The SLapH Method in tmLQCD - Part 1

Christopher Helmes
C. Jost, B. Knippschild, C. Urbach, M. Werner

May 26, 2014

Outline

Excited States in QCD

- Precise measurements of excited states in LQCD
- Examine large lattice volumes with Laplacian Heaviside Method
- Reduce variance of effective masses with stochastic ansatz
- Large operator basis by displacing operators

Stochastic LapH method - Overview

- Method to estimate quark propagation by Morningstar et al.
- Quark field smearing $\widetilde{\psi} = \mathcal{S}\psi$
  1. Reduction of contribution of excited states
  2. Efficient decomposition to "Perambulators"
  3. Computationally cheap to build large operator basis
- Combine Smearing with stochastic approach to reduce numerical costs
- Reduce variance with dilution of random vectors

Quark Field Smearing I

- **Lap**lacian **H**eaviside Smearing $\widetilde{\psi}(n) = \mathcal{S}(n,m)\psi(m)$
- Smearing kernel: $\mathcal{S}$, Heaviside function: $\Theta(x)$, Laplace operator: $\widetilde{\Delta}$

$$\mathcal{S} = \Theta\left(\sigma_s^2 + \widetilde{\Delta}\right)$$

  σ_s^2: cutoff for spectrum of $\widetilde{\Delta}$

- $\widetilde{\Delta}$ large sparse and hermitian matrix of dimensions $(N_s^3 \cdot 3) \times (N_s^3 \cdot 3)$

$$\widetilde{\Delta}_{nm}(t) = \sum_{j=1}^{3}\left(\widetilde{U}_j(n,t)\delta_{n+\hat{j},m} + \widetilde{U}_j^\dagger(n-\hat{j},t)\delta_{n-\hat{j},m}\right) - 6\delta_{nm}$$

- $N_s = 32 \rightarrow 9.7 \times 10^9$ complex entries in $\widetilde{\Delta}(t)$

Quark Field Smearing II

- Decomposition into eigenvalues $\Lambda_\Delta = \text{diag}(\lambda_1, \ldots, \lambda_\Delta)$:

$$\widetilde{\Delta} = V_\Delta^\dagger \Lambda_\Delta V_\Delta$$

- Only interested in N_v lowest eigenvectors of Laplace operator

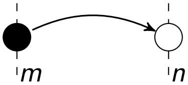
$$\mathcal{S} = V_s^\dagger \Theta \underbrace{\left(\sigma_s^2 + \Lambda_\Delta\right)}_{=\Lambda_s} V_s$$

- V_s contains N_v eigenvectors as columns
- V_s is $(N_s^3 \cdot N_t \cdot 3) \times (N_t \cdot N_v)$ matrix $\Rightarrow$ store V_s

Quark Propagation Inside Correlation Functions

- Quark propagation with smeared sources:

$$\mathcal{Q} = \overline{\psi}(n)\psi(m) = M^{-1}(n|m)$$



- Smearing $\mathcal{S}$ well approximated by $\mathcal{S} = V_s V_s^\dagger$

$$\Rightarrow \mathcal{Q} = V_s \left(V_s^\dagger M^{-1} V_s \right) V_s^\dagger$$

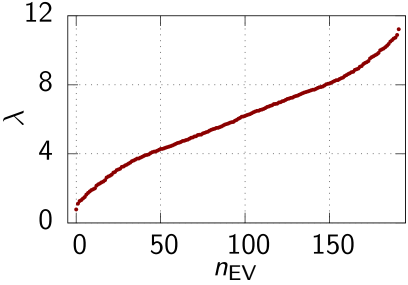
- Expensive: obtain $M^{-1} V_s$ from solving $Mx = v_s^{(k)}$ for $k \in (0, N_v)$
- $(V_s^\dagger M^{-1} V_s)$ orders of magnitude smaller in memory than M^{-1}
- Inversions: $N_v \cdot N_t \cdot 4$ per configuration and quark mass

$$N_v = 250,\ N_t = 64 \Rightarrow 64\,000$$

Eigensystems

- Decomposition into Λ_s and V_s on every timeslice for each configuration
- Fast solution: C-libraries SLEPc and PETSc
- Thick restart Lanczos algorithm
- Additionally accelerated by Chebyshev polynomials

