The Diagonal Kenney-Laub Approximation to the Overlap Dirac Operator

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The Overlap Operator

At finite lattice spacing, *chiral symmetry* for lattice Dirac operators can be realised through the Ginsparg-Wilson (GW) relation [3]:

$$\{\gamma_5, aD\} = \gamma_5\, aD + aD\gamma_5 = \frac{1}{\rho}\, aD\gamma_5\, aD\ . \tag{1}$$

The *massless* **overlap operator** satisfies it *exactly*. More generally, allowing for a nonzero bare quark mass am, its *massive* form reads:

$$aD_m^{\rm ov} = \left(\rho + \frac{am}{2}\right)\mathbb{I} + \left(\rho - \frac{am}{2}\right)\gamma_5\,{\rm sgn}[\mathbb{X}]\ , \tag{2}$$

with ${\rm sgn}[\mathbb{X}] \equiv \mathbb{X}\,(\mathbb{X}^2)^{-1/2}$, $\mathbb{X} = \gamma_5(aD_0^{\rm ker} - \rho\mathbb{I})$, $aD_0^{\rm ker}$ the overlap *kernel*, any doubler-free massless Dirac operator (e.g. Wilson-Dirac), and $\rho \in (0,2)$.

Computational bottleneck: approximating the matrix sign function ${\rm sgn}[\mathbb{X}]$. The **established** approach is the **Zolotarev** rational approximation [1], which is *minimax-optimal* on a prescribed spectral interval $\lambda_{|\mathbb{X}|} \in [\alpha, \beta]$. Therefore, α and β must be determined from estimates of the extremal eigenvalues of $|\mathbb{X}|$ on *every* gauge configuration.

This work: We investigate the *efficiency* and *practicality* of combining the "Diagonal KL" rational approximation, which requires *no* spectral input, with a chirally improved overlap kernel (the "Brillouin" operator).

The Diagonal Kenney-Laub Iterates

The Diagonal (n,n) Kenney-Laub (KL) rational iterates f_{nn} approximate the matrix sign function [4]. In partial-fraction form they read:

$${\rm sgn}[\mathbb{X}] \approx f_{nn}(\mathbb{X}) = \mathcal{N}\,\mathbb{X}\left(\mathbb{I} + \sum_{i=1}^{n}\frac{w_i}{\mathbb{X}^2 + \sigma_i}\right)\ , \tag{3}$$

with shifts σ_i and weights w_i fixed in closed form by the order n alone:

$$\sigma_i = \tan^2\left[\frac{(2i-1)\pi}{4n+2}\right]\ ,\quad \mathcal{N} = \frac{1}{2n+1},\quad w_i = \frac{2}{\cos^2\left[\frac{(2i-1)\pi}{4n+2}\right]}\ . \tag{4}$$

All n shifted systems are solved by a single multi-shift CG (MSCG) call.

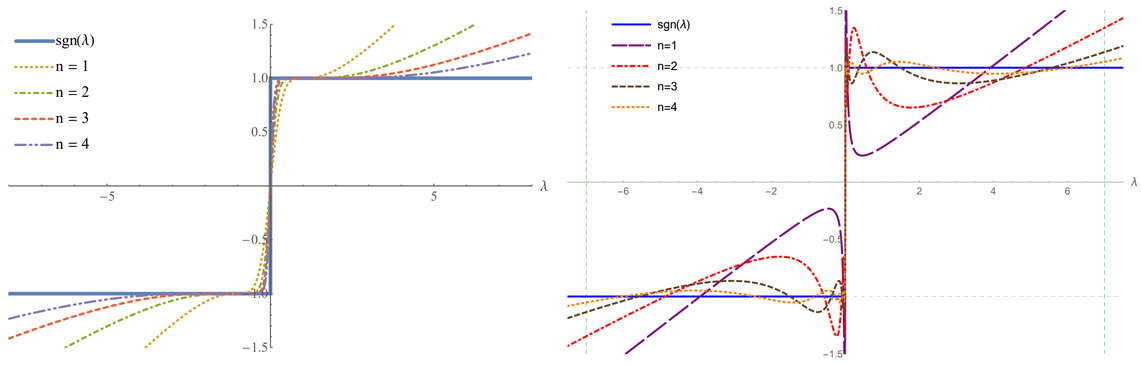

Figure 1: Scalar approximations to sgn(λ) of order $n = 1, \ldots, 4$: Diagonal KL (left) and Zolotarev (right), the latter constructed for $|\lambda| \in [10^{-3}, 7]$.

The Brillouin Kernel

A parameter-free, Wilson-like Dirac operator [2], used in this investigation as the overlap kernel. Although 3–4× more expensive per site than the Wilson-Dirac operator, its spectrum is considerably more compact:

$$\lambda_{|\mathbb{X}|}^{\rm max} \simeq 1.34\ \ \text{(Brillouin)} \qquad \text{vs.} \qquad \lambda_{|\mathbb{X}|}^{\rm max} \simeq 7.17\ \ \text{(Wilson)}\ . \tag{5}$$

The resulting condition number $\kappa_{\mathbb{X}^2}$ is reduced by 1-2 orders of magnitude.

Diagonal KL as the Degenerate Limit of Zolotarev

In the form of Eq. 3, the n Zolotarev shifts are $\sigma_i^Z = \alpha^2\, j_i(\alpha/\beta)$, with j_i's given by Jacobi elliptic functions. When the spectral interval collapses:

$$\sigma_i^Z \ \xrightarrow{\alpha,\beta\to 1}\ \tan^2\left[\frac{(2i-1)\pi}{4n+2}\right] = \sigma_i\ , \tag{6}$$

i.e. the diagonal KL iterate is the degenerate limit of the Zolotarev family. Away from this limit, the Zolotarev shifts depend on the spectral bounds, with $\sigma_i^Z \propto \alpha^{2-2/(2n+1)}$, so decreasing the smallest eigenvalue of $\mathbb{X}^2$ worsens the conditioning of the slowest MSCG system. The KL shifts are gauge-field independent, so the two methods can differ significantly in **cost** at equal n.

