Stabilised Wilson fermions – from large-scale to master-field simulations

パトリック・フリッツシュ

日立 助教授 で 高性能 コンピューティング

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

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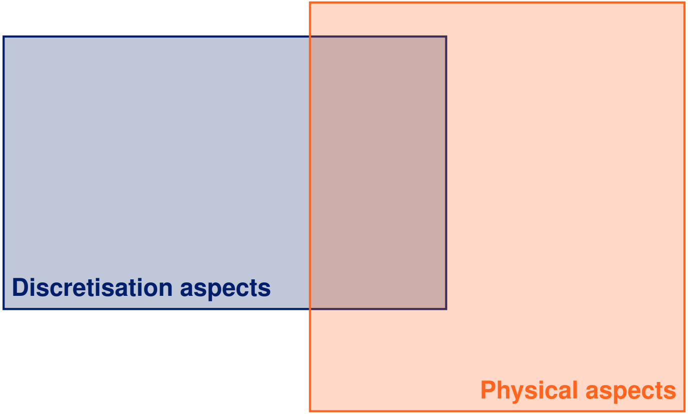
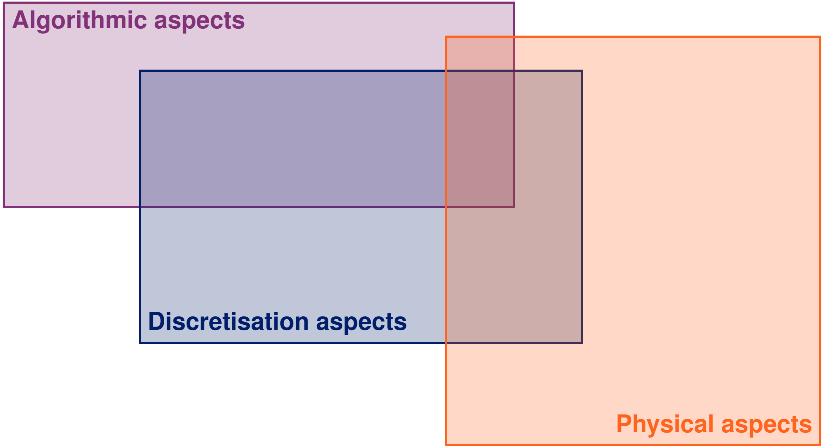
Seek balance in numerical simulations



Seek balance in numerical simulations



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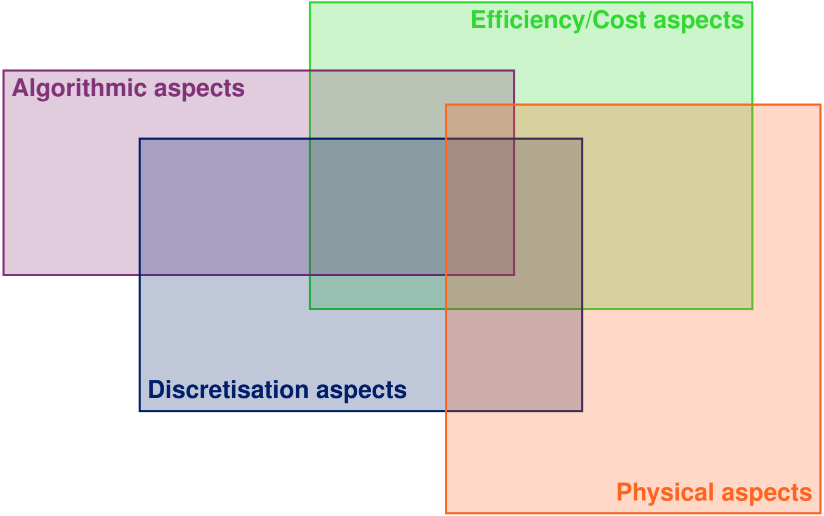

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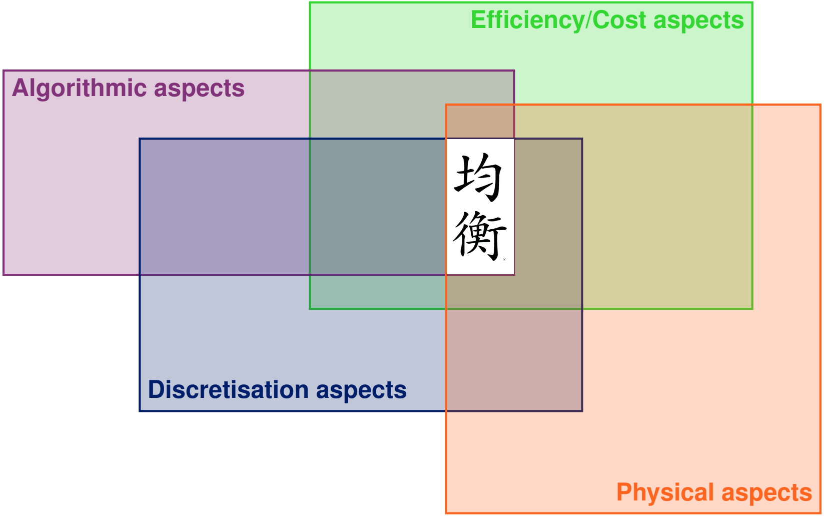

Lattice QCD

4D Euclidean space with gauge group $\mathrm{SU}(3)$ and N_f quark flavours:

$$\mathcal{L}^{\mathrm{QCD}} = -\frac{1}{2g^2}\mathrm{Tr}[F_{\mu\nu}F_{\mu\nu}] + \sum_{i=1}^{N_\mathrm{f}} \overline{\psi}_i[\gamma_\mu D_\mu + m_i]\psi_i$$

- gauge invariant
- $N_\mathrm{f}+1$ free parameters $\left\{\begin{array}{ll}\text{strong coupling} & g^2 \\ \text{quark masses} & m_i, i=1,\ldots,N_\mathrm{f}\end{array}\right\}$ require physical input

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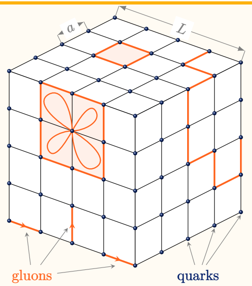
Lattice regularization

- lattice spacing (a) and physical volume ($V_4 = L^4$) $\rightarrow$ finite lattice Λ
- fermions ψ, $\overline{\psi}$ on lattice sites $x \in \Lambda$
- gluons $U(x+a\hat{\mu}, x) \sim e^{-iA_\mu(x)}$ on lattice links
- a variety of lattice actions $\mathcal{S} = \mathcal{S}_\mathrm{G} + \mathcal{S}_\mathrm{F}$



Choose a lattice discretisation

Only minor differences in discretised gauge actions.

Fermion action	Advantages	Disadvantages
Clover-improved Wilson	computationally fast	breaks chiral symmetry needs operator improvement
Twisted-mass Wilson	computationally fast automatic improvement	breaks chiral symmetry flavour breaking effects
staggered type	computationally fast	fourth root problem complicated contractions
domain wall	improved chiral symmetry	computationally demanding needs tuning
overlap	exact chiral symmetry	computationally expensive

These actions differ at order a^2.

$$\Longrightarrow \langle O \rangle_{\mathrm{lat}} = \langle O \rangle_{\mathrm{cont}} + \mathrm{O}(a^2)$$

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Here we use Clover-improved Wilson fermions.

Markov Chain Monte Carlo simulations of QCD

Goal: produce sequence of gauge fields $\{U_i | i = 1, \ldots, N_U\}$

$\Rightarrow$ expectation values of physical observables $\mathcal{O}$ from ensemble-average

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U] \, \mathcal{O} \, e^{-\mathcal{S}_{\mathrm{G}}[U] - \mathcal{S}_{\mathrm{eff}}[U]}$$

$$\approx \frac{1}{N_U} \sum_{i=1}^{N_U} \mathcal{O}[U_i] \, ,$$

with Wilson–Dirac operator Q and

$$e^{-\mathcal{S}_{\mathrm{eff}}} \simeq \prod_f \det(Q_f) \, , \qquad f \in \{u, d, s, \ldots\}$$

The standard lattice QCD approach

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employs **Hybrid Monte-Carlo (HMC) algorithm**

- with importance sampling
- draw conjugate momenta π & integrate molecular dynamics (MD) equations
- made exact by (global) Metropolis accept-reject step ($\Delta H = \Delta \mathcal{S}$)
- ergodicity maintained by redrawing the momenta

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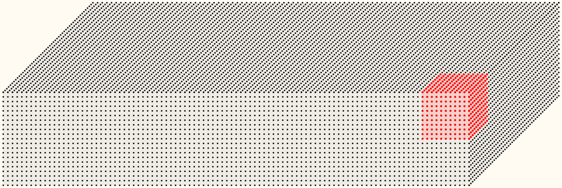
and **advanced techniques to solve large linear systems**:

- various (Krylov) solvers
- precondition techniques (eo, det-splitting, ...)
- mixed-precision arithmetic
- symplectic integrators w/ multiple time-scales
- architecture dependent optimisations
- ...

