Flavor Physics from Lattice QCD: 1

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Symmetry Breaking in Fundamental Interactions
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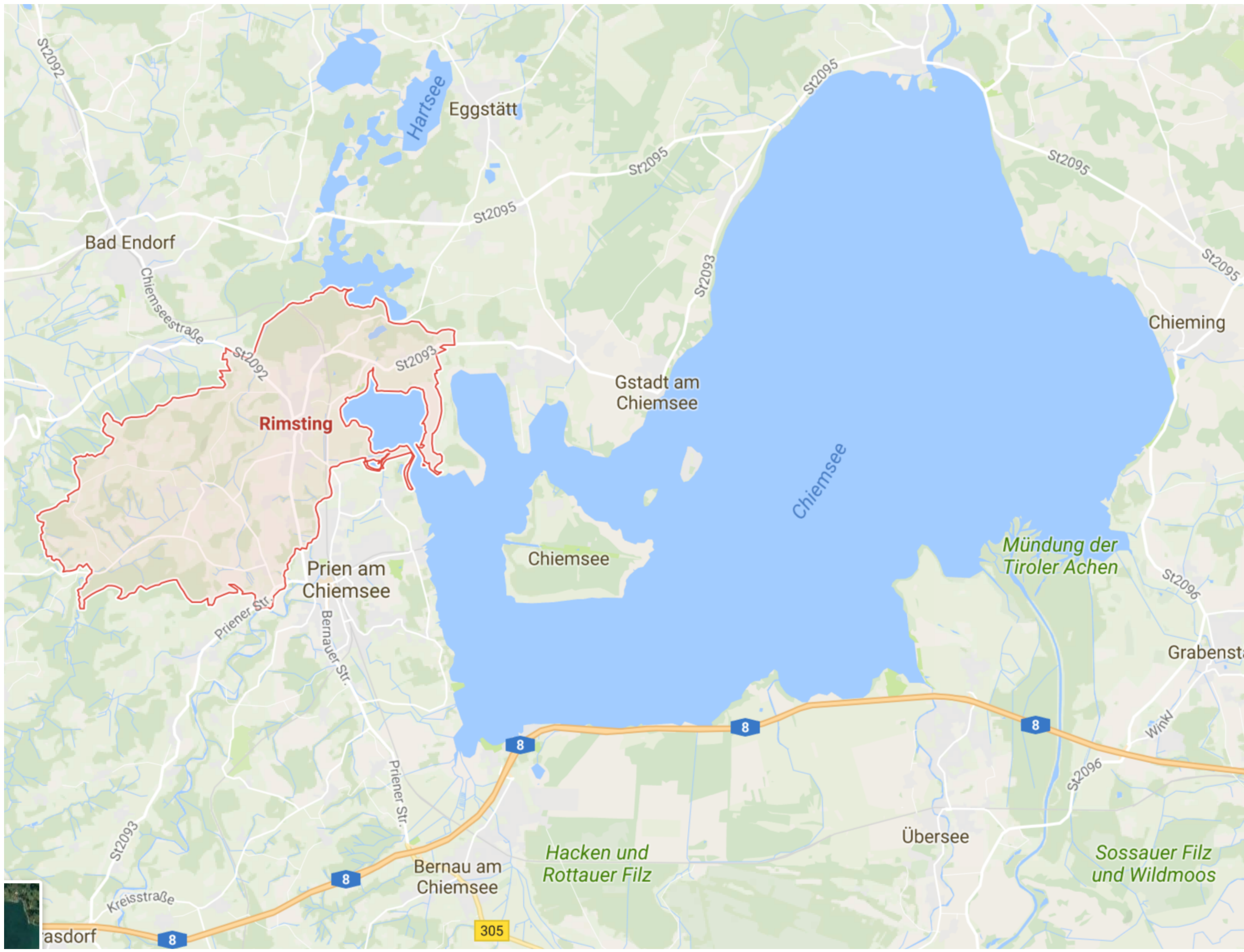
Kloster Frauenwörth

Ein Einheimischer unter den Rednern?



Outline

- Lecture 1—Lattice Gauge Theory:
  - Origins;
  - Formalism;
  - Numerical methods.
- Lecture 2—Lattice QCD Results:
  - Decay constants (leptonic decays);
  - Semileptonic form factors & neutral-meson mixing:
    - CKM determination and search for non-SM FCNC

Quantum Field Theory = Lattice Field Theory

Lots of Degrees of Freedom

- Essence of field theory is uncountably many degrees of freedom:
  - but UV divergences stem from the intrinsic problem of counting the uncountable—
  - especially so when scale invariance is key (as it is in 3+1 dim).
- Necessary to tame the counting problem, but want:
  - generality (not something limited, say, to perturbation theory);
  - computability (results different from 0 or 1).

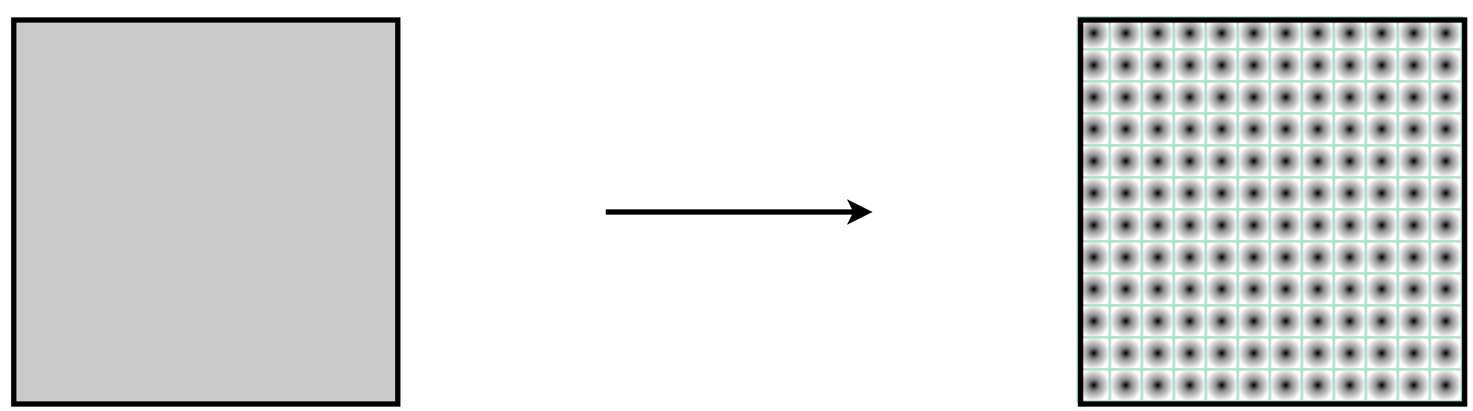
Canonical Quantization of QFT

W. Heisenberg & W. Pauli, *Z. Phys.* **56** (1929) 1

- H. & P. wanted to extend canonical quantization, $[p_j, q_k] = i\hbar\delta_{jk}$, which works for countable sets (as infinite as $\mathbb{Z}$) to continuous sets (as infinite as $\mathbb{R}$).

- Right-hand side of $[\pi(x), \phi(y)] = i\hbar\delta(x{-}y)$ was a bit too new.

- Divide space into cells, with one field variable per cell:



- # dof is now countable, reducing QFT to quantum mechanics.

- H&P: *In der Tat kann man den Fall kontinuierlich vieler Freiheitsgrade, wo die Zustandsgrößen Raumfunktionen sind, stets durch Grenzübergang aus dem Fall endlich vieler Freiheitsgrade gewinnen.*

- Indeed, one can always obtain the case of continuously many degrees of freedom, where the state variables are functions of space, through a limit of the case of finitely many degrees of freedom. (my translation)

- Wenzel (1940) and Schiff (1953) used spatial lattice to study strong coupling, treating the kinetic term as a perturbation.

Path Integral in Quantum Mechanics

R. Feynman, *Rev. Mod. Phys.* **20** (1948) 367

- Propagator in QM, with Hamiltonian $H = p^2/2m + V(x)$:

$$\langle x(T)|x(0)\rangle = \langle x_T|e^{-i\hat{H}T}|x_0\rangle = \sum_n \langle x_T|n\rangle e^{-iE_nT}\langle n|x_0\rangle$$

- Divide the time interval into many small steps, $\delta = T/N$. Insert $\int dx_n |x_n\rangle\langle x_n|$ N–1 times. Then

$$\langle x(T)|x(0)\rangle = \int \prod_{n=1}^{N-1} dx_n \prod_{n=0}^{N-1} \langle x_{n+1}|e^{-i\hat{H}\delta}|x_n\rangle$$

- Now want to work out the matrix element on RHS.

- Factorize the operator (Trotter formula):

$$\langle x_{n+1}|e^{-i\hat{H}\delta}|x_n\rangle \approx \langle x_{n+1}|e^{-iV(\hat{x})\delta/2}e^{-i\hat{p}^2\delta/2m}e^{-iV(\hat{x})\delta/2}|x_n\rangle$$
$$= e^{-iV(x_{n+1})\delta/2}\langle x_{n+1}|e^{-i\hat{p}^2\delta/2m}|x_n\rangle e^{-iV(x_n)\delta/2}$$

- Work out the factor in the middle ($\delta \to -ia$):

$$\langle x_{n+1}|e^{-\hat{p}^2 a/2m}|x_n\rangle = \sqrt{\frac{m}{2\pi a}}\,e^{-m(x_{n+1}-x_n)^2/2a}$$

- Assemble factors:

$$\langle x_T|e^{-\hat{H}\tau}|x_0\rangle = \lim_{N\to\infty}\int \mathscr{D}x \exp\left(\frac{\tau}{N}\sum_{n=0}^{N-1} L_n\right), \qquad \mathscr{D}x = \prod_{n=1}^{N-1} dx_n\sqrt{\frac{mN}{2\pi\tau}}$$

$$L_n = -\frac{1}{2}m\left(\frac{x_{n+1}-x_n}{\tau/N}\right)^2 - \frac{1}{2}V(x_{n+1}^2) - \frac{1}{2}V(x_n^2)$$

analytically continue $\tau \to iT$ after taking $N \to \infty$.

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- Assemble factors:

$$\langle x_T|e^{-\hat{H}\tau}|x_0\rangle = \lim_{N\to\infty}\int \mathscr{D}x \exp\left(\quad -S \quad \right), \qquad \mathscr{D}x = \prod_{n=1}^{N-1} dx_n \sqrt{\frac{mN}{2\pi\tau}}$$

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analytically continue $\tau \to iT$ after taking $N \to \infty$.

