Algorithms for overlap fermions

Stefan Schaefer

NIC, DESY

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Overview

1. Chiral symmetry
2. Construction of the overlap operator
3. Solution of linear equations

Chiral symmetry in the continuum

$$D(m=0)\gamma_5 + \gamma_5 D(m=0) = 0$$

- spontaneously broken by interactions: $\langle \Sigma \rangle = -\langle \bar{q} q \rangle \neq 0$
- explicitly broken by quark mass
- index theorem

Important for understanding of low-energy physics

- light meson spectrum
- chiral perturbation theory
- instantons

$\Longrightarrow$ Want to keep it on the lattice

Chiral symmetry on the lattice

Ginsparg, Wilson '82

$$D_0\gamma_5 + \gamma_5 D_0 = \frac{a}{R_0} D_0\gamma_5 D_0$$

D_0 : massless Dirac operator
a : lattice spacing
R_0 : radius of the GW–circle

- correct chiral and flavor symmetries
- $\mathcal{O}(a)$ improvement
- topology can be defined by index of the Dirac operator
- simplified renormalization
- strictly positive fermion determinant

Solutions to the Ginsparg–Wilson Equation

- overlap fermions (Neuberger)
- Domain Wall fermions (Kaplan, Shamir)
- Perfect Action (Hasenfratz, Niedermayer,..)
- approximate solutions (Gattringer et al, Bietenholz)

Use the overlap if you want chiral symmetry to machine precision.