Master-field lattice

single master-field replaces classical (Markov chain) ensemble

$$N_V = \frac{V_4^{\mathrm{mf}}}{V_4} = \prod_{i=0}^{3} N_i \simeq 100 - 1000 \approx N_U$$



$\Rightarrow$ expectation values from translation average $\langle\!\langle \mathcal{O} \rangle\!\rangle$

$$\langle \mathcal{O}(x) \rangle = \langle\!\langle \mathcal{O}(x) \rangle\!\rangle + \mathrm{O}(N_V^{-1/2}) \,,$$

$$\langle\!\langle \mathcal{O}(x) \rangle\!\rangle = \frac{1}{N_V} \sum\nolimits_z \mathcal{O}(x+z)$$

based on **stochastic locality** due to short-range interaction

- QCD field variables in distant regions fluctuate largely independent
- their distribution is everywhere the same (with periodic bc.)
- translation averages replace ensemble averages provided localisation range of $\mathcal{O} \ll L$ (lattice extent)
- uncertainties estimated using standard methods through correlations in space

Concept successfully applied to SU(3) YM theory.[2]

It isn't straightforward to simulate QCD on very large lattices!

A (naive) stochastic picture of Lattice QCD

Sketch employs Gaussian for simplicity

Simulating QCD $\rightsquigarrow$ induces sampling distribution of gauge potential $A_\mu(x)$ $\leftrightsquigarrow$ (a random variable)

Requires solving the lattice-Dirac equation

$$D\psi(x) = \eta(x)\ , \quad \text{with} \quad D(M_0) = \tfrac{1}{2}\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\tfrac{1}{2}\nabla^*_\mu\nabla_\mu + M_0 + ac_{\rm sw}\,\tfrac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

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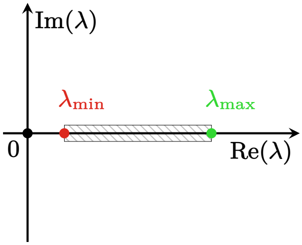
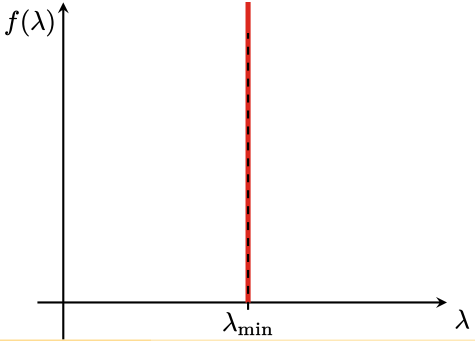
Bounded spectrum of $\gamma_5 D$:



$$g_0^2 = 0$$

Lowest eigenvalue distribution:



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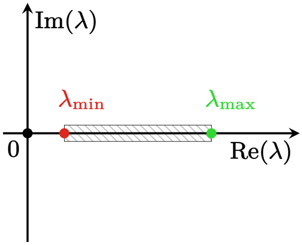
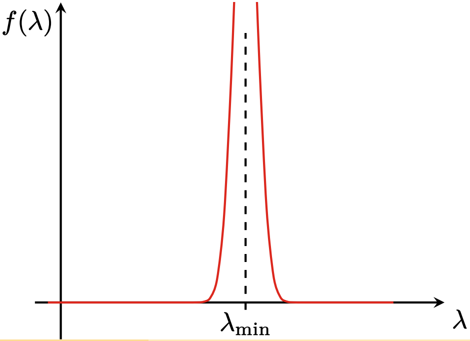


$$g_0^2 \gtrsim 0$$

Lowest eigenvalue distribution:



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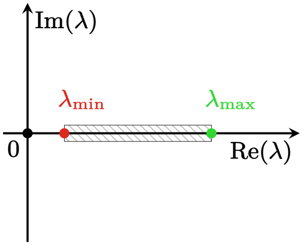
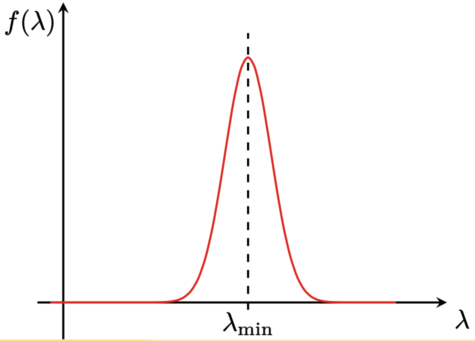


$g_0^2 > 0$

Lowest eigenvalue distribution:



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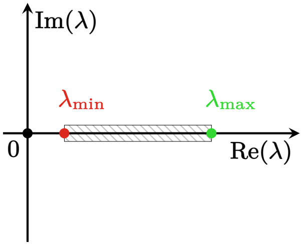
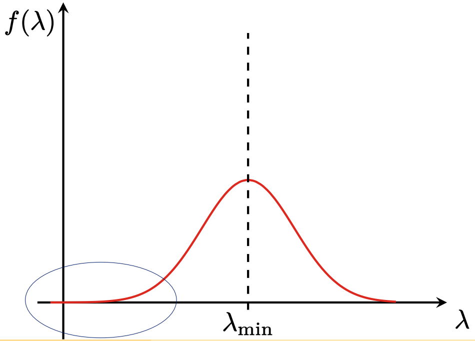


$g_0^2 \gg 0$

Lowest eigenvalue distribution:



increased change of encountering near-zero mode

Critical aspects of lattice QCD simulations

Various choices (strongly) impact simulation cost and reliability of a simulation.

Discretisation aspects

- gauge action (impacts UV fluctuations)
- fermion action (lattice Dirac operator D)
- spectral gap of $D \sim \lambda_{\rm min}$ (near zero-modes in MD evolution)

Algorithmic aspects

- update algorithm: Hybrid Monte-Carlo (exploration of phase space)
- integration schemes and length (symplectic integrators)
- numerical precision, e.g. in global sums (Metropolis step) (double precision)
- solver parameters (stability & performance)

Physical aspects

- coarse a $\rightsquigarrow$ promote large fluctuations of gauge field (roughness of U fields)
- small $m_{\rm ud}$ $\rightsquigarrow$ result in small eigenvalues $\lambda_{\rm min}(m_{\rm ud})$ of lattice Dirac operator
- large $(L/a)^4$ $\rightsquigarrow$ increase risk of exceptional behaviour (e.g. from MD force)

Large potential for algorithmic instabilities and precision issues. $\Rightarrow$ Additional stability measures required.[3]

Stabilising measures for QCD

a.k.a.

Stabilised
Wilson
Fermions

Stabilising measures for QCD[1, 3]

include …

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- new fermion action / Wilson–Dirac operator
- new algorithm: stochastic molecular dynamics (SMD) algorithm[4–7]
- solver stopping criteria

$$\|D\psi - \eta\|_2 \leq \rho\|\eta\|_2 \ ,$$

$$\|\eta\|_2 = \left(\sum\nolimits_x \big(\eta(x), \eta(x)\big)\right)^{1/2} \propto \sqrt{V}$$

✓ V-independent uniform norm: $\|\eta\|_\infty = \sup_x \|\eta(x)\|_2$

$\|\eta\|_\infty$ for all forces ($\mathrm{res}_F = 10^{-12} \ldots 10^{-10}$) and some actions ($\mathrm{res}_\phi = 10^{-12}$)

- global Metropolis accept-reject step

(numerical precision must increase with V)

$$\Delta H \propto \epsilon^p \sqrt{V}$$

✓ quadruple precision in global sums

- well-established techniques

✓ Schwarz Alternating Procedure, local deflation, multi-grid, …
even-odd & mass-preconditioning, multiple time-scales, …

New Wilson–Dirac operator[3]

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with exponential clover term

$$D = \tfrac{1}{2}\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\tfrac{1}{2}\nabla_\mu^*\nabla_\mu + \underline{M_0 + ac_{\rm sw}\tfrac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}}$$

Even-odd preconditioning:

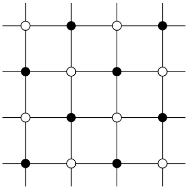
$$\hat{D} = D_{\rm ee} - D_{\rm eo}(D_{\rm oo})^{-1}D_{\rm oe}$$

with diagonal part[8] $(M_0 = 4 + m_0)$

$$D_{\rm ee} + D_{\rm oo} = M_0 + c_{\rm sw}\tfrac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

✗ not protected from arbitrarily small eigenvalues

small mass, rough gauge field, large lattice promote instabilities in $(D_{\rm oo})^{-1}$



$$D = \tfrac{1}{2}\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\tfrac{1}{2}\nabla_\mu^*\nabla_\mu + \underline{M_0 + ac_{\mathrm{sw}}\tfrac{\mathrm{i}}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}}$$