Many degrees of freedom

- Two: $V(x_1, x_2) = V(x_1) + V(x_2) - \varkappa x_1 x_2$: just repeat manipulations.
- Infinite chain, $j \in \mathbb{Z}$: $V(\phi) = \sum_j \mathscr{V}(\phi_j) - \frac{1}{2}\kappa\phi_j(\phi_{j-1} + \phi_{j+1})$
- Combine spatial lattice and path integral—before the infinitesimal cell-size & time-step limits—to get a spacetime lattice:
  - the focus of most lattice field theory.
- Need to work out the relation between $\varkappa$ and usual properties of (scalar) field theory, writing $\mathscr{V} = \frac{1}{2}\mu^2\phi_j + \ldots$.
- Then spatial lattice spacing $b = \varkappa^{-1/2}$ and $m^2 = \mu^2 - 2d\varkappa$.

- Propagator as function of time t, 3-momentum $\boldsymbol{p}$ is interesting.

- Set spatial and temporal lattice spacings equal:

$$S = a^d \sum_x \left\{ \frac{1}{2} \sum_\mu a^{-2} \left[\phi(x+ae_\mu) - \phi(x)\right]^2 + \frac{1}{2} m^2 \phi(x)^2 + \frac{1}{4!} \lambda \phi(x)^2 \right\}, \quad x = na,$$

$$= \sum_n \left\{ \frac{1}{2} \kappa \sum_\mu \varphi_n \left[\varphi_{n+e_\mu} + \varphi_{n-e_\mu}\right] + \frac{1}{2} \varphi_n^2 + \frac{1}{4} g \varphi_n^4 \right\}, \quad n \in \mathbb{Z}^d, \; e_\mu = \text{unit vector.}$$

- Compute via contour integration: (see back-up slide)

$$G(t, \boldsymbol{p}) = \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{e^{ip_4 t}}{2a^{-2}(1 - \cos p_4 a) + \hat{\boldsymbol{p}}^2 + m^2},$$

$$= \frac{a e^{-E|t|}}{2 \sinh Ea}, \quad \cosh Ea = 1 + \frac{1}{2}\left(\hat{\boldsymbol{p}}^2 + m^2\right)$$

which yields 1-particle state, with some discretization effects.

Finite Volume

- With lots of field variables, in practice, it is convenient to set the final configuration equal to the initial configuration and integrate over it:

$$Z = \int d\phi \, \langle \phi | e^{-\hat{H}\tau} | \phi \rangle = \int \mathcal{D}\phi \, e^{-S} = \mathrm{Tr}\, e^{-\hat{H}\tau}$$

  which "looks like" a partition function in statistical mechanics.

- The spatial lattice can also be finite, with suitable boundary conditions, often periodic (or a generalization).

- Finite spacetime lattice reduces quantum field theory to quantum mechanics of a large, but finite, collection of degrees of freedom.

- Used in mathematical physics to "construct" QFT [Glimm & Jaffe].

Observables

- In QFT, all information can be obtained from correlation functions:

$$\langle Q(x_t)\rangle = \frac{1}{Z}\int \mathcal{D}x\, Q(x_t)\, e^{-S(\{x_i\})}$$

$$\langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle = \frac{1}{Z}\int \mathcal{D}x\, Q_1(x_{t_1})Q_2(x_{t_2})\, e^{-S(\{x_i\})}$$

- For large time extent τ: (proofs as exercise)

$$Z \overset{\text{large }\tau}{\longrightarrow} e^{-E_0\tau}$$

$$\langle Q(x)\rangle \overset{\text{large }\tau}{\longrightarrow} \langle 0|Q(\hat{x})|0\rangle$$

yields vacuum energy E_0 and the vacuum expectation value (vev).

- For $\tau > t_1 > t_2 > 0$ and large time extent τ: (proofs as exercise)

$$\langle Q_1(t_1) Q_2(t_2)\rangle_c \xrightarrow{\text{large } \tau} \sum_{n\neq 0} \langle 0|\hat{Q}_1(t_1)|n\rangle\langle n|\hat{Q}_2(t_2)|0\rangle e^{-(E_n-E_0)(t_1-t_2)} + \sum_{n\neq 0} \langle 0|\hat{Q}_2(t_2)|n\rangle\langle n|\hat{Q}_1(t_1)|0\rangle e^{-(E_n-E_0)(\tau+t_2-t_1)}$$

yielding excited-state energies and transition matrix elements.

- When $t_1 - t_2$ and $\tau - (t_1 - t_2)$ are also large:

$$\langle Q_1(t_1) Q_2(t_2)\rangle_c \xrightarrow{\text{large } \tau,\,(t_1-t_2)} \langle 0|\hat{Q}_1(t_1)|1\rangle\langle 1|\hat{Q}_2(t_2)|0\rangle e^{-(E_1-E_0)(t_1-t_2)} + \langle 0|\hat{Q}_2(t_2)|1\rangle\langle 1|\hat{Q}_1(t_1)|0\rangle e^{-(E_1-E_0)(\tau+t_2-t_1)}$$

- And similarly for three-point functions (for, *e.g.*, form factors).

QFT as Statistical Mechanics

- Combination of the lattice and the path integral opens up new tools:
  - mean-field approximations;
  - strong coupling ("high temperature") expansions;
  - Monte Carlo methods.
- Also opens up QFT tools for condensed matter physics:
  - Feynman diagrams, *e.g.*, to calculate critical exponents;
  - renormalization group, *e.g.*, to solve Kondo problem.

Lattice Gauge Fields

Local Gauge Invariance

- Global symmetries simply tag along in the correspondence between path integrals and canonical quantization.

- Suppose there is a local symmetry, $g(x) \in$ Lie group:

$$\phi(x) \mapsto g(x)\phi(x), \qquad \phi^\dagger(x) \mapsto \phi^\dagger(x) g^{-1}(x)$$

- Couplings among different points transform like

$$\phi^\dagger(x)\phi(y) \mapsto \phi^\dagger(x) g^{-1}(x) g(y)\phi(y)$$

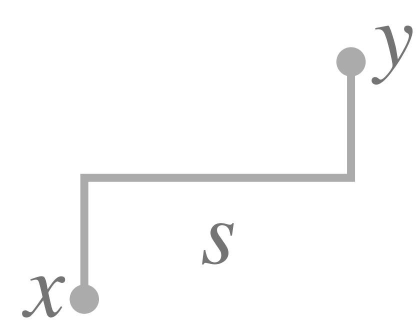
- Need object transforming like $U(x,y) \mapsto g(x)U(x,y)g^{-1}(y)$; then

$$\phi^\dagger(x)U(x,y)\phi(y) \mapsto \phi^\dagger(x)g^{-1}(x)\; g(x)U(x,y)g^{-1}(y)\; g(y)\phi(y) = \phi^\dagger(x)U(x,y)\phi(y)$$

Parallel Transport

- If $A^\mu(x)$ is the gauge potential, then define

$$U_s(x,y) = \mathbb{P}_s \exp \int_x^y dz_\mu A^\mu(z)$$



where $A^\mu(x) \mapsto g(x)\,(\partial^\mu + A^\mu(x))\,g^{-1}(x)$

no i: $t_a^\dagger = -t_a$
no g_0: normalization

- Parallel transporters along adjacent paths compose.

- These transform in the desired way. (proof as an exercise)

- Obviously, $\mathrm{tr}[U_s(x,x)]$ is gauge invariant: called Wilson loop.

Lattice Gauge Theory

- Instead of $A_\mu(x)$, gauge d.o.f. in lattice gauge theory are $U(x, x{+}ae_\mu)$, where a is the lattice spacing and e_μ is a unit vector along μ.

- Integration measure is "Haar measure": $\int dU = 1, \quad \int dU\,U = 0$

$$\int dU\, f(U) = \int dU\, f(UV) \quad \Rightarrow \quad \int dU\, U_{ij} U^*_{kl} = \frac{1}{N}\delta_{ik}\delta_{jl}$$

- For SU(2), this can be expressed via Euler angles; for SU(3) and higher, it is too cumbersome to write it out.

- Simplest Wilson loop (hypercubic lattice) goes around a 1×1 square.

- Plaquette action $\mathrm{Re}\,\mathrm{tr}[1 - U_{1\times1}]$ tends to $\mathrm{tr}[F_{\mu\nu}F^{\mu\nu}]$ as $a \to 0$.

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- For SU(2), this can be expressed via Euler angles; for SU(3) and higher, it is too cumbersome to write it out.
- Simplest Wilson loop (hypercubic lattice) goes around a plaquette.
- Plaquette action $\mathrm{Re}\,\mathrm{tr}[1 - U_{1\times1}]$ tends to $\mathrm{tr}[F_{\mu\nu}F^{\mu\nu}]$ as $a \to 0$.

Confinement of Quarks

K. Wilson, *PRD* **10** (1974) 2445

- LGT invented to understand asymptotic freedom without gauge-fixing and ghosts [Wilson, hep-lat/0412043].
- Consider a large $R \times T$ Wilson loop.
- Boltzmann weight ("plaquette action"):

$$\prod_p \exp\left(-\frac{2N}{g_0^2}\,\mathrm{Re}\,\mathrm{tr}[1 - U_p]\right)$$

- Leading term when each plaquette is covered by it's U_p: area law.
- Potential energy $V(R) = R\ln(g^2/2N)$.
- Lowest-order strong coupling expansion demonstrates color confinement.

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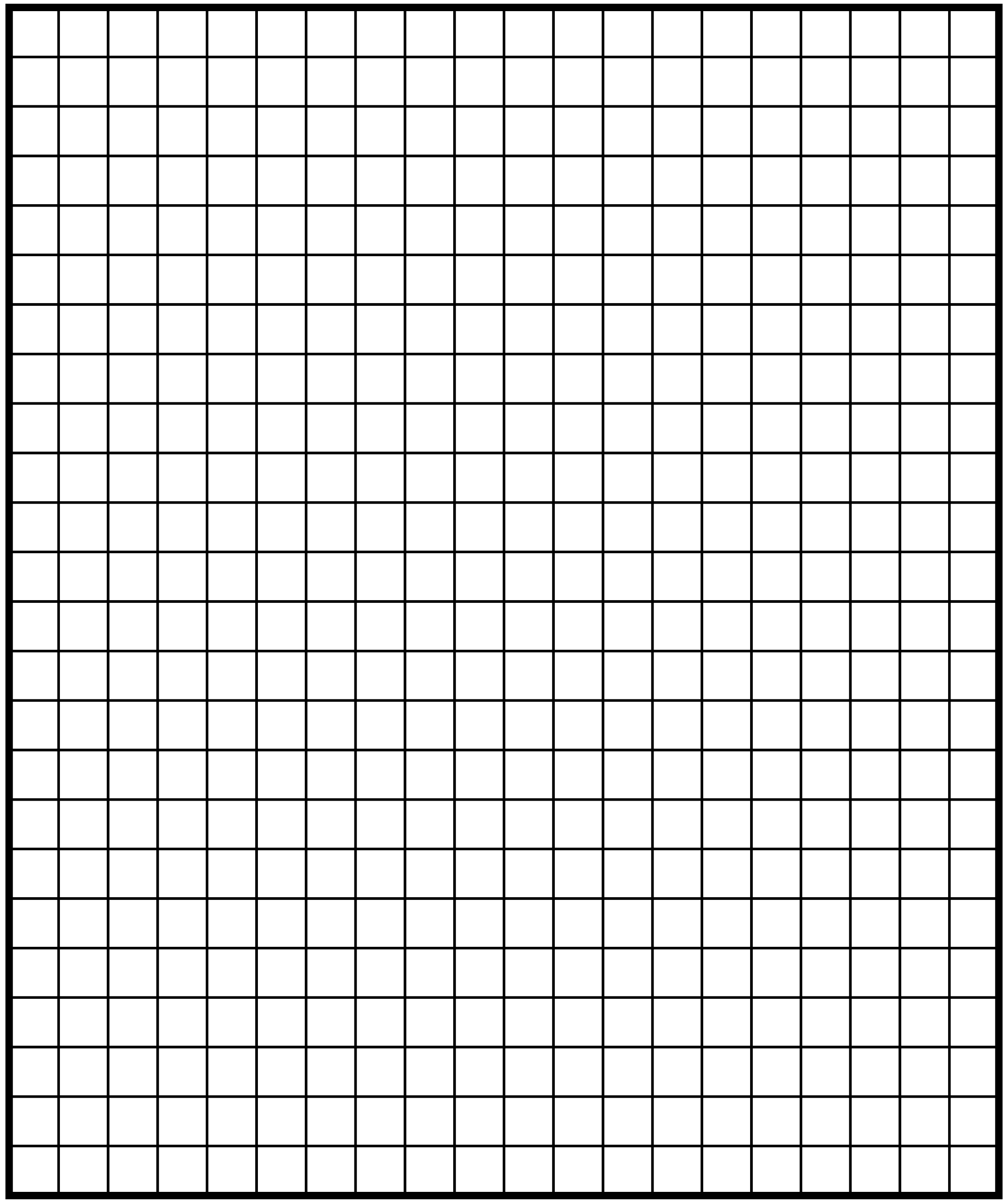