Neuberger's overlap operator

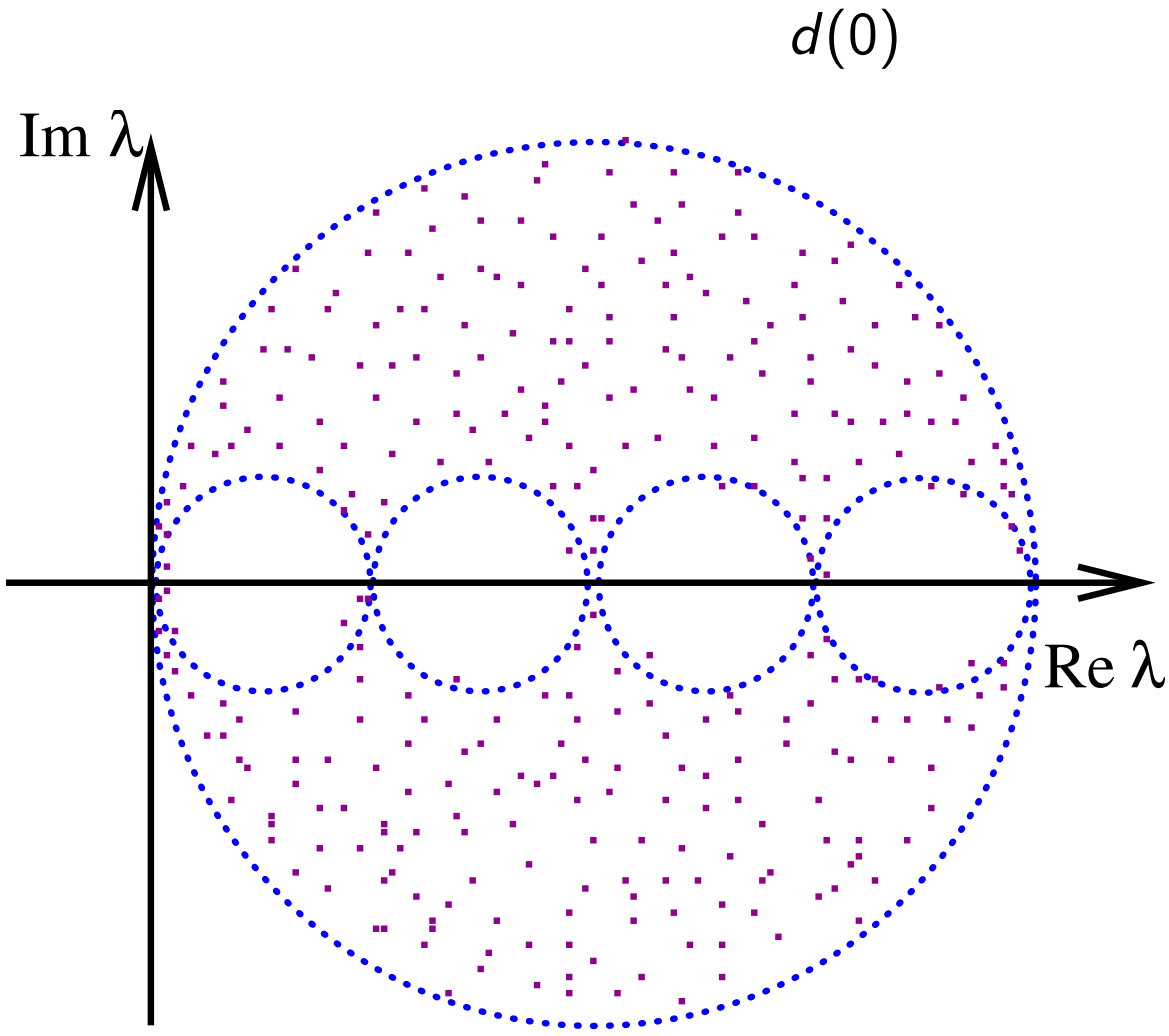
Neuberger '97, '98

$$D_{ov}(m=0) = R_0\Big[\ 1\ +\ d(-R_0)\frac{1}{\sqrt{d^\dagger d(-R_0)}}\ \Big] \qquad (1)$$
$$= R_0\Big[\ 1\ +\ \gamma_5\ \epsilon(h(-R_0))\ \Big]$$

