

# Tunneling HMC algorithm

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We propose a variant of the HMC algorithm, dubbed Tunneling HMC (THMC) algorithm, which allows for real eigenvalues of a fermion matrix to change sign during the molecular dynamics evolution. We describe two implementations: for overlap and for domain-wall fermions. The partition function is first augmented by the determinant-squared of the corresponding super-critical Wilson operator, which is beneficial. However, with ordinary HMC, the price is that the global topology cannot change. When the new algorithm is applied to the “auxiliary” Wilson determinant, the tunneling between different topological sectors is made possible.

\* not tested yet!

but first, a word on the

## domain-wall quark's wave function

$$\chi(s) \simeq \underbrace{|1 - M + \delta M|^s + \frac{g^2}{s^{2+O(g^2)}} \exp\left(-(\alpha_0 + O(g^2))s\right) + \rho(0)/s}_{\text{re-summed perturbation theory}}$$

tadpole improvement: Aoki & Taniguchi 1999, Blum, Soni & Wingate 1999  
one loop: YS, 2000

usually adjust  $M$  such that  $1 - M + \delta M \approx 0$ .

if we forget to re-sum:

$$(1 - M + \delta M)^s = (1 - M)^s \left(1 + s \frac{\delta M}{1 - M} + \frac{s(s-1)}{2} \left(\frac{\delta M}{1 - M}\right)^2 + \dots\right)$$

for example  $M = 1.7$ ,  $\delta M = 0.8$ , get  $0.1^s = 0.7^s (1 - s 1.14 + \dots)$

# Why?

Near zero Wilson eigenvalues – a problem for DWF and overlap

DWF: bigger  $m_{res}$

overlap: higher cost

solution (Vranas, JLQCD):

include  $\det(D^\dagger D)$  in the path integral

where  $D$  = supercritical Wilson operator

⇒ suppresses near zero Wilson eigenvalues "surgically"!

new problem:

global topology is frozen

(changing it requires a Wilson eigenvalue to go through zero).

THMC: recover global topology change

# The basic idea

[From now on, ignore the DWF/overlap dets.]

Partition function:

[ $\det(D^\dagger D) = \det(\mathcal{M})\det(\mathcal{A})$  from RG blocking]

$$\begin{aligned} Z &= \int \mathcal{D}\mathcal{U} \exp(-S_g) \det(D^\dagger D) \\ &= \int \mathcal{D}\mathcal{U} \mathcal{D}\phi^* \mathcal{D}\phi \exp(-S_g - S_{pf}) \det(\mathcal{A}) \end{aligned}$$

$$\begin{aligned} S_{pf} &= \phi^\dagger \mathcal{M}^{-1} \phi & \mathcal{M} &= D^\dagger D + \alpha \sum_{i=1}^n |\chi_i\rangle \langle \chi_i|, \\ (\mathcal{A}^{-1})_{ij} &= \alpha^{-1} \delta_{ij} + \langle \chi_i | (D^\dagger D)^{-1} | \chi_j \rangle \end{aligned}$$

choose  $|\chi_i\rangle \approx |\psi_i\rangle$  hence MD is blind to the near zero eigenvalues of  $\psi_i$

$$\begin{aligned} H_{\text{Molecular Dynamics}} &= S_\pi + S_g + S_{pf} \\ H_{\text{accept/reject}} &= H_{\text{Molecular Dynamics}} + S_{\text{zero modes}} \end{aligned}$$

# Overlap implementation (set $\chi_i = \psi_i$ )

$$\begin{aligned} Z &= \int \mathcal{D}\mathcal{U} \exp(-S_g) \det(D^\dagger D) \\ &= \int \mathcal{D}\mathcal{U} \mathcal{D}\phi^* \mathcal{D}\phi \exp(-S_g - S_{pf}) \det(\mathcal{A}) \end{aligned}$$

$$\begin{aligned} S_{pf} &= \phi^\dagger \mathcal{M}^{-1} \phi & \mathcal{M} &= D^\dagger D + \alpha \sum_{i=1}^n |\psi_i\rangle \langle \psi_i|, \\ D^\dagger D \psi_i &= \lambda_i \psi_i & (\mathcal{A}^{-1})_{ij} &= (\alpha^{-1} + \lambda_i^{-1}) \delta_{ij} \end{aligned}$$

$$H_{\text{Molecular Dynamics}} = S_\pi + S_g + S_{pf}$$

$$H_{\text{accept/reject}} = H_{\text{Molecular Dynamics}} - \log \det(\mathcal{A})$$

Requires  $\psi_i$  and  $\delta\psi_i/\delta U$  at each MD step;  
but they are computed anyway in an overlap simulation!