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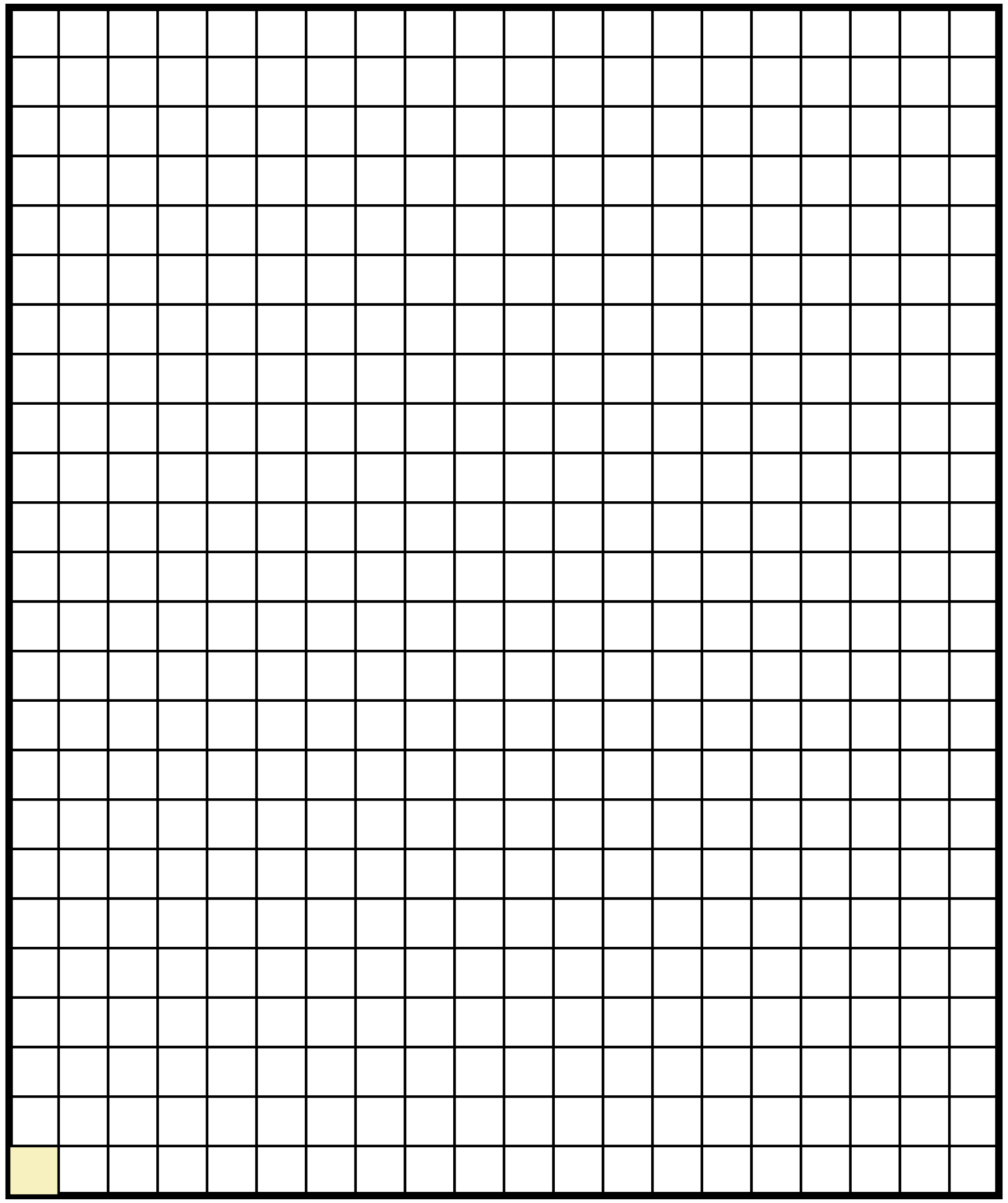

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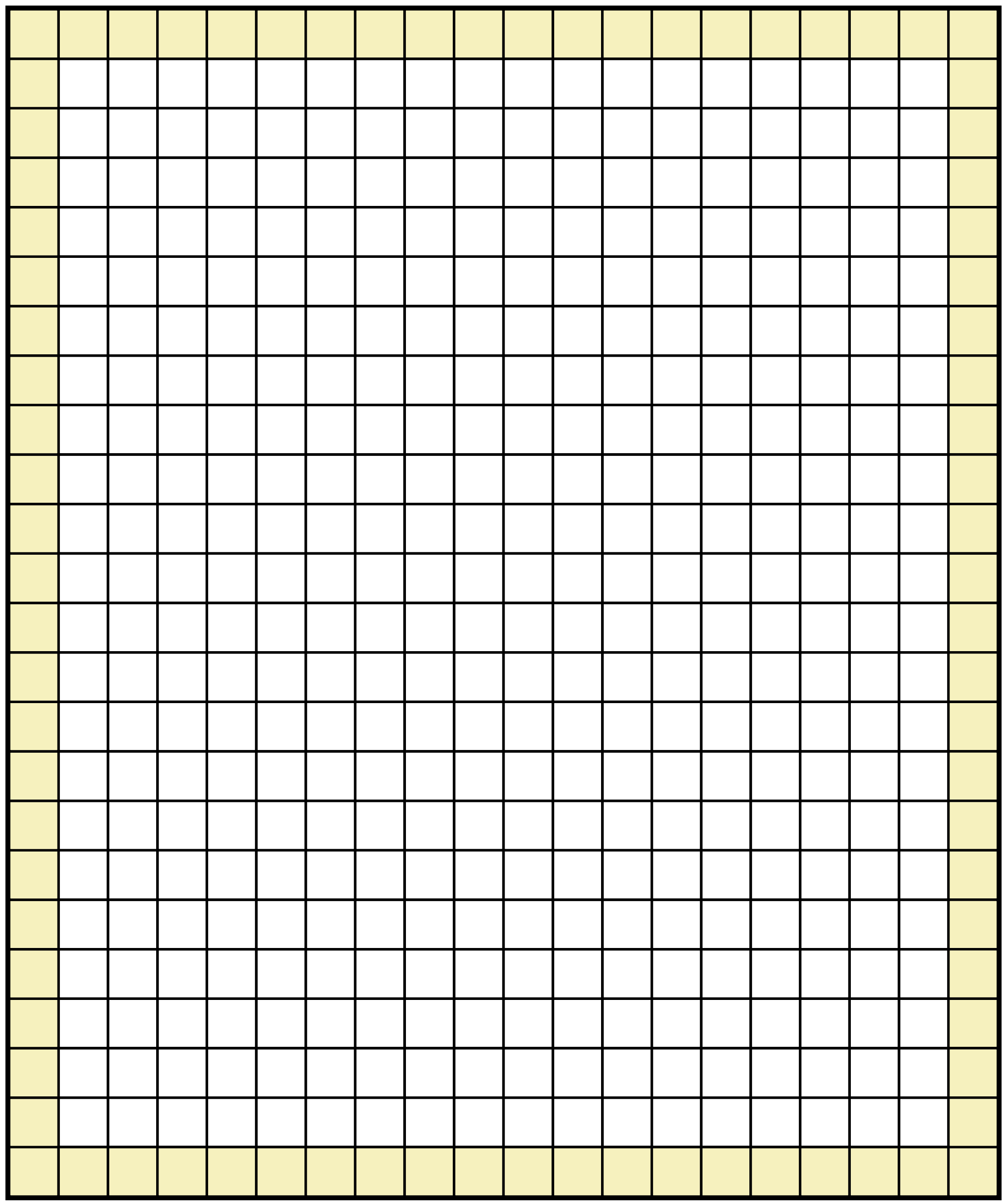