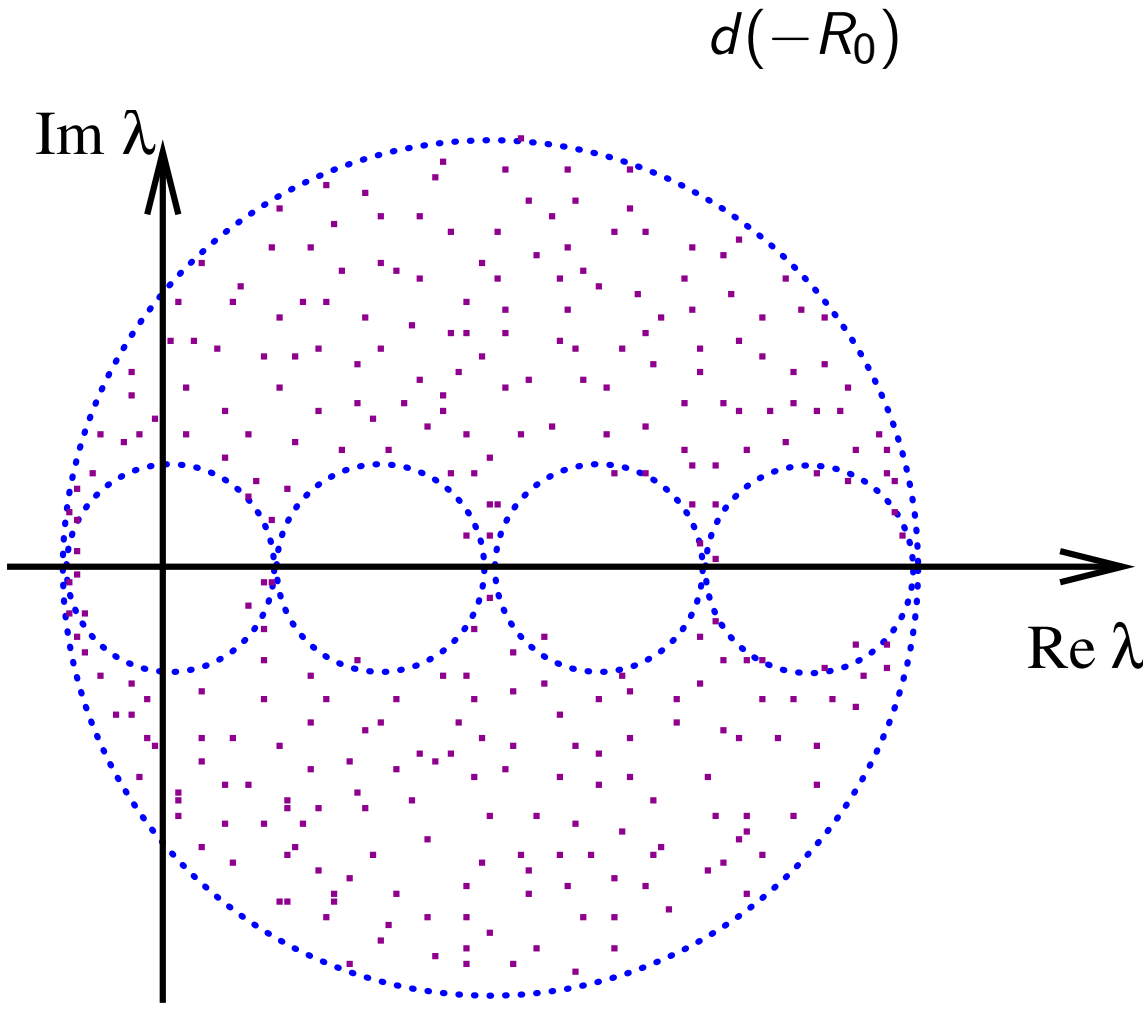
with

- $h = \gamma_5 d$ Hermitian (Wilson) Dirac operator
- $-R_0$ negative mass shift $\propto 1/a$
- ϵ is the matrix sign function