Even-odd preconditioning:

$$\hat{D} = D_{\mathrm{ee}} - D_{\mathrm{eo}}(D_{\mathrm{oo}})^{-1}D_{\mathrm{oe}}$$

with diagonal part[8] $(M_0 = 4 + m_0)$

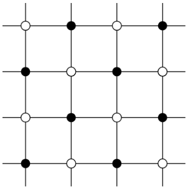
$$D_{\mathrm{ee}} + D_{\mathrm{oo}} = M_0 + c_{\mathrm{sw}}\tfrac{\mathrm{i}}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \quad \sim \quad \boxed{M_0 \exp\left\{\frac{c_{\mathrm{sw}}}{M_0}\frac{\mathrm{i}}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right\}}$$

✗ not protected from arbitrarily small eigenvalues

small mass, rough gauge field, large lattice promote instabilities in $(D_{\mathrm{oo}})^{-1}$

✓ Employ exponential mapping

- regulates UV fluctuations
- valid Symanzik expansion/improvement
- guarantees invertibility



New Wilson–Dirac operator[3]

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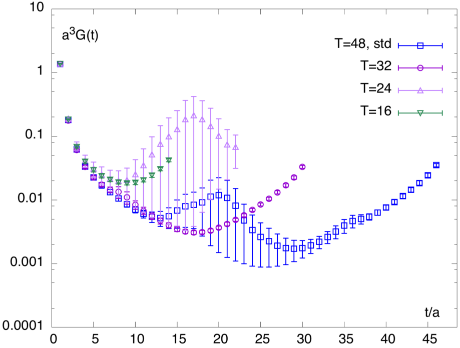
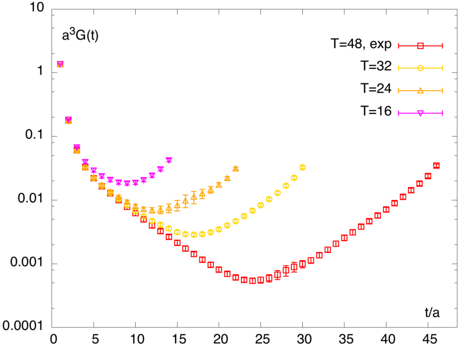
$$D = \tfrac{1}{2}\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\tfrac{1}{2}\nabla^*_\mu\nabla_\mu + \underline{M_0 + ac_{\rm sw}\tfrac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}} \sim \boxed{M_0 \exp\left\{\frac{c_{\rm sw}}{M_0}\frac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right\}} \qquad (M_0 = 4 + m_0)$$

Pion correlator in pure Yang–Mills theory $(N_{\rm f} = 0, m_\pi \simeq 200\,{\rm MeV}, \beta = 6.0, a \simeq 0.094\,{\rm fm})$:

std. Wilson–Dirac operator



new Wilson–Dirac operator



Stochastic Molecular Dynamics (SMD) algorithm[4–7]

Refresh $\pi(x,\mu)$, $\phi(x)$ by random field rotation

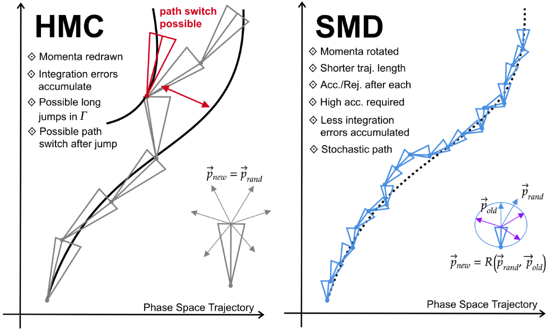
$$\pi \to c_1\pi + c_2 v\,, \qquad c_1 = e^{-\epsilon\gamma}\,,\quad c_1^2 + c_2^2 = 1\,,\qquad v(x,\mu),\eta(x) \in \mathcal{N}(0,1)$$

$$\phi \to c_1\phi + c_2 D^\dagger\eta\,,$$

($\gamma > 0$: friction parameter; ϵ: MD integration time)

+ MD evolution + accept-reject step + repeat. If rejected: $\{\tilde{U},\tilde{\pi},\tilde{\phi}\} \to \{U,-\pi,\tilde{\phi}\}$

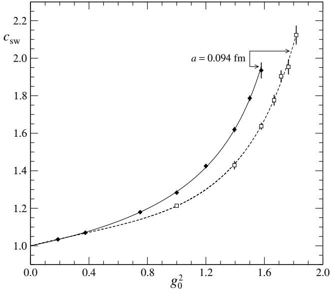
- ergodic[9] for sufficiently small ϵ (typically $\epsilon < 0.35$ vs. $\tau = 1-2$)
- exact algorithm
- significant reduction of unbounded energy violations $|\Delta H| \gg 1$
- a bit “slower“ than HMC but compensated by shorter autocorrelation times
- smooth changes in ϕ_t, U_t improve update of deflation subspace



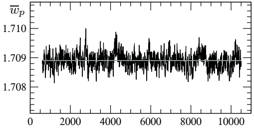
Comparison to traditional Wilson–Clover action

e.g: $N_\mathrm{f} = 2+1$ data of Coordinated Lattice Simulations (CLS) effort[10–12]

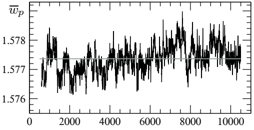
Non-perturbative improvement:



plaquette (energy density) with SMD: $a = 0.095\,\mathrm{fm}$



exp. clover (A_1)

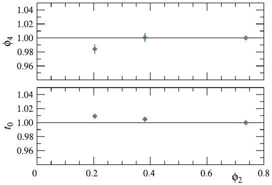


std. clover (X_1)

Chiral trajectory:

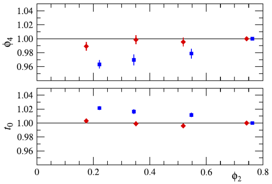
$$t_0 \text{ and } \phi_4 \equiv 8t_0(\tfrac{1}{2}m_\pi^2 + m_\mathrm{K}^2) = 1.11 \sim \mathrm{Tr}[M_\mathrm{q}]$$

Stabilised Wilson



$a = 0.095\,\mathrm{fm}$

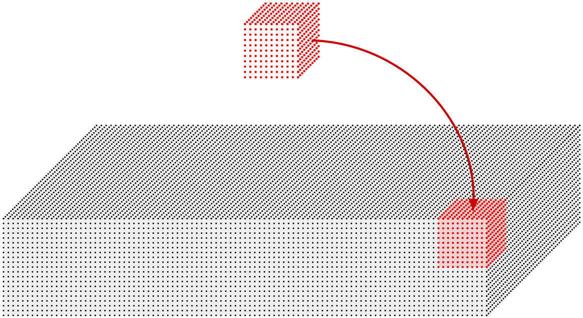
Standard Wilson



$a = 0.064, 0.086\,\mathrm{fm}$

key observation

- smoother fluctuations
- smaller lattice spacing effects

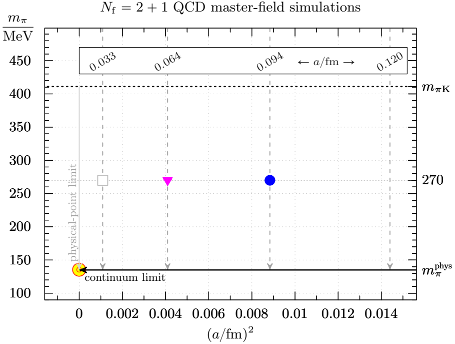


- *negligible finite-volume effects*
- *evade topological-freezing problem*
- *access to new kinematic regimes*
- *ideal for position-space methods*
- *new tool to perform different/new calculations*

$N_f = 2 + 1$+all stabilising measures[3]

- M. Cé, M. Bruno, J. Bulava, A. Francis, P. F., J. Green, M. Lüscher, A. Rago, M. Hansen
- $m_\pi = 270\,\mathrm{MeV} = 2m_\pi^{\text{phys}}$
- `openQCD-2.0`, `openQCD-2.4`[13]
- Master-field error estimation discussed in `JHEP11(2023)167`[14]
- In preparation:
  paper on master-field simulations & spectrum

Summary of $N_f = 2+1$ master-field simulations



Std. lattice: $m_\pi = 270\,\text{MeV}$, $V_4 = 32^4$, $L = 3\,\text{fm}$, $m_\pi L = 4.1$

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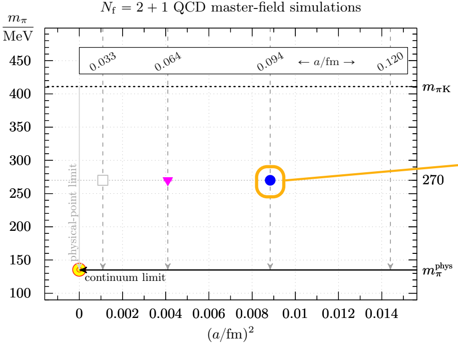