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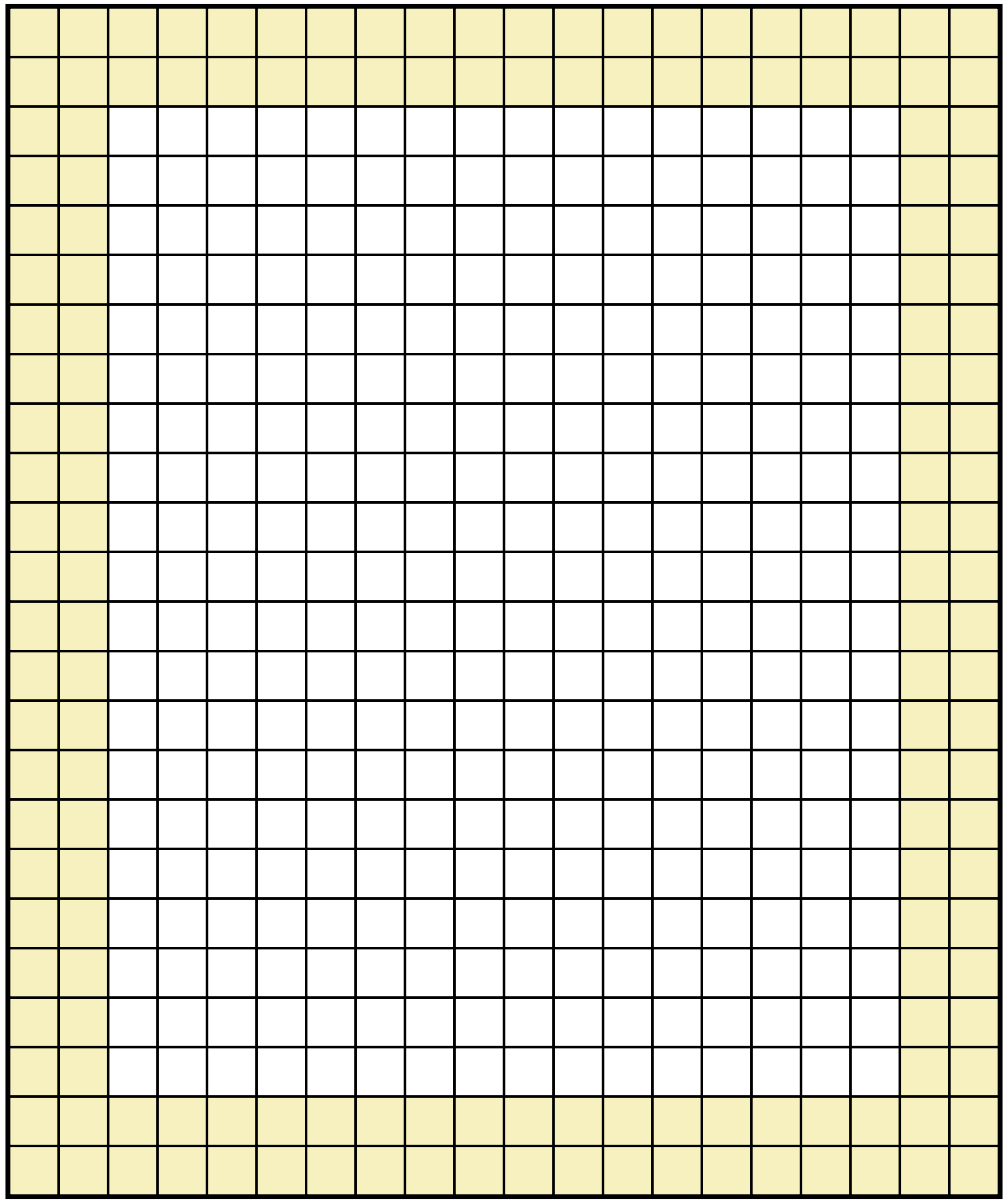

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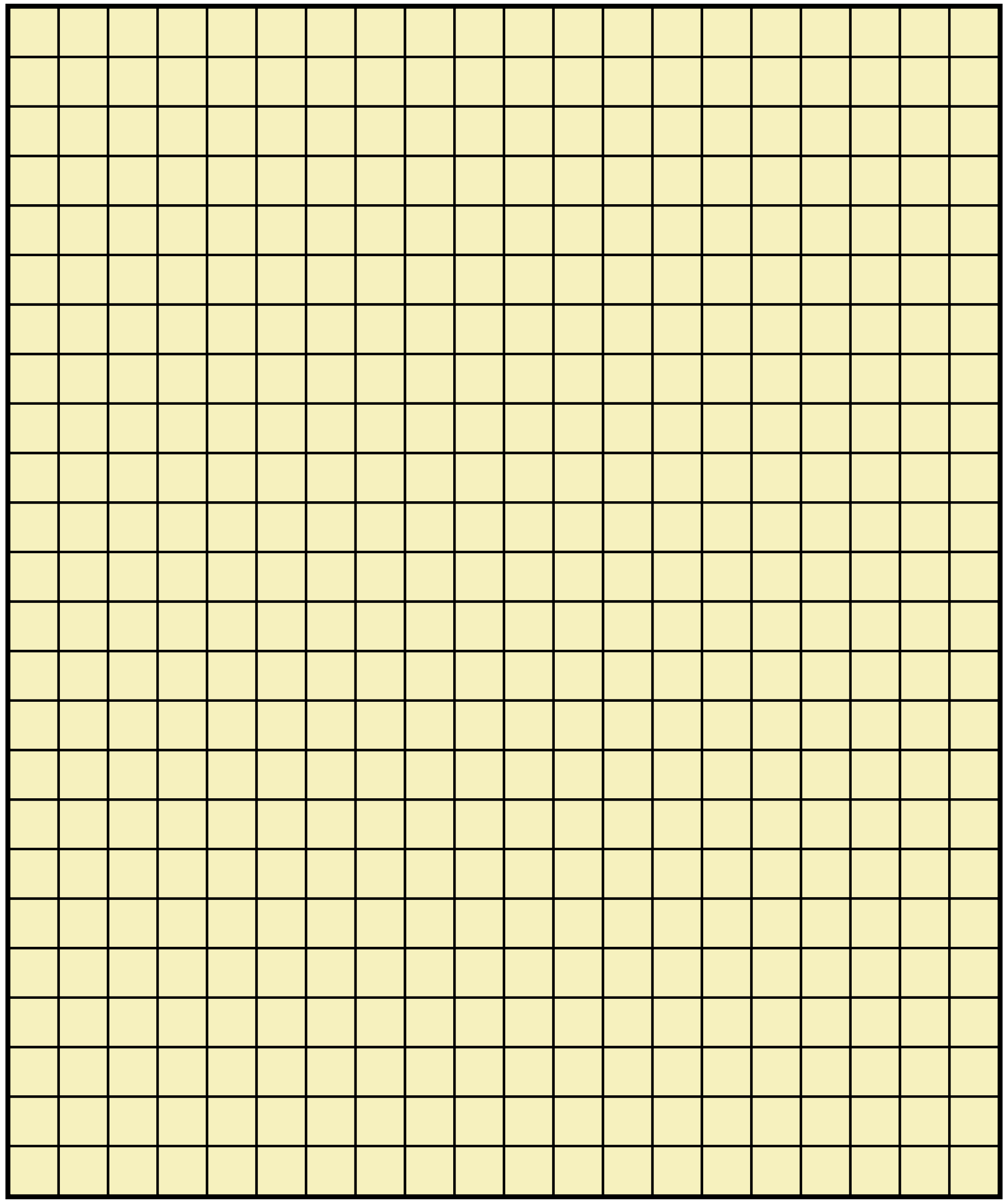

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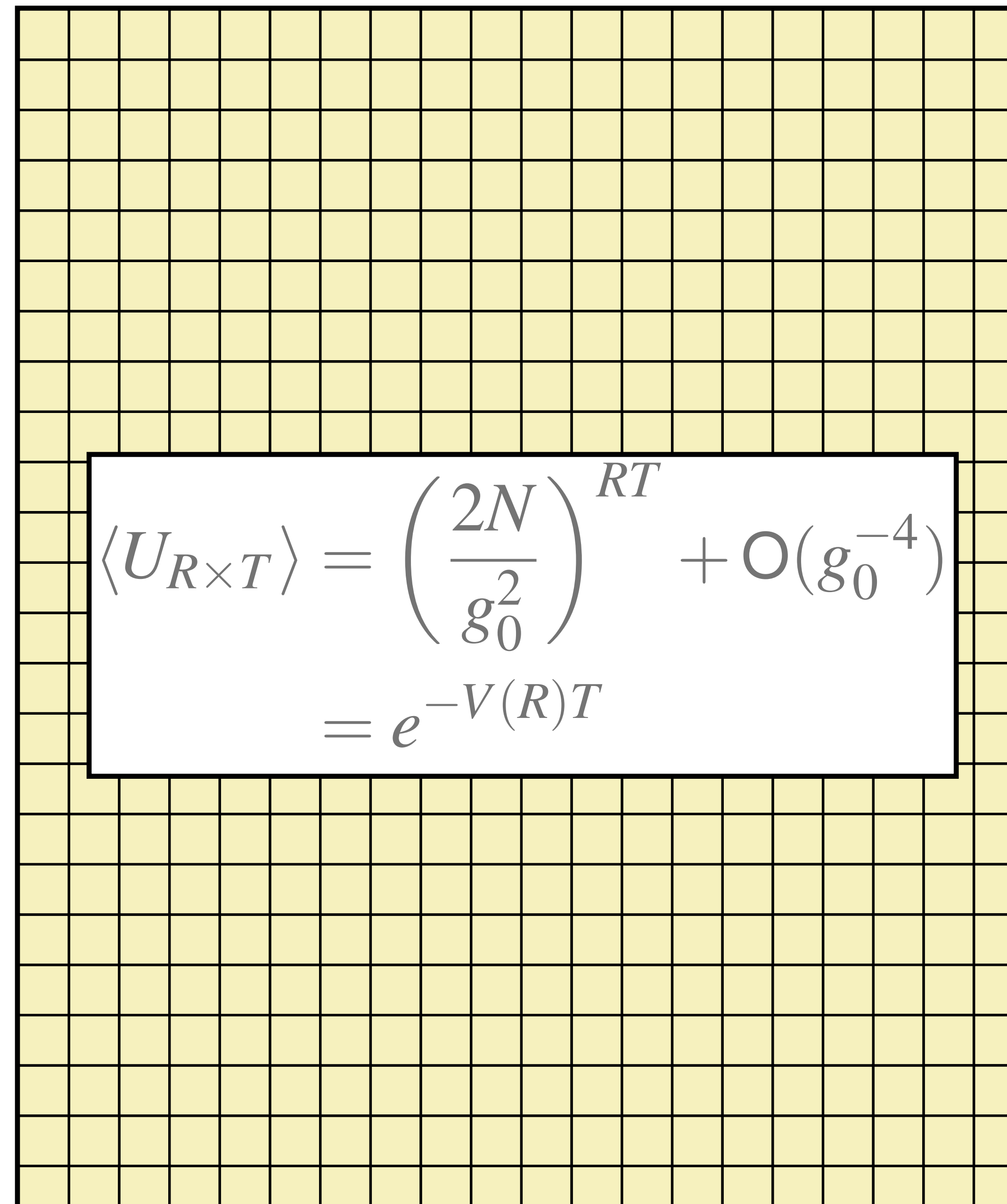


Fermion Path Integrals

Grassmann Variables

- Take a collection of fermions $\{\hat{\psi}_\alpha^\dagger, \hat{\psi}_\beta\} = \delta_{\alpha\beta}$, $\{\hat{\psi}_\alpha, \hat{\psi}_\beta\} = \{\hat{\psi}_\alpha^\dagger, \hat{\psi}_\beta^\dagger\} = 0$.

