

Deflation and polynomial preconditioning in the application of the overlap operator at nonzero chemical potential

Lattice Conference, July 2024, Liverpool

Gustavo Ramirez-Hidalgo

(Bergische Universität Wuppertal)

&

Jacob Finkenrath

(CERN)



BERGISCHE
UNIVERSITÄT
WUPPERTAL

Table of Contents

The overlap discretization

Preconditioning at the solver level

Preconditioning at the sign-function level

“Modern” overlap solver



The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice



The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator



The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator
- ▶ then, the overlap operator is:
$$D_N = \rho I + \Gamma_5 \text{sign} \left(Q(m_0^{ker}) \right),$$
with $\text{sign}(A) = A(A^2)^{-1/2}$ and
$$Q(m_0^{ker}) = \Gamma_5 D_w(m_0^{ker})$$



The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator
- ▶ then, the overlap operator is:

$$D_N = \rho I + \Gamma_5 \text{sign} \left(Q(m_0^{ker}) \right),$$
 with $\text{sign}(A) = A(A^2)^{-1/2}$ and

$$Q(m_0^{ker}) = \Gamma_5 D_w(m_0^{ker})$$
- ▶ we further equip here the Dirac operator with a chemical potential i.e. $D_w(\mu, m_0^{ker})$, and then

$$Q_\mu^H = Q_{-\mu}$$



The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator
- ▶ then, the overlap operator is:
$$D_N = \rho I + \Gamma_5 \text{sign} (Q(m_0^{ker})),$$
with $\text{sign}(A) = A(A^2)^{-1/2}$ and
$$Q(m_0^{ker}) = \Gamma_5 D_w(m_0^{ker})$$
- ▶ we further equip here the Dirac operator with a chemical potential i.e. $D_w(\mu, m_0^{ker})$, and then
$$Q_\mu^H = Q_{-\mu}$$
- ▶ **task**: solve linear systems with
$$D_N$$

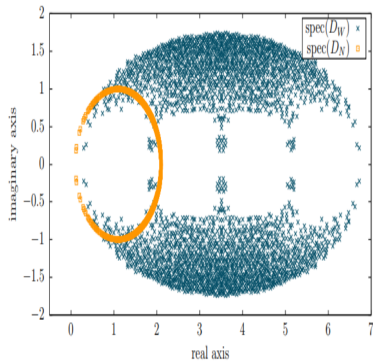


The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator
- ▶ then, the overlap operator is:

$$D_N = \rho I + \Gamma_5 \text{sign} (Q(m_0^{ker})),$$
 with $\text{sign}(A) = A(A^2)^{-1/2}$ and $Q(m_0^{ker}) = \Gamma_5 D_w(m_0^{ker})$
- ▶ we further equip here the Dirac operator with a chemical potential i.e. $D_w(\mu, m_0^{ker})$, and then $Q_\mu^H = Q_{-\mu}$
- ▶ **task**: solve linear systems with D_N

- ▶ on a 4^4 lattice (no chemical potential):

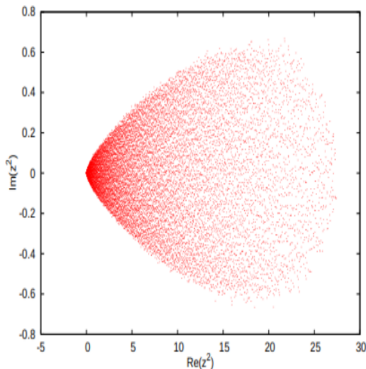


The overlap discretization

- ▶ keeps chiral symmetry when moving to the lattice
- ▶ take D_w to be the usual Wilson-Dirac operator
- ▶ then, the overlap operator is:

$$D_N = \rho I + \Gamma_5 \text{sign} (Q(m_0^{ker})),$$
 with $\text{sign}(A) = A(A^2)^{-1/2}$ and $Q(m_0^{ker}) = \Gamma_5 D_w(m_0^{ker})$
- ▶ we further equip here the Dirac operator with a chemical potential i.e. $D_w(\mu, m_0^{ker})$, and then $Q_\mu^H = Q_{-\mu}$
- ▶ **task**: solve linear systems with D_N

- ▶ on a 6^4 lattice ($\mu = 0.3, \beta_g = 5.1$), spectrum of $Q_\mu^2(m_0^{ker})$:



Preconditioning at the solver level

- ▶ a first approach at boosting these computations is preconditioning at the level of D_N , i.e. solving linear systems with

$$D_N \cdot \text{AMG}(D_w(m_0^{prec}), \epsilon)$$



Preconditioning at the solver level

- ▶ a first approach at boosting these computations is preconditioning at the level of D_N , i.e. solving linear systems with

$$D_N \cdot \text{AMG}(D_w(m_0^{\text{prec}}), \epsilon)$$

- ▶ motivation for this: if we assume that $D_w(m_0^{\text{prec}})$ is normal, then:

$$\text{spec}(D_N(D_w(m_0^{\text{prec}}))^{-1}) = \left\{ \frac{\rho + c \text{sign}(\lambda + m_0^{\text{ker}})}{\lambda + m_0^{\text{prec}}}, \lambda \in \text{spec}(D_w(0)) \right\},$$

and there is an analytic expression for m_0^{prec} which is quite close to optimal



Preconditioning at the solver level

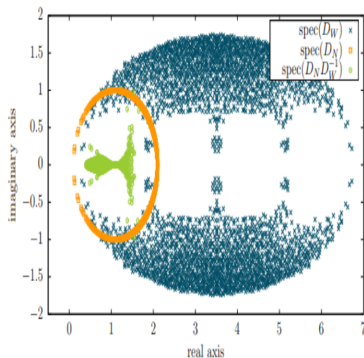
- ▶ a first approach at boosting these computations is preconditioning at the level of D_N , i.e. solving linear systems with

$$D_N \cdot \text{AMG}(D_w(m_0^{\text{prec}}), \epsilon)$$

- ▶ motivation for this: if we assume that $D_w(m_0^{\text{prec}})$ is normal, then:

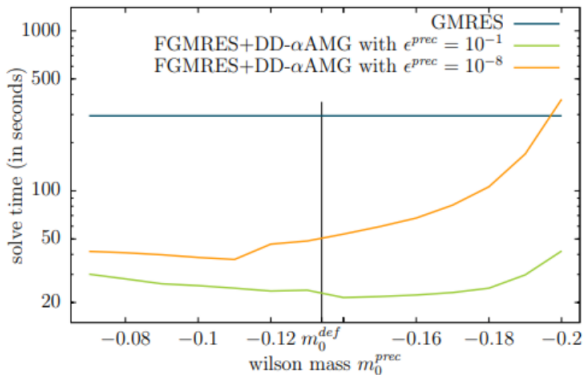
$$\text{spec}(D_N(D_w(m_0^{\text{prec}}))^{-1}) = \left\{ \frac{\rho + c \text{sign}(\lambda + m_0^{\text{ker}})}{\lambda + m_0^{\text{prec}}}, \lambda \in \text{spec}(D_w(0)) \right\},$$
 and there is an analytic expression for m_0^{prec} which is quite close to optimal

- ▶ on a 4^4 lattice (no chemical potential):



Preconditioning at the solver level

Impact of preconditioning, at the level of D_N , via $\text{AMG}(D_w(m_0^{prec}), \epsilon)$ (no chemical potential, 32×32^3 , smeared, work by [Brannick, Frommer, Kahl, Leder, Rottmann, Strebel - 2014](#)):



Preconditioning at the sign-function level

But, the sign function still has to be applied and that is the most expensive part.



Preconditioning at the sign-function level

But, the sign function still has to be applied and that is the most expensive part.

In recent work ([Frommer, R-H, Schweitzer, Tsolakis - 2024](#)), we have introduced polynomial preconditioning for the inverse square root:



Preconditioning at the sign-function level

But, the sign function still has to be applied and that is the most expensive part.

In recent work ([Frommer, R-H, Schweitzer, Tsolakis - 2024](#)), we have introduced polynomial preconditioning for the inverse square root:

$$A^{-1/2}b = q(A)(A(q(A))^2)^{-1/2}b \text{ with } q(A) \approx A^{-1/2}.$$



Preconditioning at the sign-function level

But, the sign function still has to be applied and that is the most expensive part.

In recent work ([Frommer, R-H, Schweitzer, Tsolakis - 2024](#)), we have introduced polynomial preconditioning for the inverse square root:

$$A^{-1/2}b = q(A)(A(q(A))^2)^{-1/2}b \text{ with } q(A) \approx A^{-1/2}.$$

In the LQCD context, this means:

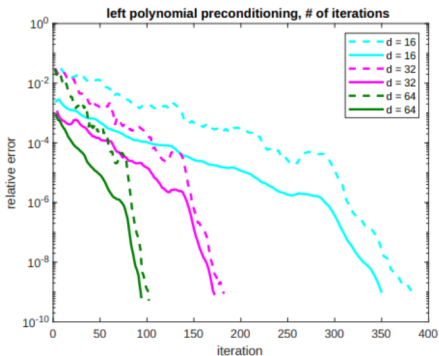
$$(Q_\mu^2)^{-1/2}b = q(Q_\mu^2)(Q_\mu^2(q(Q_\mu^2))^2)^{-1/2}b \text{ with } q(Q_\mu^2) \approx (Q_\mu^2)^{-1/2}$$

(note how Arnoldi is done with Q_μ^2).