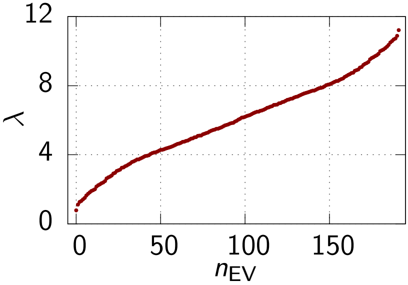
Chebyshev Acceleration: Example for 4^3 Lattice



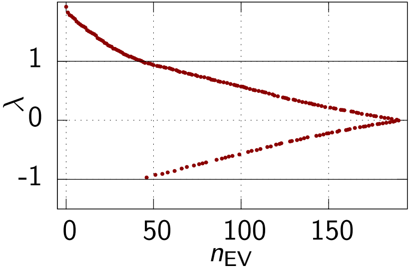
Spectrum of $\widetilde{\Delta}$

- Fast convergence if eigenvalues widely spaced
- $B = 1 + \frac{2}{\lambda_L - \lambda_C}(\widetilde{\Delta} + \lambda_C)$, λ_is tuned with boundaries of spectrum

Chebyshev Acceleration: Example for 4^3 Lattice



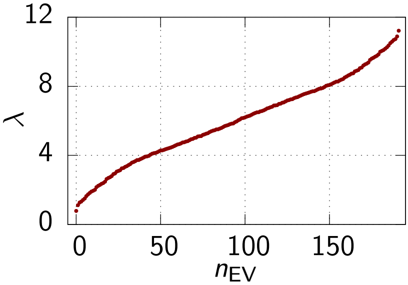
Spectrum of $\widetilde{\Delta}$



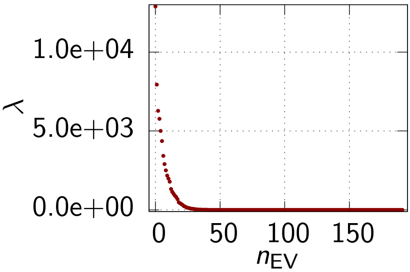
Spectrum of B

- B shifts unwanted part to $(-1, 1)$
- Chebyshev polynomial of first kind $T_8(B)$