- Define “empty” and “full” states by

$$\hat{\psi}_\alpha|\text{empty}\rangle = 0, \qquad \hat{\psi}_\alpha^\dagger|\text{full}\rangle = 0,$$
$$\langle\text{empty}|\hat{\psi}_\alpha^\dagger = 0, \qquad \langle\text{full}|\hat{\psi}_\alpha = 0.$$

- Define field eigenstates by

$$|\psi\rangle = e^{\sum_\alpha \hat{\psi}_\alpha^\dagger \psi_\alpha}|\text{empty}\rangle, \qquad |\bar{\psi}\rangle = e^{-\sum_\alpha \bar{\psi}_\alpha \hat{\psi}_\alpha}|\text{full}\rangle,$$
$$\langle\psi| = \langle\text{full}|e^{-\sum_\alpha \hat{\psi}_\alpha^\dagger \psi_\alpha}, \qquad \langle\bar{\psi}| = \langle\text{empty}|e^{\sum_\alpha \bar{\psi}_\alpha \hat{\psi}_\alpha}.$$

- These satisfy $\hat{\psi}_\alpha|\psi\rangle = \psi_\alpha|\psi\rangle$, *etc.*, and (proofs as exercise)

$$1 = \int \prod_\alpha d\psi_\alpha \, |\psi\rangle\langle\psi| = \int \prod_\alpha d\bar{\psi}_\alpha \, |\bar{\psi}\rangle\langle\bar{\psi}|$$

- Suppose we have a Hamiltonian $\hat{H} = \sum_{\alpha\beta} \hat{\psi}^\dagger_\alpha M_{\alpha\beta} \hat{\psi}_\beta$ with $M_{\beta\alpha} = M^*_{\alpha\beta}$. Then

$$\langle \psi_N | e^{-\hat{H}\tau} | \psi_0 \rangle = \int \prod_{n=1}^{N-1} \mathcal{D}\psi_n \mathcal{D}\bar{\psi}_n \, \mathcal{D}\bar{\psi}_0 \langle \psi_N | \bar{\psi}_{N-1} \rangle \langle \bar{\psi}_{N-1} | e^{-\hat{H}a} | \psi_{N-1} \rangle \cdots \times$$

$$\langle \psi_{n+1} | \bar{\psi}_n \rangle \langle \bar{\psi}_n | e^{-\hat{H}a} | \psi_n \rangle \cdots \langle \psi_1 | \bar{\psi}_0 \rangle \langle \bar{\psi}_0 | e^{-\hat{H}a} | \psi_0 \rangle$$

- Some simple algebra shows:

$$\langle \psi_{n+1} | \bar{\psi}_n \rangle = e^{-\bar{\psi}_n \cdot \psi_{n+1}}$$

$$\langle \bar{\psi}_n | e^{-a\hat{\psi}^\dagger \cdot M \cdot \hat{\psi}} | \psi_n \rangle = e^{\bar{\psi}_n \cdot \psi_n - a\bar{\psi}_n \cdot M \cdot \psi_n} + \mathrm{O}(a^2)$$

- Assembling all the factors: (show $\langle \bar{\psi}_N | e^{-\hat{H}\tau} | \bar{\psi}_0 \rangle$ leads to the same thing)

$$Z := \int \mathcal{D}\psi_0 \, \langle \psi_0 | e^{-\hat{H}\tau} | \psi_0 \rangle = \int \prod_{n=0}^{N-1} \mathcal{D}\psi_n \mathcal{D}\bar{\psi}_n \, e^{-S}$$

$$S = a \sum_{n=0}^{N-1} \left\{ \bar{\psi}_n \cdot \frac{\psi_{n+1} - \psi_n}{a} + \bar{\psi}_n \cdot M \cdot \psi_n \right\}$$

Dirac Field

- Dirac field annihilates particles and creates antiparticles—
  - $\frac{1}{2}(1 \pm \gamma^4)\hat{\psi}_x$; so treat upper (lower) sign like $\hat{\psi}_x^{(\dagger)}$.
- Then the action becomes (Dirac $\beta = \gamma^4$)

$$S = a^d \sum_x \left\{ \bar{\psi}_x \beta \left[\gamma^4 \frac{\psi_{x+ae_4} - \psi_{x-ae_4}}{2a} - \frac{a}{2} \frac{\psi_{x+ae_4} + \psi_{x-ae_4} - 2\psi_x}{a^2} \right] \right\} + a^d \sum_{x,y} \bar{\psi}_x M_{xy} \psi_y$$

where M contains the mass and the spatial kinetic terms.

- Note the extra term: looks like a second-order time derivative.
- We will examine the contents of this action after a short comment.

gamma matrices

Transfer Matrix

- We've been "deriving" lattice field theory from canonical quantization.

- Most texts start with a (discretized) Euclidean path integral.

- Then the connection to a quantum system comes via the transfer matrix $\hat{\mathbb{T}}$ (strictly speaking an operator), playing the role of $e^{-\hat{H}a}$.

- The Hilbert space consists of eigenstates of $\hat{\mathbb{T}}$ with eigenvalue $\mathbb{T}$.

- Energy is then defined via $E = -a^{-1}\ln\mathbb{T}$; these energies are deduced from the exponential fall-off of correlation functions.

Fermion Propagators

Interaction on the Spatial Lattice

from now on $\bar{\psi}\beta = \bar{\psi}'$, drop prime

- Action is (new notation: $t_{\pm\mu}\psi_x = \psi_{x\pm ae_\mu}$)

$$S = a^d \sum_x \left\{ \bar{\psi}_x \beta \left[\gamma^4 \frac{t_4 - t_{-4}}{2a} - \frac{a}{2} \frac{t_4 + t_{-4} - 2}{a^2} \right] \psi_x \right\} + a^d \sum_{x,y} \bar{\psi}_x M_{xy} \psi_y$$

- Spatial part: $M_{xy} = m\beta\delta_{xy} + \beta\boldsymbol{\gamma}\cdot\boldsymbol{\partial}_{xy} - \frac{1}{2}\beta a \triangle_{xy}$, where

$$\partial_i = (t_i - t_{-i})/2a, \quad \triangle = \sum_i (t_i + t_{-i} - 2)/a^2$$

- $\triangle$ mimics time Wilson term, but both break chiral symmetry:
  - keep Wilson terms or omit them?

Naive Fermions

- Historically, naive fermions came first, by simply discretizing the (Euclidean) Dirac Lagrangian $\partial_\mu = (t_\mu - t_{-\mu})/2a$.

$$G(t,\boldsymbol{p}) = \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{a}{i\gamma^4 \sin p_4 a + i\sum_i \gamma^i \sin p_i a + ma} e^{ip_4 t},$$

$$= \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{a[-i\gamma^4 \sin p_4 a - i\sum_i \gamma^i \sin p_i a + ma]}{\sin^2 p_4 a + \sum_i \sin^2 p_i a + m^2 a^2} e^{ip_4 t},$$

- This expression has poles at $p_4 = iE$ and $p_4 = iE + \pi a^{-1}$
    - more than desired, and some energies not real !
    - low-energy solutions for p_i near 0, and also p_i near πa^{-1}.

Naive Fermion Energy Spectrum

$$
\begin{aligned}
G(t,\vec{p}) &= \int \frac{dp_4}{2\pi} e^{ip_4 t} \frac{a}{i\sum_\mu \gamma_\mu \sin(p_\mu a) + m_0 a} \\
&= \frac{1}{\sinh(2Ea)} \left[e^{-Et} \left(\gamma_4 \sinh(Ea) - i\sum_i \gamma_i \sin(p_i a) + m_0 a \right) \right. \\
&\quad \left. + \left(-e^{-Ea}\right)^{t/a} \left(-\gamma_4 \sinh(Ea) + i\sum_i \gamma_i \sin(p_i a) + m_0 a \right) \right]
\end{aligned}
$$

$$
\sinh^2(Ea) = \sum_i \sin^2(p_i a) + (m_0 a)^2
$$

Wilson Fermions

- Including the Wilson terms solves this “doubling” problem

$$G(t,\boldsymbol{p}) = \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{ae^{ip_4t}}{i\gamma^4 \sin p_4 a + i\sum_i \gamma^i \sin p_i a + ma + a^2 \frac{1}{2}\sum_\mu \hat{p}_\mu^2},$$

$$= \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{ae^{ip_4t}\ [-i\gamma^4 \sin p_4 a - i\sum_i \gamma^i \sin p_i a + ma + a^2 \frac{1}{2}\sum_\mu \hat{p}_\mu^2]}{\sin^2 p_4 a + \sum_i \sin^2 p_i a + (ma + a^2 \frac{1}{2}\sum_\mu \hat{p}_\mu^2)^2},$$

- This expression only has poles at $p_4 = iE$:
  - other poles have been projected out;
  - low energy solutions for p_i near 0 only.

Wilson Fermion Energy Spectrum

$$
\begin{aligned}
G(t,\boldsymbol{p}) &= \int_{-\pi/a}^{\pi/a} \frac{dp_4}{2\pi} \frac{a e^{ip_4 t}}{i\gamma^4 \sin p_4 a + i\sum_i \gamma^i \sin p_i a + ma + a^2 \frac{1}{2}\sum_\mu \hat{p}_\mu^2}, \\
&= \frac{a e^{-Et}}{2\sinh(Ea)} \frac{\gamma_4 \sinh(Ea) - i\sum_i \gamma_i \sin(p_i a) + m_0 a + \frac{1}{2}a^2\hat{\boldsymbol{p}}^2 + 1 - \cosh(Ea)}{1 + m_0 a + \frac{1}{2}a^2\hat{\boldsymbol{p}}^2},
\end{aligned}
$$

$$
\cosh(Ea) = 1 + \frac{1}{2}\frac{\sum_i \sin^2(p_i a) + (m_0 a + \frac{1}{2}a^2\hat{\boldsymbol{p}}^2)^2}{1 + m_0 a + \frac{1}{2}a^2\hat{\boldsymbol{p}}^2}
$$

- Wilson fermion action

$$S = a^d \sum_{x,\mu} \bar{\psi}_x \left[\gamma^\mu \frac{t_\mu - t_{-\mu}}{2a} - \tfrac{1}{2} a \frac{t_\mu + t_{-\mu} - 2}{a^2} \right] \psi_x + a^d \sum_x m_0 \bar{\psi}_x \psi_x$$

is almost completely satisfactory.

- Must finely tune m_0 to cancel explicit breaking of the Wilson term to reach spontaneously broken (Nambu-Goldstone) vacuum:

$$M_\pi^2 = (m_0 - m_{\mathrm{crit}}) B \to 0$$

- Alas, makes renormalization of composite operators similarly nasty: operators of different chirality can mix.

Staggered Fermions

(Banks-Kogut-)Susskind Fermions

- Another way of alleviating the doubling/chiral problem:
  - Kogut & Susskind put (anti)particles on even (odd) sites;
  - Banks, Kogut, & Susskind used 1 (not 2) component/site in $d = 1$+time;
  - Susskind studied 1 component/site in $d = 3$+time;
  - Kawamoto & Smit and Sharatchandra, Thun, & Weisz generalized Susskind fermions to 4 Euclidean dimensions.

