration):



lattices: from $8^3 \cdot 24$ to $16^3 \cdot 24$

$a \approx 0.10\text{fm}$, $m_\pi/m_\rho > 0.7$

Machine: CRAY T3E $\approx$ 1Tflop

1999 (Paper by SESAM collaboration):

lattice: $16^3 \cdot 32$ lattice

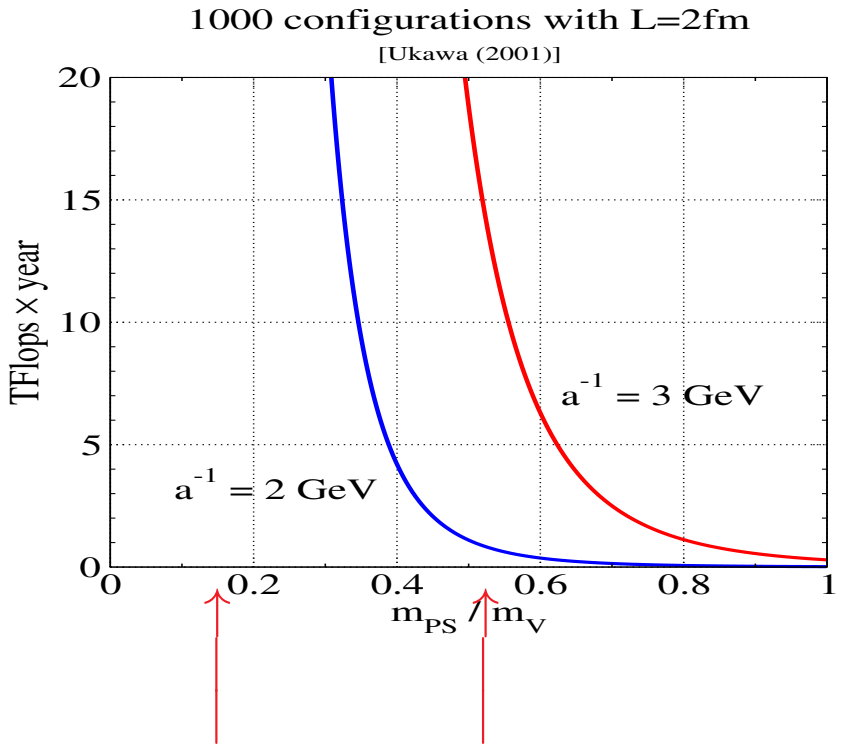
$a \approx 0.10\text{fm}$, $m_\pi/m_\rho > 0.7$

Machine: APE100 $\approx$ 100Gflop

- period of algorithm development
  - improved higher order integrators
  - multiboson algorithm
  - PHMC algorithm

Costs of dynamical fermions simulations, the "Berlin Wall"

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

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

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

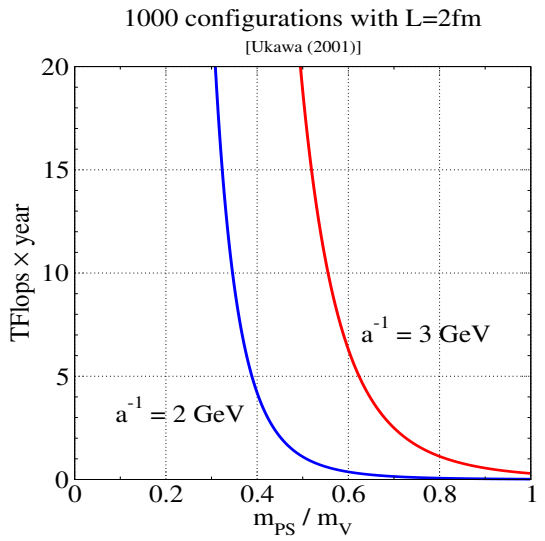
"both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place."
(Wilson, 1989)

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

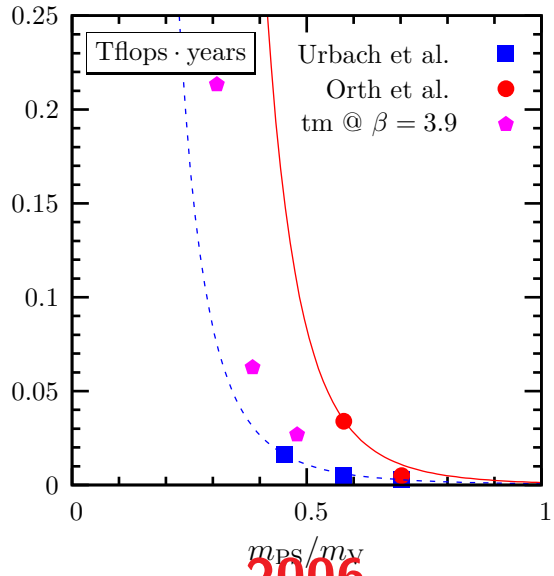
A generic improvement for Wilson type fermions

New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

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



2001



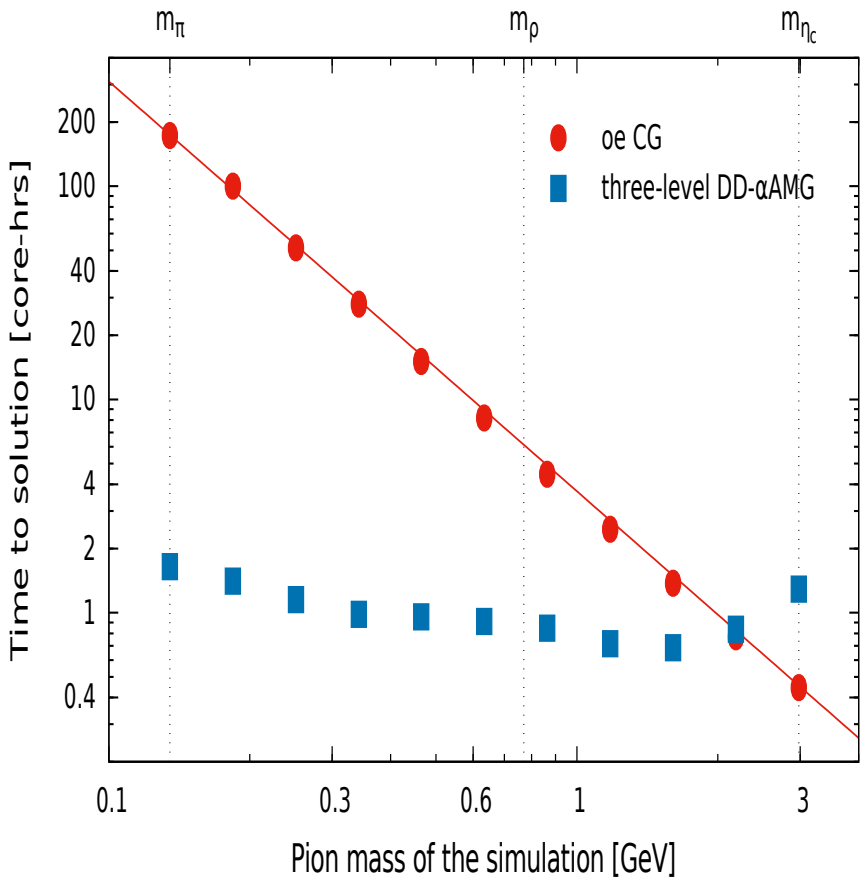
2006

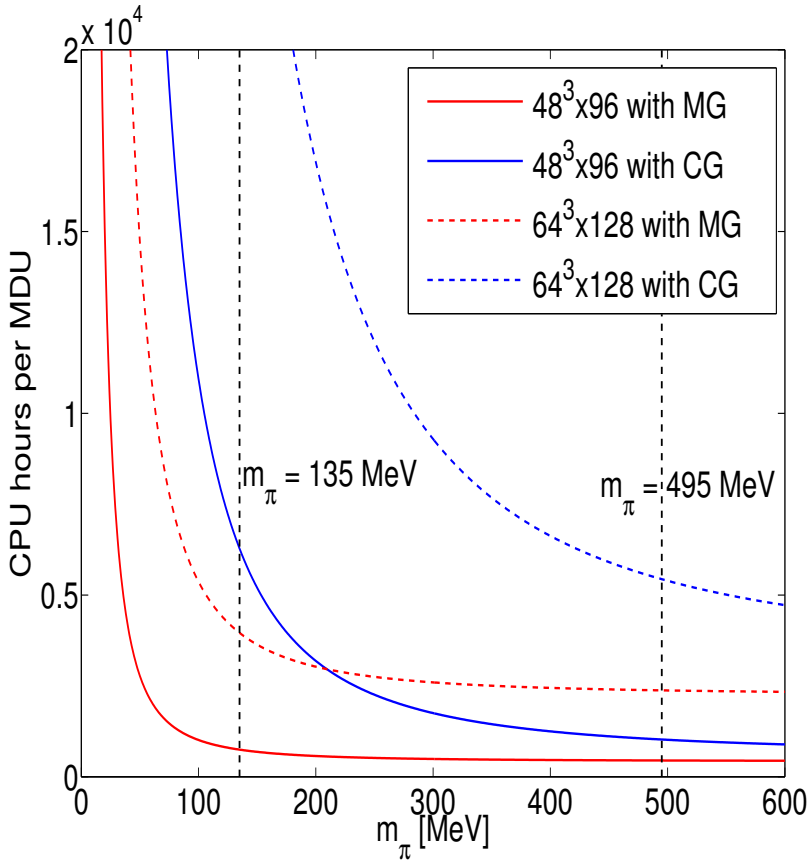
- comparable to staggered
- reach small pseudo scalar masses ≈ 300MeV

Situation today

(J. Finkenrath)

- the advance with multigrid solvers





Supercomputer

ca. 1700, Leibniz Rechenmaschine

Denn es ist eines ausgezeichneten Mannes nicht würdig, wertvolle Stunden wie ein Sklave im Keller der einfachen Rechnungen zu verbringen. Diese Aufgaben könnten ohne Besorgnis abgegeben werden, wenn wir Maschinen hätten.

Because it is unworthy for an excellent man to spent valuable hours as a slave in the cellar of simple calculations. These tasks can be given away without any worry, if we would have machines.

Supercomputer Infrastructures

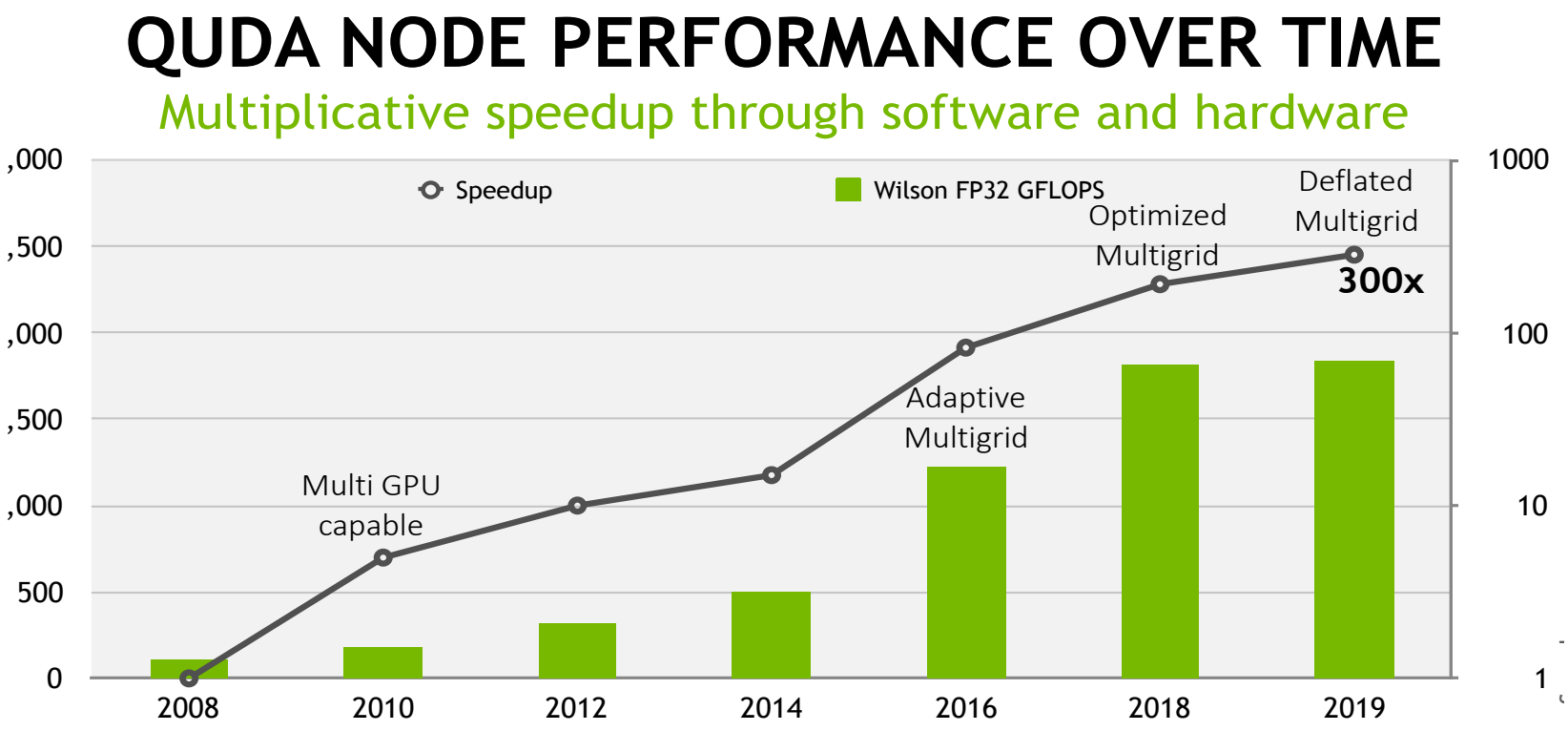
- Summit (IBM, NVIDIA),
  Oak Ridge National Laboratory, USA
  2,397,824 cores, 200 Petaflops

- Sunway TaihuLight,
  National Supercomputing Center in Wuxi, China
  10,649,600 cores, 125 Petaflops

- Piz Daint (CRAY, NVIDIA),
  Swiss National Supercomputing Centre (CSCS),
  Switzerland
  387,872 cores, 27 Petaflops