Construction of the overlap

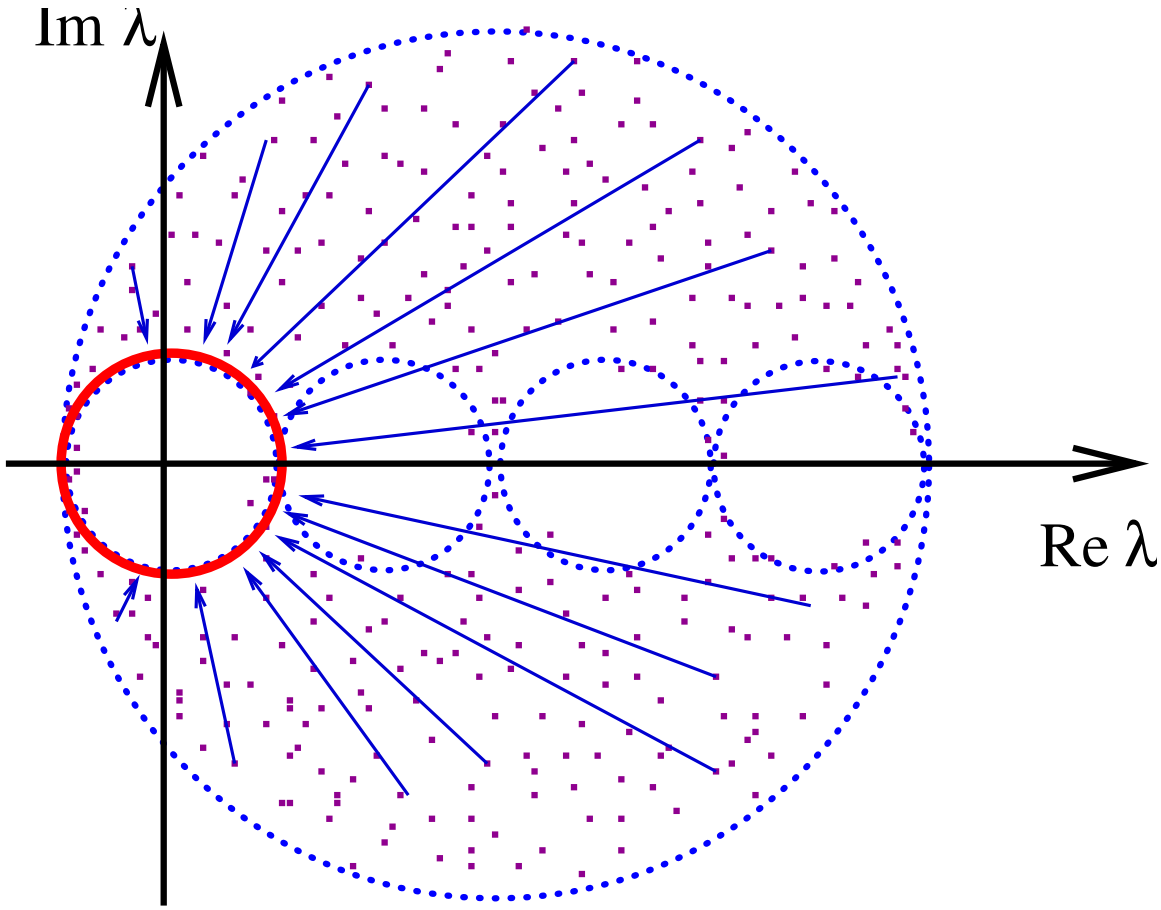


Construction of the overlap



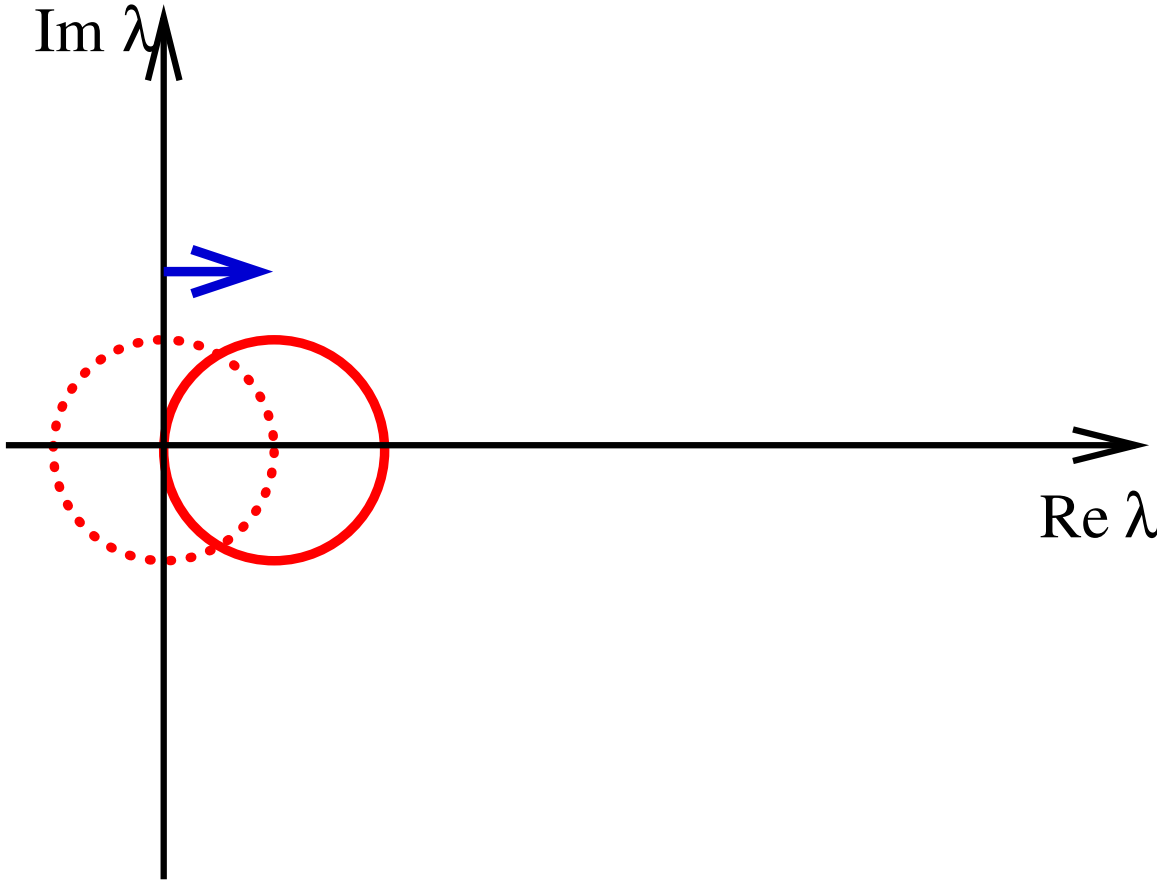
Construction of the overlap

$$d(-R_0)\frac{1}{\sqrt{d(-R_0)^\dagger d(-R_0)}} = \gamma_5 \frac{h(-R_0)}{\sqrt{h(-R_0)^2}} = \gamma_5 \epsilon(h(-R_0))$$