Naïve Fermions

- The naive action is
$$S = \frac{a^3}{2}\sum_{x,\mu}\bar{\Upsilon}(x)\gamma_\mu\left[U_\mu(x)\Upsilon(x+\hat{\mu}) - U^\dagger_{x-\mu,\mu}\Upsilon(x-\hat{\mu})\right] + m_0 a\sum_x \bar{\Upsilon}(x)\Upsilon(x)$$
with Grassmann variables Υ^i_α, $\bar{\Upsilon}^i_\alpha$ on each site.

- Invariant under $\mathrm{SU}_{\mathrm{color}}(3)$, translations, hypercubic rotations, and $\mathrm{U}_V(n_f)\times\mathrm{U}_A(n_f)$.

- The naïve action also has a remarkable “doubling” symmetry [Karsten&Smit]: $\Upsilon \mapsto B_\mu\Upsilon, \quad \bar{\Upsilon} \mapsto \bar{\Upsilon}B_\mu^{-1}, \quad B_\mu = i\gamma_\mu\gamma_5(-1)^{x_\mu/a}$

- Generates a Clifford group Γ_4: $\{B_\mu, B_\nu\} = 2\delta_{\mu\nu}$.

Ramifications

- Doubling symmetries
  - map $p \mapsto p + \pi^A/a$, where π^A is a corner of the Brillouin zone;
  - shuffle Dirac indices.
- The 16 states are really there, *e.g.*, in loops:
  - running coupling: $\beta_0 = \frac{11}{3}N_c - \frac{2}{3}(16 n_f)$;
  - axial anomaly: $\mathfrak{A}_{\textsf{naive lat}} = (1-4+6-4+1)\mathfrak{A} = 0$ (chiral symmetry exact).

Staggering Magic

- But the lattice allows a transformation [Kawamoto & Smit].

$$\Upsilon(x) \mapsto \psi(x) = \Omega(x)\Upsilon(x), \quad \Omega(x) = \gamma_1^{n_1}\gamma_2^{n_2}\gamma_3^{n_3}\gamma_4^{n_4},$$
$$\bar{\Upsilon}(x) \mapsto \bar{\psi}(x) = \bar{\Upsilon}(x)\Omega^{-1}(x), \quad n = x/a.$$

- Ω clobbers the Dirac matrices:

$$\Omega^{-1}(x)\gamma_\mu\Omega(x \pm \hat{\mu}) = (-1)^{\Sigma_{\rho<\mu} n_\rho} =: \eta_\mu(x).$$

- The naïve action assumes a simpler form (plus mass term):

$$S = \frac{a^3}{2}\sum_{x,\mu}\bar{\psi}(x)\eta_\mu(x)\left[U_\mu(x)\psi(x+\hat{\mu}) - U^\dagger_{x-\mu,\mu}\psi(x-\hat{\mu})\right]$$

- Also attained by diagonalizing a maximal subgroup of doubling symmetry [Sharatchandra, Thun, & Weisz].

- Dirac index now trivial: $\langle\Upsilon(x)\bar{\Upsilon}(y)\rangle_U = \Omega(x)\Omega^{-1}(y)\langle\chi(x)\bar{\chi}(y)\rangle_U$ where χ—the staggered fermion—has one component/color/flavor, and (kinetic) action

$$S = \frac{a^3}{2}\sum_{x,\mu}\bar{\chi}(x)\eta_\mu(x)\left[U_\mu(x)\chi(x+\hat{\mu}) - U^\dagger_{x-\mu,\mu}\chi(x-\hat{\mu})\right]$$

- But now other symmetries are entangled.

- For example, translations become shifts:

$$\begin{aligned} S_\mu : \chi(x) &\mapsto \zeta_\mu(x)\chi(x+\hat{\mu}), \quad \bar{\chi}(x) \mapsto \zeta_\mu(x)\bar{\chi}(x+\hat{\mu}) \\ U_\nu(x) &\mapsto U_\nu(x+\hat{\mu}), \forall\nu; \quad \zeta_\mu(x) = (-1)^{\sum_{\rho>\mu} n_\rho} \end{aligned}$$

- Clifford again: $\{S_\mu, S_\nu\} = 2\delta_{\mu\nu}$.

- Shifts and spatial inversion do not commute.

Species Interpretation

- After "staggering" there are enough degrees of freedom for four species of Dirac fermion ($16 \div 4 = 4$):
  - called "taste" because they aren't used for u, d, s, c flavors.
- Perturbative and nonperturbative calculations show that such a structure emerges in the continuum limit:
  - anomaly in a taste-singlet axial current;
  - agreement with various tests of chiral symmetry, e.g., eigenvalue spectrum in accord with random matrix theory.

Chiral Fermions

e.g., M. Lüscher, arXiv:hep-th/0102028

Ginsparg-Wilson Magic

- Suppose we have an operator satisfying the Ginsparg-Wilson relation:

$$\gamma^5 \not{D} + \not{D}\gamma^5 = a\not{D}\gamma^5\not{D}, \qquad \text{and } \not{D}^\dagger = \gamma^5\not{D}\gamma^5$$

  See also Hasenfratz, Laliena, & Niedermayer.

- Then we can define a gauge-field-dependent $\hat{\gamma}^5 = \gamma^5(1 - a\not{D})$

$$\hat{\gamma}^{5\,\dagger} = \hat{\gamma}^5, \qquad (\hat{\gamma}^5)^2 = 1$$

- Take chiral transformations for two definitions of chirality [Lüscher]:

$$\begin{aligned} \psi_{R/L} &= \tfrac{1}{2}(1 \pm \hat{\gamma}^5)\psi, & \psi &\mapsto \exp[i\alpha\hat{\gamma}^5/2]\psi, \\ \bar{\psi}_{R/L} &= \bar{\psi}\tfrac{1}{2}(1 \mp \gamma^5), & \bar{\psi} &\mapsto \bar{\psi}\exp[i\alpha\gamma^5/2]. \end{aligned}$$

  The action $\bar{\psi}_R \not{D} \psi_R$ then describes a Weyl fermion, up to phase.

Domain-Wall Fermions

- One implementation of the Ginsparg-Wilson relation [D.B. Kaplan] starts with a 5-dimensional spacetime.
- Take Wilson fermions with “mass” term $a^{-1}[\theta(s) - \theta(-s)]$
- In a finite system, use antiperiodic b.c. in s.
- Then a right-(left-)handed Weyl fermion is localized at $s = 0$, $s = N_s - 1$, which combine to form a Dirac fermion.
- In practice, small chiral symmetry breaking $\sim \exp(-N_s)$.

Overlap Fermions

- Narayanan & Neuberger pursued an approach to obtaining the phase in a chiral gauge theory, which involved an infinite matrix.

- Also based on Wilson fermions.

- If you give up on the phase, the construction simplifies and suggests the Dirac operator [Neuberger]:

$$\not{D} = \frac{1}{a}\left(1 - \frac{1 - a\not{D}_{\mathrm{W}}}{|1 - a\not{D}_{\mathrm{W}}|}\right)$$

- Can verify that this operator satisfies the GW relation.

- Lüscher symmetry seems to violate *CP*, transforming ψ and $\bar{\psi}$ differently.
- Considering Lüscher and his charge conjugate, Mandula uncovered a huge symmetry group, in which *CP* acts as an automorphism.
- Extra generators vanish in the spacetime continuum limit,
  - but do not go away in the limit of a spatial lattice with continuous time,
  - so GW-satisfying operators do not have a transfer operator or Hamiltonian.

Monte Carlo Integration

A Simple (Dumb) Algorithm

- Choose C random configurations of the $\{\phi\}$ variables:

$$Z = \int \mathcal{D}\phi\, e^{-S} = \lim_{C\to\infty} \frac{1}{C} \sum_{c=0}^{C-1} \exp\left[-S\left(\{\phi\}^{(c)}\right)\right],$$

$$\int \mathcal{D}\phi\, f(\{\phi\})e^{-S} = \lim_{C\to\infty} \frac{1}{C} \sum_{c=0}^{C-1} f(\{\phi\}^{(c)}) \exp\left[-S\left(\{\phi\}^{(c)}\right)\right].$$

- An estimate of the LHS is obtained for finite C.
- This method is hopeless, because S is extensive, S ~ # dof.
- Most samples make negligible contribution and are a waste of time.

Importance Sampling

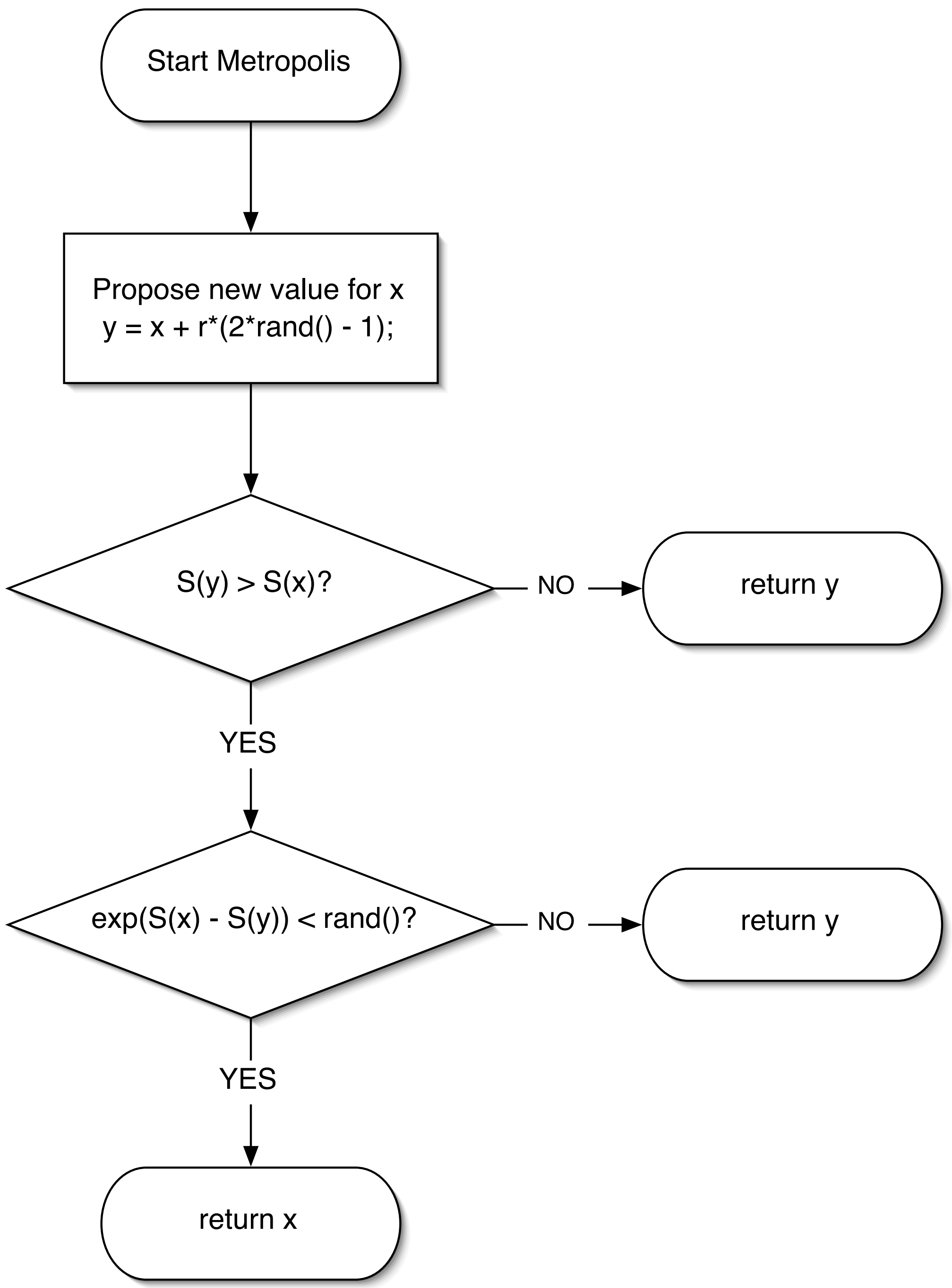
- Instead of completely random configurations, choose them with Boltzmann weight $\exp[-S(\{\phi\})]$. Then

$$\frac{1}{Z}\int \mathcal{D}\phi\, f(\{\phi\})e^{-S} = \lim_{C\to\infty}\frac{1}{C}\sum_{c=0}^{C-1} f(\{\phi\}^{(c)}).$$

- This is possible, when S is bounded below, as it is for a Euclidean action of scalar and/or gauge fields.

