First experiences with overlap fermions based on the Brillouin kernel

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In memoriam Peter Hasenfratz and Keisuke Jimmy Juge



The legacy of the "perfect action"



Perfect action: Ginsparg-Wilson spectrum, linear dispersion relation, no cut-off effects !

• Pedestrian (bottom-up) approach



$$D(x,y) = \frac{1}{2} \sum_{\mu} \left\{ (\gamma_{\mu} - I) U_{\mu}(x) \delta_{x+\hat{\mu},y} - (\gamma_{\mu} + I) U_{\mu}^{\dagger}(x-\hat{\mu}) \delta_{x-\hat{\mu},y} \right\} + \frac{1}{2\kappa} \delta_{x,y} - \frac{c_{\rm SW}}{2} \dots$$

with $\sigma_{\mu\nu} = \frac{i}{2} [\gamma_{\mu}, \gamma_{\nu}]$ and $F_{\mu\nu}$ the hermitean clover-leaf field-strength tensor equals

$$D(x,y) = \sum_{\mu} \gamma_{\mu} \nabla^{\text{std}}_{\mu}(x,y) - \frac{a}{2} \triangle^{\text{std}}(x,y) + m_0 \delta_{x,y} + \text{improvement term}$$

with the two mass parameters relating to each other through $1/(2\kappa) = 4 + am_0$.

Brillouin operator in 2D

• 4 options for Laplacian



Standard Laplacian in 2D: $\hat{\Delta} = 2\cos(k_1) + 2\cos(k_2) - 4$ Tilted Laplacian in 2D: $\hat{\Delta} = 2\cos(k_1)\cos(k_2) - 2$ Brillouin Laplacian in 2D: $\hat{\Delta} = 4\cos^2(k_1/2)\cos^2(k_2/2) - 4$ Isotropic Laplacian in 2D: $\hat{\Delta} = [2\cos(k_1)\cos(k_2) + 4\cos(k_1) + 4\cos(k_2) - 10]/3$

• 3 options for derivative



Standard Derivative in 2D: $\hat{\partial}_x = i \sin(k_1)$ Brillouin Derivative in 2D: $\hat{\partial}_x = i \sin(k_1) [\cos(k_2) + 1]/2$ Isotropic Derivative in 2D: $\hat{\partial}_x = i \sin(k_1) [\cos(k_2) + 2]/3$

Ultralocality

All 2D stencils (12 options) restricted to $[-1:1]^2$ hypercube (9 sites).

• Eigenvalues of Wilson and Brillouin operators in 2D



• Free dispersion relation for Wilson and Brillouin operators in 2D



Brillouin operator in 4D

• 4 options for Laplacian

 $\begin{array}{lll} \mbox{Standard Laplacian:} & \hat{\bigtriangleup} = 2\cos(k_1) + 2\cos(k_2) + 2\cos(k_3) + 2\cos(k_4) - 8 \\ \mbox{Tilted Laplacian:} & \hat{\bigtriangleup} = 2\cos(k_1)\cos(k_2)\cos(k_3)\cos(k_4) - 2 \\ \mbox{Brillouin Laplacian:} & \hat{\bigtriangleup} = 4\cos^2(k_1/2)\cos^2(k_2/2)\cos^2(k_3/2)\cos^2(k_4/2) - 4 \\ \mbox{Isotropic Laplacian:} & \hat{\bigtriangleup} = [2c_1c_2c_3c_4 + 7c_1c_2c_3 + ... + 20c_1c_2 + ... + 25c_1 + ... - 250]/54 \end{array}$

• 3 options for derivative

Standard Derivative: $\hat{\partial}_x = i \sin(k_1)$ Brillouin Derivative: $\hat{\partial}_x = i \sin(k_1) [\cos(k_2) + 1] [\cos(k_3) + 1] [\cos(k_4) + 1]/8$ Isotropic Derivative: $\hat{\partial}_x = i \sin(k_1) [\cos(k_2) + 2] [\cos(k_3) + 2] [\cos(k_4) + 2]/27$

(4D stencils look similar to 2D case)

• Ultralocality

All 4D stencils (12 options) restricted to $[-1:1]^4$ hypercube (81 sites).