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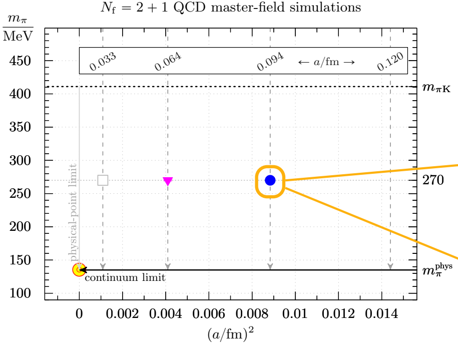
$V = 96^4$ ($L = 9\,\mathrm{fm}$, $m_\pi L \approx 12.3$)

- $V/V_4 = 3^4 = 81$ ($N_{\mathrm{core}} = 6144$)
- *Cost:* 3 Mch (thermal.) + 0.2 Mch (add. cfg.)
- *Total memory used:* 1.8 TiB (= 309.1 MiB per core)
- *On disc:* 132 GiB (= 46 GiB U + 61 GiB ϕ + 20 GiB π)

Summary of $N_f = 2 + 1$ master-field simulations



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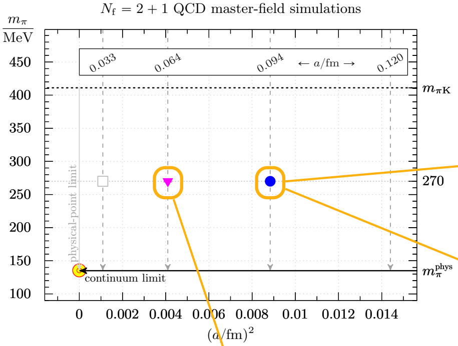
- $V/V_4 = 6^4 = 1296$ ($N_{\mathrm{core}} = 36864$)
- *Cost:* 45 Mch (thermal.) + 9 Mch (add. cfg.)
- *Total memory used:* 35.9 TiB (= 1019.8 MiB per core)
- *On disc:* 2 TiB (= 729 GiB U + 972 GiB ϕ + 324 GiB π)

Summary of $N_\mathrm{f} = 2+1$ master-field simulations



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$V = 144^4$ ($L = 9.2\,\mathrm{fm}$, $m_\pi L \approx 12.6$)

- $V/V_4 = (144/48)^3 = 81$ ($N_\mathrm{core} = 10368$)
- *Cost:* 20 Mch (thermal.) + 13 Mch (per add. cfg.)
- *Total memory used:* 11.1 TiB (= 1.1 GiB per core)
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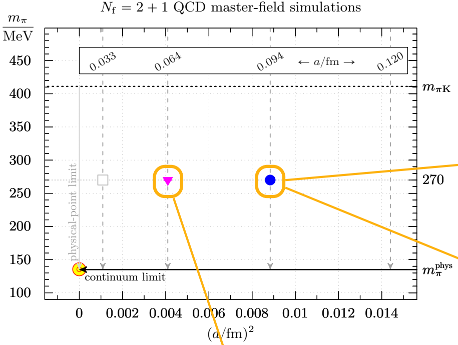
Summary of $N_f = 2 + 1$ master-field simulations



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tuning at finer lattice spacing
$a \sim 0.035\,\mathrm{fm} \implies 256^4 @ L = 9\,\mathrm{fm}$
$\rightsquigarrow$ **continuum limit**

How to (efficiently) calculate hadronic observables?

Variety of choices:

time-momentum correlators

$$C(x_0, \mathbf{p}) = \sum_{\mathbf{x}} \exp(-i\mathbf{p}\mathbf{x}) C(x, 0)$$

have large footprint in space for $\mathbf{p} = \mathbf{0}$
(inexact momentum projection $\rightsquigarrow$ more localized)

$\Rightarrow$ position-space correlators

- single point source (inefficient)
- Dirichlet b.c. on blocks[1] (induce boundary effect)
- random source (useable)
- …

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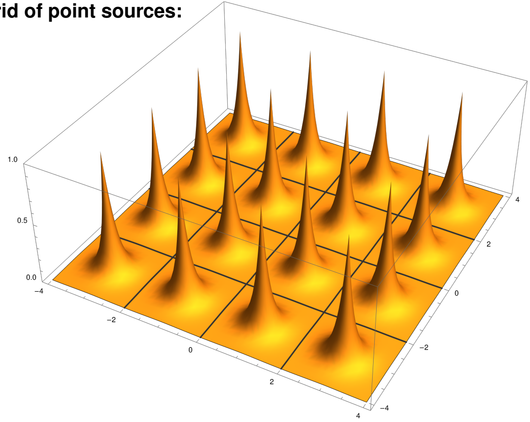
Grid of point sources:



2D sketch of exponential decay of „2-pt function“ with $(8a/2a)^2 = 4^2 = 16$ grid source points

Take away message

employ techniques compatible with MF translation average for single inversion of Dirac op.

Hadron propagators

E.g. meson 2-pt function (like pion propagator):

$$C_{\Gamma\Gamma'}(x) = -\mathrm{Tr}\{\Gamma\gamma_5 D^{-1}(x,0)\gamma_5\Gamma' D^{-1}(x,0)\}\ , \qquad ||D^{-1}(x,0)|| \sim e^{-m|x|/2}$$

with localisation range $1/m$ (not ultra-local)

- Asymptotic form of position-space correlators analytically known when $a = 0$ ($T, L = \infty$).
  For $|x| \to \infty$:

$$C_{\mathrm{PP}}(x) \to \frac{|c_{\mathrm{P}}|^2}{4\pi^2}\frac{m_{\mathrm{P}}^2}{|x|}K_1(m_{\mathrm{P}}|x|)\ ,$$

$$C_{\mathrm{NN}}(x) \to \frac{|c_{\mathrm{N}}|^2}{4\pi^2}\frac{m_{\mathrm{N}}^2}{|x|}\left[K_1(m_{\mathrm{N}}|x|) + \frac{\not{x}}{|x|}K_2(m_{\mathrm{N}}|x|)\right]$$

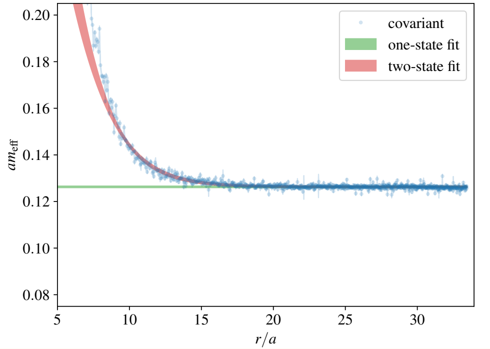
- axis/off-axis directions different cutoff effects
- correlator averaged over equivalent distances $r = |x|$:

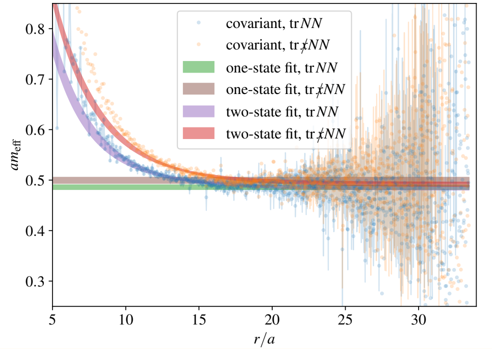
$$\overline{C}(r) = \frac{1}{\mathrm{r}_4((r/a)^2)}\sum_{|x|=r} C(x)$$

Hadronic observables

from position-space correlators & grid-points offset $b = 48a$ ($r_{\max} = 48a/\sqrt{2} \leq 34a$)

Effective masses of pion and nucleon ($a = 0.94\,\mathrm{fm}$) on 96^4





Comments:

- similar statistics (4096 noise src.) and computational effort on 96^4 ($x_{\mathrm{gs}} = 12$) and 192^4 ($x_{\mathrm{gs}} = 24$)
- different methods for proper calculations of uncertainties available (bootstrap, Γ-method)
- using empirical ansatz for excited state effects

Hadronic observables

from position-space correlators & grid-points offset $b = 48a$ ($r_{\max} = 48a/\sqrt{2} \leq 34a$)

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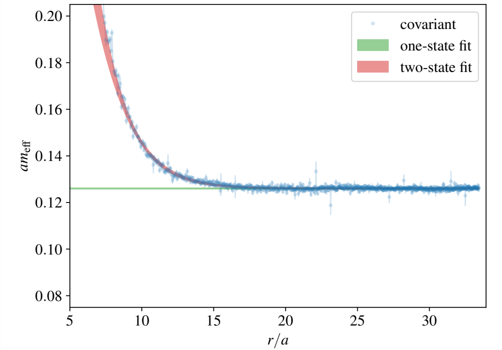

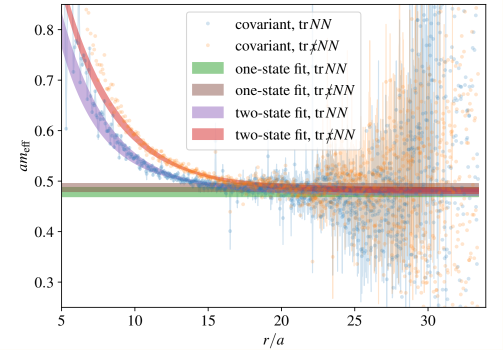

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Simulating StabWF: the standard way