Computer and algorithm development over the years

taken from K. Clarke's plenary at lattice 2019

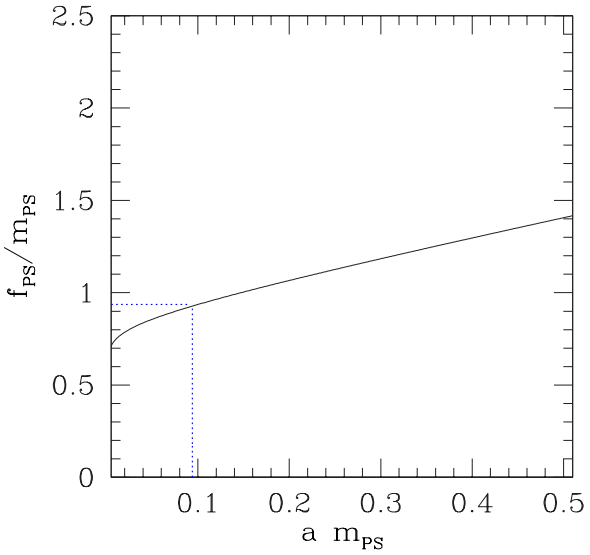


edup determined by measured time to solution for solving the Wilson operator against a random source on a V=24^{3}64 lattice, .5, M_π= 416 MeV. One node is defined to be 3 GPUs

Setting the scale

$$m_{\rm PS}^{\rm latt} = a m_{\rm PS}^{\rm phys} \ , \quad f_{\rm PS}^{\rm latt} = a f_{\rm PS}^{\rm phys}$$

$$\frac{f_{\rm PS}^{\rm phys}}{m_{\rm PS}^{\rm phys}} = \frac{f_{\rm PS}^{\rm latt}}{m_{\rm PS}^{\rm latt}} + {\rm O}(a^2)$$



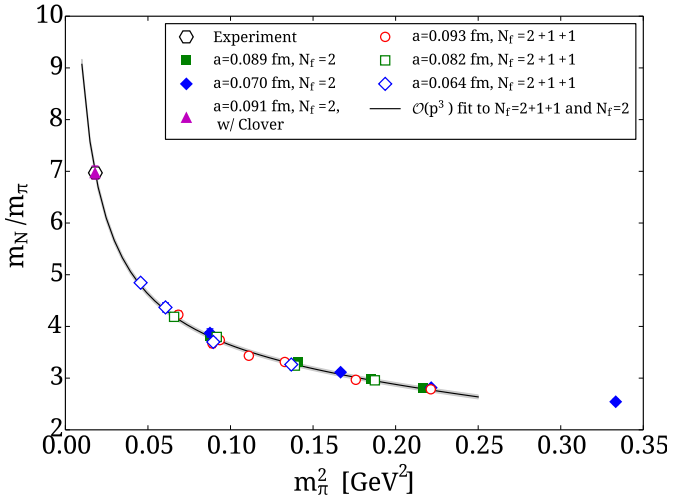
→ setting $\frac{f_{\rm PS}^{\rm latt}}{m_{\rm PS}^{\rm latt}} = 130.7/139.6$

→ obtain $m_{\rm PS}^{\rm latt} = a 139.6$[Mev]

→ value for lattice spacing a

Setting the scale from the nucleon mass

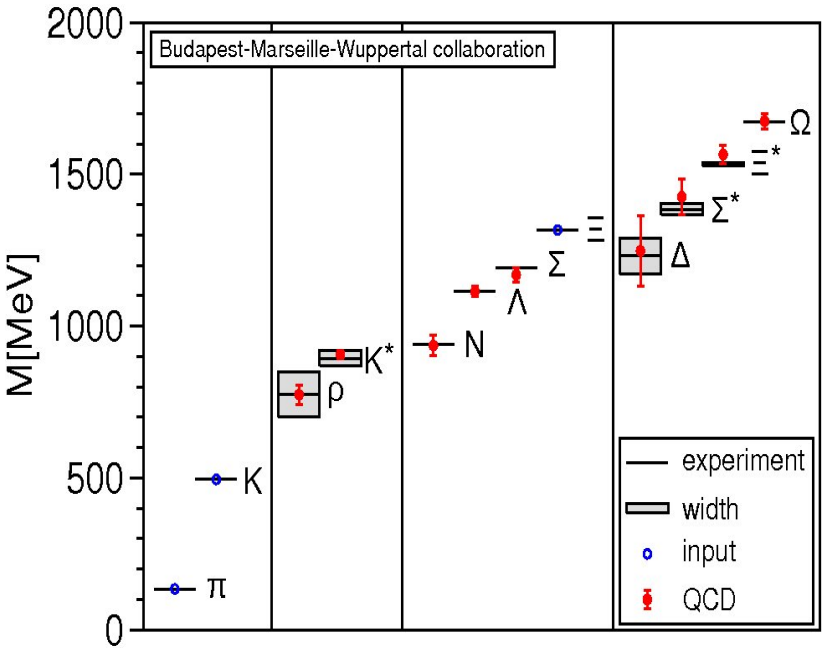
- including the nucleon mass at physical quark mass
- combining with baryon chiral perturbation theory
  → see lecture by A. Walker Loud

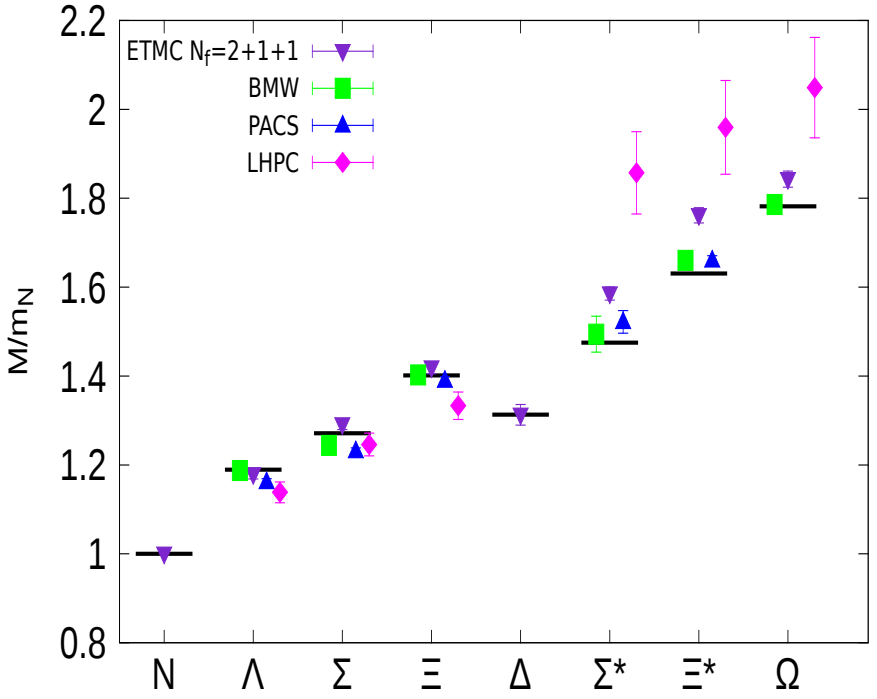


- other possibilities
  - use Ω mass
  - gradient flow observables
    → see lecture by H. Suzuki

The lattice QCD benchmark calculation: the spectrum

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





first spectrum calculation BMW

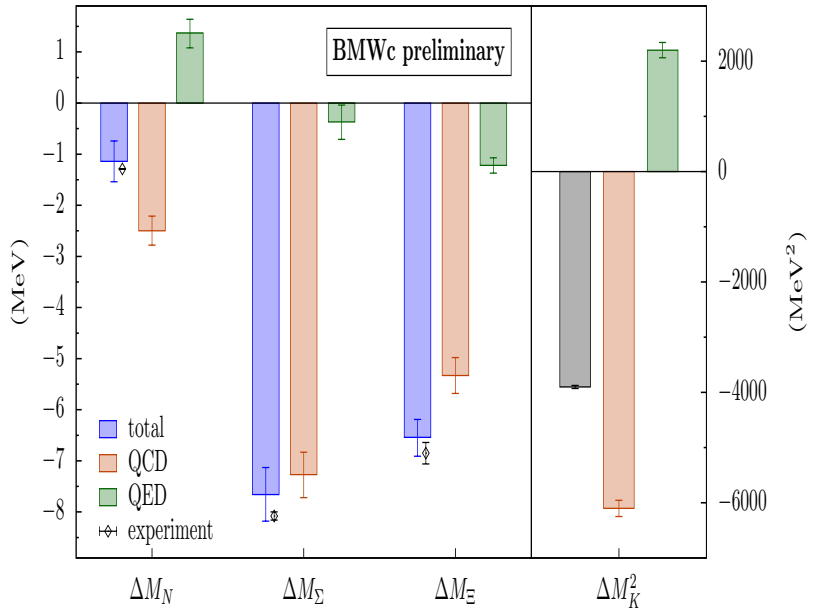
repeated by other collaborations

(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

→ see lecture by G. Martinelli

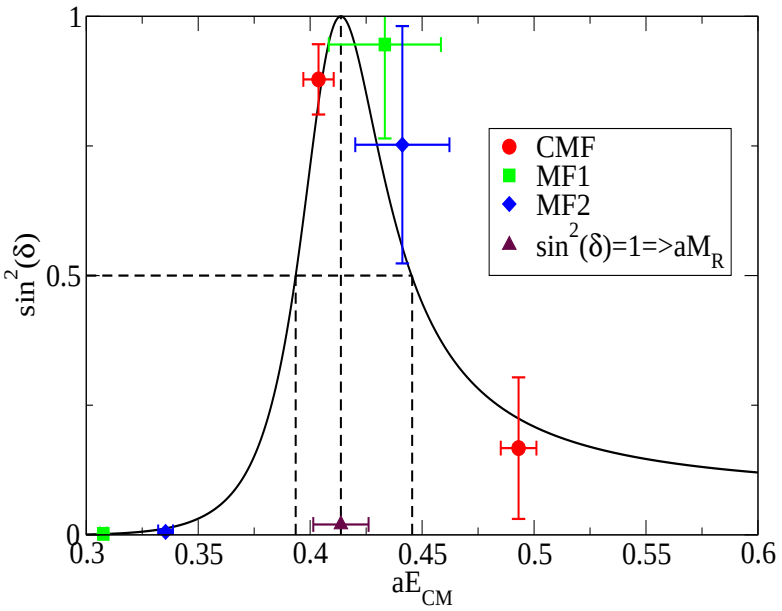


baryon spectrum with mass splitting (BMW collaboration)

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

The ρ-meson resonance: dynamical quarks at work

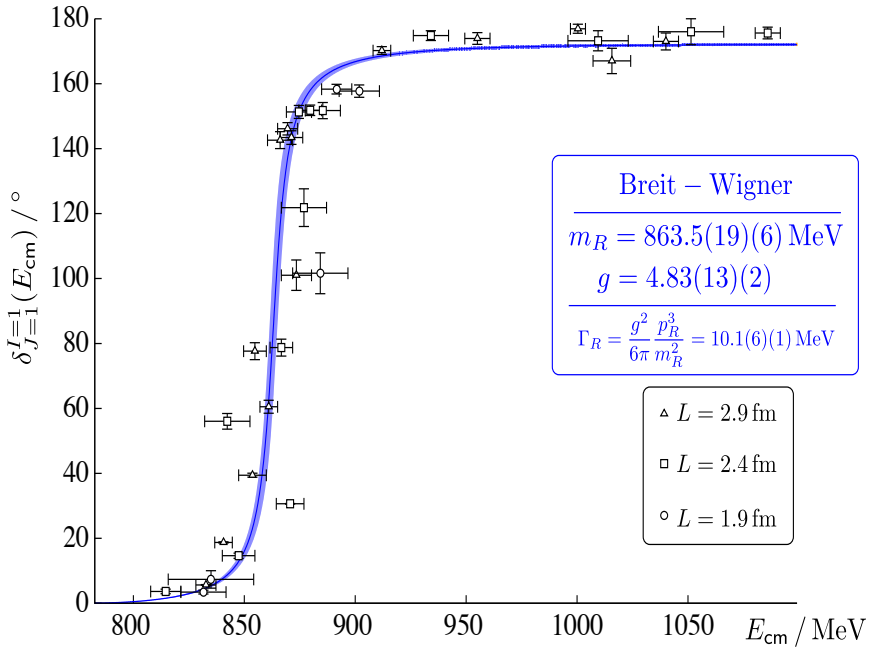
$\rightarrow$ see lecture by C. Urbach



(2010: X. Feng, D. Renner, K.J.)

$m_\rho = 1033(31)$ MeV,

$\Gamma_\rho = 123(43)$ MeV

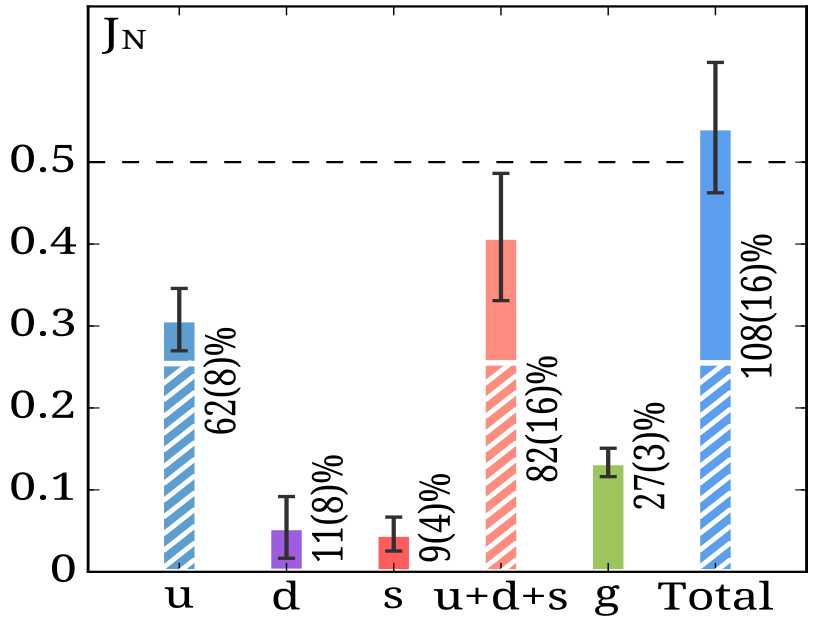


(J. Dudek, R. Edwards, C. Thomas, 2013)

Spin content of the nucleon

(C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. J.,
C. Kallidonis, G. Koutsou, A. Vaquero Aviles-Casco, C. Wiese)

- long standing puzzle: **EMC** experiment
  $\rightarrow$ surprisingly small quark contribution to proton spin of $s = \frac{1}{2}$
- dedicated effort to disentangle the different contributions of the proton spin



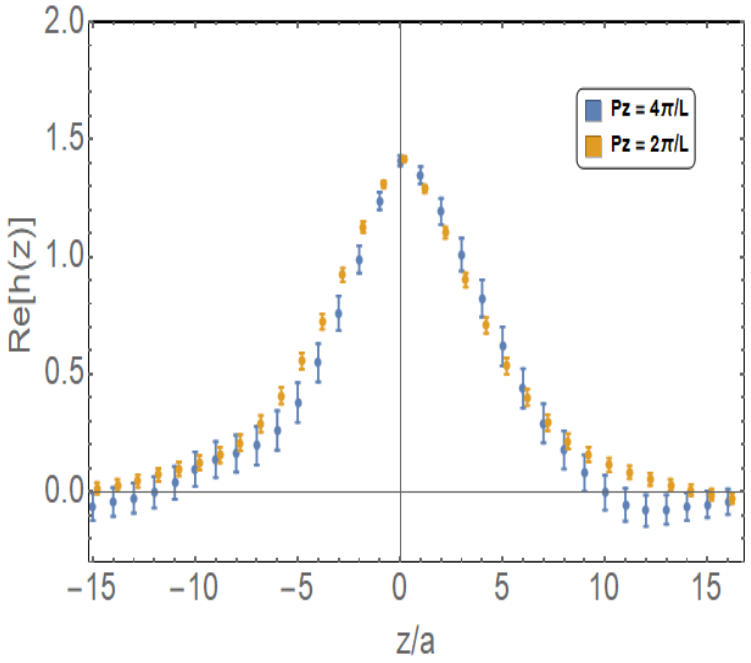
- first complete spin decomposition of proton spin
- reveal large gluon contribution

Parton distribution functions from lattice simulations

→ see lecture by X. Ji

for nucleon matrix elements: see lecture by R. Gupta

- parton distribution function:
  → determines the complete momentum distribution of quarks in the proton
- recent theoretical breakthrough:
  can be determined from simulations



(Shicheng Xia, Yahui Chai, Yuan Li et. al.)