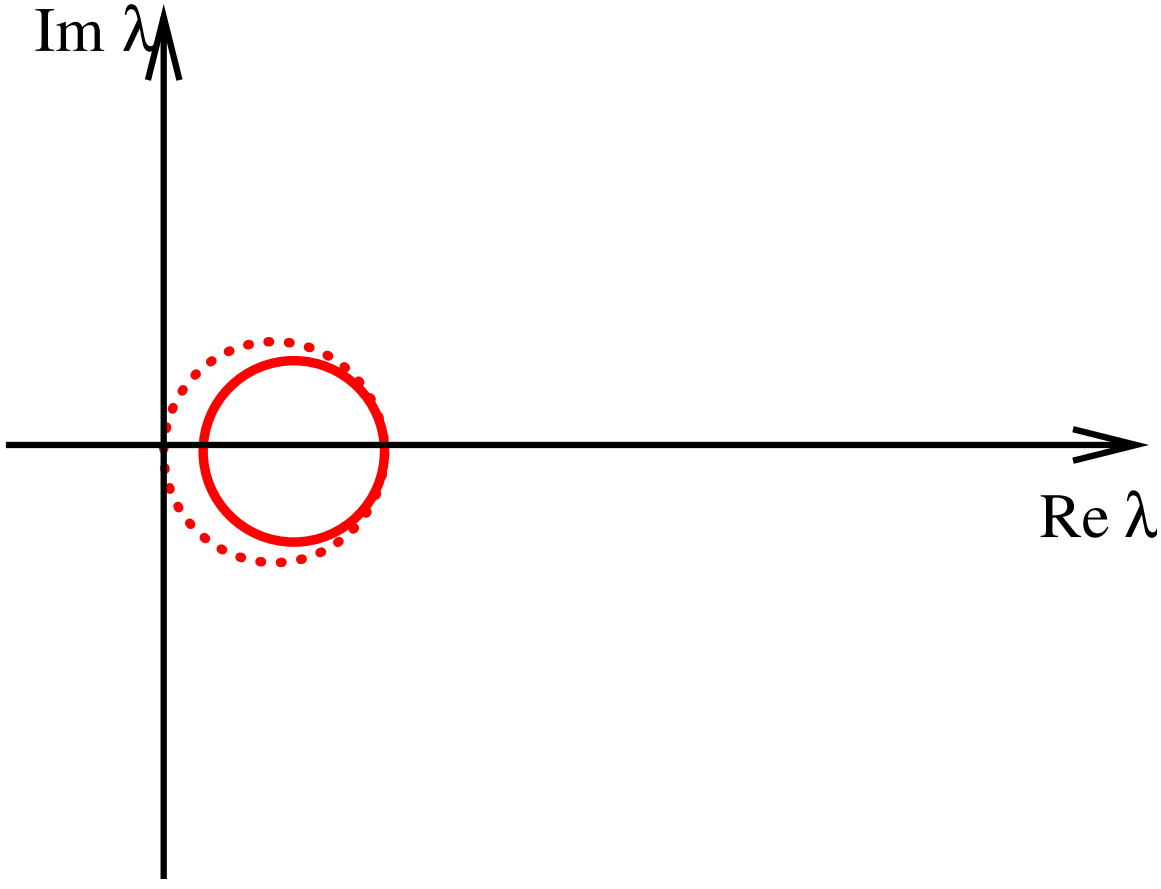
Construction of the overlap

$$D(m=0) = R_0(1+\gamma_5\epsilon(h(-R_0))$$



Construction of the overlap

$$D(m) = (R_0 - \frac{m}{2})(1 + \epsilon(h(-R_0)) + m$$

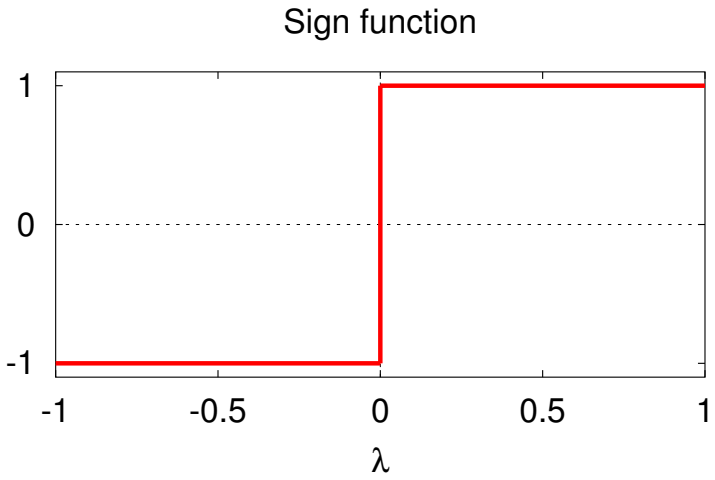


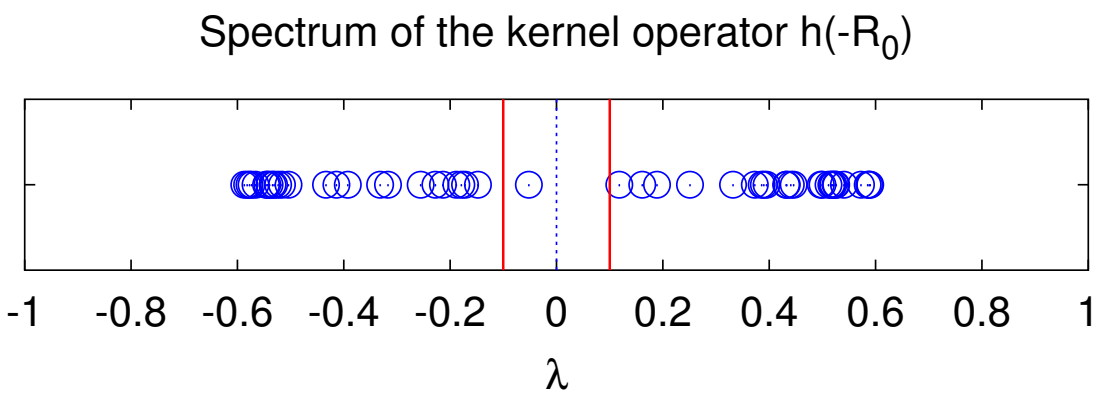
Definition of the matrix sign function

$$\epsilon(h) = \frac{h}{\sqrt{h^2}} = \sum_i \mathrm{sign}(\lambda_i)|\lambda_i\rangle\langle\lambda_i|$$

