Condensation of lighter-than-physical pions in QCD

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CRC-TR 211 Strong-interaction matter under extreme conditions

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Partition function of 2+1 flavour QCD with staggered fermions on the lattice after integration over fermion fields

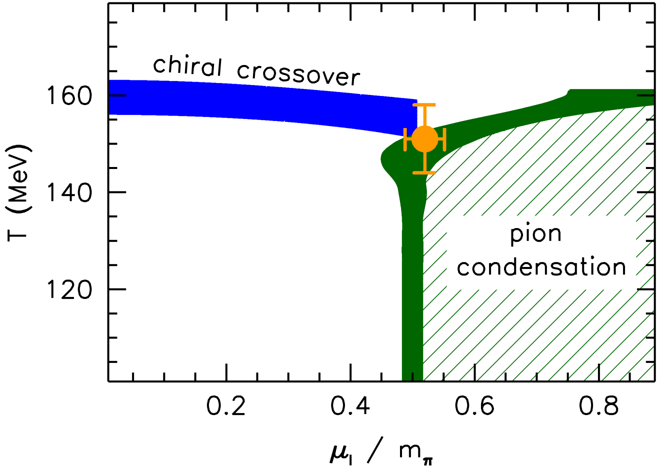
$$\mathcal{Z} = \int \mathcal{D}U_\mu \, e^{-\beta S_G} \, (\det \mathcal{M}_{ud})^{1/4} \, (\det \mathcal{M}_s)^{1/4} \, ,$$

$$\mathcal{M}_{ud} = \begin{pmatrix} \not{D}(\mu_I) + m_{ud} & \lambda \eta_5 \\ -\lambda \eta_5 & \not{D}(-\mu_I) + m_{ud} \end{pmatrix} \, , \quad \mathcal{M}_s = \not{D}(0) + m_s \, ,$$

$$\eta_5 = (-1)^{x+y+z+t} \, , \quad \not{D}(\mu_I)^\dagger = \eta_5 \not{D}(-\mu_I) \eta_5 = -\not{D}(-\mu_I) \, .$$

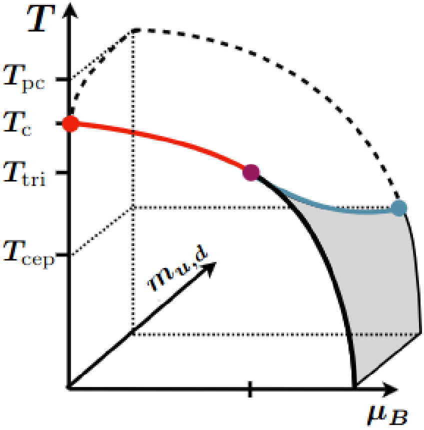
$$\det \mathcal{M}_{ud} = \det \left(\left(\not{D}(\mu_I) + m_{ud} \right)^\dagger \left(\not{D}(\mu_I) + m_{ud} \right) + \lambda^2 \right)$$

Phase diagram at physical point



Brandt, Endrődi, Schmalzbauer (2018)

Possible QCD phase diagram in T–μ_B–m_{ud} space:

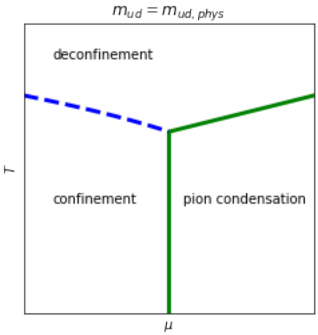


Karsch (2022)

Phase structure in chiral limit, T–μ_I

At zero temerature pion condensation happens at $\mu_I = m_\pi/2$, and for small light quark masses $m_\pi \sim m_{ud}^{1/2}$

Possible (schematic) scenario when going to chiral limit:



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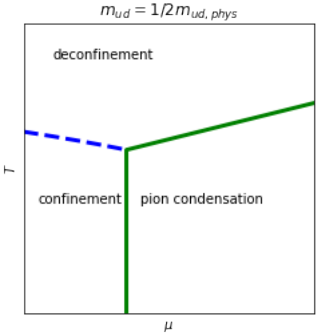

Phase structure in chiral limit

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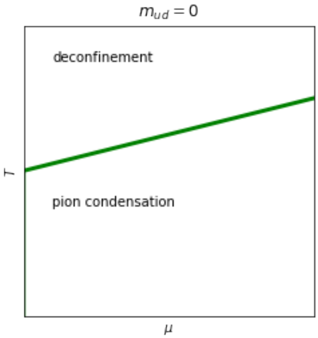
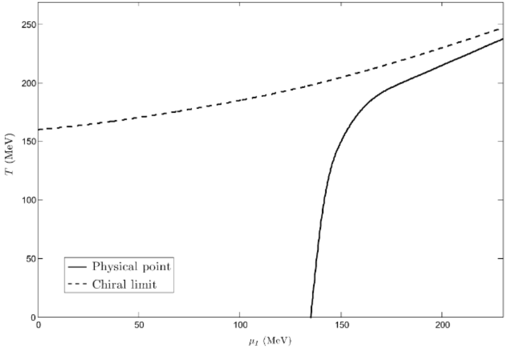


The above scenario is supported by following studies:

- NJL models He, Jin, Zhuang (2005)
- FRG study Svanes, Andersen (2011)



Simulation details

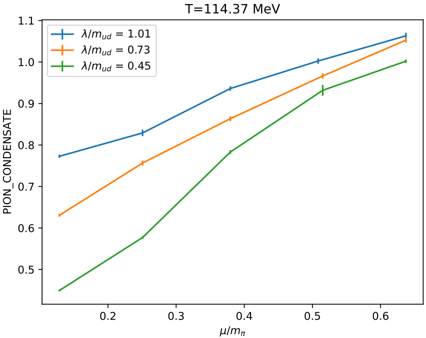
- Staggered fermions, tree-level Symanzik-improved gauge action
- $24^3 \times 8$ lattice with several checks on $32^3 \times 10$ and $36^3 \times 12$.
- 5 T values (114.37 MeV – 141.96 MeV) for μ_I scan
- at least 5 values of μ_I, $0.1 \leq \mu_I / m_{\pi,\text{phys}} \leq 0.7$
- 9 T values (114.37 MeV – 160.72 MeV) for T scan at $\mu_I / m_\pi \approx 0.72$.
- 3 values of λ, $0.4 \leq \lambda / m_{ud} \leq 1.5$
- at least 200 configurations per parameter set, 5 updates between configurations, 1000 thermalization updates.

Pion condensate

$$\left\langle \pi^{\pm} \right\rangle = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial \lambda} = \frac{T}{2V} \left\langle \mathrm{Tr} \, \frac{\lambda}{|\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2} \right\rangle$$

Renormalized condensate (additive divergence vanish at $\lambda \to 0$):

$$\Sigma_\pi = \frac{m_{ud}}{m_\pi^2 f_\pi^2} \left\langle \pi^{\pm} \right\rangle$$



Improved pion condensate

Banks-Casher type relation for the pion condensate

$$\left\langle \mathrm{Tr} \frac{\lambda}{|\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2} \right\rangle = \left\langle \sum_n \frac{\lambda}{\xi_n^2 + \lambda^2} \right\rangle ,$$

where ξ_n is the n-th singular value of the Dirac operator:

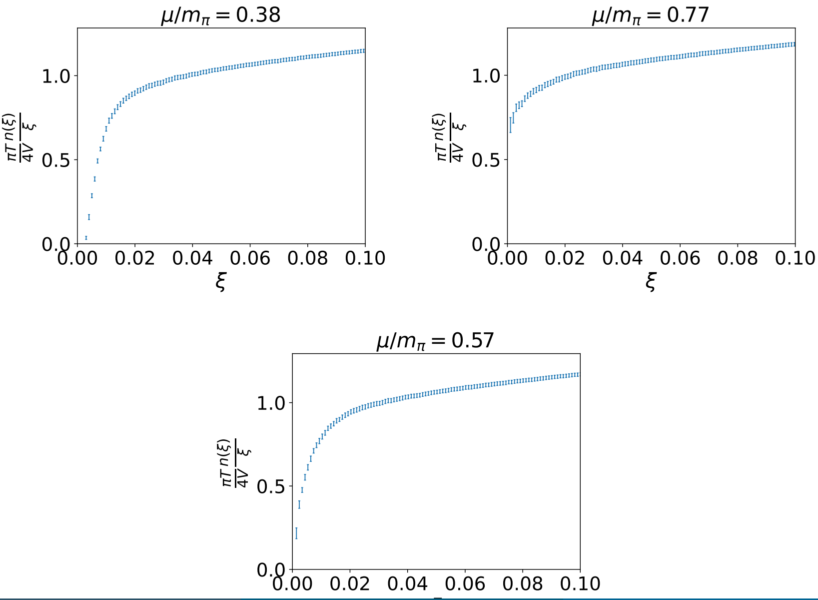
$$\left(\not{D}(\mu_I) + m_{ud}\right)^\dagger \left(\not{D}(\mu_I) + m_{ud}\right) \phi_n = \xi_n^2 \phi_n .$$

In the infinite volume limit summation can be replaced by integration

$$\left\langle \pi^\pm \right\rangle = \frac{\lambda}{2} \left\langle \int_0^\infty \mathrm{d}\xi \, \frac{\rho(\xi)}{\xi^2 + \lambda^2} \right\rangle ,$$

and taking the limit $\lambda \to 0$ we get

$$\left\langle \pi^\pm \right\rangle = \frac{\pi}{4} \left\langle \rho(0) \right\rangle .$$


$\mu/m_\pi = 0.38$
$\mu/m_\pi = 0.77$
$\mu/m_\pi = 0.57$
$\frac{\pi T}{4V}\frac{n(\xi)}{\xi}$
ξ
1.0
0.5
0.0
0.00
0.02
0.04
0.06
0.08
0.10

Ill-conditioned fermion operator

We see that in the pion condensate phase $\rho(0) > 0$

$(\not{D}(\mu_I) + m_{ud})$ has singular values close to zero.

Another reason we can not simulate at $\lambda = 0$ (only at small volumes)

At small finite λ, fermion operator condition number $\sim \lambda^{-2}$

- Need to calculate smallest singular values of $(\not{D}(\mu_I) + m_{ud})$
  - Chebyshev spectral transformation
- Need to invert an ill-conditioned operator $\mathcal{M}_{ud}$
  - Exact deflation for low modes

Leading order reweighting

Remaining dependence on λ comes from the configurations sampled at fixed λ – i.e. with weights proportional to $(\det \mathcal{M}_{ud})^{1/4} = \left(\det |\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2\right)^{1/4}$
We can try minimizing the dependence by reweighting the samples with weights

$$W(\lambda) = \frac{\left(\det |\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2_{\text{new}}\right)^{1/4}}{\left(\det \left[|\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2\right]\right)^{1/4}}$$

In the leading order one can write

$$\log W(\lambda) \approx -\frac{\lambda^2 - \lambda^2_{\text{new}}}{4} \operatorname{Tr} \frac{1}{|\not{D}(\mu_I) + m_{ud}|^2 + \lambda^2} = -\frac{\lambda^2 - \lambda^2_{\text{new}}}{\lambda} \frac{V}{2T} \pi^{\pm} \ ,$$

and use the reweighted observables

$$\langle O \rangle_{RW} = \frac{\langle O W(\lambda) \rangle}{\langle W(\lambda) \rangle}$$

Beyond leading order reweighting

We can use the expansion into singular values to calculate reweighing terms with better precision:

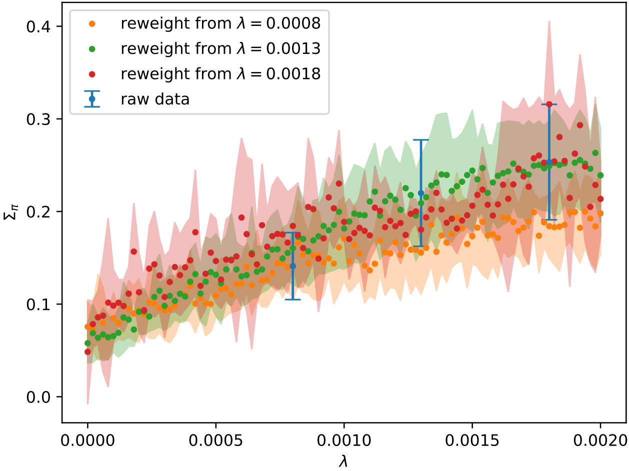
$$\log W(\lambda) = \frac{1}{4} \sum_{i=1}^{n} \log \frac{\xi_i^2 + \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2}$$

For the smaller ξ_i we can calculate the correction term, and assume that it is negligible for larger ξ_i

$$\log \frac{\xi_i^2 + \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2} = -\frac{\lambda^2 - \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2} + \log \frac{\xi_i^2 + \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2} + \frac{\lambda^2 - \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2}$$

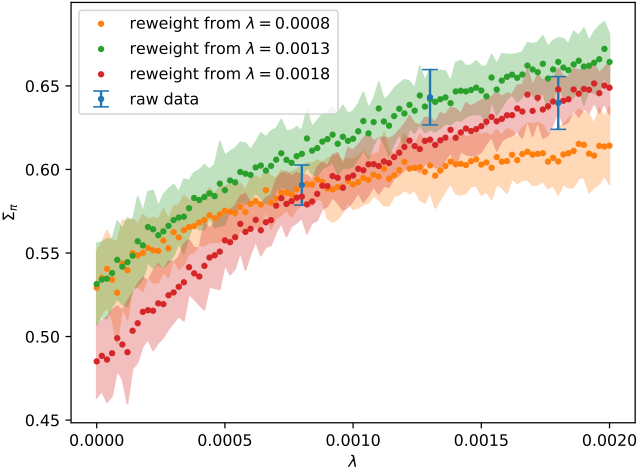
$$\log W(\lambda) \approx \log W_{LO}(\lambda) + \frac{1}{4} \sum_{i=1}^{k} \left(\log \frac{\xi_i^2 + \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2} + \frac{\lambda^2 - \lambda_{\text{new}}^2}{\xi_i^2 + \lambda^2} \right)$$

$T = 132$ MeV, $\mu = 0.53 m_\pi$



Beyond leading order reweighting

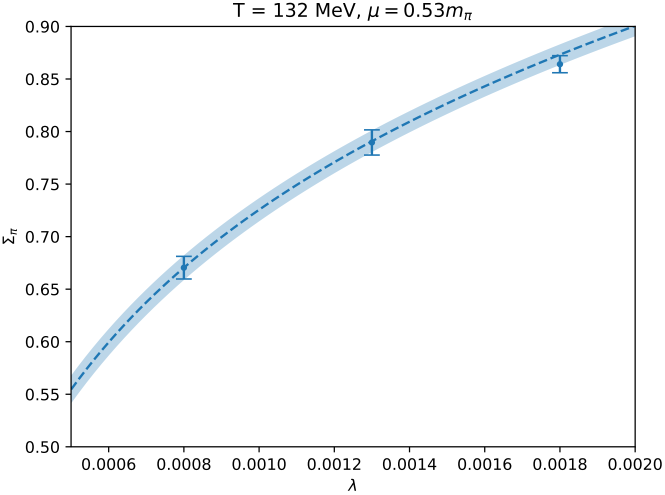
$$T = 132\ \text{MeV},\ \mu = 0.72 m_\pi$$