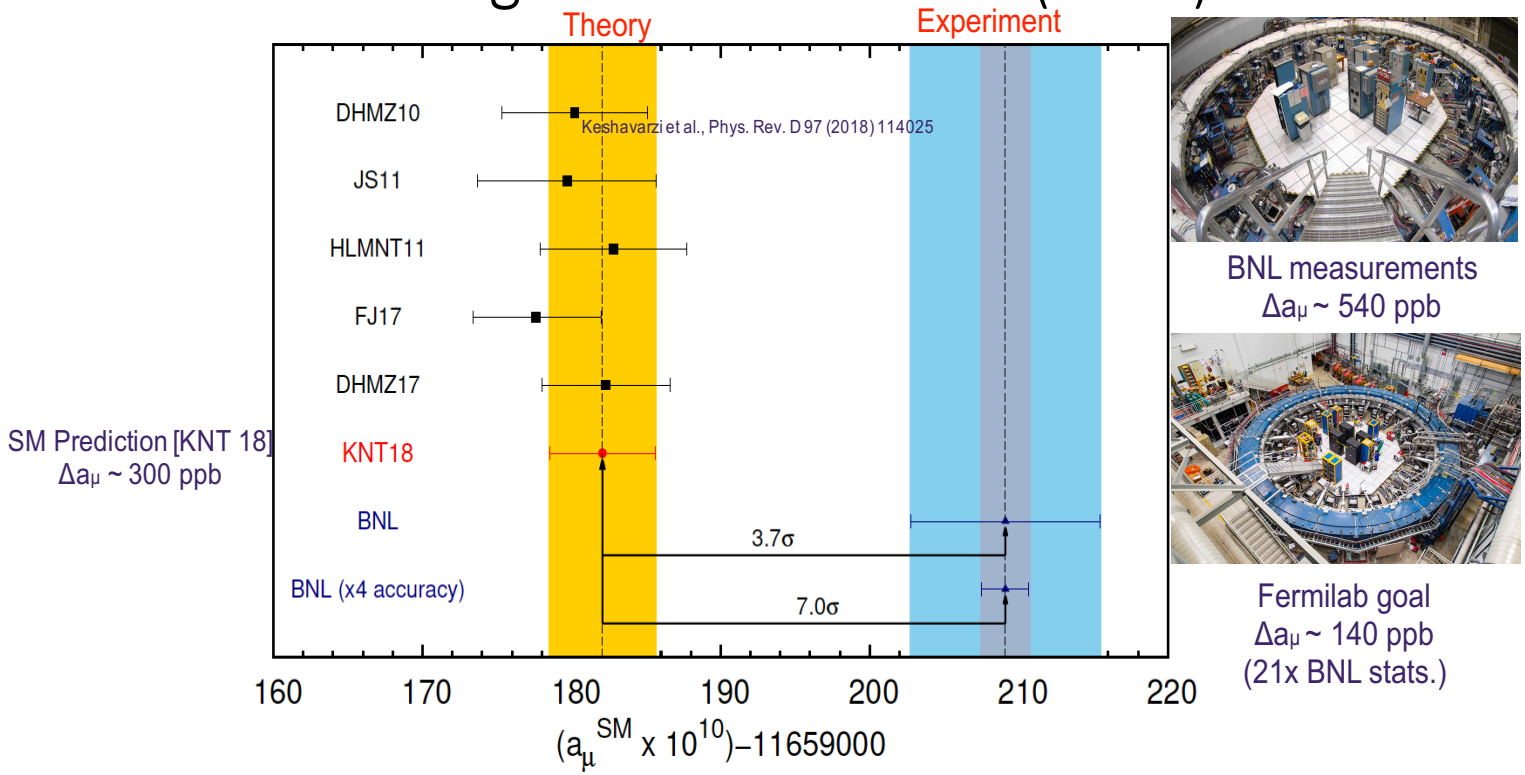
- x = quark momentum in proton
- simulation provides ab-inito information on most inner proton structure
- not accessible otherwise

The anomalous magnetic moment of the muon

(taken from Dikai Li's plenary talk at lattice 2019)

→ see lecture by L. Jin

Muon g-2: Current Status (2019)



SM Prediction [KNT 18]
$\Delta a_\mu \sim 300$ ppb

BNL measurements
$\Delta a_\mu \sim 540$ ppb

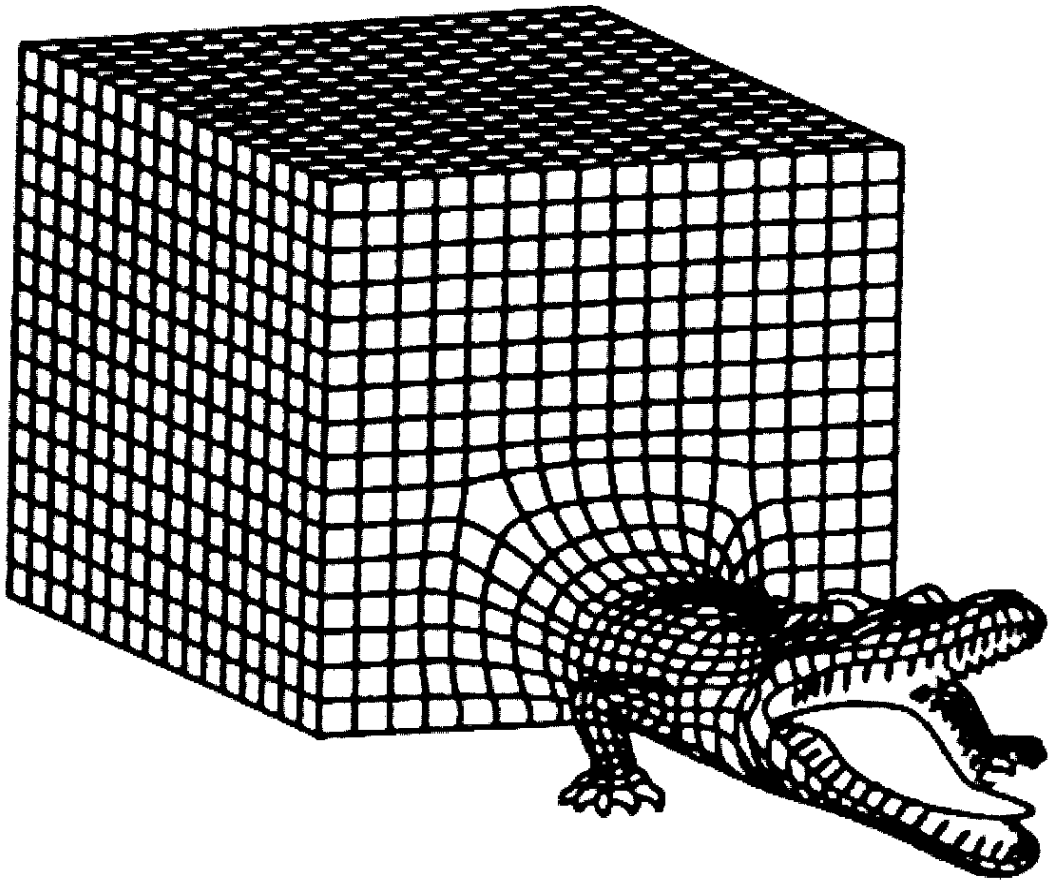
Fermilab goal
$\Delta a_\mu \sim 140$ ppb
(21x BNL stats.)

Fermilab aims at 4xBNL precision improvement, will give 7.0σ discrepancy from SM prediction (if center value stays)

Challenges

- reached high precision: need to include QED and isospin breaking effects
  → see lecture by G. Martinelli
- understand ϵ'/ϵ
  → see lecture by W. Lee
- solving the B-physics discrepancy
  → see lecture by S. Meinel
- multi-particle and multi-channel scattering
  → see lecture by S. Sharpe
- beyond standard mdoel physics
  → see lecture by D. Lin
- quantum computing
  → see lecture by D. Kaplan
- ...
  → see lecture by N.N.

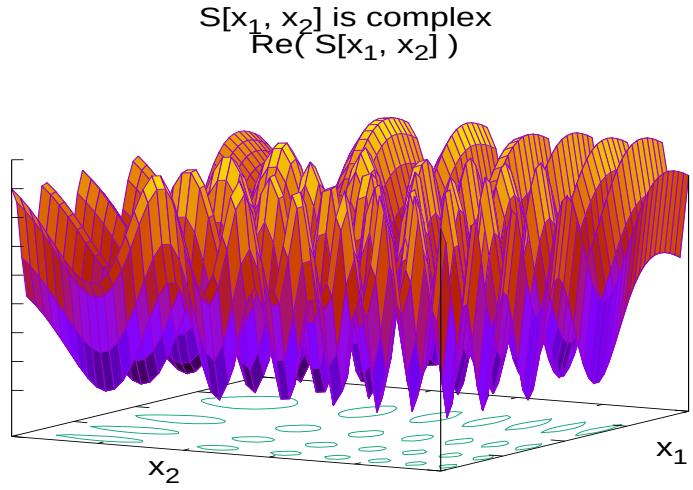
There are dangerous lattice animals

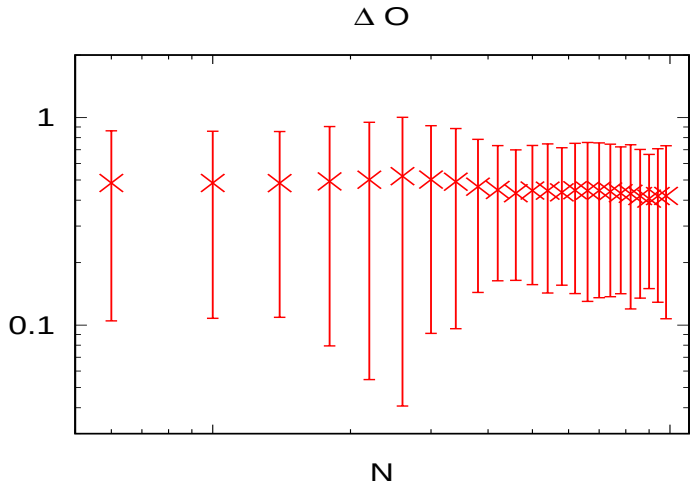


Markov Chain Monte Carlo (MCMC) Method

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

- needs real and positive probability density measure $\mathcal{D}_{\text{Fields}} e^{-S}$
- complex action not accessible to standard MCMC
  - no notion of probability distribution
  - importance sampling not possible
- constant error $O(1)$ as function of sample size N



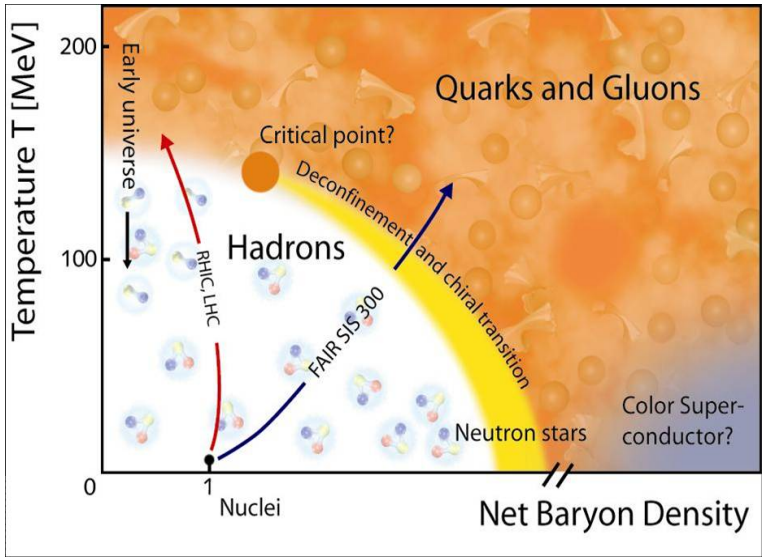


Understanding QCD phase diagram

- 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

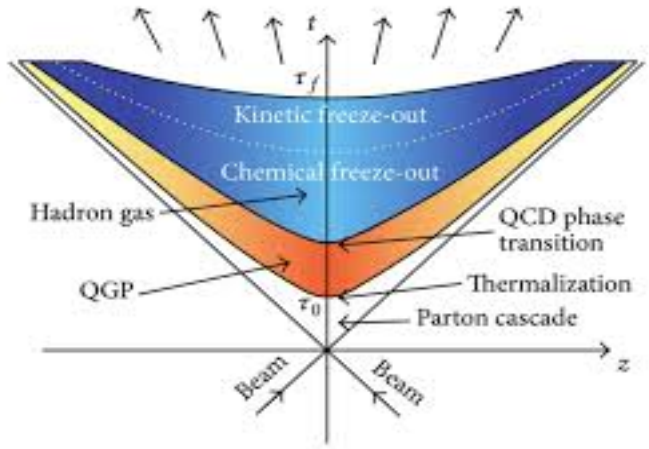
- only thermal equilibrium accessible

$\rightarrow$ no real time simulation

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

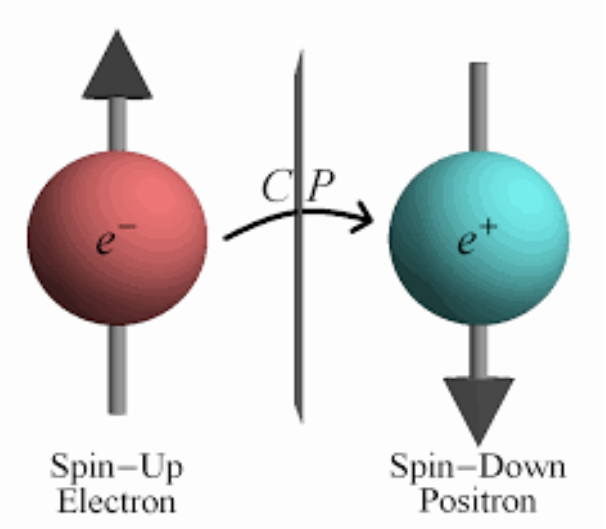
- standard way: linearize equations
  plus small fluctuations