• Free eigenvalues of Wilson and Brillouin operators in 4D



Free-field dispersion relations

Notation:
$$\hat{p}_{\mu} = \frac{2}{a} \sin(\frac{ap_{\mu}}{2}), \quad \bar{p}_{\mu} = \frac{1}{a} \sin(ap_{\mu}), \quad \tilde{p}_{\mu} = \frac{1}{27a} \sin(ap_{\mu}) \prod_{\nu \neq \mu} \{\cos(ap_{\nu}) + 2\}$$

 $\Rightarrow \nabla^{\text{std}}_{\mu} = i\bar{p}_{\mu}, \quad \Delta^{\text{std}} = -\frac{4}{a^2} \sum_{\mu} \sin^2(\frac{ap_{\mu}}{2}) = \frac{2}{a^2} \sum_{\mu} \cos(ap_{\mu}) - \frac{8}{a^2} = -\sum_{\mu} \hat{p}_{\mu}^2 = -\hat{p}^2$
 $\Rightarrow \nabla^{\text{iso}}_{\mu} = i\tilde{p}_{\mu}, \quad \Delta^{\text{bri}} = \frac{4}{a^2} \prod_{\mu} \cos^2(\frac{ap_{\mu}}{2}) - \frac{4}{a^2} = \frac{1}{4a^2} \prod_{\mu} \{\cos(ap_{\mu}) + 1\} - \frac{4}{a^2} \equiv -\check{p}^2$

• Dispersion relation for Wilson operator

$$D_{W,m} = \nabla^{\text{std}}_{\mu} \gamma_{\mu} - \frac{a}{2} \Delta^{\text{std}} + m = i\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^{2} + m$$

$$G_{W,m} = \frac{-i\bar{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\hat{p}^{2} + m}{(i\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^{2} + m)(-i\bar{p}_{\nu}\gamma_{\nu} + \frac{a}{2}\hat{p}^{2} + m)} = \frac{-i\bar{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\hat{p}^{2} + m}{\bar{p}^{2} + (\frac{a}{2}\hat{p}^{2} + m)^{2}}$$

Search for zero of denominator with $p_4 \rightarrow iE$ and $\frac{a}{2}\hat{p}^2 = -\frac{1}{a}\sum_{\mu}\cos(ap_{\mu}) + \frac{4}{a}$ yields

$$\sinh^{2}(aE) - \sum_{i} \sin^{2}(ap_{i}) = \cosh^{2}(aE) + 2\cosh(aE) \left[\sum_{i} \cos(ap_{i}) - 4 - am\right] + \left[...\right]^{2}$$

and with $\cosh^2 - \sinh^2 = 1$ this turns into a *linear equation* in $\cosh(aE)$.



 \ominus strong deviation from continuum for any $a|\mathbf{p}| > 1$ \ominus strong rotational symmetry breaking for any $a|\mathbf{p}| > 1$

 \ominus strong effect of $am \ll 1$, even at $\mathbf{p} = \mathbf{0}$

• Dispersion relation for Brillouin operator

$$D_{B,m} = \nabla^{iso}_{\mu} \gamma_{\mu} - \frac{a}{2} \Delta^{bri} + m = i \tilde{p}_{\mu} \gamma_{\mu} + \frac{a}{2} \check{p}^{2} + m$$

$$G_{B,m} = \frac{-i \tilde{p}_{\sigma} \gamma_{\sigma} + \frac{a}{2} \check{p}^{2} + m}{(i \tilde{p}_{\mu} \gamma_{\mu} + \frac{a}{2} \check{p}^{2} + m)(-i \tilde{p}_{\nu} \gamma_{\nu} + \frac{a}{2} \check{p}^{2} + m)} = \frac{-i \tilde{p}_{\sigma} \gamma_{\sigma} + \frac{a}{2} \check{p}^{2} + m}{\tilde{p}^{2} + (\frac{a}{2} \check{p}^{2} + m)^{2}}$$