# DWF implementation

Want to keep “zero modes’ lifter” fixed during each MD evolution.  
New stochastic degrees of freedom:  $\chi_i$  (much like pseudo-fermions)

$$\begin{aligned} Z &= \int \mathcal{D}U \exp(-S_g) \det(D^\dagger D) \\ &= \int \mathcal{D}U \mathcal{D}\phi^* \mathcal{D}\phi \mathcal{D}\chi^* \mathcal{D}\chi \exp(-S_g - S_{pf} - S_{ker}) \det(\mathcal{A}) \end{aligned}$$

$$\begin{aligned} S_{pf} &= \phi^\dagger \mathcal{M}^{-1} \phi & \mathcal{M} &= D^\dagger D + \alpha \sum_{i=1}^n |\chi_i\rangle \langle \chi_i|, \\ (\mathcal{A}^{-1})_{ij} &= \alpha^{-1} \delta_{ij} + \langle \chi_i | (D^\dagger D)^{-1} | \chi_j \rangle \end{aligned}$$

Kernel action:  $S_{ker} = \gamma \sum_{i=1}^n \langle \chi_i - \psi_i | \chi_i - \psi_i \rangle$

$$H_{\text{Molecular Dynamics}} = S_\pi + S_g + S_{pf}$$

$$H_{\text{accept/reject}} = H_{\text{Molecular Dynamics}} + S_{ker} - \log \det(\mathcal{A})$$

# Update

$$Z = \int \mathcal{D}U \mathcal{D}\phi^* \mathcal{D}\phi \mathcal{D}\chi^* \mathcal{D}\chi \exp(-S_g - S_{pf} - S_{ker}) \det(\mathcal{A})$$

$$S_{pf} = \phi^\dagger (\sqrt{\mathcal{M}})^{-2} \phi \qquad S_{ker} = \gamma \sum_{i=1}^n \langle \chi_i - \psi_i | \chi_i - \psi_i \rangle$$

## 1. Heat bath

$$\begin{aligned} \mathcal{P}(\xi) &= \exp(-\xi^\dagger \xi) & \phi &= r(\mathcal{M}(U)) \xi, & r(x) &\simeq \sqrt{x} \\ \mathcal{P}(\eta_i) &= \exp(-\gamma \eta_i^\dagger \eta_i) & \chi_i &= \psi_i(U) + \eta_i \end{aligned}$$

## 2. MD

$$\begin{aligned} H_{\text{Molecular Dynamics}} &= S_\pi + S_g + S_{pf} \\ H_{\text{accept/reject}} &= H_{\text{Molecular Dynamics}} + S_{ker} - \log \det(\mathcal{A}) \end{aligned}$$

## More on the kernel action

$$S_{ker} = \gamma \sum_{i=1}^n \langle \chi_i - \psi_i | \chi_i - \psi_i \rangle$$

$\gamma$  too small:  $\chi_i \not\approx \psi_i \Rightarrow$  near zero modes not lifted

$\gamma$  too large:

Initial heat bath:  $\chi_i = \psi_i + O(1/\sqrt{\gamma})$

metropolis test:

$$\langle \chi_i - \psi_i(U') | \chi_i - \psi_i(U') \rangle \simeq \langle \psi_i(U) - \psi_i(U') | \psi_i(U) - \psi_i(U') \rangle = f_i(\tau)$$

where  $f_i(\tau)$  monotonically increasing with MD time  $\tau$ .

Hence  $\exp(-S_{ker}) = \exp(-\gamma \sum_i f_i(\tau)) \ll 1$

$\Rightarrow$  always rejected for  $\gamma \rightarrow \infty$

Therefore, must choose  $\gamma = O(1)$

# (Reduction in) acceptance — a crude model

Consider overlap implementation (Ignore  $S_{ker}$ )

Assume exact energy conservation  $H_{MD}(U', \pi') = H_{MD}(U, \pi)$

In principle:  $P_{accept} = \int_0^1 dx dy P_1(x) P_2(y|x) \min\{1, y/x\}$

where  $x = \det(\mathcal{A}(U))$ ,  $y = \det(\mathcal{A}(U'))$

In THMC, molecular dynamics is blind to near zero modes;  
not unreasonable to assume the same fixed distribution  $\hat{P}$  for both  $x$  and  $y$ .

Get easily:  $P_{accept} = \int_0^1 dx dy \hat{P}(x) \hat{P}(y) \min\{1, y/x\} \geq 1/2$