- 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

Matrix representation of the tensor

- the original tensor

$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_N=1}^{d} C_{s_1,s_2,\ldots,s_N} |s_1\rangle \otimes |s_2\rangle \otimes \ldots \otimes |s_N\rangle$$

- rewrite as matrix product (e.g. by reshaping)

$$|\psi\rangle = \sum_{\alpha=1}^{D_\alpha} \sum_{\beta=1}^{D_\beta} C_{\alpha,\beta} |\alpha\rangle \otimes |\beta\rangle$$

$$C_{(s_1,s_2,\ldots,s_k),\left(s_{k+1},s_{k+2},\ldots,s_N\right)} = C_{\alpha,\beta}$$

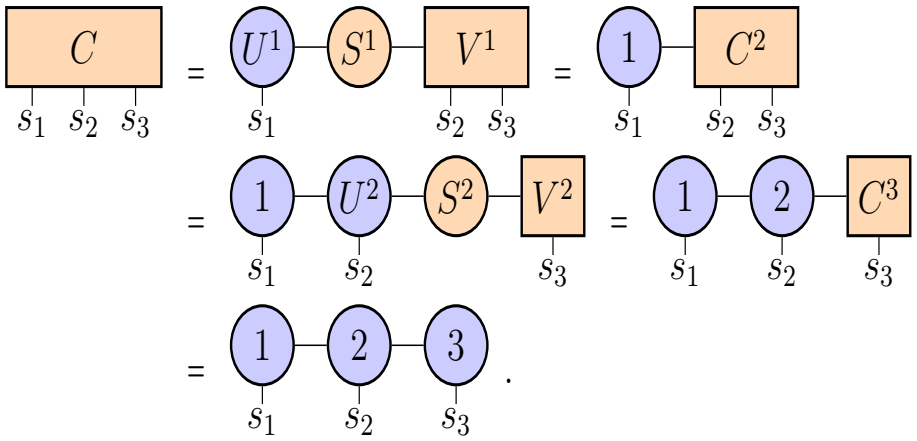
Towards a Matrix Product State (MPS): singular value decomposition

- singular value decomposition

$$C_{\alpha,\beta} = \sum_{\alpha'=1}^{D_\alpha} \sum_{\beta'=1}^{D_\beta} U_{\alpha,\alpha'} S_{\alpha',\beta'} V_{\beta',\beta} \ , \ VV^\dagger = UU^\dagger \mathbb{1}$$

- iterating the procedure

$$A^{j,s_j}_{\alpha_j,\alpha'_j} := \sum_{\beta=1}^{D_j} \sum_{\gamma=1}^{D_j} U_{\alpha_j,\beta} S_{\beta,\gamma} V^\dagger_{\gamma,\alpha'_j}$$



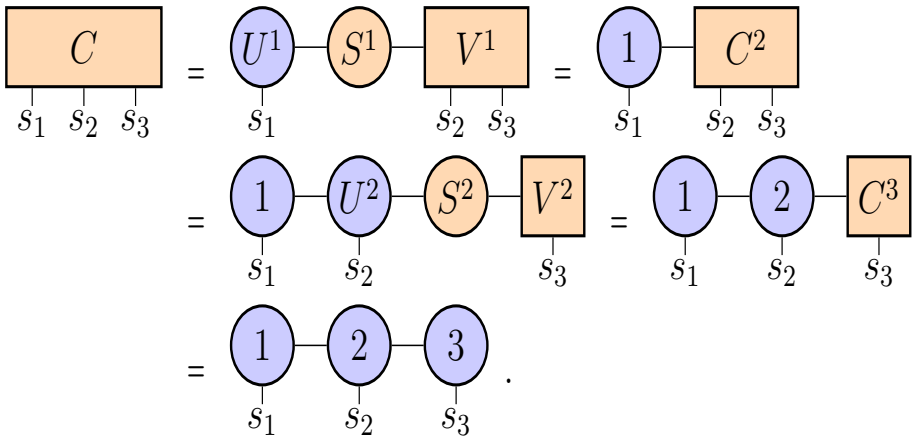
$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_N=1}^{d} A^{1,s_1} A^{2,s_2} \ldots A^{N,s_N} |s_1, s_2, \ldots, s_N\rangle$$

- tensor $\rightarrow$ matrix products always possible
- is it useful?

A Matrix Product State (MPS)

- iterating the procedure

$$A^{j,s_j}_{\alpha_j,\alpha'_j} := \sum_{\beta=1}^{D_j} \sum_{\gamma=1}^{D_j} U_{\alpha_j,\beta} S_{\beta,\gamma} V^{\dagger}_{\gamma,\alpha'_j}$$



$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_N=1}^{d} A^{1,s_1} A^{2,s_2} \ldots A^{N,s_N} |s_1, s_2, \ldots, s_N\rangle$$

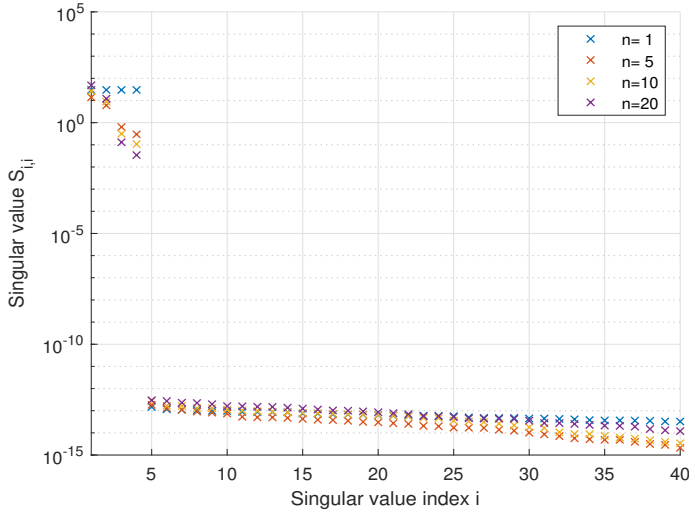
- tensor $\rightarrow$ MPS always possible

- is it useful?

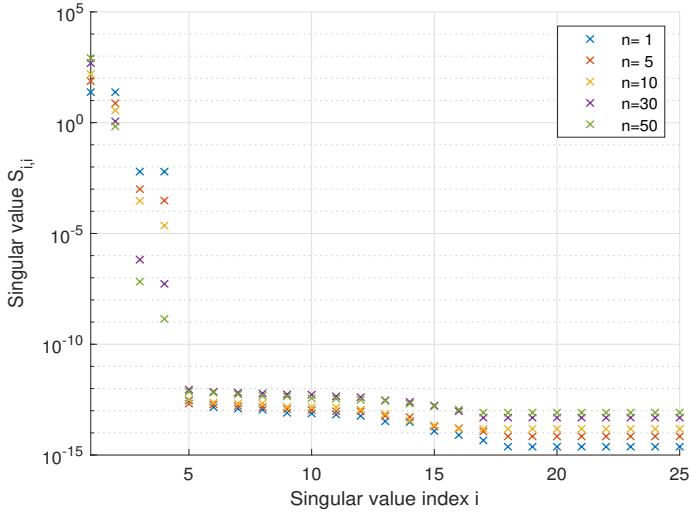
The rank of the matrices

- rank r of matrix: eigenvalue below some threshold ϵ

$$C_{\alpha,\beta} = \sum_{\alpha'=1}^{r} \sum_{\beta'=1}^{r} U_{\alpha,\alpha'} S_{\alpha',\beta'} V_{\beta',\beta}$$



Ising model



critical Heisenberg model

- many very small eigenvalues $\rightarrow$ neglect them

Summary matrix product states

A particular ansatz: matrix product state

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

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

- replace complicated tensor by matrix products
- A_i is $D \otimes D$ matrix $\rightarrow$ D *bond dimension*
- i_i physical index (e.g. spin $\pm 1/2$ for $d = 2$)
- rank of matrix A_i very small $\rightarrow$ enormously reduced cost

Some explanantion: 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 $\|\rho_{\rm exact} - \rho_{\rm approx}\| \leq \delta$

then the wavefunction

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

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

- δ scales polynomially

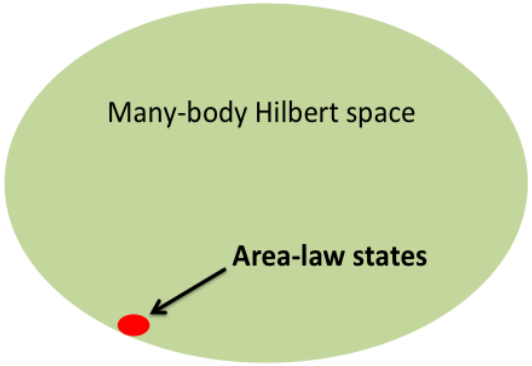
Relevant part of Hilbert space is very small

- (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?

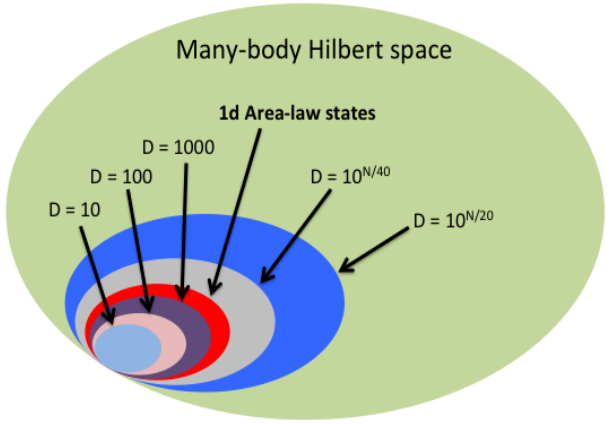


Bond dimension for ground state

- 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 to the ground state
- **controlled** and **fast** convergence to solution



The Schwinger model

- Quantum electrodynamics in 1+1 dimensions
- U(1) gauge fields coupled to fermionic matter
- confinement of charges
- bound states
- chiral symmetry breaking
- super-renormalizable
- exactly solvable in massless case

$\Rightarrow$ testbench for new methods and algorithms

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

$$D_\mu \Psi(x) \equiv (\partial_\mu - i g_0 A_\mu(x)) \Psi(x)$$

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 Hamiltonian

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

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

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

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

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

ϕ_n single component fermion field

$\theta_n = iaA_1(n)$ gauge variables

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

Gauss law and Jordan Wigner transformation

- Gauss law: $L_n - L_{n-1} = \phi_n^\dagger \phi_n - \frac{1}{2}\left[1 - (-1)^n\right]$
- Jordan-Wigner transformation

  $\phi_n = \prod_{k<n}(i\sigma_k^z)\sigma_n^-,\ \sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$
- allows formulation in spin language
- general fermion description possible

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

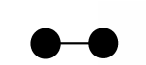
$\Rightarrow$ eliminate gauge degrees of freedom $\rightarrow$ pure spin formulation

- perfect formulation for matrix product states

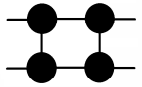
The (Feynman) Diagrams of tensor networks

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

Some contractions:

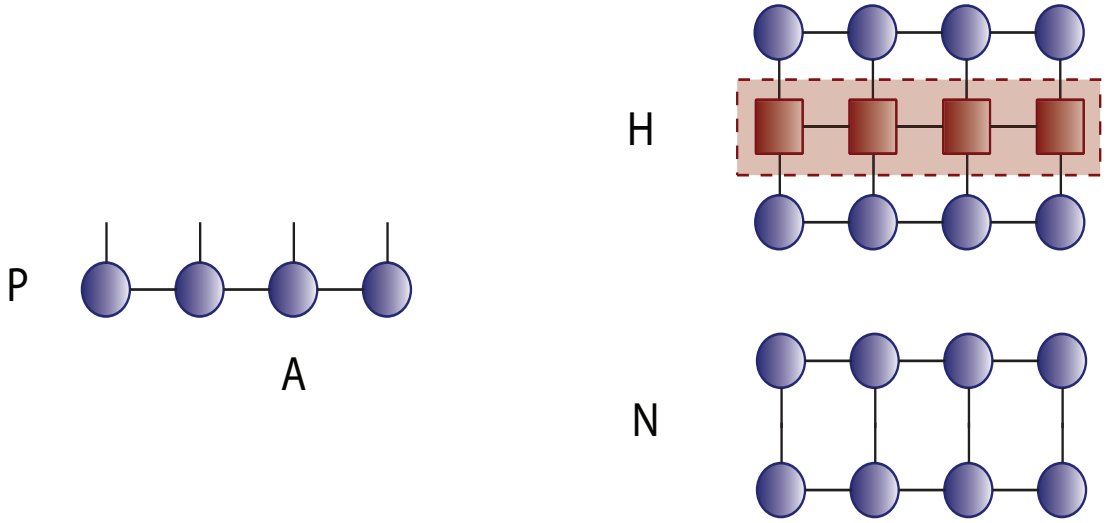

scalar $A_\alpha B_\alpha$


tensor of rank-2 $A_{\alpha\beta}B_{\beta\gamma}$


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

Finding the ground state energy

- minimize the functional $\frac{<\Psi|H|\Psi>}{<\Psi|\Psi>}$
  - graphical representation