Search for zero of denominator with $p_4 \rightarrow iE$ yields

$$\sum_{\mu} \tilde{p}_{\mu}^2 + \frac{1}{64a^2} \prod_{\mu} \{c_{\mu} + 1\}^2 - \frac{1}{4a} \prod_{\mu} \{c_{\mu} + 1\} [\frac{2}{a} + m] + [\frac{2}{a} + m]^2 = 0$$

with $\tilde{p}^2 = \frac{1}{729a^2} \sum_{\mu} s^2_{\mu} \prod_{\nu \neq \mu} \{c_{\nu} + 2\}^2$ this takes the form

$$\frac{1}{729a^2} \sum_i s_i^2 \prod_{j \neq i} \{c_j + 2\}^2 \{c_4^2 + 4c_4 + 4\} + \frac{1}{729a^2} s_4^2 \prod_i \{c_i + 2\}^2 + \frac{1}{64a^2} \prod_i \{c_i + 1\}^2 \{c_4^2 + 2c_4 + 1\} - \frac{1}{4a} \prod_i \{c_i + 1\} \{c_4 + 1\} [\frac{2}{a} + m] + [\frac{2}{a} + m]^2 = 0$$

and with $\cosh^2 - \sinh^2 = 1$ this turns into a *quadratic equation* in $\cosh(aE)$. It turns out that for any **p** explored below at most one of the solutions is real.



⊕ mild deviation from continuum up to $a|\mathbf{p}| \simeq 2$ ⊕ mild rotational symmetry breaking up to $a|\mathbf{p}| \simeq 2$ ⊖ strong effect of $am \ll 1$, especially at $\mathbf{p} = \mathbf{0}$

• Dispersion relation for overlap with Wilson kernel

$$D_{\mathrm{W},-\rho} = \mathrm{i}\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^2 - \frac{\rho}{a}$$

$$D_{\mathrm{W},-\rho}^{\dagger} D_{\mathrm{W},-\rho} = (-\mathrm{i}\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^{2} - \frac{\rho}{a})(\mathrm{i}\bar{p}_{\nu}\gamma_{\nu} + \frac{a}{2}\hat{p}^{2} - \frac{\rho}{a}) = \bar{p}^{2} + (\frac{a}{2}\hat{p}^{2} - \frac{\rho}{a})^{2}$$

$$D_{\text{NW},m} = \left(1 - \frac{am}{2\rho}\right) D_{\text{NW}} + m \quad \text{with} \quad D_{\text{NW}} = \frac{\rho}{a} \left\{1 + D_{\text{W},-\rho} [D_{\text{W},-\rho}^{\dagger} D_{\text{W},-\rho}]^{-1/2}\right\}$$

$$D_{\text{NW},m} = \underbrace{\left(\frac{\rho}{a} + \frac{m}{2}\right)}_{\equiv c} + \underbrace{\left(\frac{\rho}{a} - \frac{m}{2}\right)}_{\equiv d} \left(i\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^{2} - \frac{\rho}{a}\right) \left[\bar{p}^{2} + \left(\frac{a}{2}\hat{p}^{2} - \frac{\rho}{a}\right)^{2}\right]^{-1/2}}$$

$$G_{\text{NW},m} = \frac{c + d[\bar{p}^{2} + \left(\frac{a}{2}\hat{p}^{2} - \frac{\rho}{a}\right)^{2}]^{-1/2}(-i\bar{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\hat{p}^{2} - \frac{\rho}{a})}{\left[1 + d(\bar{p}^{2} + (\bar{q}_{\sigma}\hat{p}^{2} - \rho)^{2}) - 1/2(-i\bar{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\hat{p}^{2} - \frac{\rho}{a})\right]}$$

$$\begin{aligned} \mathcal{F}_{\text{NW},m} &= \frac{1}{\left\{c + d[\bar{p}^2 + (\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})^2]^{-1/2}(-\mathrm{i}\bar{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\hat{p}^2 - \frac{\rho}{a})\right\} \left\{c + d(\mathrm{i}\bar{p}_{\nu}\gamma_{\nu} + \frac{a}{2}\hat{p}^2 - \frac{\rho}{a})[\bar{p}^2 + (\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})^2]^{-1/2}}\right\} \\ &= \frac{c + d[\bar{p}^2 + (\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})^2]^{-1/2}(-\mathrm{i}\bar{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\hat{p}^2 - \frac{\rho}{a})}{c^2 + 2cd(\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})[\dots]^{-1/2} + d^2[\dots]^{-1/2}[\dots]^{-1/2}} \end{aligned}$$