Preconditioning at the sign-function level

With a chemical potential $\mu = 0.3$, 64×32^3 , non-smeared, d is the degree of the polynomial, the **dashed** lines are a cheap approximation of the error. Tolerances are 10^{-5} for the table and 10^{-9} for the figure.



d	iterations	mvms	inner products	time 64 nodes (in s)	time 256 nodes (in s)
1	1 600	3 200	1 279 200	127.8	105.8
8	296	8 910	42 510	25.7	9.8
16	140	8 742	9 991	12.3	7.8
32	72	9 198	3 125	11.6	7.4
64	33	8 636	2 578	10.6	5.5



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

► let: $AR_m = R_m\Lambda_m$



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

- ▶ let: $AR_m = R_m\Lambda_m$
- ▶ let: $L_m^H A = \Lambda_m L_m^H$



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

- ▶ let: $AR_m = R_m\Lambda_m$
- ▶ let: $L_m^H A = \Lambda_m L_m^H$
- ▶ then: $f(A)b = f(A)(I - R_m L_m^H)b + f(A)R_m L_m^H b$ (note:
 $f(A)R_m L_m^H b = R_m f(\Lambda_m) L_m^H b$)



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

- ▶ let: $AR_m = R_m\Lambda_m$
- ▶ let: $L_m^H A = \Lambda_m L_m^H$
- ▶ then: $f(A)b = f(A)(I - R_m L_m^H)b + f(A)R_m L_m^H b$ (note:
 $f(A)R_m L_m^H b = R_m f(\Lambda_m) L_m^H b$)

- ▶ main problem with this approach: eigensolving can be extremely expensive



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

- ▶ let: $AR_m = R_m\Lambda_m$
- ▶ let: $L_m^H A = \Lambda_m L_m^H$
- ▶ then: $f(A)b = f(A)(I - R_m L_m^H)b + f(A)R_m L_m^H b$ (note: $f(A)R_m L_m^H b = R_m f(\Lambda_m) L_m^H b$)

- ▶ main problem with this approach: eigensolving can be extremely expensive
- ▶ our numerical experiments show that expensive eigensolving is not a critical issue anymore, if we **combine polynomial preconditioning with LR deflation**



Preconditioning at the sign-function level

A short note on LR deflation for the sign function (Bloch, Frommer, Lang, Wettig - 2007):

- ▶ let: $AR_m = R_m\Lambda_m$
- ▶ let: $L_m^H A = \Lambda_m L_m^H$
- ▶ then: $f(A)b = f(A)(I - R_m L_m^H)b + f(A)R_m L_m^H b$ (note: $f(A)R_m L_m^H b = R_m f(\Lambda_m) L_m^H b$)

- ▶ main problem with this approach: eigensolving can be extremely expensive
- ▶ our numerical experiments show that expensive eigensolving is not a critical issue anymore, if we **combine polynomial preconditioning with LR deflation**

Analyzing the interplay of polynomial preconditioning with deflation, in the context of the sign function, is **ongoing work**.

"Modern" overlap solver

```

1: while not converged do
2:   for  $i = 1 : m_{out}$  do
3:     ...
4:     for  $j = 1 : m_{in}$  do
5:       ...
6:        $v_{in}^{(1)} \leftarrow \text{AMG}(D_w(m_0^{prec}, \epsilon)) w_{in}^{(1)}$  (hp)
7:       ...
8:        $v_{in}^{(2)} \leftarrow \left(Q_\mu^2 (q(Q_\mu^2))^2\right)^{-1/2} \left(w_{in}^{(2)} - R_m L_m^H w_{in}^{(2)}\right)$  (sp/hp)
9:       ...
10:    end for
11:    ...
12:     $v_{out} \leftarrow \left(Q_\mu^2 (q(Q_\mu^2))^2\right)^{-1/2} \left(w_{out} - R_m L_m^H w_{out}\right)$  (dp)
13:    ...
14:  end for
15: end while

```



Thank you!