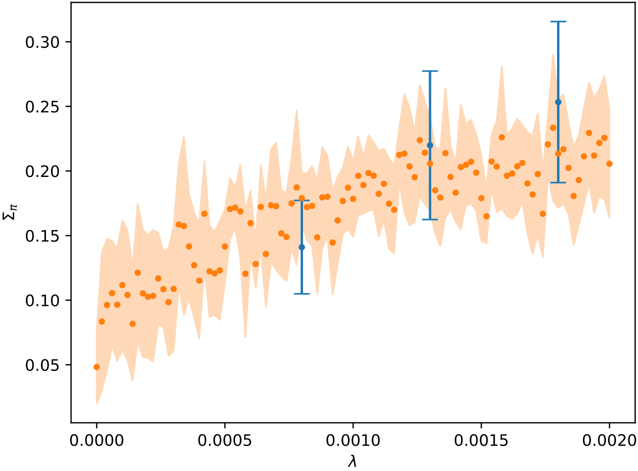
Beyond leading order reweighting

If the observable explicitly depends on λ it has to be taken into account

$$\mathrm{Tr}\,\frac{\lambda_{\mathrm{new}}}{|\not{D}(\mu_I)+m_{ud}|^2+\lambda_{\mathrm{new}}^2} \approx$$
$$\lambda_{\mathrm{new}}\left(\mathrm{Tr}\,\frac{1}{|\not{D}(\mu_I)+m_{ud}|^2+\lambda^2}+\mathrm{Tr}\,\frac{\lambda^2-\lambda_{\mathrm{new}}^2}{(|\not{D}(\mu_I)+m_{ud}|^2+\lambda^2)^2}+\right.$$
$$\left.+\sum_{k=1}^{m}\left(\frac{1}{\xi_k^2+\lambda_{\mathrm{new}}^2}-\frac{1}{\xi_k^2+\lambda^2}-\frac{\lambda^2-\lambda_{\mathrm{new}}^2}{\left(\xi_k^2+\lambda^2\right)^2}\right)\right)$$

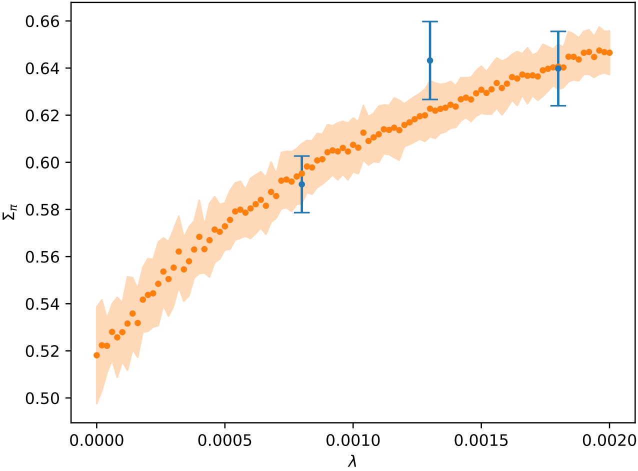

T = 132 MeV, $\mu = 0.53 m_\pi$
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
Σ_π
0.0006
0.0008
0.0010
0.0012
0.0014
0.0016
0.0018
0.0020
λ