End up searching for zero in $c^2 + 2cd(\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})[\bar{p}^2 + (\frac{a}{2}\hat{p}^2 - \frac{\rho}{a})^2]^{-1/2} + d^2 = 0$ with

$$\bar{p}^2 = \frac{1}{a^2} \sum_{\mu} s_{\mu}^2 \quad \text{with} \quad s_{\mu} \equiv \sin(ap_{\mu})$$

$$\hat{p}^2 = \frac{8}{a^2} - \frac{2}{a^2} \sum_{\mu} c_{\mu} \quad \text{with} \quad c_{\mu} \equiv \cos(ap_{\mu})$$

and the inverse sqare root renders this a *transcendental equation* in $\cosh(aE)$.

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 \ominus strong deviation from continuum for any $a|\mathbf{p}|>1$

 \ominus strong rotational symmetry breaking for any $a|\mathbf{p}| > 1$

 \oplus mild effect of $am \ll 1$, at least at $\mathbf{p} = \mathbf{0}$

• Dispersion relation for overlap with Brillouin kernel

$$D_{\mathrm{B},-\rho} = \mathrm{i}\tilde{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\check{p}^{2} - \frac{\rho}{a}$$

$$D_{\mathrm{B},-\rho}^{\dagger} D_{\mathrm{B},-\rho} = (-\mathrm{i}\tilde{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\check{p}^{2} - \frac{\rho}{a})(\mathrm{i}\tilde{p}_{\nu}\gamma_{\nu} + \frac{a}{2}\check{p}^{2} - \frac{\rho}{a}) = \tilde{p}^{2} + (\frac{a}{2}\check{p}^{2} - \frac{\rho}{a})^{2}$$

$$D_{\text{NB},m} = \left(1 - \frac{am}{2\rho}\right) D_{\text{NB}} + m \quad \text{with} \quad D_{\text{NB}} = \frac{\rho}{a} \left\{1 + D_{\text{B},-\rho} [D_{\text{B},-\rho}^{\dagger} D_{\text{B},-\rho}]^{-1/2} \right\}$$
$$D_{\text{NB},m} = \underbrace{\left(\frac{\rho}{a} + \frac{m}{2}\right)}_{\equiv c} + \underbrace{\left(\frac{\rho}{a} - \frac{m}{2}\right)}_{\equiv d} \left(i\tilde{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\check{p}^{2} - \frac{\rho}{a}\right) \left[\tilde{p}^{2} + \left(\frac{a}{2}\check{p}^{2} - \frac{\rho}{a}\right)^{2}\right]^{-1/2}$$
$$c + d[\tilde{p}^{2} + \left(\frac{a}{2}\check{p}^{2} - \frac{\rho}{a}\right)^{2}]^{-1/2} (-i\tilde{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\check{p}^{2} - \frac{\rho}{a})$$

$$G_{\text{NB},m} = \frac{c + a[p + (\frac{1}{2}p - \frac{1}{a})] - (-1p_{\sigma}\gamma_{\sigma} + \frac{1}{2}p - \frac{1}{a})}{\left\{c + d[\tilde{p}^{2} + (\frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})^{2}]^{-1/2}(-i\tilde{p}_{\mu}\gamma_{\mu} + \frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})\right\}\left\{c + d(i\tilde{p}_{\nu}\gamma_{\nu} + \frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})[\tilde{p}^{2} + (\frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})^{2}]^{-1/2}\right\}}$$
$$= \frac{c + d[\tilde{p}^{2} + (\frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})^{2}]^{-1/2}(-i\tilde{p}_{\sigma}\gamma_{\sigma} + \frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})}{c^{2} + 2cd(\frac{a}{2}\tilde{p}^{2} - \frac{\rho}{a})[...]^{-1/2} + d^{2}[...]^{-1/2}[...]^{-1/2}}$$

End up searching for zero in $c^2 + 2cd(\frac{a}{2}\check{p}^2 - \frac{\rho}{a})[\tilde{p}^2 + (\frac{a}{2}\check{p}^2 - \frac{\rho}{a})^2]^{-1/2} + d^2 = 0$ with

$$\tilde{p}^2 = \frac{1}{729a^2} \sum_{\mu} s_{\mu}^2 \prod_{\nu \neq \mu} \{c_{\nu} + 2\}^2$$
$$\check{p}^2 = \frac{4}{a^2} - \frac{1}{4a^2} \prod_{\mu} \{c_{\mu} + 1\}$$

and the inverse sqare root renders this a *transcendental equation* in $\cosh(aE)$.