Chebyshev Acceleration: Example for 4^3 Lattice



Spectrum of $\widetilde{\Delta}$



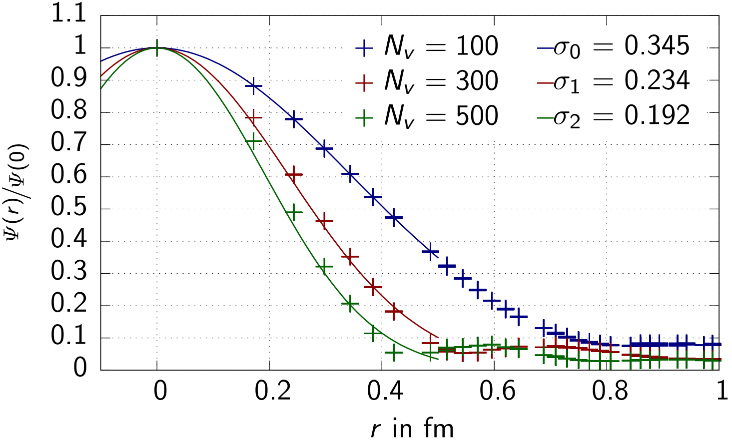
Spectrum of $T_8(B)$

- Eigenvectors unchanged
- Speedup of factor 4 despite application of T_8

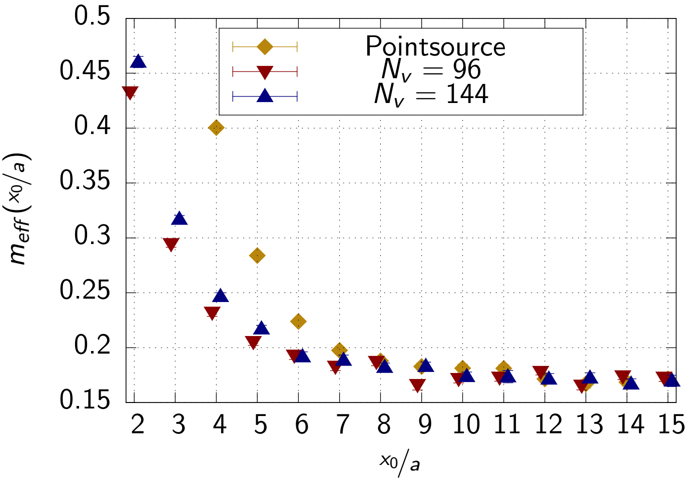
Distillation Operator and Sourceshape

- Measure effect of Distillation with Sourceshape $\Psi(r,t)$

$$\Psi(r,t) = \sum_n \sqrt{\mathrm{tr}\left(\square_{n,n+r}(t)\square_{n+r,n}(t)\right)}, \quad \square(t) = V_s(t)V_s^\dagger(t)$$

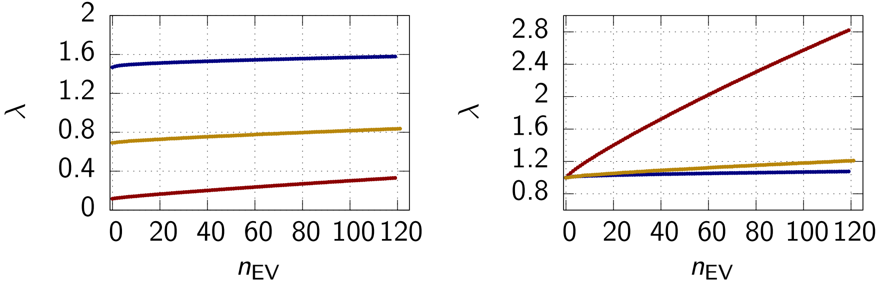


Influence of N_v on C_π



Gauge Link Smearing and Eigenspectrum

Influence of ideal HYP-, badly tuned HEX- and No gauge link Smearing on spectrum of $\widetilde{\Delta}$



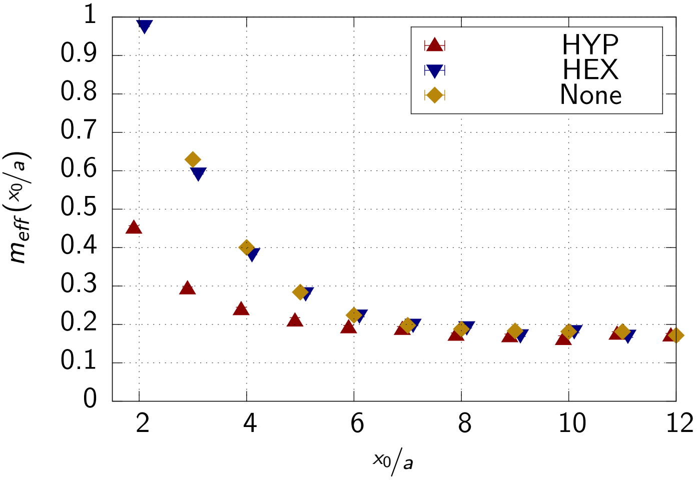
Eigenspectrum

Normalised to lowest λ

Figure: Data: 24^3 lattice, lattice spacing $a = 0.086\,\mathrm{fm}$

Influence of Gauge Link Smearing

Ideal HYP-, badly tuned HEX- and No gauge link Smearing influence $m_{eff}\left({x_0}/{a}\right)$