$$T = 132 \text{ MeV}, \ \mu = 0.53 m_\pi$$

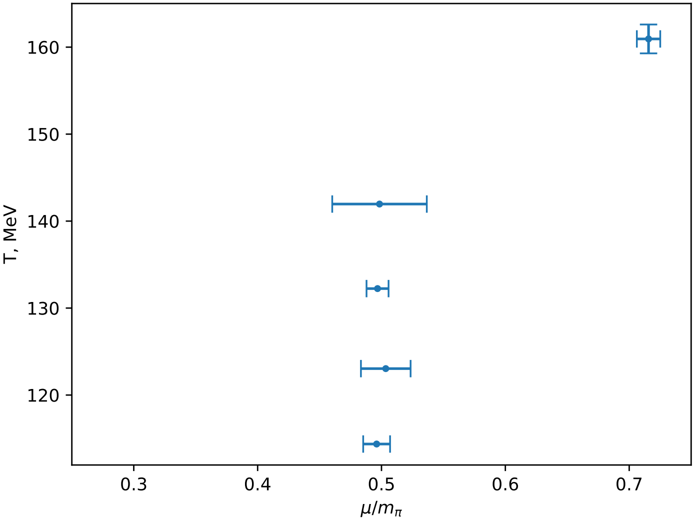


Multihistogram reweighting

$T = 132$ MeV, $\mu = 0.72 m_\pi$

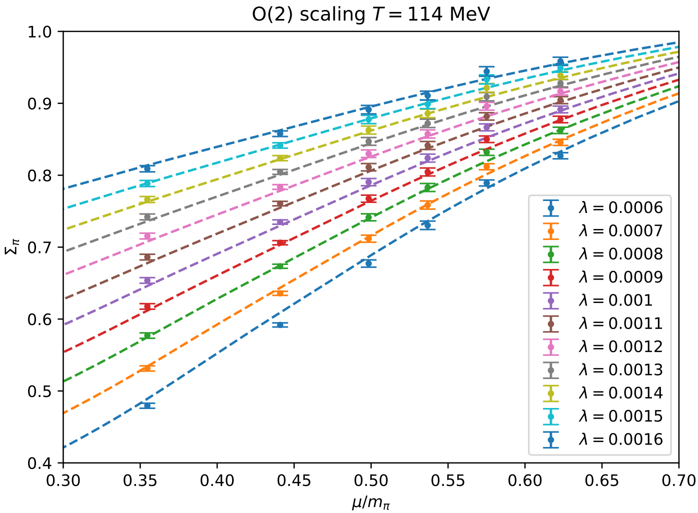


Location of the phase transition



O(2) scaling

$$\Sigma_\pi = h^{1/\delta} f_G(t/h^{1/(\beta\delta)}) + a_1 t h + b_1 h,$$
$$t = (\mu_c - \mu)/t_0,\ h = \lambda/\lambda_0$$



Summary

- Improved pion condensate observable using the Banks-Casher type relation for the pion condensate is less dependent on λ, and allows to use $\lambda \sim m_{ud}$.
- Reweighting can improve $\lambda \to 0$ extrapolation.
- At half physical light quark mass, the pion condensation boundary remains vertical up to $T = 140$ MeV. The transition is of the second order, belonging to the O(2) universality class.
- This supports the scenario for the chiral limit, in which the pion condensation phase appears at arbitrary small nonzero μ_I.

Appendix

Extracting singular value density at zero

We measure $m = 150$ smallest singular values on each sampled configuration. To obtain an estimate of the singular value density at zero we calculate $n(\xi)$ – number of singular values below ξ and take $\rho(0)$ as

$$\rho(0) = \lim_{\xi \to 0} \lim_{V \to \infty} \frac{T}{V} \frac{n(\xi)}{\xi}$$

In practice we assume that the lattice volume used is high enough to estimate $\frac{T}{V}\frac{n(\xi)}{\xi}$ for the set of ξ sampling points, and extrapolate the densities to $\xi = 0$.
A check comparing the integrated densities at two lattice volumes shows that if $n(\xi) > 4$ on both lattices the resulting values agree with each other within errors.