 \oplus mild deviation from continuum up to $a|\mathbf{p}| \simeq 2$ \oplus mild rotational symmetry breaking up to $a|\mathbf{p}| \simeq 2$ \oplus mild effect of $am \ll 1$ as long as $|\mathbf{p}|$ not loo large

• Interim summary on dispersion relations



 \rightarrow Brillouin kernel improves DR w.r.t. momenta, but *not* w.r.t. quark masses \rightarrow Overlap recipe improves DR w.r.t. quark masses, but *not* w.r.t. momenta \Rightarrow Brillouin-Overlap shows reasonable DR w.r.t. both masses and momenta

Brillouin kernel: Implementation details

"prohibitively expensive" or "just expensive" ?

• Overall smearing

Use same smearing in covariant derivative and Laplacian and improvement term. Practical solution: smeared gauge field copy, i.e. create V(Nc,Nc,4,Nx,Ny,Nz,Nt) alongside original U_{ρ} , and evaluate Wilson/Brillouin operator on V_{ρ} . For $c_{\rm SW} \neq 0$ precompute $F_{\mu\nu}$ from V_{ρ} , i.e. create F(Nc,Nc,6,Nx,Ny,Nz,Nt).

• Gauging strategy

To maintain γ_5 -hermiticity: sum over all paths of equal length [1 path for 1-hop, 2 paths for 2-hop, 6 paths for 3-hop, 24 paths for 4-hop, average or SU(3)-project]. Practical solution: off-axis-link precomputed, i.e. create W(Nc,Nc,40,Nx,Ny,Nz,Nt).

• Bandwidth saturation

Practical solution: multiple-vector strategy, i.e. use vec(Nc,4,Nvec,Nx*Ny*Nz*Nt)