λ_i : eigenvalues of h

$|\lambda_i\rangle$: associated eigenvectors

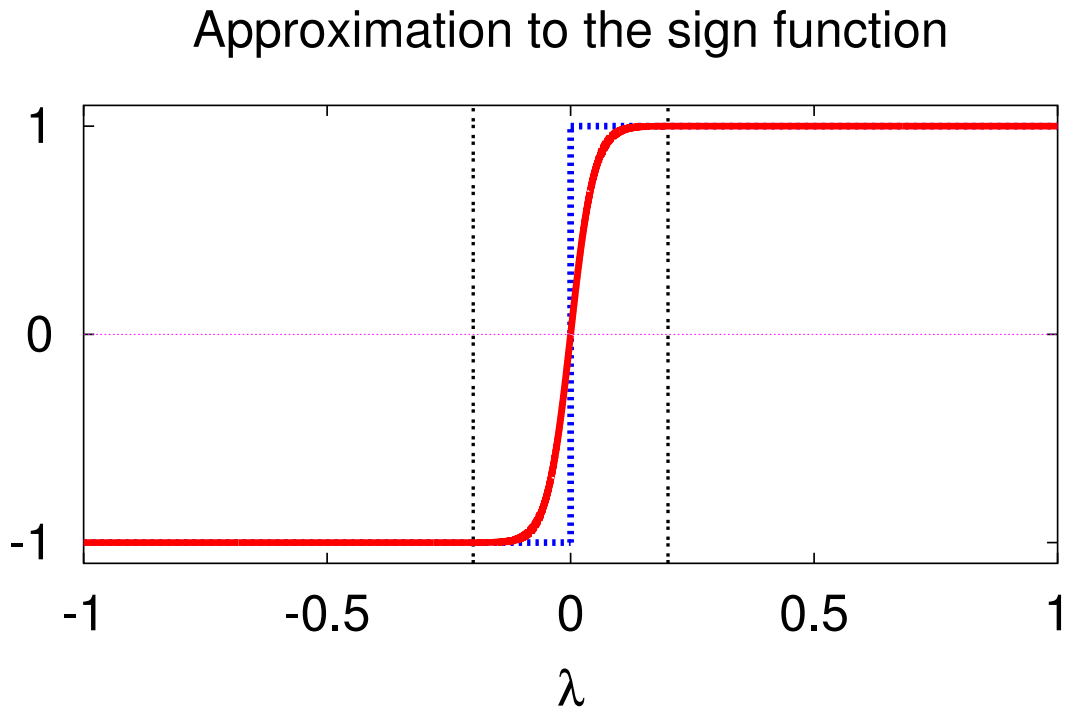




Implementation of the sign function

- Use spectral representation for $|\lambda| < |\lambda_{\min}|$
- Use approximation for the rest of the spectrum.
- Cost of approximation increases for smaller $\lambda_{\min}$

$$\epsilon(h) = \sum_{n=1}^{N} \mathrm{sign}(\lambda_i)|\lambda_i\rangle\langle\lambda_i| + (1 - \sum_{n=1}^{N} |\lambda_i\rangle\langle\lambda_i|)\epsilon_{\mathrm{app}}(h)$$

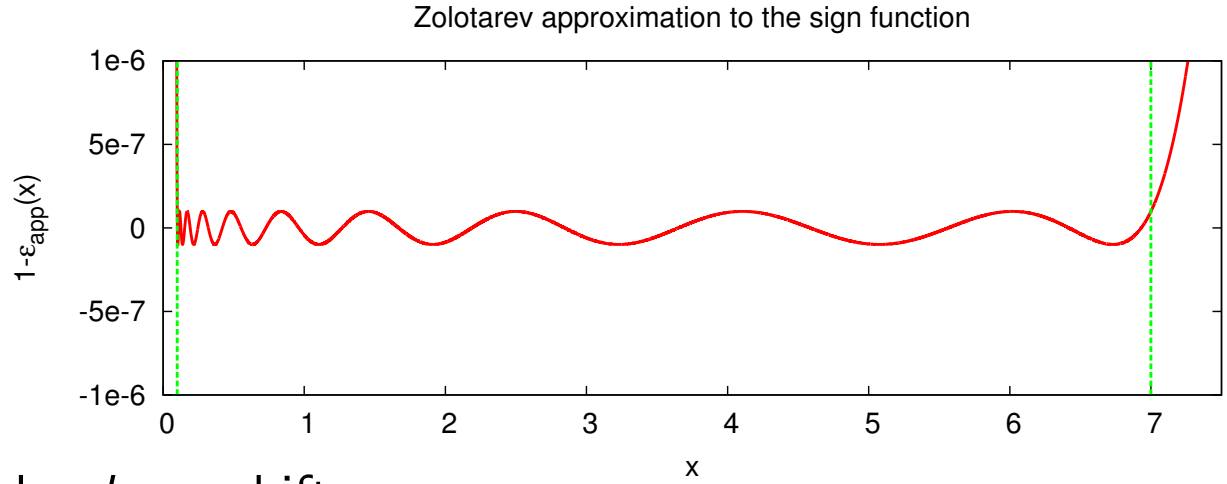


The sign function: Rational approximations

$$\epsilon(h) = h \sum_{i=1}^{M} \frac{b_i}{h^2 + c_i}$$

- coefficients determined by accuracy and range of the approximation
- need to solve systems $(h^2 + c_i)\, x \;=\; v$
- multi-mass
- interplay between accuracy of the solver & precision of the scalar approximation
- need several hundred h on vector multiplications for on D_{ov}.

Example: Zolotarev approximation



n	residue b_n	shift c_n
0	0.037	0.0008
1	0.050	0.009
2	0.078	0.037
3	0.132	0.124
4	0.229	0.395
5	0.406	1.240
6	0.741	3.941
7	1.472	13.244
8	3.841	54.340
9	32.04	601.173

$$\epsilon_{app}(x) = x \sum_n \frac{b_n}{x^2 + c_n}$$

- 10 shifts, $x \in [0.1, 7] \Rightarrow 1 \cdot 10^{-7}$ accuracy
- cost determined by smallest shift
- smallest shift decreases with larger range of approx.