OPEN
LATtice
initiative

$N_\mathrm{f} = 2 + 1$ Stabilised Wilson-Fermion simulations

- perform standard-sized lattice simulations
- exploit all stabilising measures[15] (Exp-Clover action, SMD, …)
- various lattices $\{a/L, \beta, m_\pi\}$ to complement master-field simulations
- `https://openlat1.gitlab.io`

OPEN LATtice initiative

This is an effort within the Lattice QCD community (started in 2019) for the production and sharing of dynamical gauge field ensembles to study physical phenomena of the strong interaction. We are aware that not every young researcher can be in the favourable position to belong to one of the big collaborations with access to large scale simulations to pursue new ideas. We want to close this gap by forming the present initiative centered around latest developments in the field. We offer

Francesca Cuteri

Anthony Francis

Patrick Fritzsch

Giovanni Pederiva

Antonio Rago

Andrea Shindler

André Walker-Loud

Savvas Zafeiropoulos

Jangho Kim

Dimitra Pefkou

OPEN LATtice initiative

Physics projects:

- Moments of parton distribution functions
- Neutron electric dipole moment
- Nucleon elastic and inelastic resonant structure
- QCD thermodynamics
- Heavy quark physics
- Renormalisation & $\mathrm{O}(a)$-improvement

$N_\mathrm{f} = 2 + 1$ Stabilised Wilson-Fermion simulations

OpenLat large-scale simulations


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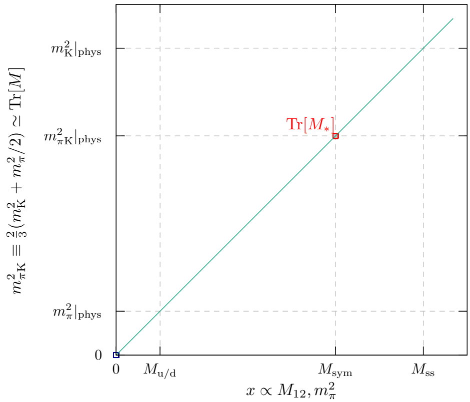
Open for new members, collaborations, joint ventures, …

OpenLat gauge ensembles

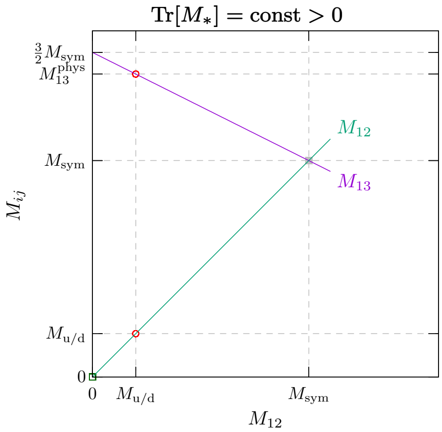
Physical run parameters from hadronic scheme

- Tree-level Symanzik improved gauge action
- Non-perturbatively improved exponential Wilson-Clover fermion action with $M = \mathrm{diag}(m_\ell, m_\ell, m_s)$
- All stabilising measures implemented

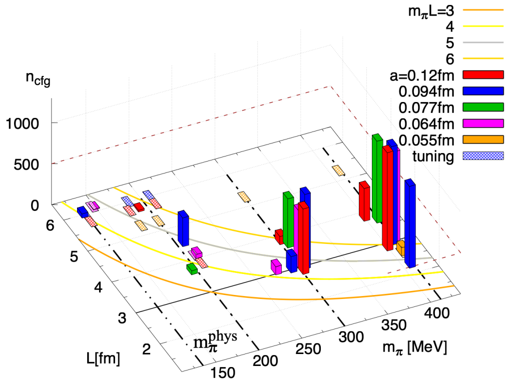
$N_\mathrm{f} = 3$



$N_\mathrm{f} = 2 + 1$



$N_f = 2 + 1$ Stabilised Wilson-Fermion simulations

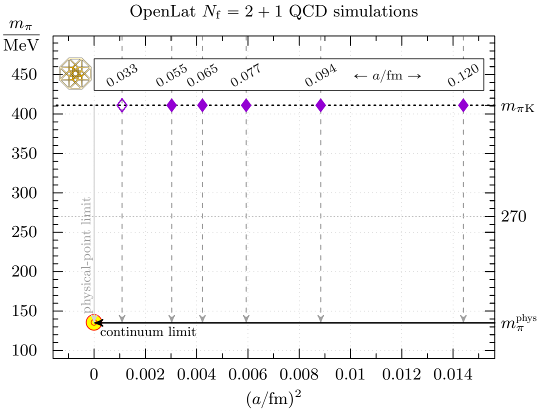


Target:

- 1000 independent gauge configs
- 5-6 lattice spacings at $SU(3)$-flavour-symmetric point
- 4 lines of approx. const. pion mass:
  $m_\pi/\text{MeV} \simeq 410, 300, 200, 135$
- approaching physical points at coarse lattice spacings
  $a/\text{fm} = 0.078, 0.094, 0.12$
- $m_\pi L \gtrsim 4.0$

Supported by:

Following QCDSF, CLS strategy at $\mathrm{Tr}[M] = \mathrm{const}$



symmetric point ensembles

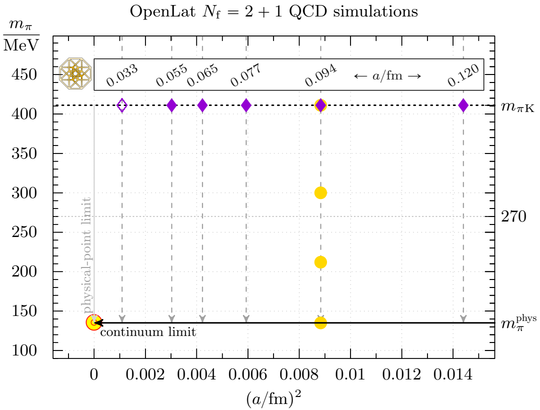
β	g.b.c.	T/a	L/a	a/fm	L/fm	$Lm_{\pi K}$
4.37	O	192	96	0.033	3.2	6.6
4.1	O	128	64	0.055	3.5	7.3
4.0	P	96	48	0.065	3.1	6.5
3.9	P	96	48	0.077	3.7	7.7
3.8	P	96	32	0.095	3.0	6.3
3.685	P	96	24	0.120	3.8	8.0

$$\phi_4 = 8t_0 \tfrac{3}{2} m_{\pi K} = 1.115\,, \qquad m_{\pi K} = 410.9(2)\ \mathrm{MeV}$$

$$m_{\pi K} = \tfrac{2}{3}(m_K^2 + m_\pi^2/2)\,, \qquad \sqrt{8t_0} = 0.414(5)\ \mathrm{fm}$$

OpenLat continuum and chiral trajectories

Following QCDSF, CLS strategy at $\mathrm{Tr}[M] = \mathrm{const}$



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chiral trajectory at $a = 0.095\,\mathrm{fm}$
$(\beta = 3.8, \mathrm{Tr}[M_0] = -1.205759)$

preliminary

T/a	L/a	$\frac{L}{\mathrm{fm}}$	$\frac{m_{\mathrm{PS}}}{\mathrm{MeV}}$	Lm_{PS}
96	32	3.04	410	6.32
96	32	3.04	300	4.62
128	48	4.56	200	4.62
128	72	6.84	135	4.68

Tuning large-scale StabWF simulations

Goal: Gaussian distributed ΔH (no spikes)

Advantage: short integration length ϵ vs. $\tau = 2$ MDU $P_{\text{acc}} = 98\%$ at $\epsilon \simeq 0.25$ MDU $\implies$ $2/\epsilon \simeq 8\times$ **more data**

My claims:

- speeds up tuning process significantly
  (UV fluctuations important, not autocorrelations)
- helps determining likelihood of unwanted spikes
- better mass-preconditioning through eigenvalue computation
- high-acceptance SMD $\iff$ less spikes in ΔH
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Typical simulation setup: keep it simple, but not too simple

- 2-level OMF4 integrators (gauge, fermions)
- $N_{\rm pf} \simeq 5 + 4$ pseudofermion fields
  - 5: mass-preconditioning $(\mu_0 = 0.00005 - 0.00012)$
  - 4: RHMC 11-15 poles
- mostly 2nd form of mass-reweighting $(\mu_1 = \sqrt{2}\mu_0)$
- $\mu_0(,\mu_1) < \lambda_{\rm min}(|\gamma_5 D|)$
- RHMC: somewhat more conservative than `ms2` suggestion
- $\|\eta\|_\infty$ for all forces (res$_F = 10^{-12} \ldots 10^{-10}$) and some actions (res$_\phi = 10^{-12}$)
- …

$$
\begin{aligned}
a &\simeq 0.095\,\mathrm{fm} \\
m_\pi &\simeq 210\,\mathrm{MeV}
\end{aligned}
$$