• Routine app_bril_sp/dp

GK: OpenMP+MPI routine in C++, see https://github.com/g-koutsou/qpb. SD: OpenMP-only routine in F2008, discussed on following two slides.

```
!$OMP PARALLEL DO DEFAULT(private) FIRSTPRIVATE(Nx,Ny,Nz,Nt,Nvec,mass) SHARED(old,new,W) SCHEDULE(static)
do l=1,Nt
do k=1,Nz
do j=1,Ny
do i=1,Nx
  n=(((l-1)*Nz+(k-1))*Ny+(j-1))*Nx+i
  site(:,:,:)=mass*old(:,:,:,n) !!! note: site is Nc*4*Nvec
  !!! visit all 81 sites within hypercube (distances 0 to 4 in taxi-driver metric)
  do go_l=-1,1; lsh=modulo(l+go_l-1,Nt)+1
  do go_k=-1,1; ksh=modulo(k+go_k-1,Nz)+1
  do go_j=-1,1; jsh=modulo(j+go_j-1,Ny)+1
  do go_i=-1,1; ish=modulo(i+go_i-1,Nx)+1
     nsh=(((lsh-1)*Nz+(ksh-1))*Ny+(jsh-1))*Nx+ish
     dir=(go_l+1)*27+(go_k+1)*9+(go_j+1)*3+go_i+2
      select case(dir)
        case(01:40); tmp=W(:,:,dir,i,j,k,l)
        case( 41); tmp=color_eye() !!! note: yields Nc*Nc identity matrix
        case(42:81); tmp=conjg(transpose(W(:,:,82-dir,ish,jsh,ksh,lsh)))
      end select
     select case(abs(go_i)+abs(go_j)+abs(go_k)+abs(go_l))
        case(0); fac_i=
                                    0.0; fac_j= 0.0; fac_k= 0.0; fac_l= 0.0; fac=(-240.0/128.0)
        case(1); fac_i=go_i*(64.0/432.0); fac_j=go_j*(...); fac_k=go_k*(...); fac_l=go_l*(...); fac=(
                                                                                                        8.0/128.0)
        case(2); fac_i=go_i*(16.0/432.0); fac_j=go_j*(...); fac_k=go_k*(...); fac_l=go_l*(...); fac=(
                                                                                                        4.0/128.0
        case(3); fac_i=go_i*( 4.0/432.0); fac_j=go_j*(...); fac_k=go_k*(...); fac_l=go_l*(...); fac=(
                                                                                                        2.0/128.0
        case(4); fac_i=go_i*( 1.0/432.0); fac_j=go_j*(...); fac_k=go_k*(...); fac_l=go_l*(...); fac=(
                                                                                                        1.0/128.0)
      end select
     do idx=1,Nvec
        tmg=matmul(tmp,old(:,:,idx,nsh)) !!! note: tmg is Nc*4
        !!! add terms proportional to isotropic derivative operators
        if (go_i.ne.0) then
           site(:,1,idx)=site(:,1,idx)-cmplx(0.0,fac_i)*tmq(:,4) !!! transpose(gamma1)=
                                                                                            0
                                                                                                  0
                                                                                                        0
                                                                                                             i
           site(:,2,idx)=site(:,2,idx)-cmplx(0.0,fac_i)*tmq(:,3) !!!
                                                                                            0
                                                                                                 0
                                                                                                        i
                                                                                                             0
           site(:,3,idx)=site(:,3,idx)+cmplx(0.0,fac_i)*tmq(:,2) !!!
                                                                                            0
                                                                                                 -i
                                                                                                        0
                                                                                                             0
           site(:,4,idx)=site(:,4,idx)+cmplx(0.0,fac_i)*tmq(:,1) !!!
                                                                                           -i
                                                                                                 0
                                                                                                        0
                                                                                                              0
        end if
```

```
if (go_j.ne.0) then
            site(:,1,idx)=site(:,1,idx)-fac_j*tmq(:,4)
                                                                   !!! transpose(gamma2)=
                                                                                               0
                                                                                                     0
                                                                                                           0
                                                                                                                 -1
            site(:,2,idx)=site(:,2,idx)+fac_j*tmq(:,3)
                                                                   !!!
                                                                                               0
                                                                                                     0
                                                                                                           1
                                                                                                                 0
            site(:,3,idx)=site(:,3,idx)+fac_j*tmq(:,2)
                                                                                                     1
                                                                                               0
                                                                                                           0
                                                                                                                 0
                                                                   !!!
            site(:,4,idx)=site(:,4,idx)-fac_j*tmq(:,1)
                                                                   111
                                                                                              -1
                                                                                                     0
                                                                                                           0
                                                                                                                 0
         end if
         if (go_k.ne.0) then
            site(:,1,idx)=site(:,1,idx)-cmplx(0.0,fac_k)*tmq(:,3) !!! transpose(gamma3)=
                                                                                               0
                                                                                                     0
                                                                                                           i
                                                                                                                 0
            site(:,2,idx)=site(:,2,idx)+cmplx(0.0,fac_k)*tmq(:,4) !!!
                                                                                               0
                                                                                                     0
                                                                                                                 -i
                                                                                                           0
            site(:,3,idx)=site(:,3,idx)+cmplx(0.0,fac_k)*tmq(:,1) !!!
                                                                                              -i
                                                                                                     0
                                                                                                           0
                                                                                                                 0
            site(:,4,idx)=site(:,4,idx)-cmplx(0.0,fac_k)*tmq(:,2) !!!
                                                                                                     i
                                                                                               0
                                                                                                           0
                                                                                                                 0
         end if
         if (go_l.ne.0) then
            site(:,1,idx)=site(:,1,idx)+fac_l*tmq(:,3)
                                                                   !!! transpose(gamma4)=
                                                                                               0
                                                                                                     0
                                                                                                           1
                                                                                                                  0
            site(:,2,idx)=site(:,2,idx)+fac_l*tmq(:,4)
                                                                   !!!
                                                                                               0
                                                                                                     0
                                                                                                           0
                                                                                                                  1
            site(:,3,idx)=site(:,3,idx)+fac_l*tmq(:,1)
                                                                   !!!
                                                                                               1
                                                                                                     0
                                                                                                           0
                                                                                                                 0
            site(:,4,idx)=site(:,4,idx)+fac_l*tmq(:,2)
                                                                                               0
                                                                                                     1
                                                                                                           0
                                                                   !!!
                                                                                                                 0
         end if
         !!! subtract 1/2 times brillouin laplacian
         site(:,:,idx)=site(:,:,idx)-fac*tmq !!! note: factor 0.5 excluded here but shuffled into "fac"
      end do ! idx=1,Nvec
   end do ! go_i=-1,1
   end do ! go_j=-1,1
   end do ! go_k=-1,1
   end do ! go_l=-1,1
   !!! plug everything into new vector
   do idx=1,Nvec
      new(:,:,idx,n)=site(:,:,idx)
   end do ! idx=1,Nvec
end do ! i=1,Nx
end do ! j=1,Ny
end do ! k=1,Nz
end do ! l=1.Nt
!$OMP END PARALLEL DO
```