Chebychev Polynomials

Approximate $1/\sqrt{h^2}$ by a sum over Chebychev polynomials

$$\epsilon(h) \approx h \sum_{n=0}^{N} c_n T_n(h^2)$$

- sum is computed with the (recursive) Clenshaw algorithm: numerically very stable
- need several hundred terms
- one parameter determines the accuracy of the approximation

Summary I: Contruction of the overlap operator

$$D_{\mathrm{ov}}(m) = (R_0 - \frac{m}{2})\left[1 + \gamma_5 \epsilon(h(-R_0))\right] + m$$

- expensive part is the application of the sign function on a vector
- project low modes of the kernel operator $h(-R_0)$
- use rational or polynomial approximation for the rest of the spectrum
- several hundred times more expensive than applying Wilson operator
- for larger volume, there are more modes to project

Solving systems of linear equations

$$D_{\mathrm{ov}}^{\dagger}(m) D_{\mathrm{ov}}(m) x = b$$

- use an iterative solver: many tried, best depends on physical situation
- $D_{\mathrm{ov}}^{\dagger} D_{\mathrm{ov}}$ has strict upper bound for conditioning number $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}} = \frac{R_0^2}{m^2}$
- total cost $n_{iter} \times n_{construct}$
- application of $D^{\dagger} D$ as expensive as application of D

Improvements I: adaptive / relaxed precision

Strategy for improvement:

- Krylov methods build solution from $\{(D^\dagger D)^n v; n = 0, ..., N\}$

$$x = \sum_{n=0}^{N} c_i (D^\dagger D)^n v$$

- identify less important contributions and compute $\epsilon(h)w$ with reduced accuracy
  - lower order polynomial
  - less accurate rational approximation / reduced inner solver precision

Recent publications:
Cundy et al, CPC 165:221-242,2005
Chiarappa et al, hep-lat/0609023

Example RelCG

Taken from Cundy et al, CPC 165:221-242,2005

compute x such that $\|D_{\mathrm{ov}}^{\dagger} D_{\mathrm{ov}} x - b\| \leq \epsilon \cdot \|b\|$

$x = 0$; $r = b$; $p = r$;

$\gamma_{old} = \gamma = r^{\dagger} \cdot r$; $\zeta = 1/\gamma$;

while $\sqrt{\gamma} > \epsilon \cdot \|b\|$ **do**

compute q with $\|D_{\mathrm{ov}}^{\dagger} D_{\mathrm{ov}} p - q\| \leq \epsilon \cdot \|b\| \cdot \|p\| \cdot \sqrt{\zeta}$;

$\beta = q^{\dagger} \cdot p$;

$\alpha = \gamma/\beta$;

$x = x + \alpha \cdot p$;

$r = r - \alpha \cdot q$;

$\gamma = r^{\dagger} \cdot r$;

$\zeta = \zeta + 1/\gamma$;

$p = r + \gamma/\gamma_{old} \cdot p$;

$\gamma_{old} = \gamma$;

end while

- Many algorithms can be modified in this way
- key is to find a strategy to relax accuracy and keep convergence under control
- gain depends on the situation and the solver: up to factor 5 reported
- Cundy et al, CPC 165:221-242,2005
- Chiarappa et al, hep-lat/0609023 (computation of inverse 30-120 times more expensive than TM)

Improvements II: Low mode preconditioning

Same trick as used for the construction of the sign function

$$(D_{\mathrm{ov}}^{\dagger}(m)D_{\mathrm{ov}}(m))^{-1}v = \sum_{i=1}^{N} \frac{1}{\lambda_i}\psi_{\lambda_i}\psi_{\lambda_i}^{\dagger}v + (1-P)(D_{\mathrm{ov}}^{\dagger}D_{\mathrm{ov}}(m))^{-1}v$$

- Can be made exact by Schur complement technique (Chiarappa et al, hep-lat/0609023)
- even relatively poor eigenvectors can lead to significant speed-up
- best suited if system is solved for many sources

Conclusions

- chiral symmetry simplifies many lattice computations
- chiral fermions are expensive: need to construct sign function
- state of the art: low-mode projection + rational (Zolotarev) or polynomial (Chebychev) approximation
- solver can be greatly improved my relaxing the accuracy of the sign function
- many solvers have been tested; best setup depends on physical situation
- total cost 30–100 times of twisted mass fermions — in quenched
- dynamical simultations: coarse lattice should be possible