P: $|\Psi\rangle$ **H:** $\langle\Psi|H|\Psi\rangle$ **N:** $\langle\Psi|\Psi\rangle$

- procedure for MPS solution $|\Psi>=\sum_{i_1,i_2,\cdots i_N=1}^{d} \mathrm{Tr} A_1^{i_1} A_2^{i_2} \cdots A_N^{i_N} |i_1 i_2 \cdots i_N>$
  - fix all matrices besides one $A_k^{i_j}$
  - minimize energy with respect to this matrix only
  - sweep through the whole lattice
  - repeat procedure until convergence

Algorithm

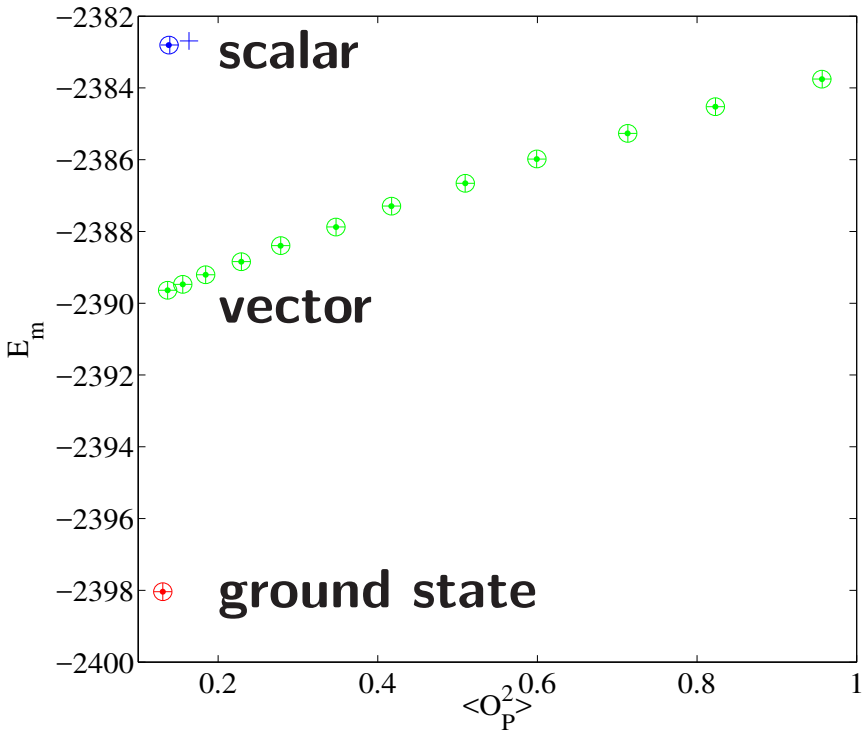
Require: Hamiltonian for an N-site chain, H; bond dimension, D; tolerance, ϵ
Ensure: MPS approximation to the ground state, $|\Psi\{A_k\}\rangle_D$, with energy E

$\{A_0, \ldots A_{N-1}\} \leftarrow$ initial guess
$E \leftarrow \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$
$\delta E \leftarrow 1$
$sweeping\_direction \leftarrow$ right
while $\delta E > \epsilon$ **do**
  $k \leftarrow$ first site for $sweeping\_direction$
  while $0 \leq k \leq N-1$ **do**
    compute contraction without tensor A_k
    solve eigenvalue problem $\mathcal{H}A_k = \lambda_{\min}A_k$
    $A_k \leftarrow A$, $E_k \leftarrow \lambda_{\min}$
    $k \leftarrow$ next site according to $sweeping\_direction$
  end while
  $\delta E \leftarrow \left|\frac{E-E_{\text{iter}}}{E}\right|$
  $E \leftarrow E_{\text{iter}}$
  flip $sweeping\_direction$ {left $\leftrightarrow$ right}
end while

Higher lying states

- project out the already found M eigenstates

$$H_{eff} = H - \sum_{k=1}^{M} E_k |\Psi_k >< \Psi_k|$$



- dispersion relation
- O_P discretized momentum operator
  $P = \int dx \Psi^\dagger(x) i\partial_x \Psi(x)$

Finding the ground state energy with MPS

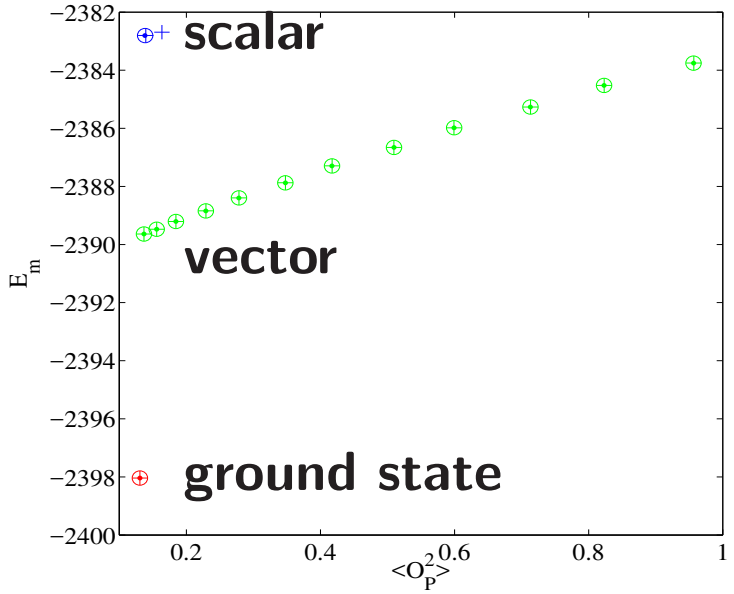
- minimize the functional $\frac{<\Psi|H|\Psi>}{<\Psi|\Psi>}$

- procedure for MPS solution $|\Psi>=\sum_{i_1,i_2,\cdots i_N=1}^{d} \mathrm{Tr} A_1^{i_1} A_2^{i_2} \cdots A_N^{i_N} |i_1 i_2 \cdots i_N>$
  - fix all matrices besides one $A_k^{i_j}$
  - minimize energy with respect to this matrix only
  - sweep through the whole lattice
  - repeat procedure until convergence

- Higher lying states: project out the already found M eigenstates

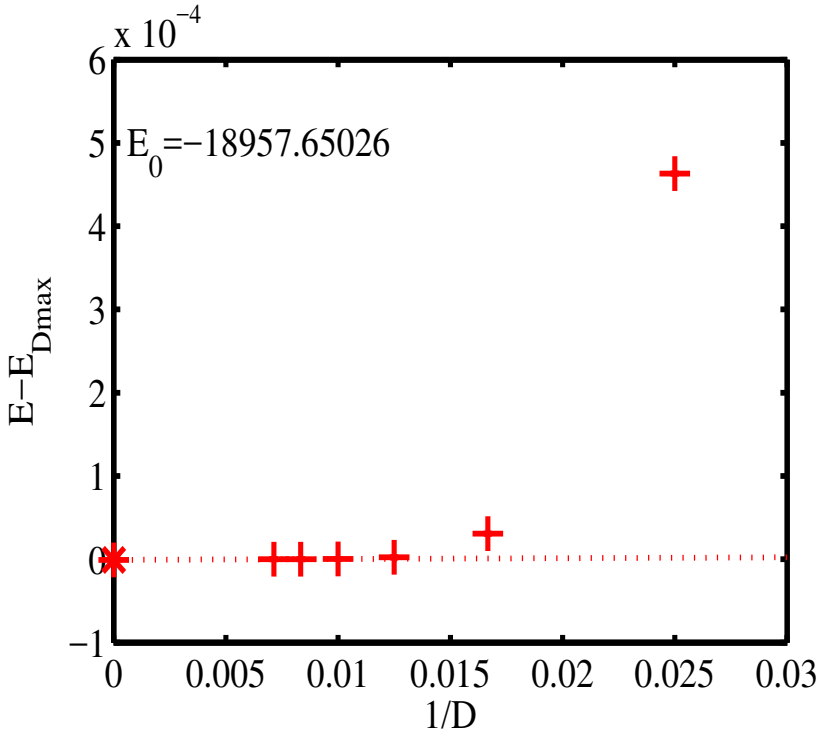
  $H_{eff} = H - \sum_{k=1}^{M} E_k |\Psi_k><\Psi_k|$

- obtain complete dispersion relation



Controlling systematic errors: bond dimension

- rapid convergence to infinite bond dimension



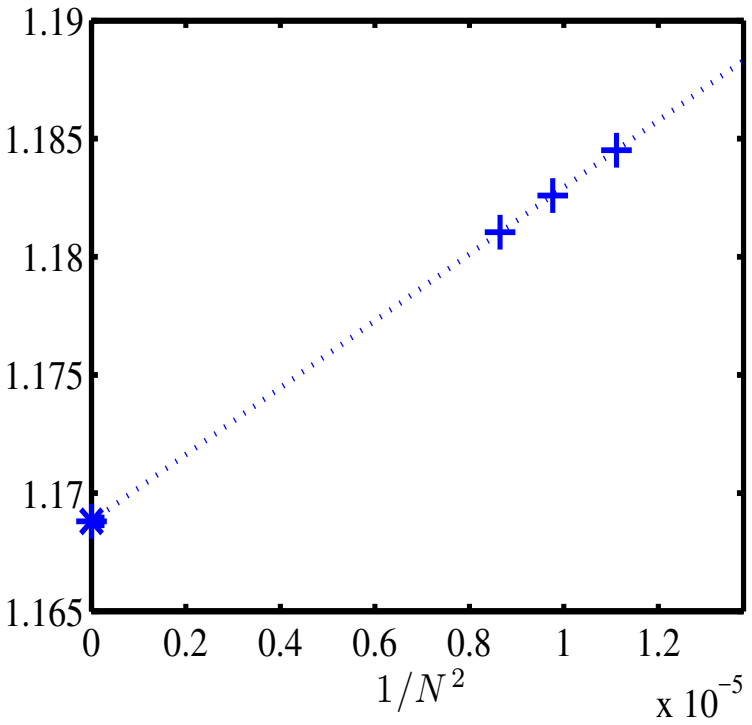
- linear extrapolation in $1/D$

- error: difference between extrapolated and largest bond dimension value

Controlling systematic errors: finite size effects

- mass gap (E_0 ground state energy)

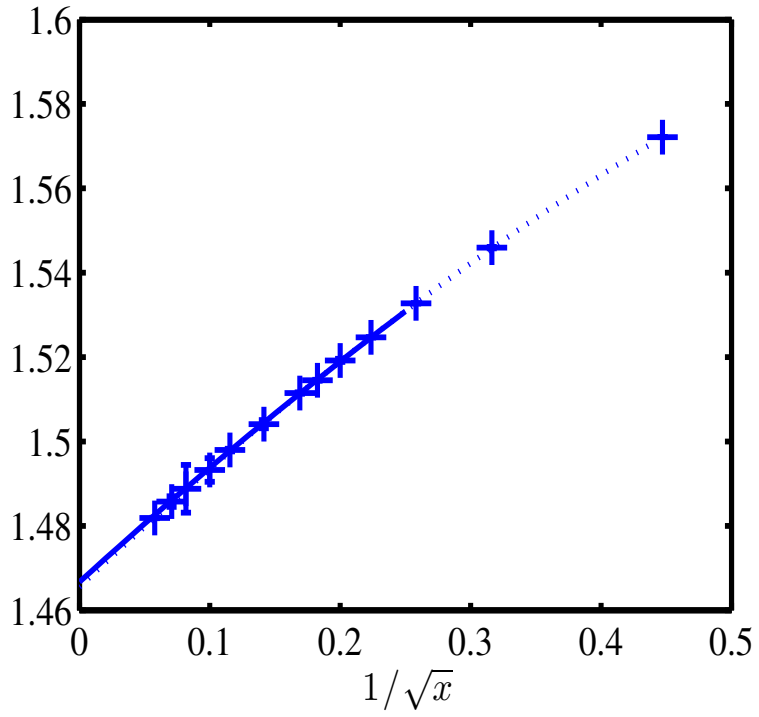
$$\frac{E_{\rm gap}-E_0}{2\sqrt{x}} = \omega_\infty + a_1/N^2 + a_2/N^3$$



Controlling systematic errors: continuum limit

- continuum extrapolation

$$E(1/\sqrt{x} = ag) = E_{\text{cont}} + a_1 \frac{1}{\sqrt{x}} + a_2 \frac{1}{(\sqrt{x})^2} + \cdots$$



- error: from distribution of many fit results

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

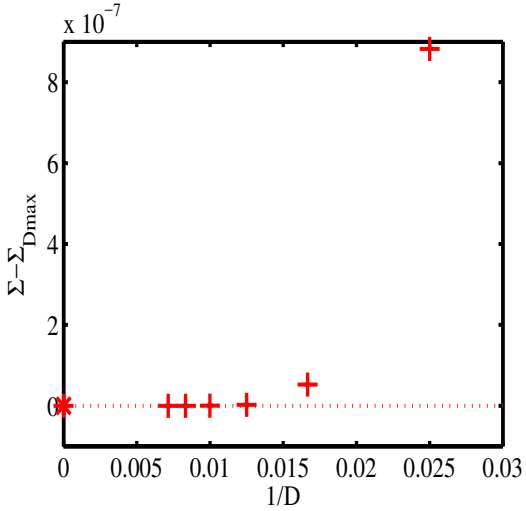
	Scalar binding energy		
m/g	MPS with OBC	SCE result	exact
0	1.1279(12)	1.11(3)	1.12838
0.125	1.2155(28)	1.22(2)	-
0.25	1.2239(22)	1.24(3)	-
0.5	1.1998(17)	1.20(3)	-

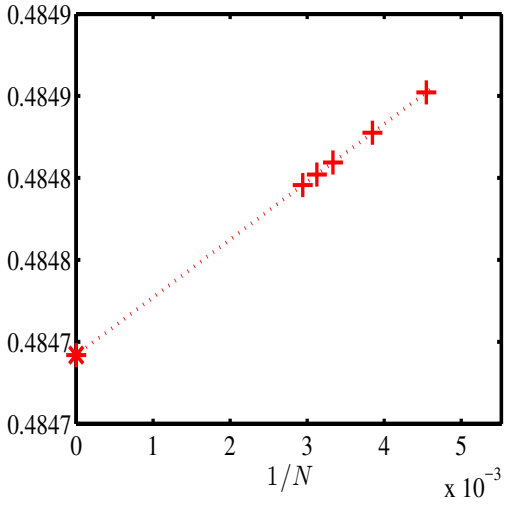
- scalar case: accurate determination of energy
- MPS approach works for gauge theories!