Stochastic Approximation

- Estimate $\mathcal{Q}$ up to accuracy of gauge noise limit
- N_R random vectors ρ in V_s, T, D
- $E(\rho) = 0$ and $E(\rho\rho^\dagger) = \mathbb{1}$
- Dilution projections $P^{(b)}\rho$ zero many offdiagonal elements of $\rho\rho^\dagger$

Dilution Schemes

- Each $P^{(b)}$ combines dilution in Time, Dirac space and LapH space
- Statistical errors of correlation functions
  - Random vectors $\propto \frac{1}{\sqrt{N_R}}$
  - Dilution vectors $\propto \frac{1}{N_D}$

  $\Rightarrow$ Find balance between N_R and N_D for best signal in dependence of number of inversions
- Inversions: typically between 1500 and 2500 per configuration

Quarklines

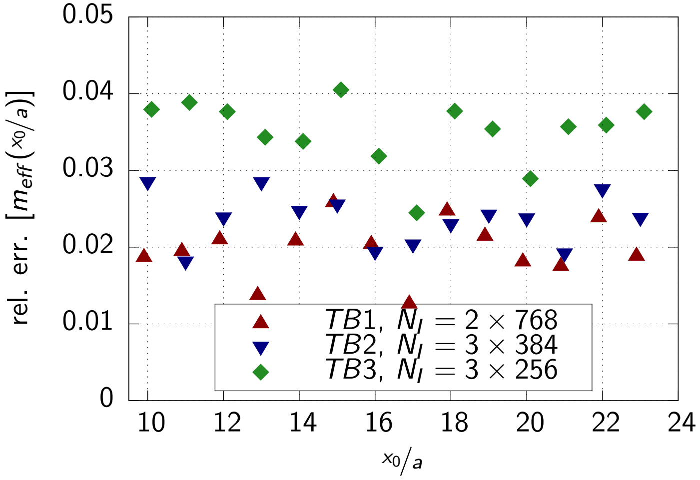
- Use $\sum_b P^{(b)} P^{(b)\dagger} = E(\rho\rho^\dagger) = \mathbb{1}$ in $\mathcal{Q}$

$$\begin{aligned}\mathcal{Q} &= \mathcal{S} M^{-1} V_s V_s^\dagger \\ &= \sum_b \mathcal{S} M^{-1} V_s P^{(b)} E(\rho\rho^\dagger) P^{(b)\dagger} V_s^\dagger \\ &= \sum_b E\left(\mathcal{S} M^{-1} V_s P^{(b)} \rho \left(V_s P^{(b)} \rho\right)^\dagger\right)\end{aligned}$$

- Reuse sources $V_s P^{(b)} \rho$ and "Perambulators" $V_s^\dagger M^{-1} V_s P^{(b)} \rho$
- Each $\mathcal{Q}$ needs independent ρ for unbiased estimation
- Possible tuning via N_R and dilution scheme

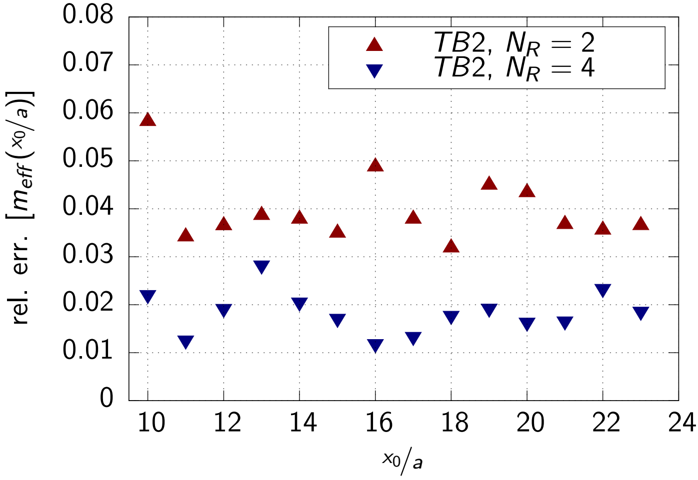
Influence of Number of inversions on C_π