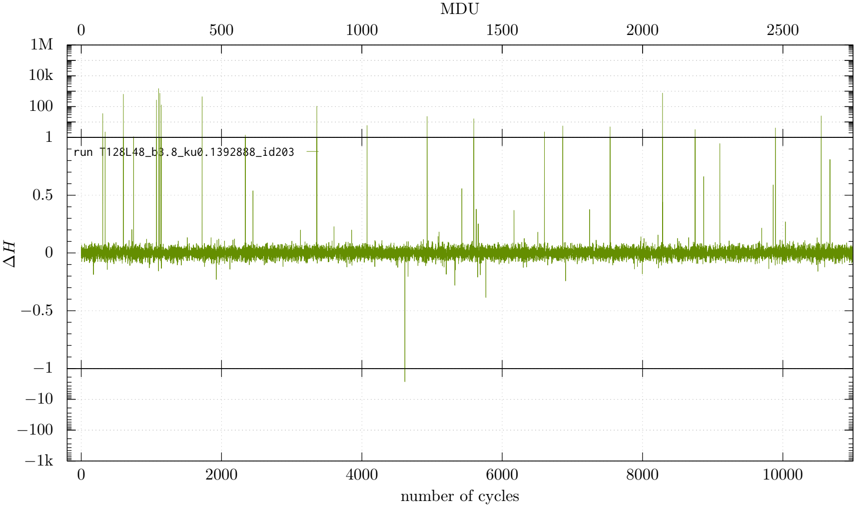
Towards the physical point.

Tuning large-scale StabWF simulations

Example: $a = 0.095\,\mathrm{fm}$, 128×48^3, $m_\pi \simeq 210\,\mathrm{MeV}$, $Lm_\pi \simeq 4.8$ ($\epsilon = 0.25$, $\epsilon\Delta_{\mathrm{cfg}} = 4$ MDU, $\mu_0 = 0$)

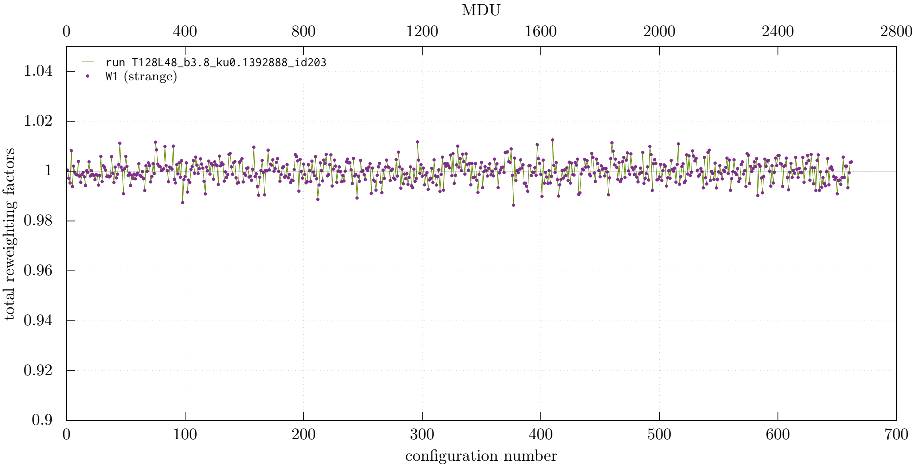
WORK IN PROGRESS

Energy violation ΔH: No regions of meta-stability!



WORK IN PROGRESS

reweighting factors: `RHMC ([0.016,8.6] w/ 11 poles)`



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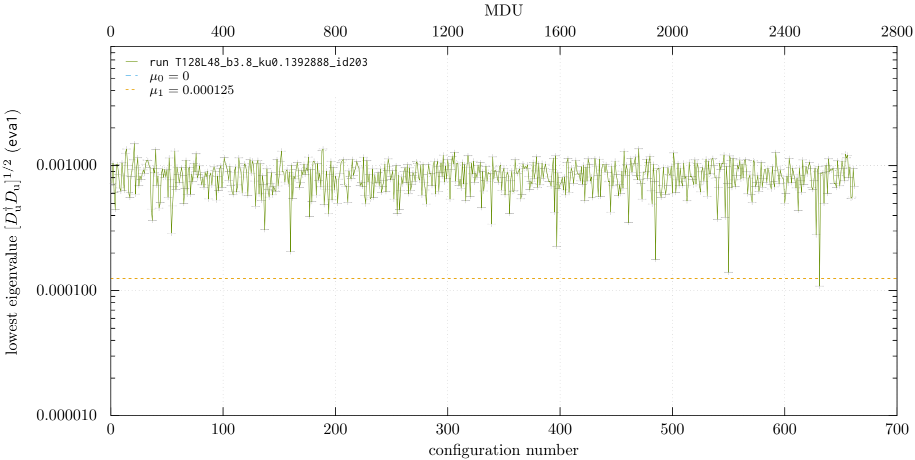
WORK IN PROGRESS

lowest eigenvalue of $|D_u^\dagger D_u|$:



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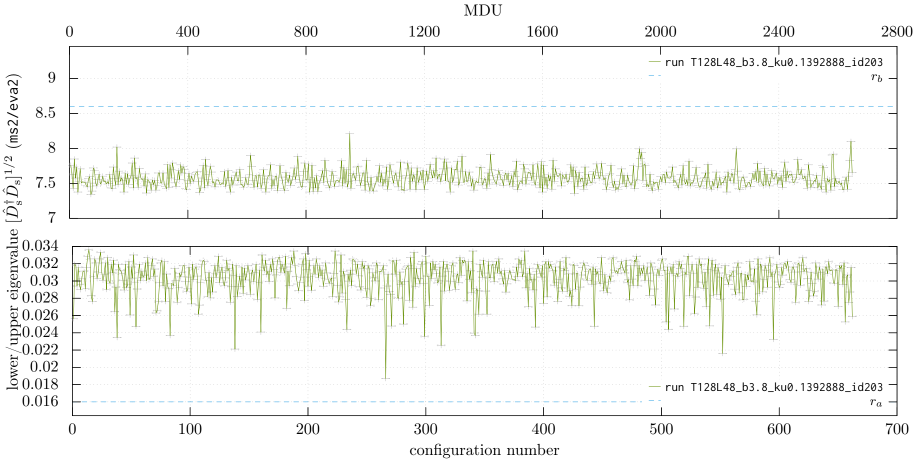
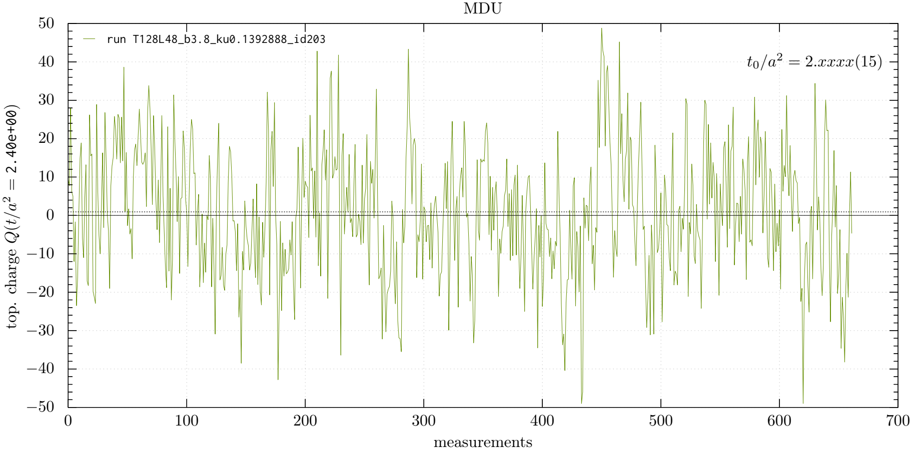
WORK IN PROGRESS

lowest eigenvalue of $|\hat{D}_s^\dagger \hat{D}_s|$:



WORK IN PROGRESS

topological charge:



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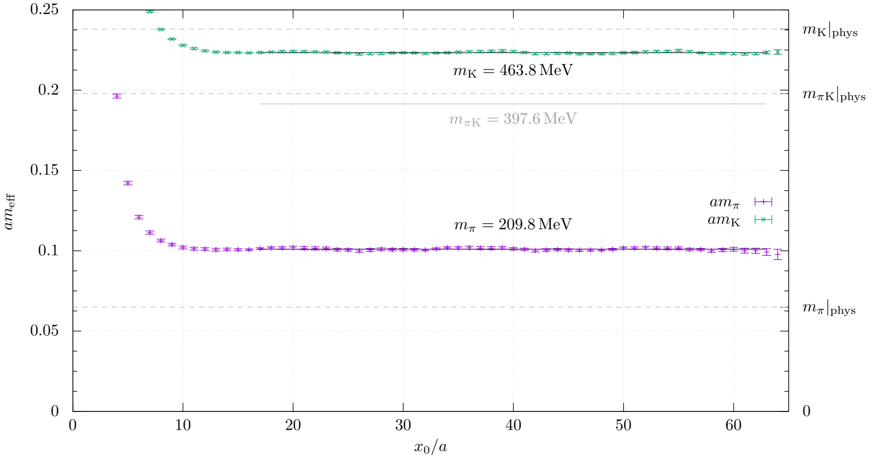
WORK IN PROGRESS

effective masses:



No fully-fledged autocorrelation analysis!