- Quantum field theory has been reduced to the design of random number generators.

Metropolis Method



- Requires only $e^{-S} \geq 0$.
- Visit each x_i in turn; follow flow chart.
- `rand()` $\in [0,1)$.
- Choose r to accept 40–50%.
- Keep configurations after enough sweeps to decorrelate.
- Adapt update step for other degrees of freedom (*e.g.*, gauge fields).

Lattice Gauge Theory

- QCD functional integral can always be simplified:

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \, \mathcal{D}\psi \mathcal{D}\bar{\psi} \exp\left(-S\right) [\bullet]$$

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \prod_{f=1}^{n_f} \det(\not{D} + m_f) \exp\left(-S_{\text{gauge}}\right) [\bullet']$$

- Fermion determinant is computationally extremely challenging:
    - brute force would require many operations;
    - nonlocal influence on gauge field $\mathrm{Det}(\not{D} + m_f) = e^{\mathrm{Tr}\ln(\not{D} + m_f)}$

Lattice Gauge Theory

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Lattice Gauge Theory

- QCD functional integral can always be simplified:

$$\langle \bullet \rangle = \frac{1}{Z} \int \underbrace{\boxed{\mathcal{D}U}}_{\text{MC}} \underbrace{\boxed{\mathcal{D}\psi \mathcal{D}\bar{\psi}}}_{\text{hand}} \exp\left(-S\right) [\bullet]$$

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \prod_{f=1}^{n_f} \det(\not{D} + m_f) \exp\left(-S_{\text{gauge}}\right) [\bullet']$$

- Fermion determinant is computationally extremely challenging:
  - brute force would require many operations;
  - nonlocal influence on gauge field $\mathrm{Det}(\not{D} + m_f) = e^{\mathrm{Tr}\ln(\not{D} + m_f)}$

Hybrid Monte Carlo

Propose new value for x
y = x + r*(2*rand() - 1);

- Introduced new fictitious momentum, conjugate to the $U_\mu(x)$:
  - "time" is computer time;
  - Hamilton's equations for the momentum $\Pi_\mu(x)$ and $U_\mu(x)$:

$$\dot{U}_\mu(x) = \Pi_\mu(x), \quad \dot{\Pi}_\mu(x) = -\frac{\partial[S - \operatorname{Tr}\ln(\not{D} + m)]}{\partial U_\mu(x)}$$

    with care taken to keep $U_\mu(x)$ in the Lie group.

  - At the end of a "trajectory", accept or reject with Metropolis.
  - Then refresh with new, random $\Pi_\mu(x)$.

Monte Carlo “Simulation”

- Choose sequence of bare couplings $g_0(a)$ and $am_0(a)$, such that physical quantities are independent of a:
  - gauge coupling ↔ lattice spacing a in MeV^{-1};
  - quark masses ↔ suitable meson mass $M_\pi^2, M_K^2, M_{D_s}, M_{B_s}$
- Generate large ensemble of lattice gauge fields
- Obtain statistical estimate of correlation functions from the averages and covariance in the ensemble.

Correlators Yield Masses & Matrix Elements

- Two-point functions for masses, $\pi(t) = \sum_{\boldsymbol{x}} \bar{\psi}_d \gamma^5 \psi_d(\boldsymbol{x}, t)$:

$$\langle \pi(t)\pi^\dagger(0)\rangle = \sum_n |\langle 0|\hat{\pi}|\pi_n\rangle|^2 \exp(-\boxed{m_{\pi_n}}t)$$

- Two-point functions for decay constants:

$$\langle J(t)\pi^\dagger(0)\rangle = \sum_n \boxed{\langle 0|\hat{J}|\pi_n\rangle}\langle \pi_n|\hat{\pi}^\dagger|0\rangle \exp(-m_{\pi_n}t)$$

- Three-point functions for form factors, mixing:

$$\langle \pi(t)J(u)B^\dagger(0)\rangle = \sum_{mn} \langle 0|\hat{\pi}|\pi_m\rangle \boxed{\langle \pi_n|\hat{J}|B_m\rangle}\langle B_m|\hat{B}^\dagger|0\rangle \times \exp[-m_{\pi_n}(t-u) - m_{B_m}u]$$

- LHS needs supercomputers; RHS needs students, postdocs, ….

Statistics for Masses and Matrix Elements

- Hadron masses and, consequently, hadronic matrix elements are nonlinear functions of the correlation functions:
  - function defined implicitly by the fitting function.
- To compute their statistic errors need to repeat the simulation?
- Create pseudo-ensembles from the original one:
  - eliminate individual (or pairs, …) configurations—jackknife;
  - draw configurations at random, allowing repeats—bootstrap.

- Bootstrap and jackknife have numerous nice and understood properties [Efron]:
    - cumulants of bootstrap distribution reproduce underlying cumulants;
    - cumulants of jackknife distribution differ from underlying cumulants by factor C^{-k}.
- Practical: arbitrarily complicated analysis can be repeated on the set of pseudo-ensembles, yielding a histogram for the output of the analysis.
- Computationally demands large but small compared to the whole enterprise.

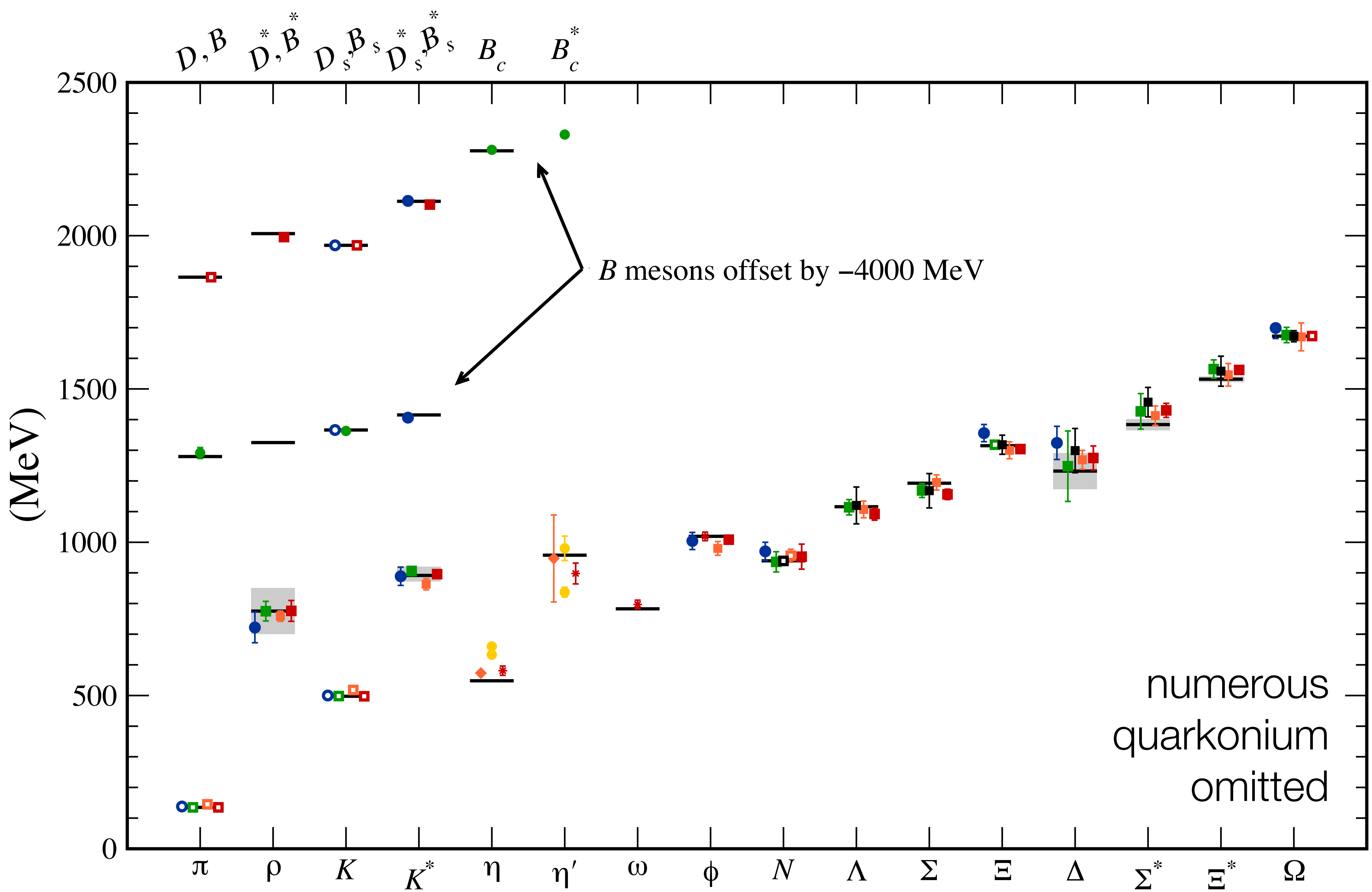
Lattice Data and Effective Field Theory

- Discretization effects of lattice described w/ Symanzik effective field theory.
- The finite volume provides an IR cutoff: effective field theory in a box:
    - loop integrals become finite sums;
    - these effects are either very small or very useful (absorptive parts).
- Sometimes the light quarks aren't light enough: chiral perturbation theory:
    - replace the computer's pion cloud with Nature's.
- Sometimes heavy-quark masses have $m_Q a \approx 1$: HQET or NRQCD.

Verflixtes Zeug! Does It Work?