Setup

Quenched 48×24^3 ensemble, $\beta = 6.20$, $a \approx 0.066$ fm; 1 APE step, $\alpha_{\rm APE} = 0.72$; $\rho = 1$, $c_{SW} = 0$. Identical solvers and tolerances.

Result 1: GW Relation Violation

For the *massless* overlap operator, an approximate sgn[$\mathbb{X}$] violates Eq. 1. We quantify this violation on random vectors η through the difference Δ_{GW}:

$$\delta_{GW} = \frac{\|\Delta_{GW}\,\eta\|^2}{\|\eta\|^2}\ ,\qquad \Delta_{GW} \equiv \gamma_5\, aD^{\rm ov} + aD^{\rm ov}\gamma_5 - \frac{1}{\rho}\, aD^{\rm ov}\gamma_5\, aD^{\rm ov}\ . \tag{7}$$

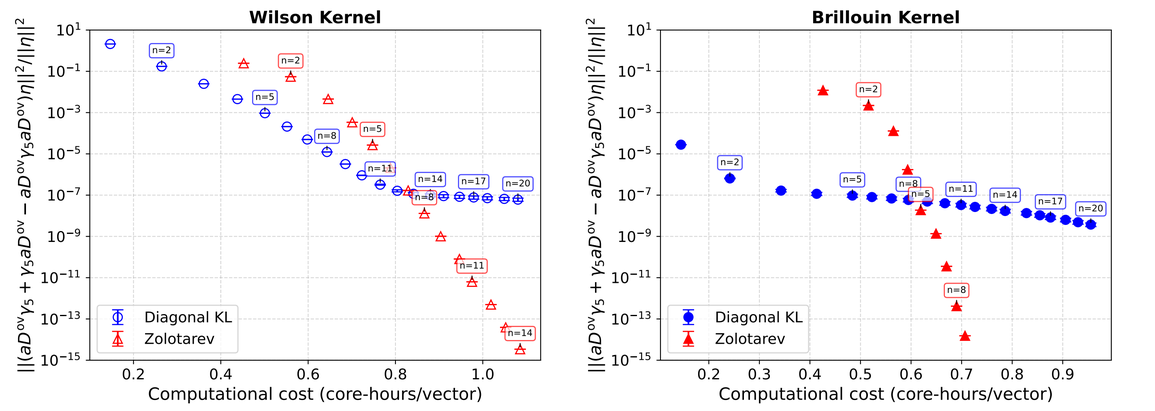

Figure 2: GW relation violation Vs. computational cost per random vector for Wilson (left) and Brillouin (right) kernels, on a poorly-conditioned configuration. Averages over 10 random vectors.

- The **Brillouin kernel** reaches a given violation at lower cost with *either* approximation method.
- At moderate precision, Diagonal KL is cheaper because its shifted systems are better conditioned; at higher precision, Zolotarev converges faster.

Result 2: Residual Chiral Symmetry Breaking

Using the *massive* overlap operator, plateau values of $am_{\rm PCAC}$ at several bare masses are extracted, then extrapolated to $am_{\rm PCAC} = 0$. The corresponding $am_{\rm bare}^{\rm critical}$ is the additive mass shift of the operator: it *vanishes* for an exactly chiral operator, so its magnitude measures the residual chiral symmetry breaking of the approximate overlap operator.

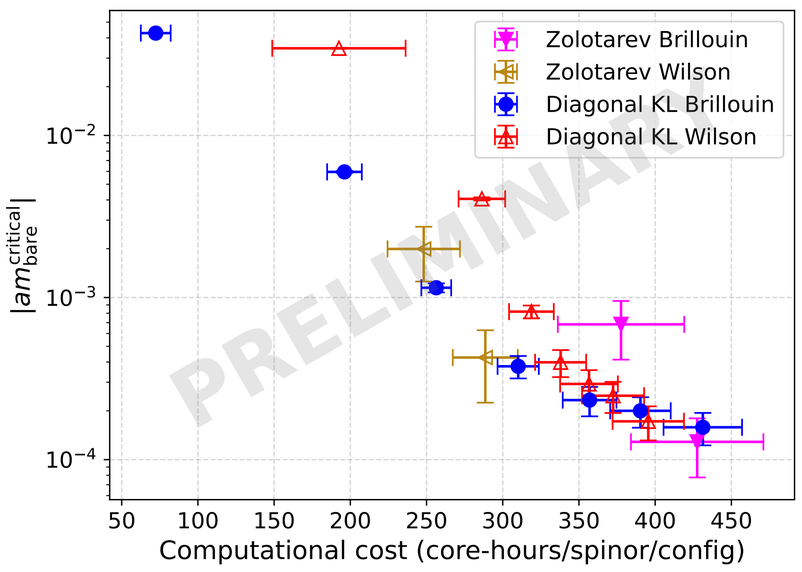

Figure 3: $|am_{\rm bare}^{\rm critical}|$ Vs. cost (core-hours per spinor per configuration at $aM_\pi \approx 300$ MeV), for both approximations and both kernels. Jackknife errors, propagated through the extrapolation. *Preliminary.*

- At $|am_{\rm bare}^{\rm critical}| \sim 10^{-4}$, both approximations require comparable cost. The **Diagonal KL**, however, needs no spectral estimation, is algorithmically simpler, and converges monotonically, hence predictably, in order n.

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