• Timings on $24^3 \times 48$ lattice

ifort [...] -openmp -O2 -xavx -opt-mem-bandwidth1 -c modulename.f90

Matrix-vector multiplication in sp/dp on 4-core CPU [sec/vec]:

	Wilson	Brillouin	ratio
$c_{\rm SW} = 0$	0.033	0.611	18.5
$c_{\rm SW} = 1$	0.059	0.636	10.8

BiCGstab unpreconditioned inversion in mp/dp [sec/rhs]:

	Wilson	Brillouin	ratio
$c_{\rm SW} = 0$	18.6	88.7	4.8
$c_{\rm SW} = 1$	40.9	179.7	4.4
iterations	45+28+35=108	57	
iterations	74+53+57=184	112	

 $(c_{\rm SW}=0 \text{ with } am=0.1 \text{ and } 7 \text{ stout steps results in } aM_{\pi} \simeq 0.65 \text{ in both cases})$ $(c_{\rm SW}=1 \text{ with } am=0.1 \text{ and } 7 \text{ stout steps results in } aM_{\pi} \simeq 0.45 \text{ in both cases})$

Summary: matrix-vector is **10-20** times more expensive with Brillouin action, but a factor **2-4** comes back (reduced iteration count, fixed linalg), hence overall factor **5**.

• Wilson flop count

For matrix-times-vector operation we must (per site):

- (i) spin-project (from 4 to 2) for each direction $\longrightarrow 12 \cdot 8 = 96$ flops
- (*ii*) SU(3)-multiply (spin-reduced) for each direction $\rightarrow 6 \cdot 22 \cdot 8 = 1056$ flops
- (*iii*) accumulate 8+mass 1 contributions to out-spinor $\longrightarrow 24 \cdot 9 = 216$ flops

All together 1368 flops per site and $24^3 \times 48 = 663552$ sites. Performance in simple OpenMP implementation is $1368 \cdot 663552/0.033$ flops per second or 27.5 Gflops.

• Brillouin flop count

For matrix-times-vector operation we must (per site):

(*i*) SU(3)-multiply (spin-full) for each direction $\rightarrow 12 \cdot 22 \cdot 80 = 21120$ flops

(*ii*) multiply with fac_i/.../fac: $24 \cdot (54+54+54+54+81) = 7128$ flops

(*iii*) accumulate 80+mass 1 contributions to out-spinor $\rightarrow 24 \cdot 81 = 1944$ flops

All together 30192 flops per site and $24^3 \times 48 = 663552$ sites. Performance in simple OpenMP implementation is $30192 \cdot 663552/0.611$ flops per second or 32.8 Gflops.

• Summary

The Brillouin-to-Wilson ratio of flops is **22.1**, while observed timing ratio was **18.5**.

• Wilson memory traffic

For matrix-times-vector operation we must (per site, with #rhs=1):

- (i) read one sp-spinor for each direction $\longrightarrow 24 \cdot 9 = 216$ floats
- (*ii*) read one sp-gauge matrix V per direction $\rightarrow 18 \cdot 8 = 144$ floats
- (iii) write one sp-spinor $\longrightarrow 24$ floats

All together 384 floats of traffic per site, i.e. 1536 bytes in sp (1.12 bytes/flop).