Tuning large-scale StabWF simulations

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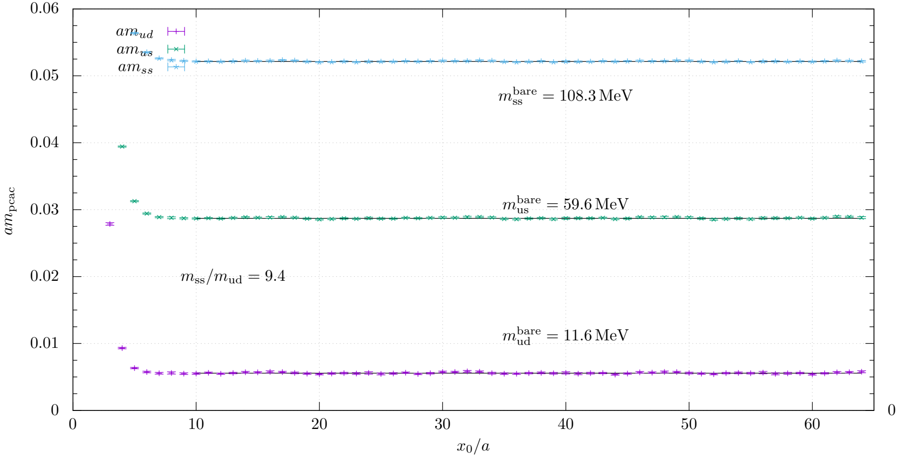
WORK IN PROGRESS

bare current quark masses:



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$$a \simeq 0.095\,\mathrm{fm}$$
$$m_\pi \simeq 135\,\mathrm{MeV}$$

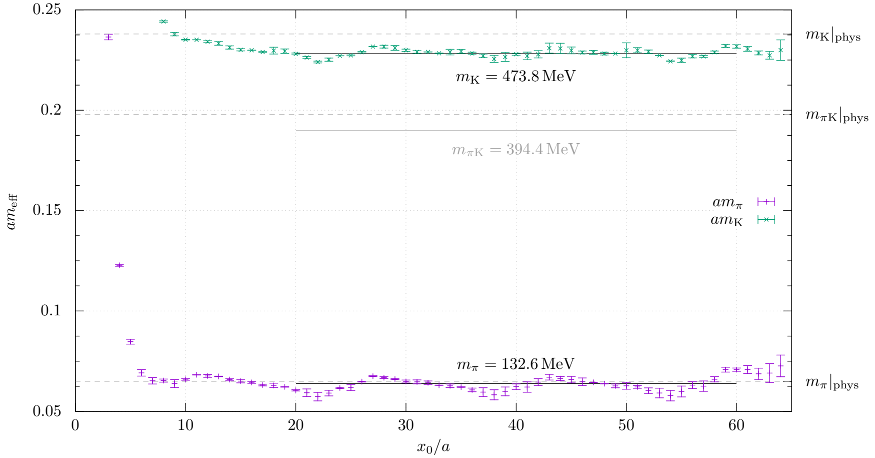
Latest, most stable tuned simulation.
Very short run so far.

Tuning large-scale StabWF simulations

Example: $a = 0.095\,\mathrm{fm}$, 128×72^3, $m_\pi \simeq 135\,\mathrm{MeV}$ ($\epsilon = 0.25$, $\epsilon\Delta_{\mathrm{cfg}} = 1$ MDU)

WORK IN PROGRESS

effective masses:



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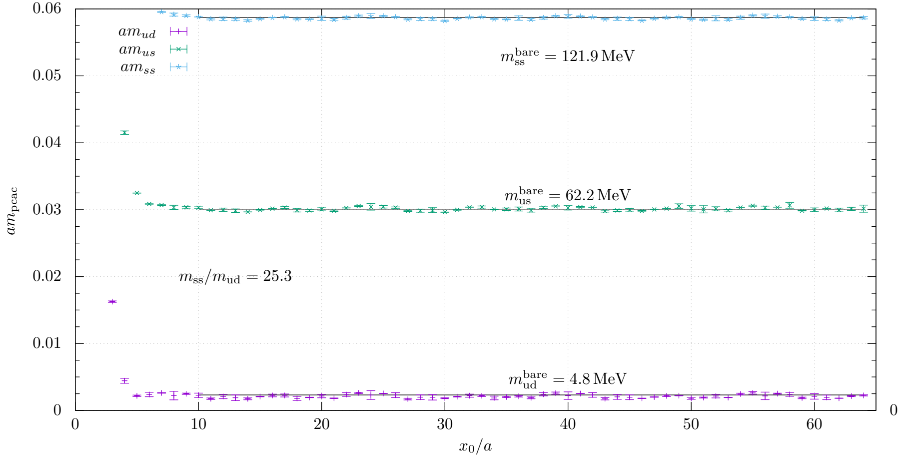


FLAG: $m_s/m_{ud} = 27.4$

No fully-fledged autocorrelation analysis!

Renormalisation and improvement in the SF

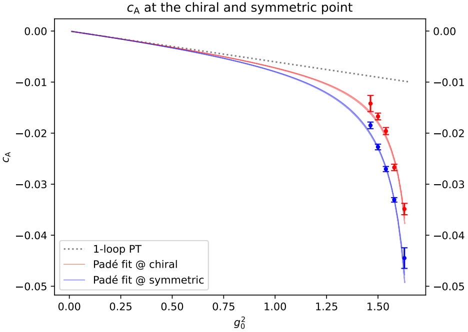
In collaboration with J.Heitger and J.Kuhlmann

Goal:

- Massless vs massive scheme
  2 LCP's: $\mathrm{Tr}[M] = 0$ and $\mathrm{Tr}[M] > 0$
- enter hadronic regime with SF simulations
  (i.e. close volume gap between SF and LV runs)
- t_0 vs. $\bar{g}^2_{\mathrm{GF}}(L)$ scale setting
- reduce ambiguities of Z_X, c_X, b_X
- confirm ren. & improvement pattern of Wilson fermions

$$M_\mathrm{q} \simeq 0 \quad \text{at} \quad L \approx 3\,\mathrm{fm}$$

L/a	β	a/fm	L/fm	$\delta L[3\,\mathrm{fm}]$
96	4.37	0.033	3.168	+5.6%
56	4.1	0.055	3.080	+2.6%
48	4.0	0.065	3.120	+4.0%
40	3.9	0.077	3.080	+2.6%
32	3.8	0.095	3.040	+1.3%
24	3.685	0.120	2.880	−4.0%



Summary

Master-fields require stabilising measures

- Modified fermion action (a.k.a. exponential clover)
- Stochastic Molecular dynamics (SMD) algorithm
- Uniform norm & quadruple precision
- Multilevel deflation

So far:

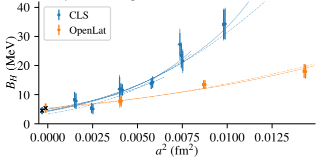
- stabilising measures (action, SMD, …) work excellent, especially at coarse lattice spacing ✓
- 96^4, 192^4 ($a = 0.095\,\mathrm{fm}$) and 144^4 ($a = 0.065\,\mathrm{fm}$) master-field ready for physics applications ✓
- master-field prefers traget partition function ✓
- very large volumes like $(18\,\mathrm{fm})^4$ still challenging but doable (or m_π^{phys}) ✓
- position-space correlators ⇝ hadron masses, decay constants, …

Ongoing:

- continuum limit scaling behaviour (3rd lattice spacing)
- master-fields: natural setup to study spectral reconstruction
- complementary large-scale lattice simulations (OpenLat)
- exploration of physical calculations & benchmarking

H dibaryon: $a \to 0$ universality (PRELIMINARY)

BaSc: Baryon Scattering collaboration — combined effort of "Mainz" and sLapHnn



Three exp-clover ensembles with $L \approx 3$ fm.

Second action at SU(3) point: exponentiated clover / stabilized Wilson (OpenLat). Smaller lattice artifacts than standard clover (CLS).

We just start to uncover new possibilities.