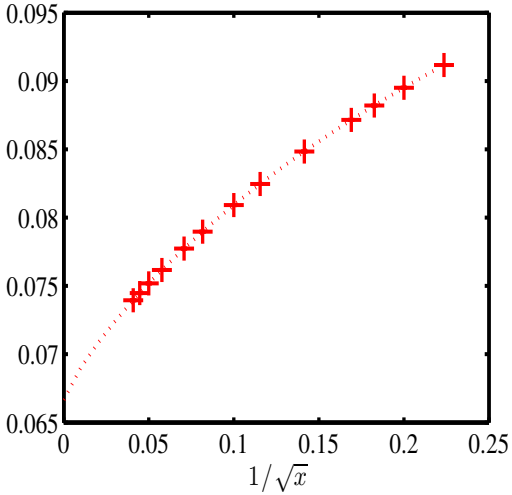
Zero tmperature chiral consensate $\leftarrow$ chiral anomaly

- spin representation of chiral condensate: $\Sigma = \frac{\sqrt{x}}{N} \sum_n (-1)^n \frac{1+\sigma_n^z}{2}$

- systematics







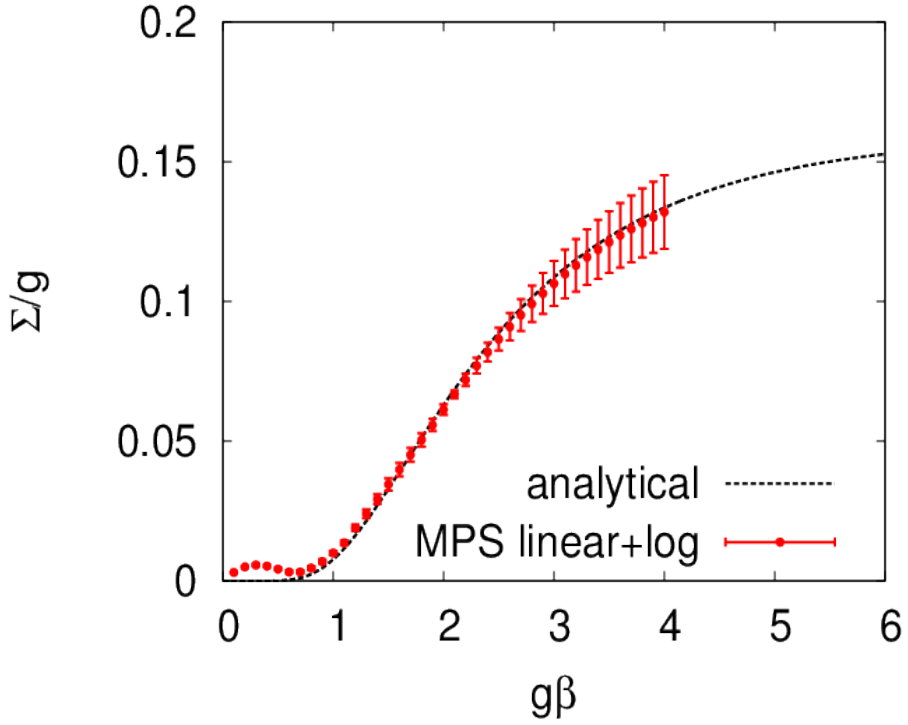
- results

	Substracted condensate		
m/g	**MPS with OBC**	exact	Hosotani
0	**0.159930(8)**	0.159929	-
0.125	**0.092023(4)**	-	0.0918
0.25	**0.066660(11)**	-	-
0.5	**0.042383(22)**	-	-

Temperature dependence of chiral condensate

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

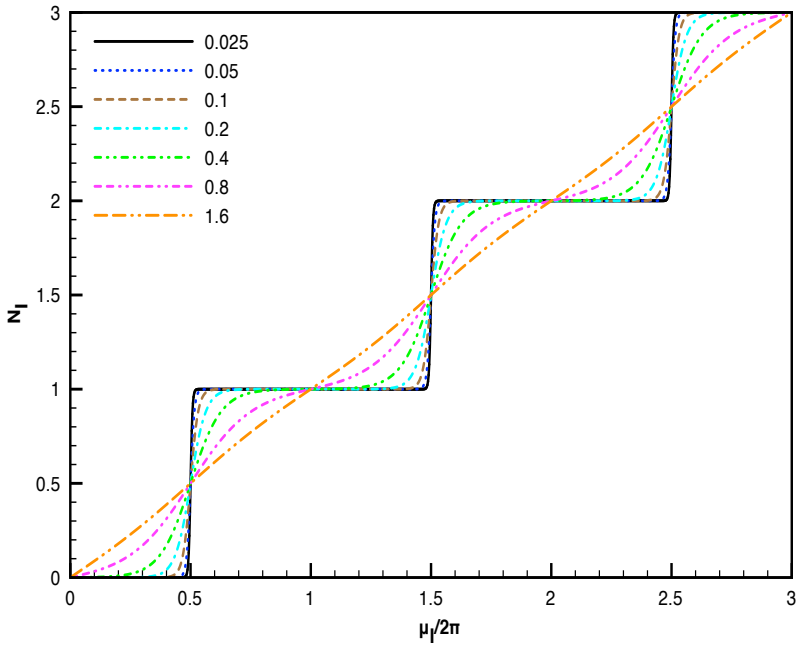
- imaginary time evolution with Matrix Product States (MPS)



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 $T > 0$

Hamiltonian lattice formulation

$$H = -ix \sum_{n=0}^{N-2} \sum_{f=0}^{F-1} \left(\phi^\dagger_{n,f} \phi_{n+1,f} - \text{h.c.} \right)$$

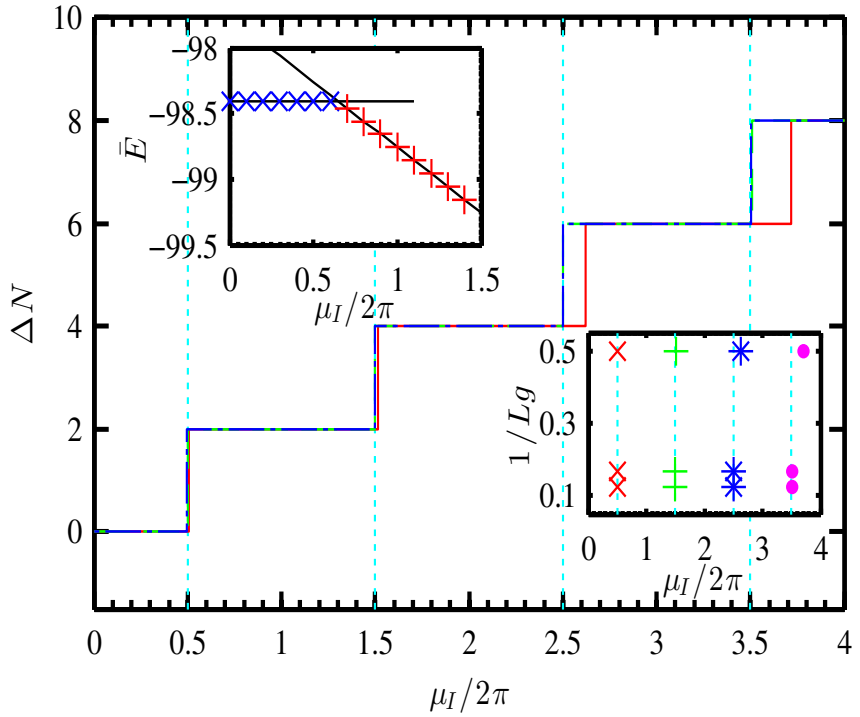
$$+ \sum_{n=0}^{N-1} \sum_{f=0}^{F-1} \left(\mu_f (-1)^n + \nu_f \right) \phi^\dagger_{n,f} \phi_{n,f}$$

$$+ \sum_{n=0}^{N-2} \left(\sum_{k=0}^{n} \left(\sum_{f=0}^{F-1} \phi^\dagger_{k,f} \phi_{k,f} - \frac{F}{2}(1 - (-1)^k) \right) \right)^2 ,$$

- $x = 1/(ag)^2$ parameter controlling continuum limit
- $\mu_f = 2\sqrt{x} m_f / g$ fermion mass
- ν_f chemical potential
- isospin chemical potential for $N_f = 2$: $\mu_I / 2\pi = N/4\pi x \cdot (\nu_1 - \nu_0)$
  $\leftarrow$ contact to Narayanan's work

Location of phase transitions in massless case

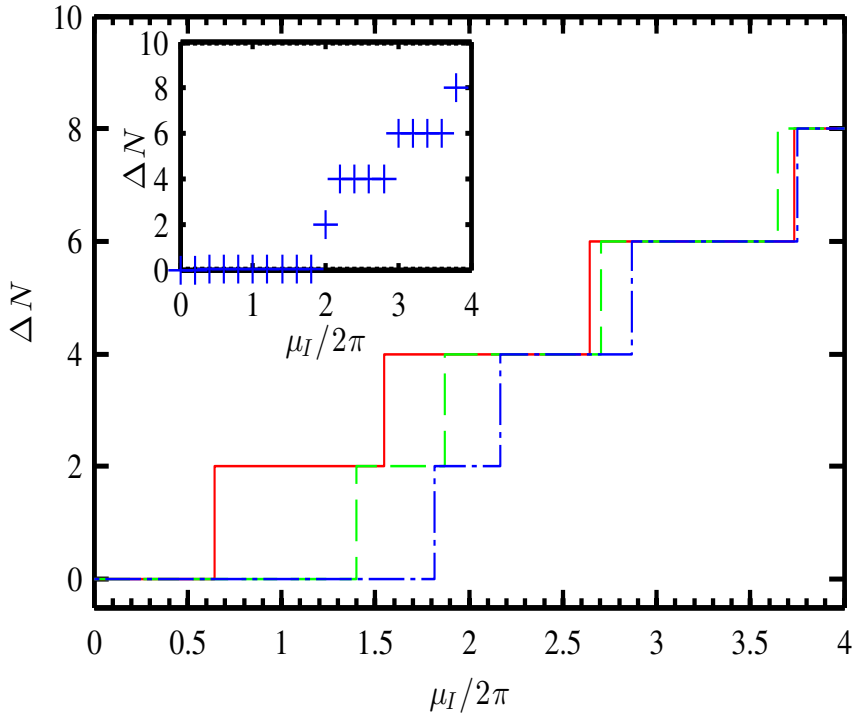
- change in particle number ΔN
- energy in given phase $E \propto \frac{\Delta N}{2}\mu_I/2\pi$
  $\Rightarrow$ slope of E changes as function of μ_I
- analytical prediction: no finite volume effect
- as usual: $D \to \infty, N \to \infty, x \to 0$

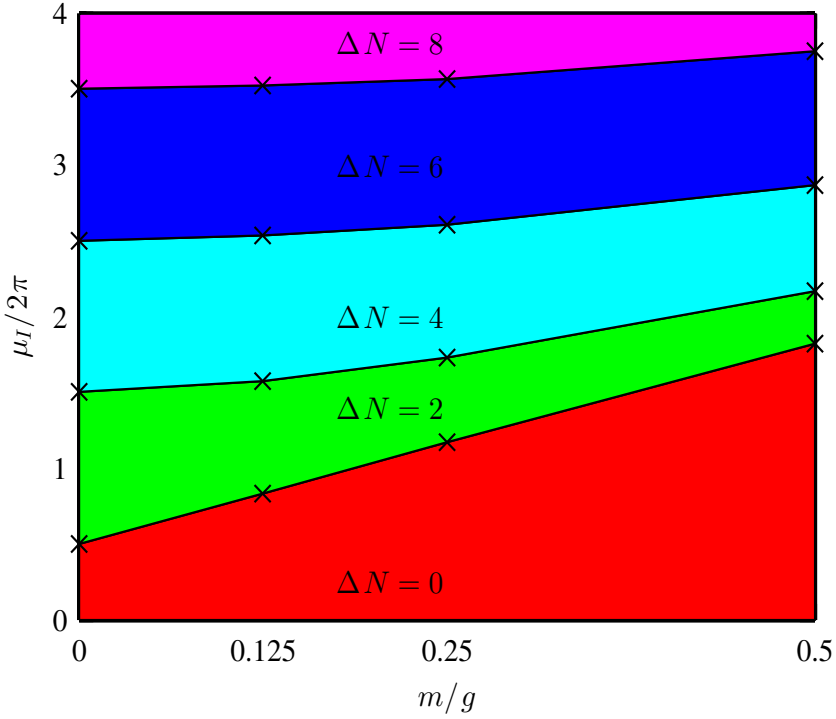


- intersection point:
  $\to$ location of jump
- no noticeable fse
- reproduce phase diagram
- no sign of sign problem