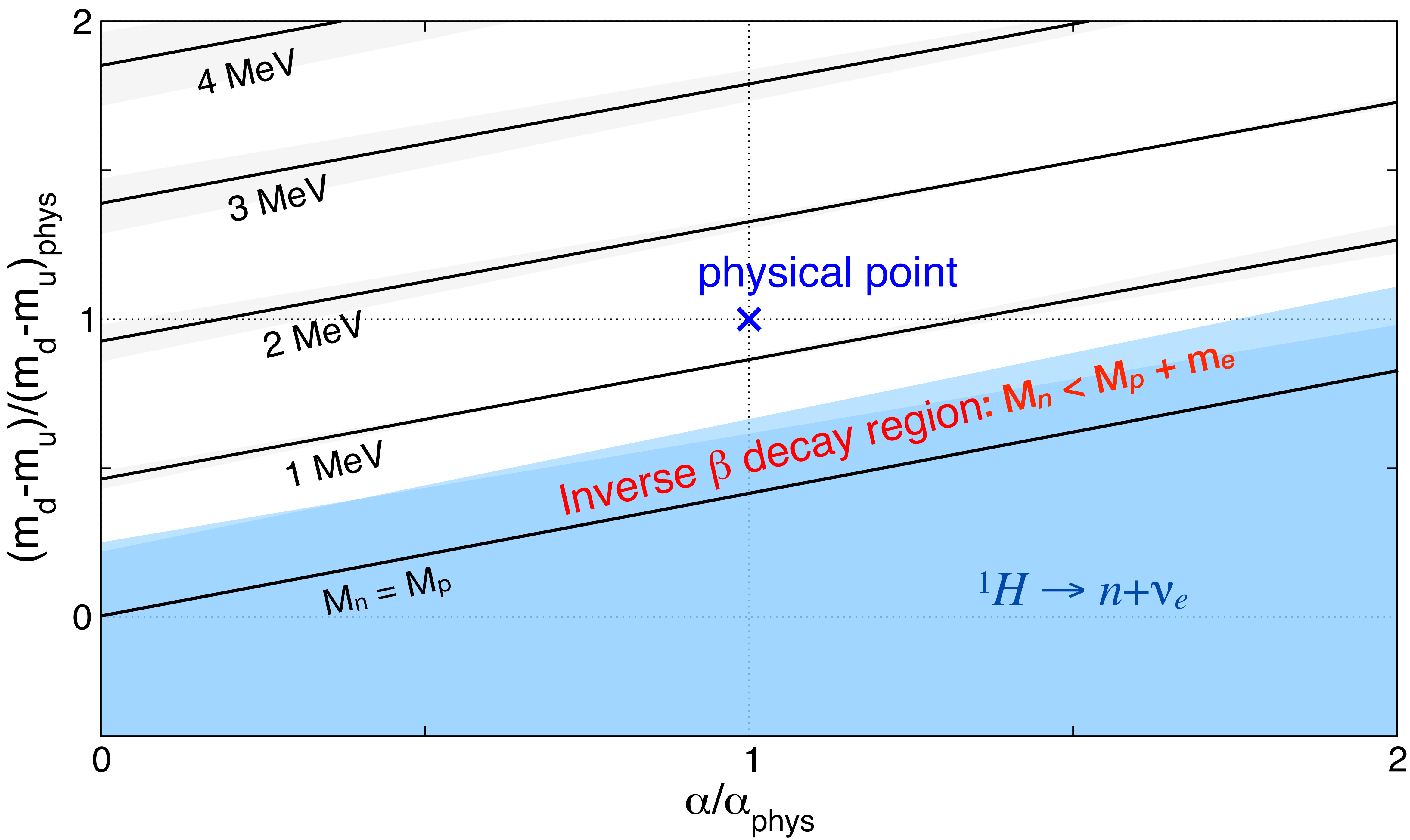
QCD Hadron Spectrum

π…Ω: BMW, MILC, PACS-CS, QCDSF; ETM (2+1+1);
η-η′: RBC, UKQCD, Hadron Spectrum (ω);
D, B: Fermilab, HPQCD, Mohler&Woloshyn



Neutron-Proton Mass Difference

BMW Collab., arXiv:1406.4088 (see also Horsley *et al*. arXiv:1508.06401)



Tomorrow: more numerical results, focusing on flavor physics. Till then, vielen herzlichen Dank!

Solutions to Some Exercises

Correlation Functions

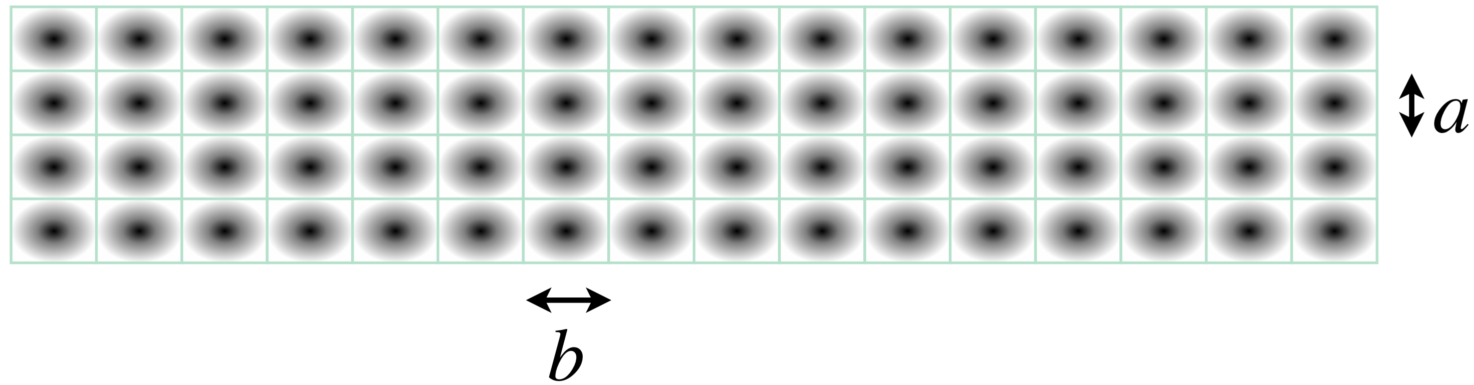
- One idea: insert complete sets of states of the Hamiltonian (or transfer operator):

$$Z = \mathrm{Tr}\, e^{-\hat{H}\tau} = \sum_n \langle n|e^{-\hat{H}\tau}|n\rangle = \sum_n e^{-E_n\tau} \overset{\text{large } \tau}{\rightarrow} e^{-E_0\tau}$$

$$\langle Q(x)\rangle = \frac{1}{Z}\,\mathrm{Tr}\, Q(\hat{x})e^{-\hat{H}\tau} = \frac{1}{Z}\sum_n e^{-E_n\tau}\langle n|Q(\hat{x})|n\rangle \overset{\text{large } \tau}{\rightarrow} \langle 0|Q(\hat{x})|0\rangle$$

$$\begin{aligned}\langle Q_1(t_1)Q_2(t_2)\rangle_c &= \frac{1}{Z}\sum_{nn'}\langle n|e^{-\hat{H}(\tau-t_1)}\hat{Q}_1(t_1)|n'\rangle\langle n'|e^{-\hat{H}(t_1-t_2)}\hat{Q}_2(t_2)e^{-\hat{H}t_2}|n\rangle \\ &\quad - \frac{1}{Z}\sum_n\langle n|e^{-\hat{H}(\tau-t_1)}\hat{Q}_1(t_1)e^{-\hat{H}t_1}|n\rangle\frac{1}{Z}\sum_{n'}\langle n'|e^{-\hat{H}(\tau-t_2)}\hat{Q}_2(t_2)e^{-\hat{H}t_2}|n'\rangle \\ &\overset{\text{large } \tau}{\rightarrow} \sum_{n'\neq 0}\langle 0|\hat{Q}_1(t_1)|n'\rangle\langle n'|\hat{Q}_2(t_2)|0\rangle e^{-(E_{n'}-E_0)(t_1-t_2)} + \sum_{n\neq 0}\langle 0|\hat{Q}_2(t_2)|n\rangle\langle n|\hat{Q}_1(t_1)|0\rangle e^{-(E_n-E_0)(\tau+t_2-t_1)} \\ &\overset{\text{large } \tau,(t_1-t_2)}{\rightarrow} \langle 0|\hat{Q}_1(t_1)|1\rangle\langle 1|\hat{Q}_2(t_2)|0\rangle e^{-(E_1-E_0)(t_1-t_2)} + \langle 0|\hat{Q}_2(t_2)|1\rangle\langle 1|\hat{Q}_1(t_1)|0\rangle e^{-(E_1-E_0)(\tau+t_2-t_1)}\end{aligned}$$

- Try this for a three-point function, too.



Action:

$$S = ab \sum_{n,j} \left\{ \tfrac{1}{2} \left(\frac{\phi_{n+1,j} - \phi_{n,j}}{a} \right)^2 + \tfrac{1}{2}\mu^2 \phi_{n,j}^2 - \tfrac{1}{2}\kappa \phi_{n,j} \left(\phi_{n,j-1} + \phi_{n,j+1} \right) \right\},$$

Fourier transform:

$$\phi_{n,j} = \int_{-\pi/a}^{\pi/a} \frac{d\omega}{2\pi} \int_{-\pi/b}^{\pi/b} \frac{dk}{2\pi} e^{i[na\omega + jbk]} \varphi(\omega, k),$$

Plug in and collect terms:

$$S = \tfrac{1}{2} \int_{-\pi/a}^{\pi/a} \frac{d\omega}{2\pi} \int_{-\pi/b}^{\pi/b} \frac{dk}{2\pi} \, \varphi^*(\omega, k) \left[\hat{\omega}^2 + \kappa b^2 \hat{k}^2 + (\mu^2 - 2\kappa) \right] \varphi(\omega, k)$$

where $\hat{\omega} = 2a^{-1} \sin \tfrac{1}{2}\omega a$, $\hat{k} = 2b^{-1} \sin \tfrac{1}{2} kb$. Identify $\mu^2 - 2\kappa = m^2$, $\kappa = b^{-2}$.

return

Dirac Matrix Conventions

- Euclidean indices, $1, 2, 3, 4$; metric $\delta^{\mu\nu} = \mathrm{diag}(1,1,1,1)$.
- Clifford algebra $\{\gamma^\mu,\gamma^\nu\} = 2\delta^{\mu\nu}$; all γ^μ are Hermitian.
- Chiral $\gamma^5 = \gamma^1\gamma^2\gamma^3\gamma^4$; also Hermitian.
- Spin $[\gamma^\mu,\gamma^\nu] = -2i\sigma^{\mu\nu}$; $\sigma^{\mu\nu}$ is also Hermitian.
- Continue back to Minkowski with $g^{\mu\nu} = \mathrm{diag}(-1,1,1,1)$,
  - and time components $x^0 = -ix^4$; $\gamma^0 = -i\gamma^4$; $p^0 = E = -ip^4$.

$$\gamma^4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix},$$

$$\gamma^5 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

return