Relative error on effective mass



Influence of N_R on C_π

Relative error on effective mass



Multiple Operators With Same J^{PC}

- Spatially extend Interpolators

$$\overline{\psi}(\vec{x},t)\Gamma\overleftrightarrow{D}\psi(\vec{x},t), \quad \overleftrightarrow{D} = \overleftarrow{D} - \overrightarrow{D}$$

- Fermion bilinears using gamma matrices and $\overleftrightarrow{D}_m$

$$\overleftrightarrow{D}_{m=-1} = \frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x - i\overleftrightarrow{D}_y\right), \quad \overleftrightarrow{D}_{m=+1} = -\frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x + i\overleftrightarrow{D}_y\right),$$
$$\overleftrightarrow{D}_{m=0} = i\overleftrightarrow{D}_z$$

- Clebsch-Gordan-coefficients for definite J, PC via Γ structure
- Example: $J = 0, 1, 2$:

$$\left(\Gamma \times D^{[1]}_{J=1}\right)^{J,M} = \sum_{m_1,m_2} \langle 1, m_1; 1, m_2 | J, M\rangle \, \overline{\psi}(\vec{x},t)\Gamma_{m_1}\overleftrightarrow{D}_{m_2}\psi(\vec{x},t)$$

Realisation

- Correlation functions (stochastic contribution suppressed)

$$C_{ij}(t,t') = \left\langle \left[V^\dagger \Gamma_i \overleftrightarrow{D} V \right]_t \left[V^\dagger M^{-1} V \right]_{t,t'} \left[V^\dagger \Gamma_j \overleftrightarrow{D} V \right]_{t'} \left[V^\dagger M^{-1} V \right]_{t',t} \right\rangle$$

- Expansion:

$$V^\dagger \overleftrightarrow{D}_i V = V^\dagger \overleftarrow{D}_i V - V^\dagger \overrightarrow{D}_i V$$

- Sufficient to calculate second term:

$$V^\dagger \overleftarrow{D}_i V = \left(V^\dagger \overrightarrow{D}_i V \right)^\dagger$$

Correlation Matrix for π^+

- Non-vanishing pseudoscalar contributions:

$$\mathcal{O}_1(t) = \overline{d}(t)\gamma_5 u(t), \quad \mathcal{O}_2(t) = \overline{d}(t)\gamma_0\gamma_5 u(t)$$
$$\mathcal{O}_3(t) = \overline{d}(t)\left[\epsilon_{ijk}\gamma_j\gamma_k \overleftrightarrow{D}_i\right] u(t)$$

- Construct C_{lm}

$$C_{lm}(t,t') = \begin{pmatrix} \langle\mathcal{O}_1(t)\mathcal{O}_1(t')\rangle & \langle\mathcal{O}_1(t)\mathcal{O}_2(t')\rangle & \langle\mathcal{O}_1(t)\mathcal{O}_3(t')\rangle \\ \langle\mathcal{O}_2(t)\mathcal{O}_1(t')\rangle & \langle\mathcal{O}_2(t)\mathcal{O}_2(t')\rangle & \langle\mathcal{O}_2(t)\mathcal{O}_3(t')\rangle \\ \langle\mathcal{O}_1(t)\mathcal{O}_3(t')\rangle & \langle\mathcal{O}_3(t)\mathcal{O}_2(t')\rangle & \langle\mathcal{O}_3(t)\mathcal{O}_3(t')\rangle \end{pmatrix}$$

- Solve associated GEVP

Summary

- Tuning of Stochastic LapH method:
  - N_v for suppression of excited states
  - N_R for small number of inversions
  - Dilution scheme for optimal variance reduction in inversions
- Work in progress: Implementation of Displacement