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





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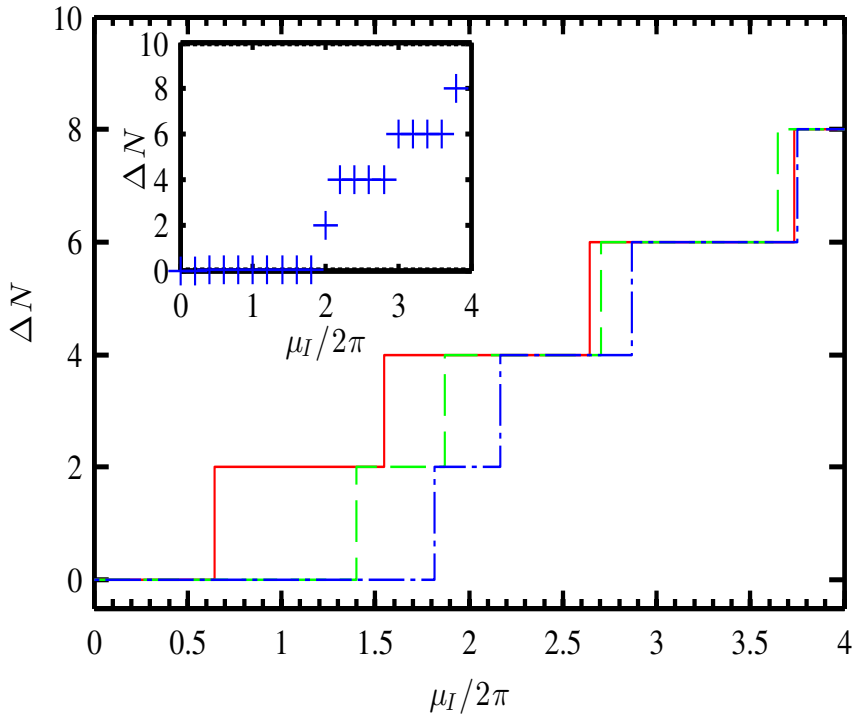
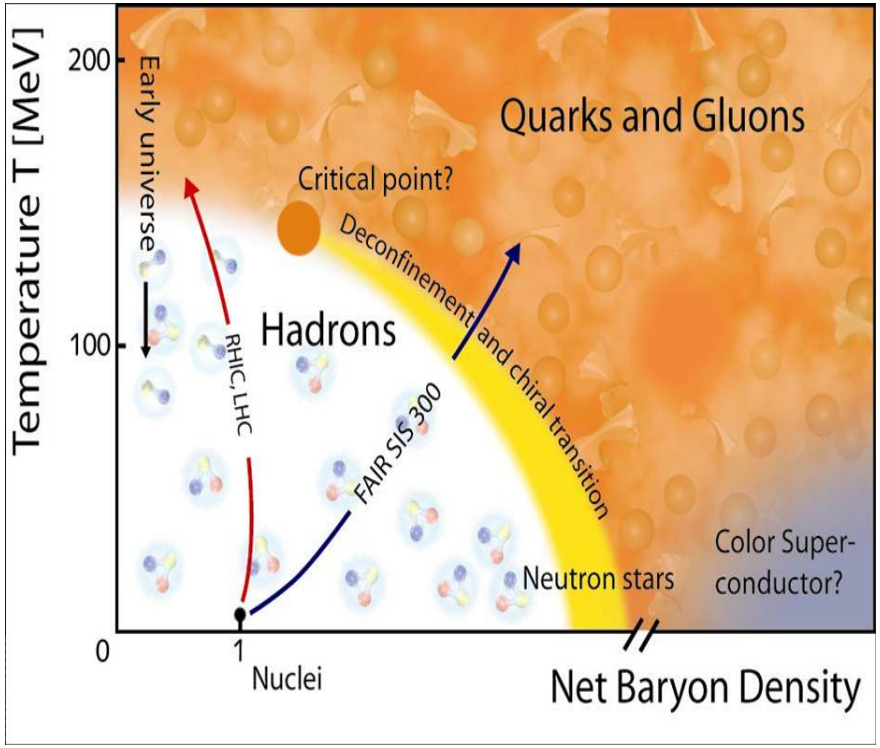
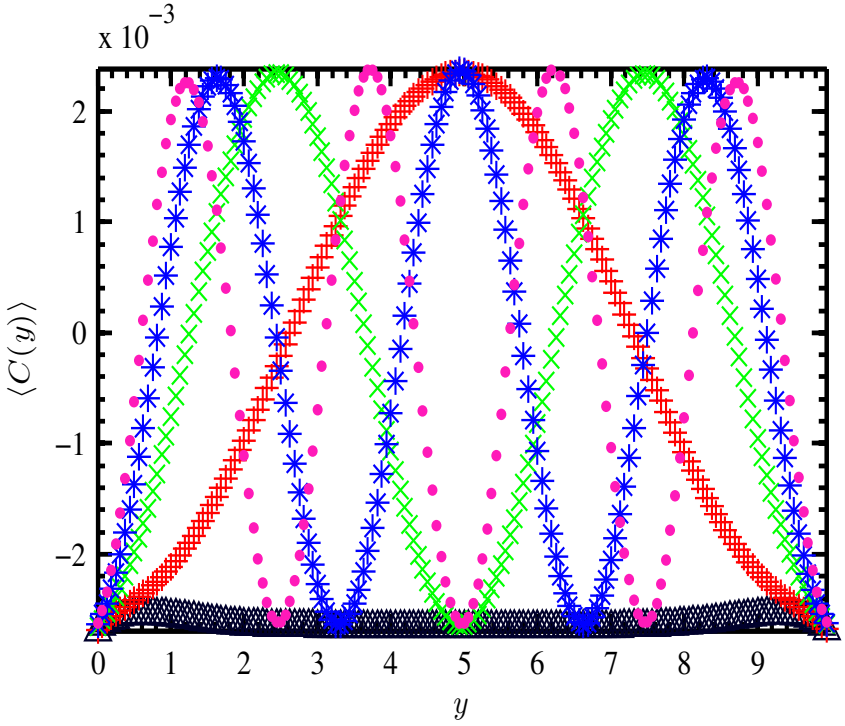
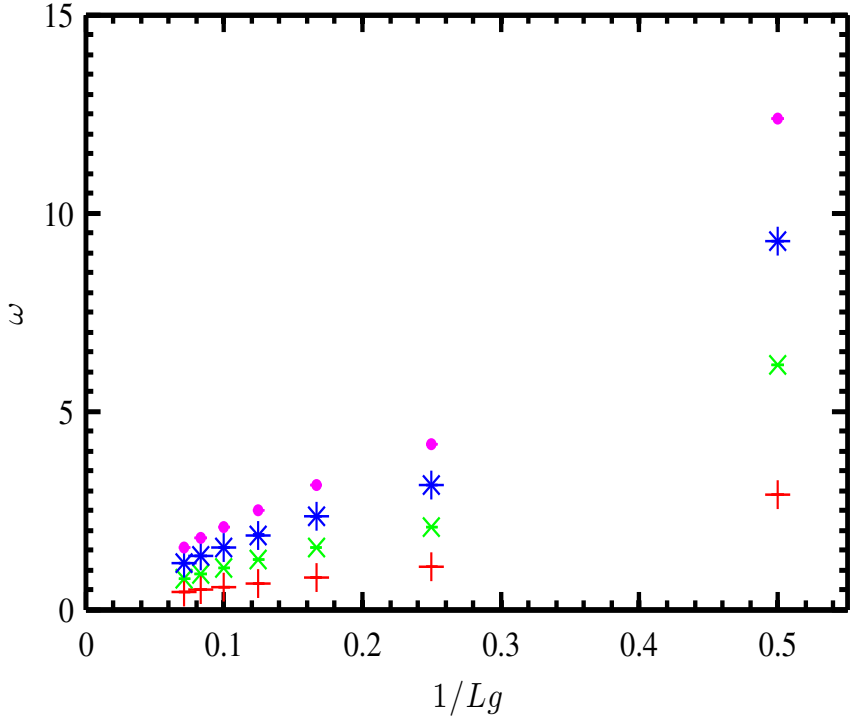




Inhomogenuous chiral condensate

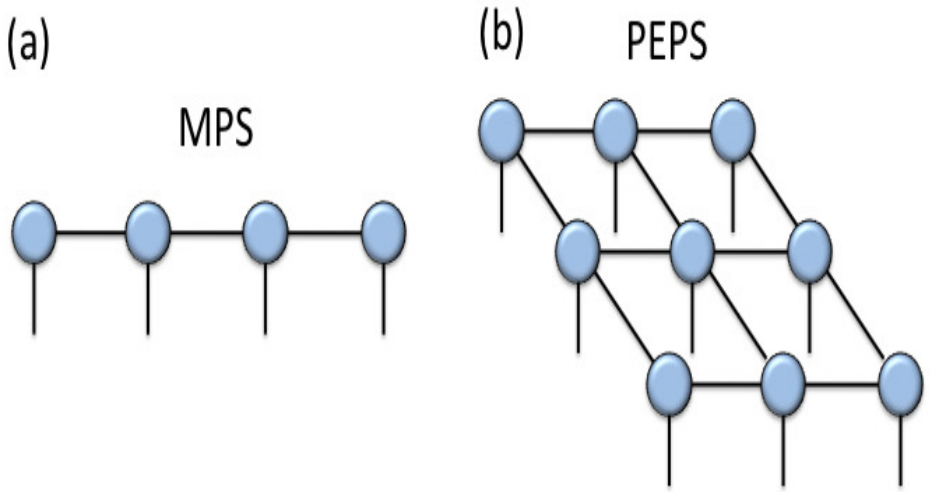
- condensate at non-zero chemical potential:
  prediction: standing wave $\bar{\Psi}(x)\Psi(x) = \bar{\Psi}(0)\Psi(0)\cos(\kappa x)$
- condensate: $C_{n,f} = \frac{\sqrt{x}}{N}(-1)^n \phi^\dagger_{n,f}\phi_{n,f}$
- we see oscillations, fit
  $\langle C(y)\rangle = A\cos(\omega y + \theta) + B$





Higher dimensions

- Projected Entangled Pair States (PEPS)



- PEPS are tensor networks for 2-d systems
- computational cost $\propto D^{10}$

$\rightarrow$ need new ideas for tensor networs

$\rightarrow$ ... or **alternatives: quantum simulations in ζ regularized path integral**

Example: hydrogen atom

- Hamiltonian

$$H = -\frac{\partial^2}{2m} + U(x)\ ,\quad U = \begin{cases} x & ; x \in (0,\pi) \\ 0 & ; x \in (-\pi, 0] \end{cases}$$

- Hilbert space: $L_2(-\pi,\pi)$ with discretization

$$\varphi_k(x) := \frac{1}{\sqrt{2\pi}} e^{ikx}$$

- orthogonal projection

$$P_n[\mathcal{H}] = lin\,\{\varphi_k; -n \le k \le n-1\}$$

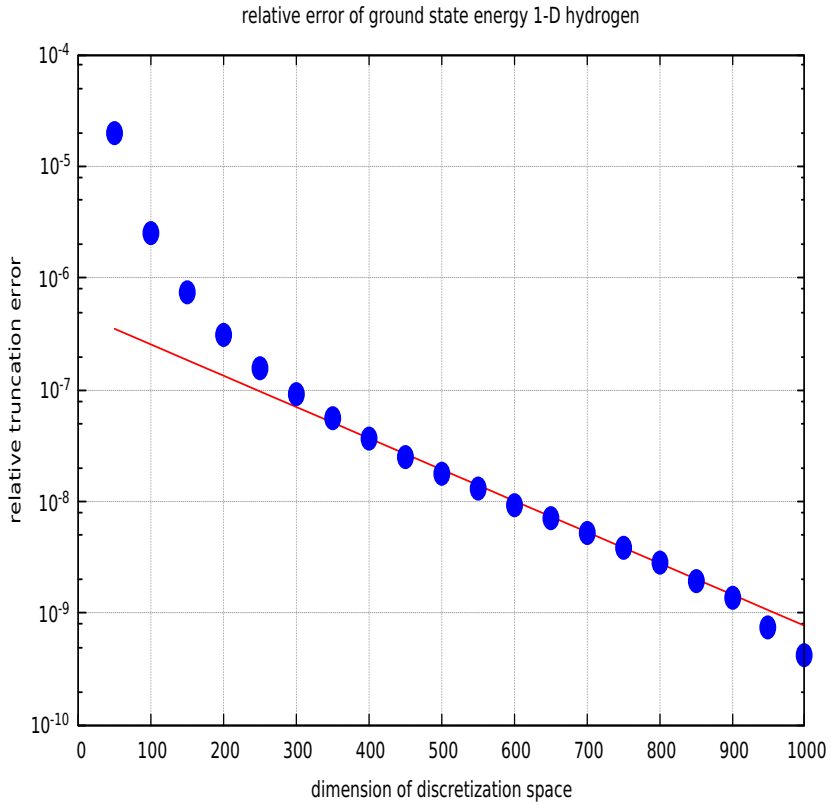
- matrix elements (for $m = 1$)

$$\langle \varphi_l, H\varphi_k \rangle = \frac{\left((-1)^{k-l}(1-i\pi(k-l))-1\right)}{2\pi(k-l)^2}$$

Truncation error

- exact diagonalization of matrix with elements

$$\langle \varphi_l, H\varphi_k \rangle = \frac{\left((-1)^{k-l}(1-i\pi(k-l))-1\right)}{2\pi(k-l)^2}$$



- relative error $\frac{E(j)-E(1024)}{E(1024)}$
- blue points: exact diagonalization
- red line: exponential fit
- find exponentially fast convergence

Hamiltonian for quantum computation

- the qubit Hamiltonian

$$H_q := \langle e_j, He_k \rangle_{j,k \in 2^Q}$$

- Pauli basis $[(1), \sigma_x, \sigma_y, \sigma_z]$

$$\left\{ S^q = \sigma^{q_{Q-1}} \otimes \sigma^{q_{Q-2}} \otimes \ldots \otimes \sigma^{q_0}; q \in 4^Q \right\}$$

- projecting H_q onto Pauli basis

$$H_Q = \sum_{q \in 4^Q} \frac{\mathrm{tr}\left(H_q S^q\right)}{2^Q} S^q$$

Variational quantum simulation

- start with some initial state $|\Psi_{\text{init}}\rangle$
- apply succesive gate operations $\equiv$ unitary operations $e^{-iS\theta}$
- examples for S: σ_x, σ_y, σ_z, parametric CNOT

$$|\Psi(\vec{\theta})\rangle = e^{-iS_{(n)}\theta_n} \dots e^{-iS_{(1)}\theta_1} |\psi_{\text{init}}\rangle$$

- with $R_j := e^{-iS_{(j)}\theta_j}$ we obtain cost function

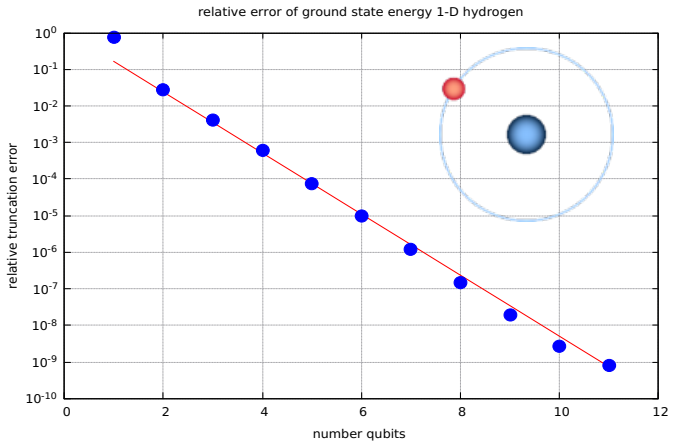
$$C := \left\langle \psi_{\text{init}} \left| \left(\prod_{j=1}^{n} R_j \right)^{\dagger} H \prod_{j=1}^{n} R_j \right| \psi_{\text{init}} \right\rangle$$

- goal: minimize C over the angles $\vec{\theta}$
  $\rightarrow$ obtain minimal energy, i.e. ground state
- in original paper:
  - minimization on classical computer
  - minimize over one angle at a time
  - loop several times over the complete set of angle