• Brillouin memory traffic

For matrix-times-vector operation we must (per site, with #rhs=1):

- (*i*) read one sp-spinor for each direction $\longrightarrow 24 \cdot 81 = 1944$ floats
- (*ii*) read one sp-gauge matrix W per direction $\rightarrow 18 \cdot 80 = 1440$ floats
- (iii) write one sp-spinor $\longrightarrow 24$ floats

All together 3408 floats of traffic per site, i.e. 13632 bytes in sp (0.45 bytes/flop).

• Summary/Comments

The Brillouin-to-Wilson ratio of memory traffic is 3408/384=8.9 or 2088/252=8.9. With 12 rhs W changes to 216+12+24=252 floats from/to memory per site. With 12 rhs B changes to 1944+120+24=2088 floats from/to memory per site. Worst case scenario assumed, i.e. everything to be read afresh, since no cache. S. Dürr, BUW/JSC Lattice 2016, 25.7.2016 24

Brillouin kernel: Spectroscopy tests

Throughout this section: 1 APE step with $\alpha = 0.72$ in $\nabla^{iso}, \Delta^{bri}, F_{\mu\nu}$ and $c_{SW} = 1$

• Additive mass renormalization



Lattice 2016, 25.7.2016

• Ratios of decay constants





• BiCGstab convergence history



Brillouin overlap: Implementation details

$$D_{\text{overlap},0} = \frac{\rho}{a} \left\{ 1 + \gamma_5 \text{sign}(\gamma_5 D_{\text{kernel},-\rho/a}) \right\}$$
$$= \frac{\rho}{a} \left\{ 1 + D_{\text{ker},-\rho/a} (D_{\text{ker},-\rho/a}^{\dagger} D_{\text{ker},-\rho/a})^{-1/2} \right\}$$

Kenney-Laub family of iterates for matrix sign function / inverse square root:

$$f_{11}(x) = x \frac{3+x^2}{1+3x^2}, \quad f_{22}(x) = x \frac{5+10x^2+1x^4}{1+10x^2+5x^4}, \quad \dots, \quad f_{11}(f_{11}(x)) = f_{44}(x)$$

Special features: no wiggles, no eigenvalue info required (but still useful for speed-up) Other options (Zolotarev polynomial/rational, ...) possible and arguably faster.



Brillouin overlap: Spectroscopy tests

• Normality



 \implies B-overlap closer to normality than W-overlap, and advantage grows for $a \rightarrow 0$ Note: here "overlap" denotes the fixed-order (low-grade) approximation KL11

• GW defect



 \implies B-overlap much more chiral than W-overlap, and advantage grows for $a \rightarrow 0$ Note: here "overlap" denotes the fixed-order (low-grade) approximation KL11

• Operator locality



 \implies B-overlap much better localized than W-overlap, and better rotational symmetry

• Meson spectroscopy

$$D_{
m kern}$$
 (red), $D_{
m KL11}$ (blue), $D_{
m KL44}$ (green)
 $c_{
m SW} = 1$ (left) and $c_{
m SW} = 0$ (right)
3 APE smearings throughout

 $40^3 \times 64$ lattices, various bare quark masses Inversion with BiCGstab





 am_{bare}

Summary

- Brillouin action shows better [more continuum-like] dispersion relation than Wilson action for large momenta but *not* for large quark masses.
- Overlap recipe improves [shown for two kernels, conjectured for any kernel] dispersion relation for large quark masses but *not* for large momenta.
- Brillouin-Overlap/DomainWall yields down-to-earth approximation to "perfect action" concept by Peter Hasenfratz and collaborators, which is universally applicable for small/large quark masses, as well as small/large momenta.
- Implementation details:

Cost of matrix-vector with Brillouin is 10-20 times higher than with Wilson kernel. About a factor 2-4 comes back from reduced iteration count for non-chiral action. About a factor 2-4 comes back from reduced iteration count in $\gamma_5 \operatorname{sign}(\gamma_5 D_{-\rho})$.

o Cheap it is not, but the convenience may be worth it !!!

Dürr and Koutsou arXiv:1012.3615/1108.1650/1208.6270/forthcoming Cho et al arXiv:1504.01630, Gattringer et al, Bietenholz et al, Hasenfratz et al