Backup slides

Exponential clover implementation

Apply **Cayley–Hamilton theorem** for 6×6 hermitean matrices.

$$\tfrac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x) = \begin{pmatrix} A_+(x) & 0 \\ 0 & A_-(x) \end{pmatrix} ,$$

$$\mathrm{tr}\{\mathrm{A}\} = 0 \quad \Rightarrow \quad A^6 = \sum_{k=0}^{4} p_k A^k$$

Any polynomial in A of degree $N \geq 6$ can be reduced to

$$\sum_{k=0}^{5} q_k A^k ,$$

with A-dependent coefficients q_k, calculated recursively.

Expansion coefficients ($p_k \in \mathbb{R}$)

$$p_0 = \tfrac{1}{6}\mathrm{tr}\{\mathrm{A}^6\} - \tfrac{1}{8}\mathrm{tr}\{\mathrm{A}^4\}\mathrm{tr}\{\mathrm{A}^2\} - \tfrac{1}{18}\mathrm{tr}\{\mathrm{A}^3\}^2 + \tfrac{1}{48}\mathrm{tr}\{\mathrm{A}^2\}^3$$

$$p_1 = \tfrac{1}{5}\mathrm{tr}\{\mathrm{A}^5\} - \tfrac{1}{6}\mathrm{tr}\{\mathrm{A}^3\}\mathrm{tr}\{\mathrm{A}^2\} ,$$

$$p_2 = \tfrac{1}{4}\mathrm{tr}\{\mathrm{A}^4\} - \tfrac{1}{8}\mathrm{tr}\{\mathrm{A}^2\}^2 ,$$

$$p_3 = \tfrac{1}{3}\mathrm{tr}\{\mathrm{A}^3\} ,$$

$$p_4 = \tfrac{1}{2}\mathrm{tr}\{\mathrm{A}^2\} ,$$

$$\exp(A) = \sum_{k=0}^{N} \frac{A^k}{k!} + r_N(A)$$ converges rapidly with bound $$||r_N(A)|| \leq \frac{||A||^{N+1}}{(N+1)!}\exp(||A||)$$

$\Rightarrow \exp\left(\tfrac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)\right)$ easily obstained to machine precision.

Master fields prefer the target partition function

Reweighting of observables not available

QCD simulations necessitate frequency-splitting methods

- Hasenbusch (mass-)preconditioning for quark doublet $(\mu_n > \ldots > \mu_0)$

$$S_{\rm pf} = (\phi_0, \frac{1}{D^\dagger D + \mu_n^2}\phi_0) + \sum_{k=1}^{n}(\phi_k, \frac{D^\dagger D + \mu_{n-k+1}^2}{D^\dagger D + \mu_{n-k}^2}\phi_k)$$

requires mass-reweighting if regulator mass $\mu_0 \neq 0$ $\Rightarrow$ ✓ if $\mu_0 = 0$

- rational approximation of strange (or charm) quark determinant is given by

$$\det(D_{\rm s}) = W_{\rm s}\det(R^{-1})\ , \quad R = C\prod_{k=0}^{m-1}\frac{D_{\rm s}^\dagger D_{\rm s} + \omega_k^2}{D_{\rm s}^\dagger D_{\rm s} + \nu_k^2}$$

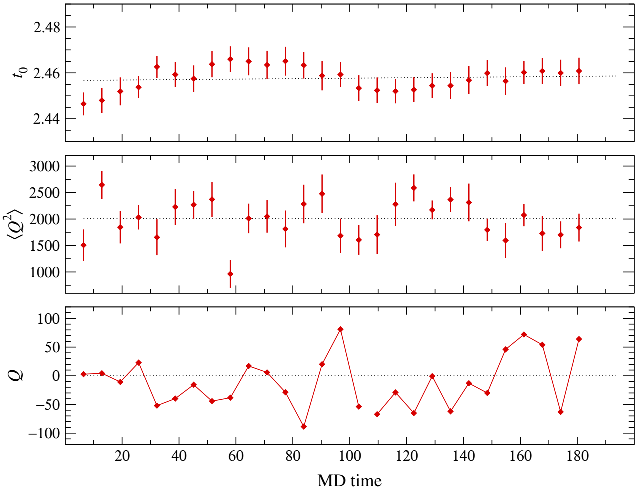
: Zolotarev optimal rat. approx.

with reweighting factor $W_{\rm s} = \det(D_{\rm s}R)$ to
correct approximation error ($m =$degree of $[D_{\rm s}^\dagger D_{\rm s}]^{-1/2}$) $\Rightarrow$ ✓ if approximation is sufficiently accurate

Complying with strict bound $\frac{\sigma(W_{\rm s})}{\langle W_{\rm s}\rangle} \leq 0.1$ guarantees unbiased results in all observables.

Monitoring observables (thermalisation)

$96^4 : a = 0.095\,\text{fm},\ m_\pi = 270\,\text{MeV},\ Lm_\pi = 12.5\ (L = 9\,\text{fm})$



Simulations without TM-reweighting:

- no spikes in ΔH
- $\langle e^{-\Delta H} \rangle = 1$ within errors
- acceptance rate 98% or higher
- checked that $\sigma(\hat{D}_s) \in [r_a, r_b]$ of Zolotarev rational approximation
- adapt solver tolerances to exclude statistically relevant effects of numerical inaccuracies
- autocorrelation times: 20-30 MDU

Master-field simulations

Thermalising 192^4 ($a = 0.094\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$) at LRZ using 768 nodes (36864 cores)

openQCD-2.0.2: multilevel DFL solver (full double prec.)

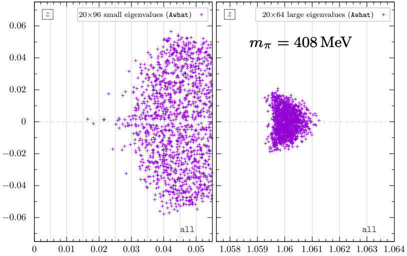
```
SMD parameters:
actions = 0 1 2 3 4 5 6 7 8
npf = 8
mu = 0.0 0.0012 0.012 0.12 1.2
nlv = 2
gamma = 0.3
eps = 0.137
iacc = 1

...

Rational 0:
degree = 12
range = [0.012,8.1]

Level 0:
4th order OMF integrator
Number of steps = 1
Forces = 0

Level 1:
4th order OMF integrator
Number of steps = 2
Forces = 1 2 3 4 5 6 7 8
```

```
Update cycle no 48
dH = -1.4e-02, iac = 1
Average plaquette = 1.708999
Action  1: <status> = 0
Action  2: <status> = 0 [0,0|0,0]
Action  3: <status> = 0 [0,0|0,0]
Action  4: <status> = 0 [0,0|0,0]
Action  5: <status> = 2 [5,2|7,6]
Action  6: <status> = 271
Action  7: <status> = 21 [3,2|5,3]
Action  8: <status> = 22 [3,2|5,3]
Field   1: <status> = 139
Field   2: <status> = 31 [3,2|6,4]
Field   3: <status> = 38 [5,3|8,7]
Field   4: <status> = 33 [5,2|7,6]
Field   5: <status> = 267
Field   6: <status> = 26 [3,2|5,3]
Field   7: <status> = 24 [3,2|5,3]
Force   1: <status> = 91
Force   2: <status> = 22 [3,2|6,4];23 [3,2|5,4]
Force   3: <status> = 28 [5,3|7,6];30 [5,3|7,6]
Force   4: <status> = 29 [5,2|7,6];32 [5,2|7,6]
Force   5: <status> = 28 [5,2|7,5];30 [5,2|7,6]
Force   6: <status> = 303
Force   7: <status> = 22 [3,2|5,3];23 [3,2|5,3]
Force   8: <status> = 23 [3,2|5,3];26 [3,2|5,3]
Modes   0: <status> = 0,0|0,0
Modes   1: <status> = 4,2|5,5 (no of updates = 4)
Acceptance rate = 1.000000
Time per update cycle = 4.34e+03 sec (average = 4.38e+03 sec)
```

Master-field simulations

Study deflation subspace ($a = 0.095\,\mathrm{fm}$)

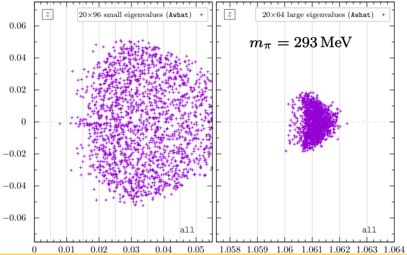
Small/Large eigenvalue spectrum of eo-preconditioned DFL operator **`Awhat`** on A-lattices (96×32^3):

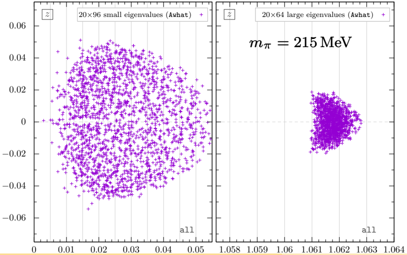


Deflation subspace ⇔ „low-modes“ $\{\psi_1, \cdots, \psi_{N_s}\}$

$$A_w = P_0 D P_0 \qquad \text{: restricted Dirac op.}$$

P_0: orthogonal projector to DFL subspace





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