Simulation

- noise free simulation on Rigetti's QVM

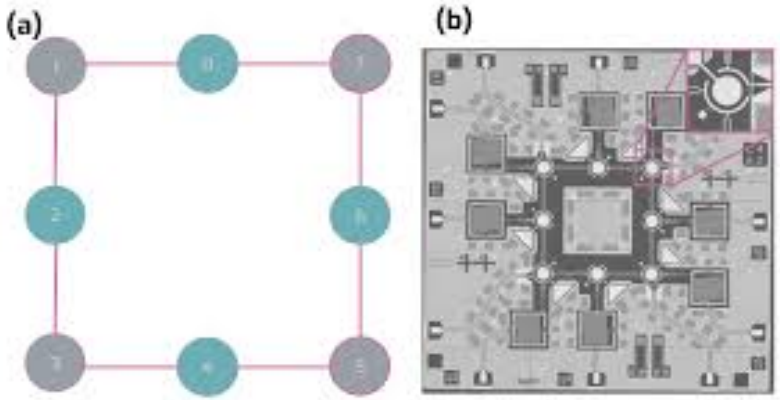
Q qubits	min. eig. H_Q	$\langle \psi_{2Q}, H_Q \psi_{2Q} \rangle$
1	.392108816647	.392108816647
2	.229395425745	.229395425968
3	.224258841712	.224258841747
4	.223452200306	.223452200445
5	.223336689755	.223336690423



- relatice error $\Delta E = \frac{E(q) - E(q=12)}{E(q=12)}$
- blue points: quantum simulator results
- find exponentially fast convergence
- line: fit $\Delta E(q) \approx 1.14 \cdot e^{-1.92q}$

Running on the Rigetti hardware

- Practical example: compute ground state energy of 1-dimensional hydrogen atom on Rigetti's 8-qubit Agave chip
  - performed variational quantum simulation



Agave chip

- hardware performance
  - select the qubit of the day
  - found gate fidelity $F_{1Q} = 0.982$, readout fidelity $F_{RO} = 0.94$
  - ground state energy with 4.9% error
  - more qubits: no significant result

Implement better algorithm

(T. Hartung, P. Stornati, KJ)

- new algorithm: quantum gradient descent
  - example for 2 unitaries, cost function:

$$C := \left\langle \psi_{\text{init}} \left| \left(e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}\right)^\dagger H e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2} \right| \psi_{\text{init}} \right\rangle$$

  - derivative D of $R = e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}$

    $D = (\frac{\partial R}{\partial \theta_1}, \frac{\partial R}{\partial \theta_2})$
  - obtain gradient of cost function

$$\partial/\partial\theta_1 C = \left\langle \psi_{\text{init}} \left| \left(e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2}\right)^\dagger \left[H i\sigma_x^\dagger + i\sigma_x H\right] e^{i\sigma_x\theta_1} e^{i\sigma_y\theta_2} \right| \psi_{\text{init}} \right\rangle$$

- can re-use generated state vector, measure $H i\sigma_x^\dagger + i\sigma_x H$
- obtain new vector of angles: $\vec{\theta}^{new} := \vec{\theta}^{old} - \eta \nabla C \left(\vec{\theta}^{old}\right)$
- tune "learning rate" η

Generalization

- general form of the quantum gradient descent algorithm
  - cost function, $R_j = e^{iS_{(j)}\theta_j}$

$$C := \left\langle \psi_{\text{init}} \left| \left(\prod_{j=1}^{n} R_j \right)^{\dagger} H \prod_{j=1}^{n} R_j \right| \psi_{\text{init}} \right\rangle$$

  - define derivative operator

$$D_k := \left(\prod_{j=k+1}^{n} R_j \right) R'_k \left(\prod_{j=k+1}^{n} R_j \right)^{\dagger}$$

  - express CNOT gate in Pauli matrices

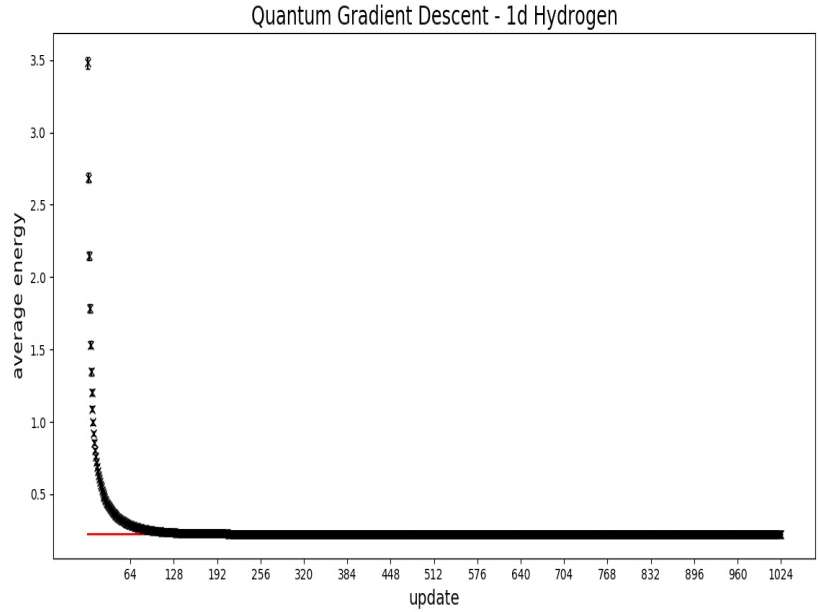
$$CNOT_{1\to 2} = \frac{\mathbb{1}_1 + \sigma_1^z}{2} \otimes \mathbb{1}_2 + \frac{\mathbb{1}_1 - \sigma_1^z}{2} \otimes \sigma_2^x$$

  - obtain kth-component of gradient

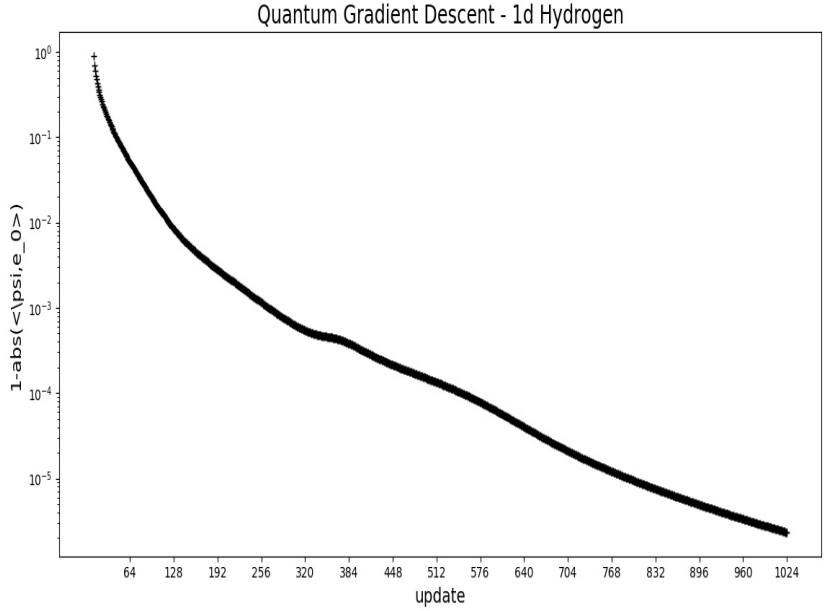
$$\partial_k C = \left\langle \prod_{j=1}^{n} R_j \psi_{\text{init}} \left| HD_k + (HD_k)^{\dagger} \right| \prod_{j=1}^{n} R_j \psi_{\text{init}} \right\rangle$$

- can re-use generated state vector, measure $HD_k + (HD_k)^{\dagger}$
- obtained new vector of angles: $\vec{\theta}^{new} := \vec{\theta}^{old} - \eta \nabla C \left(\vec{\theta}^{old} \right)$

Testing the algorithm



- average energy
  - simulator
  - no noise
  - 3 qubits
  - red line: exact result

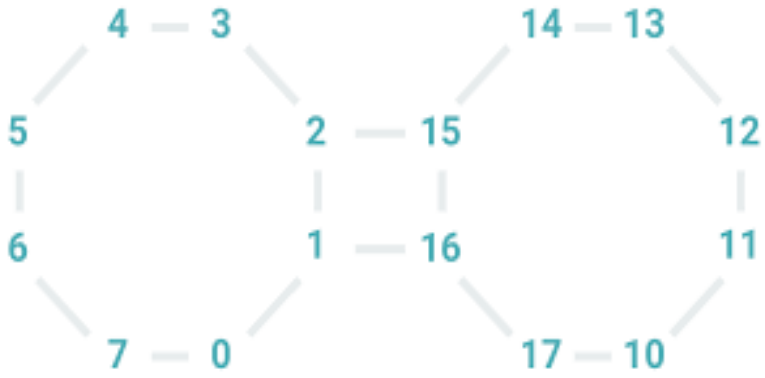


- distance to groundstate
- $|1 - \langle\Psi(j)|\Psi_0\rangle|$

  Ψ_0 ground state wave function

New hardware

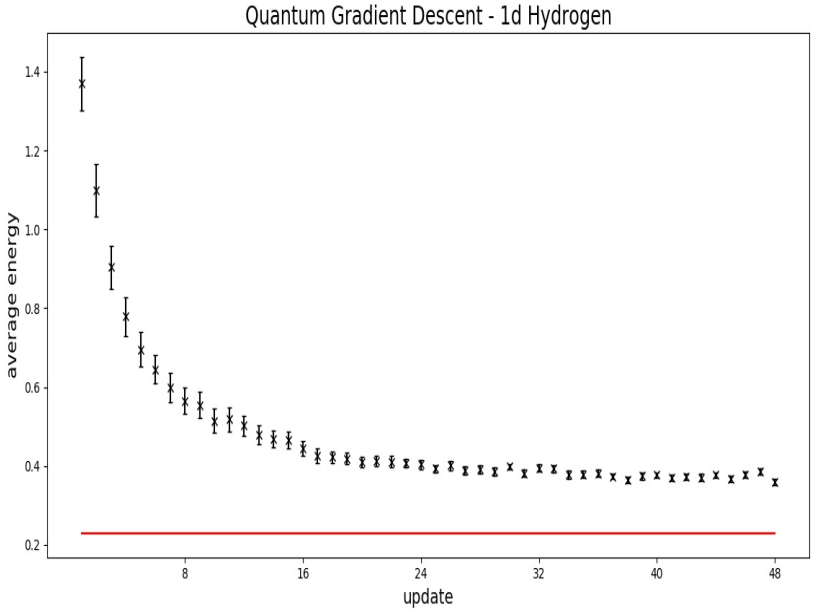
- new hardware: Aspen line (up to 128 qubits)



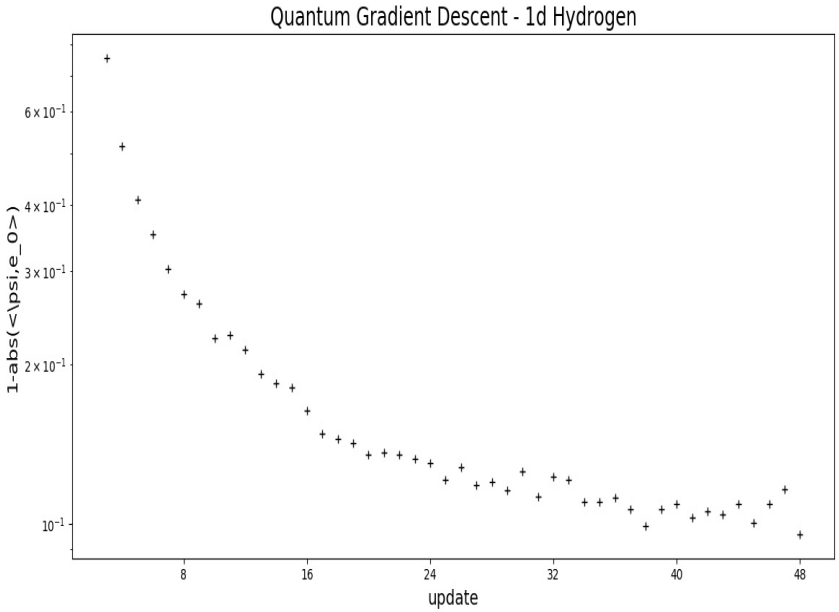
Aspen layout

- Rigetti's setup
  - Quantum Cloud Service
  - Pyquil (Python based) program enviroment
  - mean single qubit fidelity 95.5%

Running on Rigetti's Aspen hardware



- average energy
  - 2 qubits
  - red line: exact result
  - 60% fidelity



- distance to groundstate
- 90% fidelity
- reaching machine precision

Remarks

- with new hardware and better algorithm
  from impossible (2 qubits) $\rightarrow$ 90% fidelity for ground state

- still, 3 qubits: no significant result

- quantum gradient descent very expensive
  - justified for 1-d hydrogen atom (expensive itself)
  - for local Hamiltonians (e.g. Heisenberg)
    $\rightarrow$ need better algorithm (... and we are working on this)
    $\rightarrow$ can reach O(10) qubits

- quantum simulations of Schwinger model on real hardware
  - E.A. Martinez et.al., Nature 534 (2016) 516 (trapped ions)
  - N. Klco et.al., Phys.Rev. A98 (2018) no.3, 032331 (IBMQ)
  - C. Kokail et.al., Nature 569 (2019) no.7756, 355 (trapped ions, > 10 qubits)

General articles

Lectures, review articles

- R. Gupta
  Introduction to Lattice QCD, hep-lat/9807028
- C. Davies
  Lattice QCD, hep-ph/0205181
- M. Lüscher
  Advanced Lattice QCD, hep-lat/9802029
  Simulation strategies, hep-lat/xxxxxxx
  Chiral gauge theories revisited, hep-th/0102028
- A.D. Kennedy
  Algorithms for Dynamical Fermions, hep-lat/0607038

Books about Lattice Field Theory

- **C. Gattringer and C. Lang**
  Quantum Chromodynamics on the Lattice
  Lecture Notes in Physics 788, Springer, 2010

- **T. DeGrand and C. DeTar**
  Lattice methods for Quantum Chromodynamics
  World Scientific, 2006

- **H.J. Rothe**
  Lattice gauge theories: An Introduction
  World Sci.Lect.Notes Phys.74, 2005

- **J. Smit** *Introduction to quantum fields on a lattice: A robust mate*
  Cambridge Lect.Notes Phys.15, 2002

- **I. Montvay and G. Münster**
  Quantum fields on a lattice
  Cambridge, UK: Univ. Pr., 1994

- **Yussuf Saad**
  Iterative Methods for sparse linear systems
  Siam Press, 2003