Thank you

1. Wick Rotation of Real Minkowski Space

- Wick rotate Minkowski space to euclidean space introducing imaginary times

$$t = -i\tau \Rightarrow ds^2 = -(dt^2) + dx^2 + dy^2 + dz^2$$
$$= d\tau^2 + dx^2 + dy^2 + dz^2$$

- Path integral then becomes:

$$\langle O_2(t) O_1(0) \rangle = \frac{1}{Z} \int \mathcal{D}\left[\overline{\psi}, \psi\right] \mathcal{D}\left[U\right] e^{-S_E} O_2 O_1$$
$$Z = \int \mathcal{D}\left[\overline{\psi}, \psi\right] \mathcal{D}\left[U\right] e^{-S_E}$$

- Ocillating imaginary part has vanished in favour of exponential decay

2. Discretization of Euclidean Space

- Introduce periodic 4-dimensional Euclidean lattice Λ

$$\Lambda = \{n = (n_0, n_1, n_2, n_3) \,|\, n_i = 0, \ldots, N_S - 1\,;\; n_0 = 0, \ldots, N_T - 1\}$$

- My calculations: N_S from 20 to 48, N_T from 40 to 96
- Distance of neighboring points a, "lattice spacing", usually $a \approx 0.1\,\text{fm}$
- Used as automatic UV-cutoff

Wilson tmLQCD: Fermionic Action

- Framework: Wilson twisted mass lattice QCD for $N_f = 2 + 1 + 1$

$$S_F^{tm}\left[\overline{\chi}_l, \chi_l, U\right] = a^4 \sum_{k,n \in \Lambda} \overline{\chi}_l(k) \left(M(k|n)\mathbb{1}_2 + m\mathbb{1}_2\delta_{kn} + i\mu\gamma_5\tau^3\delta_{kn}\right)\chi_l(n)$$

- Twisted mass μ as an infrared regulator for exceptional configurations

- Automatic $\mathcal{O}(a)$ improvement on observables at maximal twist

Stochastic Approximation

- Estimate $\mathcal{Q}$ up to accuracy of statistical fluctuations of $\widetilde{U}_\mu(n)$
- R Random vectors η_r obeying $E(\eta_i) = 0$ and $E(\eta_i \eta_j^*) = 1$

$$M_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} x_i^r \eta_j^{r*}, \quad x^r = M^{-1} \eta^r$$

- Problem: too large variances in estimation of M_{ij}^{-1}
- Solution: dilution of η_r by Projections $P^{[b]}$, $\eta^{[b]r} = P^{[b]} \eta^r$

$$M_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{b} x_i^{[b]r} \eta_j^{[b]r*}, \quad x^{[b]r} = M^{-1} \eta^{[b]r}$$

Stochastic Quarklines

- Quarklines read:

$$\mathcal{Q} = \sum_b E\left(\mathcal{S}M^{-1}V_s P^{(b)}\rho\left(V_s P^{(b)}\rho\right)^\dagger\right)$$

- Define:

$$\varphi_u^{[b]}(\rho) = \mathcal{S}M^{-1}V_s P^{(b)}\rho$$
$$\varrho_v^{[b]}(\rho) = V_s P^{(b)}\rho$$

- Quarklines now approximable using smeared diluted sources $\varrho^{[b]}(\rho)$ and sinks $\varphi^{[b]}(\rho)$

$$\mathcal{Q}_{uv}^{AB} \approx \frac{1}{N_R}\delta_{AB}\sum_{r=1}^{N_R}\sum_b \varphi_u^{[b]}(\rho)\varrho_v^{[b]*}(\rho)$$