Smallest singular values without inversion

- Extract largest singular values of A^{-1} – not possible due to diverging condition number.
- Krylov-Schur methods converge starting on edges of the spectrum – small ξ^2 are denser than large ones, thus converge slower
- Polynomial spectral transformation – needs to keep the region of interest at the edge of the spectrum and reduce the singular value density in the region of interest

$$P(A^\dagger A)\psi = P(\xi^2)\psi$$

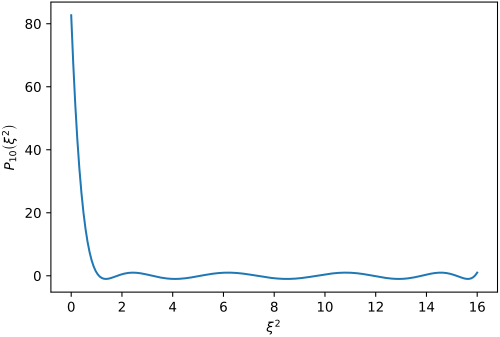
Rate of convergence for ξ_k^2 is governed by the spectral gap ρ_k:

$$\rho_k = \frac{|\xi_{k+1}^2 - \xi_k^2|}{|\xi_{k+1}^2 - \xi_n^2|}$$

Smallest singular values without inversion

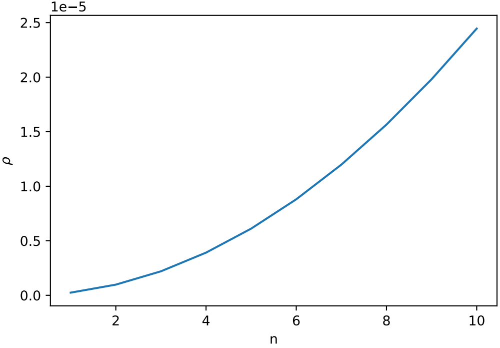
Assume we are interested in singular values in $\xi^2 \in [0, a]$, while the whole spectrum is $\xi^2 \in [0, b]$.

The polynomial $P_n(x) = T_n\left(\frac{2x-a-b}{b-a}\right)$ transforms all 'uninteresting' ξ^2 to $[-1, 1]$, and the 'interesting' ones quickly grow away from $[-1, 1]$



Smallest singular values without inversion

Increasing n grows spectral gap ρ, but also increases time to calculate $P_n(A^\dagger A)$ and increases numerical errors.
Empirically best n for our problems is in range 1 – 10 (depending on parameters).



Inversion with exact deflation

To calculate $\mathcal{M}_{ud}^{-1}\psi$ we can use calculated smallest singular values ξ_i^2 and corresponding singular vectors ϕ_i

$$\psi = \psi_r + \sum_{i=1}^{k} a_i \phi_i \ , \quad a_i = \phi_i^\dagger \psi$$

$$\mathcal{M}_{ud}^{-1}\psi = \mathcal{M}_{ud}^{-1}\psi_r + \sum_{i=1}^{k} \frac{a_i}{\xi_i^2 + \lambda^2}\phi_i$$

Since ψ_r does not contain singular vectors corresponding to the smallest singular values, the effective condition number of the problem is 150 smallest singular values at $\beta = 3.6, \lambda = 8 \cdot 10^{-4}, \mu = 0.081$ reduces κ from $6 \cdot 10^6$ to $5 \cdot 10^3$

- Needs singular vectors with high precision.
- Sensitive to precision of calculation ψ_r and a_i – needs extended precision summation, and sometimes iterated orthogonalization.

Inversion with exact deflation

For stochastic trace estimation can also reduce fluctuations:

$$\mathrm{Tr}\,\mathcal{M}_{ud}^{-1} = \lim_{n\to\infty}\frac{1}{n}\sum_{j=1}^{n}\psi_j^\dagger\mathcal{M}_{ud}^{-1}\psi_j$$

$$\mathrm{Tr}\,\mathcal{M}_{ud}^{-1} = \sum_{i=1}^{k}\frac{1}{\xi_i^2+\lambda^2} + \lim_{n\to\infty}\frac{1}{n}\sum_{j=1}^{n}\psi_{j,r}^\dagger\mathcal{M}_{ud}^{-1}\psi_{j,r}$$

- Implemented for measurements – large speed-up since we do many inversions with the same matrix
- Not implemented yet for updates – most probably will not result in speedup, but can allow simulations at smaller λ