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Non-Hermitian Polynomial Hybrid Monte Carlo

Employing the

Non-Hermitian Dirac-Wilson operator [Wilson 1974]

in an HMC-type update [Duane et al. 1987]

and approximating its inverse polynomially [Lüscher 1994, de Forcrand and Takaishi 1996, Frezzotti and Jansen 1997]

Non-Hermitian Polynomial Hybrid Monte Carlo

Based on the PHMC with reweighting [Frezzotti and Jansen 1997]

$$\det\{MM^\dagger\} = \det\{[MP_n][MP_n]^\dagger\} \cdot [\det\{P_n P_n^\dagger\}]^{-1}$$

$$P_n(M) \approx M^{-1} \qquad \text{and} \qquad R_{n+1}(M) = \mathbb{1} - MP_n(M)$$

- The pseudo-fermion action: $S_{\mathrm{PF}} = \phi^\dagger P_n^\dagger P_n \phi$
- Create pseudo-fermion fields: $\phi = P_n^{-1}\eta = (\mathbb{1} - R_{n+1})^{-1} M\eta$
- Bosonic force requires the variation of S_{PF} – a cumbersome sum
- Estimate the reweighting factor:
  $$\widehat{C} = \exp\{\eta^\dagger[\mathbb{1} - ((MP_n)^\dagger(MP_n))^{-1}]\eta\}$$

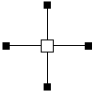
The non-Hermitian Dirac-Wilson Operator

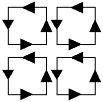
- is given in matrix notation and hopping parameter representation by

$$M_{xy} = \delta_{xy} - K_{xy}$$

with

$$K_{xy} = \kappa \left(\underbrace{H_{xy}}_{\text{hopping operator}} - \underbrace{\frac{i}{2} c_{\text{sw}} \sigma_{\mu\nu} \mathcal{F}_{\mu\nu}(x) \delta_{xy}}_{\text{Sheikholeslami}-\text{Wohlert term}} \right)$$



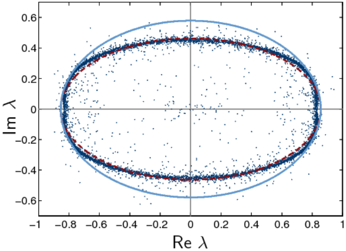


- has a complex spectrum –
  advantageous for polynomial approximation [Borelli et al. 1996]
- allows for simple and stable recursive implementation
- is in general non-normal

Spectral Boundaries of the non-Hermitian Operator

Quenched configurations on a 8^4 lattice at $\beta = 6.0$ and $\kappa = 0.13458$

without clover



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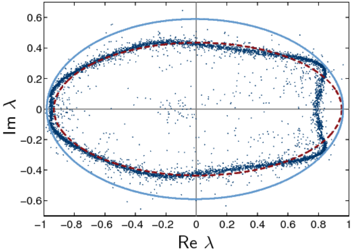
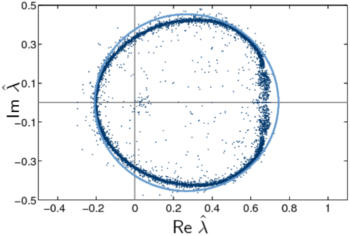
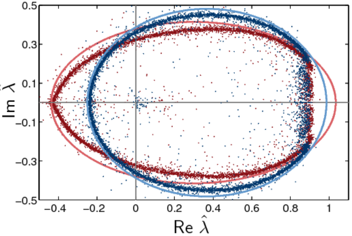




with even-odd preconditioning



Approximation using Chebyshev Polynomials

- Introduce polynomial for inverse Dirac-Wilson operator $P_n \approx M^{-1}$
- Build up a "small quantity" (remainder) $R_{n+1}(M) = \mathbb{1} - MP_n$
- Use scaled and translated Chebyshev polynomials [Manteuffel 1977]
  - provide an optimal approximation with respect to the L_∞ norm
  - are small on an elliptical region containing the spectrum of M

$$R_{n+1}(M) = \frac{T_{n+1}(K/e)}{T_{n+1}(d/e)} \quad \text{with} \quad K = d - M$$

Recursions

- The Cheybshev polynomials obey the recurrence relations

$$T_{n+1}(z) = 2zT_n(z) - T_{n-1}(z); \quad T_1 = z; \quad T_0 = 1$$

- Exploiting these we find for R_{n+1} and P_n

$$R_{n+1} = a_n K R_n + b_n R_{n-1}; \quad R_1 = K/d; \quad R_0 = \mathbb{1}$$

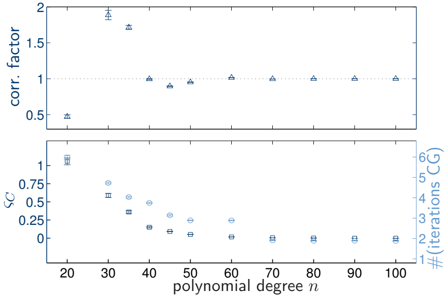
$$P_n = a_n(\mathbb{1} + KP_{n-1}) + b_n P_{n-2}; \quad P_1 = a_1(\mathbb{1} + K/d); \quad P_0 = \mathbb{1}/d$$

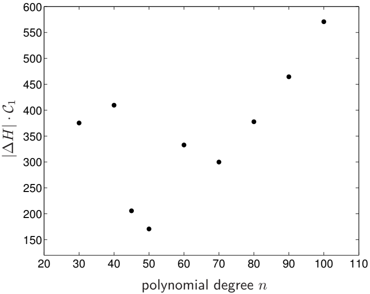
$$a_n = (d - a_{n-1}e^2/4)^{-1}; \quad a_1 = d(d^2 - e^2/2)^{-1}; \quad b_n = 1 - da_n$$

- All recurrences are numerically stable and lead to repeated matrix $\times$ vector - multiplications.

Dependence on Polynomial Parameters

- *d* and *e* do not require fine tuning
- polynomial degree *n* is crucial:
  - Quality of the approximation
  - Deviation from importance sampling
  - Fluctuations of correction factor
  - How many CG iterations are required
  - Numerical costs





Conclusion

- One pseudo-fermion NPHMC performs slightly better than a one pseudo-fermion HMC
- Simple and stable recursions – no special root ordering like for the PHMC [Bunk et al. 1999]
- Two pseudo-fermion HMC is nevertheless superior (Hasenbusch-trick, MTSI) [Hasenbusch 2001, Urbach et al. 2006]

Two Pseudo-Fermion NPHMC

- Incorporating the Hasenbusch-trick is possible
- Requires an involved tuning of the polynomial degrees
- Appears to be not too promising