Gerschgorin-circles

$$M = \begin{pmatrix} -5 & -1 & 0 & 1 \\ 0.2 & 8 & 0.2 & 0.2 \\ 1 & 1 & 2 & 1 \\ -1 & -1 & -1 & -8 \end{pmatrix} \qquad \mathrm{EV} = (-7.53, -5.33, 1.86, 8.00)$$

$$S_1 = (-5, 2)\,; \quad S_2 = (8, 0.6)\,; \quad S_3 = (2, 1.2)\,; \quad S_4 = (-8, 2.2)$$

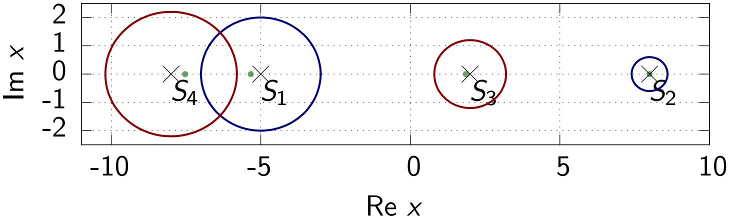


Figure: Gerschgorin-circles corresponding to M

PETSc and SLEPc

- Two libraries specialized for solving large sparse eigenvalue problems
- Numerous algorithms available
- Highly customizable via Shell method for introducing own operations
- Testing lead to Krylov-Schur method with no preconditioning

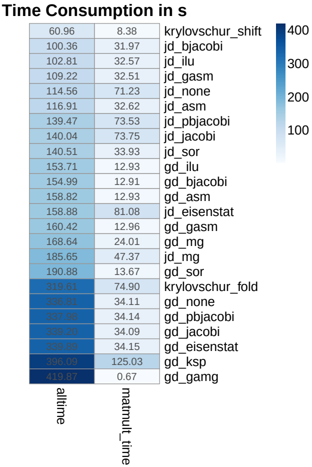


Figure: Time consumption of solving algorithms

Sourceshape and Lattice Volume

$\Psi(r)$ scales with lattice volume, for same σ factor of $\frac{N_{s1}^3}{N_{s2}^3}$

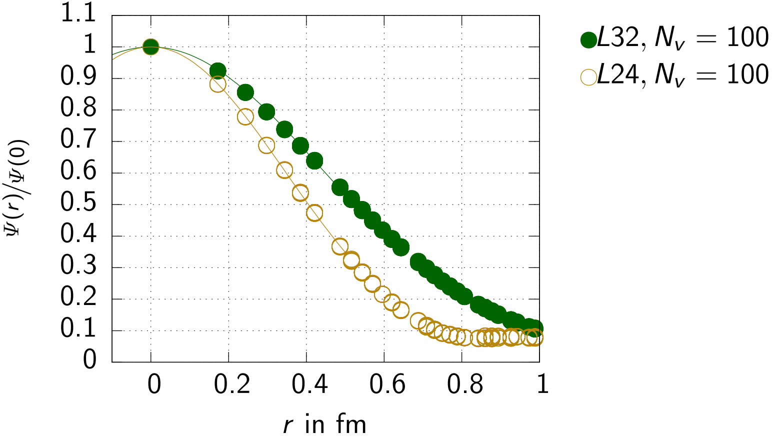


Figure: Data: Lattice spacing $a = 0.086\,\text{fm}$

Sourceshape and Lattice Volume

$\Psi(r)$ scales with lattice volume, for same σ factor of $\frac{N_{s1}^3}{N_{s2}^3}$

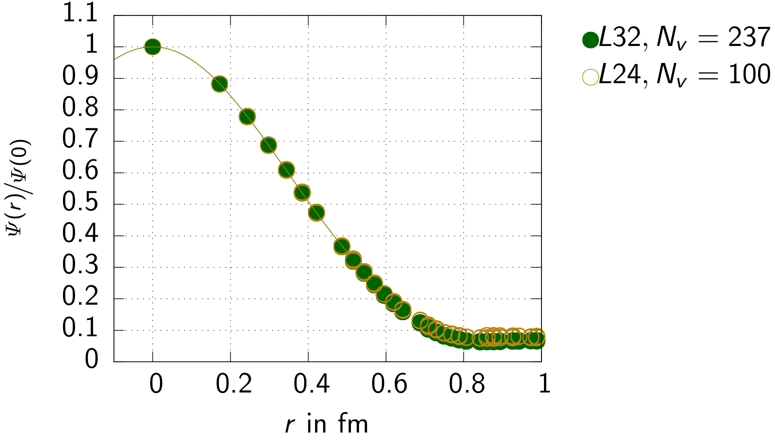
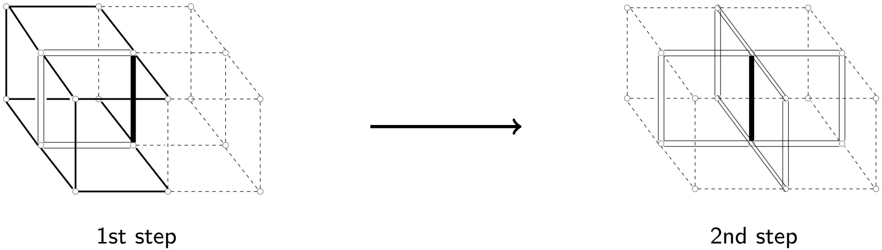


Figure: Data: Lattice spacing $a = 0.086\,\text{fm}$

Hypercubic Blocking[1]



- Smoothes gauge field $U_\mu(n)$
- Improves eigenspectrum of $\widetilde{\Delta}$
- 3 parameters: "staple weights" α_1, α_2 and iterations n_i

[1]A.Hasenfratz, F.Knechtli, Phys. Rev. D64 (2001) 034504

Tuning α_1 and α_2

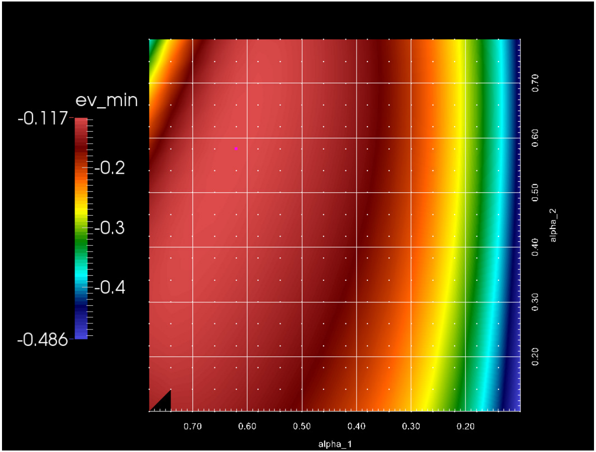


Figure: scan through the parameter plane (α_1, α_2)

Optimal parameters: $n_i = 3, \alpha_1 = 0.62, \alpha_2 = 0.58 \Rightarrow \lambda_1 = 0.118$

Thermal States

- Total time extent T, Partition function $Z = \mathrm{tr}(e^{-HT})$

$$\langle \mathcal{O}(t)\overline{\mathcal{O}}(0)\rangle = \frac{1}{Z}\sum_{m,n} |\langle n|\mathcal{O}|m\rangle|^2 \, e^{-(E_m+E_n)T/2} \cosh\left((E_m - E_n)(t - T/2)\right)$$

- For finite T contributions from $\langle n| = \langle \pi^+|$ and $\langle m| = \langle \pi^-|$

$$\frac{1}{Z}\left|\langle \pi^+|\mathcal{O}_{\pi\pi}|\pi^-\rangle\right|^2 e^{-m_\pi T}$$

- Comparable to standard contribution at $t = T/2$

$$\frac{1}{Z}\left|\langle \pi^+\pi^+|\mathcal{O}_{\pi\pi}|0\rangle\right|^2 e^{-E_{\pi\pi}^{I=2}T/2} \cosh(E_{\pi\pi}^{I=2}(t - T/2))$$