

Scalar Content of Nucleon with the Gradient Flow and Machine Learning

August 4th, 2023 | Giovanni Pederiva, Jangho Kim, Andrea Shindler | Lattice 2023

Calculation of Hadronic Matrix Elements that Couple to Dark Matter

- A weakly interacting massive particle (WIMP) is a very popular dark matter (DM) candidate, with various ongoing experiments around the world provide rather severe constraints for the parameters of the models.
- A WIMP type of DM particles, due to its assumed large mass, produces a Higgs boson that couples to the various quark flavor scalar density operators taken between nucleon states.
- At zero momentum transfer, the cross section for spin independent elastic WIMP–nucleon (χN) scattering reads

$$\sigma_{\chi N} \sim \left| \sum_f G_f(m_\chi^2) f_{T_f} \right|^2 \quad \text{with} \quad f_{T_f} = \frac{m_f}{m_N} \langle N | \bar{q}_f q_f | N \rangle = \frac{m_f}{m_N} g_S^f. \quad (1)$$

Lattice Calculation

- Lattice QCD determination of the nucleon matrix elements from first principles.
- Direct calculation is numerically very challenging (disconnected diagrams).
- Gradient flow helps to reduce the statistical error.¹
- The matrix element we are interested in

$$g_S^\ell = \frac{G_\pi}{G_{\pi,t}} \cdot \left[\langle \mathcal{N} S^\ell(t) \bar{\mathcal{N}} \rangle^{con} + \langle \mathcal{N} S^\ell(t) \bar{\mathcal{N}} \rangle^{disc} - \langle S^\ell(t) \rangle \langle \mathcal{N} \bar{\mathcal{N}} \rangle \right]. \quad (2)$$

$$g_S^s = \frac{G_\pi}{G_{\pi,t}} \cdot \left[\langle \mathcal{N} S^s(t) \bar{\mathcal{N}} \rangle^{disc} - \langle S^s(t) \rangle \langle \mathcal{N} \bar{\mathcal{N}} \rangle \right]. \quad (3)$$

¹See DOI:10.22323/1.214.0251 and A. Shidler talk from Monday 31/7 for more details.

Numerical Strategy

- We compute the quark disconnected diagrams stochastically using the Hutchinson trace method.

$$\text{Tr}[A] \approx \frac{1}{N_\xi} \sum_{\xi}^{N_\xi} z_\xi^\dagger A z_\xi \quad (4)$$

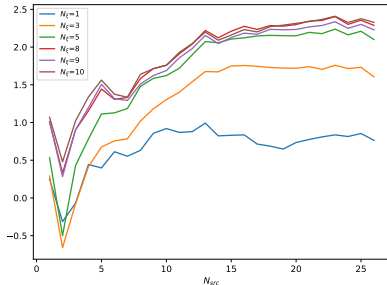
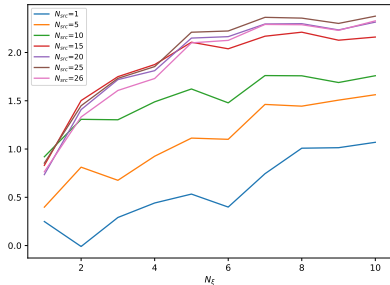
- Here z_ξ is one of $\{1, -1, i, -i\}$ as in a Z_4 random noise source.
- We apply the gradient flow and we define $A = K(t)SK^\dagger$, where K^\dagger is the adjoint kernel which flows the source of the propagator S , while K flows the propagator sink.
- Hence, $KS K^\dagger = S(t, t)$.

$$\text{Tr}[S(t)] \approx \frac{1}{N_\xi} \sum_{\xi}^{N_\xi} z_\xi^\dagger K(t, 0)SK^\dagger(0, t)z_\xi. \quad (5)$$

- The gradient flow has the added benefit of a noise reduction effect.

Signal to Noise Ratio Study

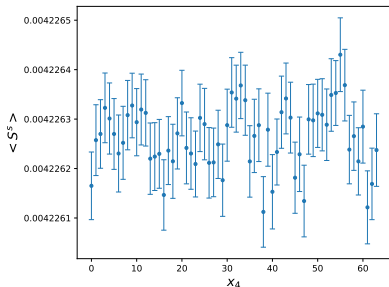
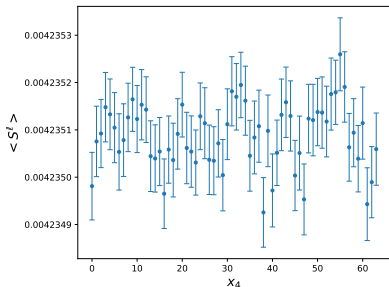
- We combine the disconnected diagram calculation with their respective nucleon-nucleon 2-pt function.
- We study the signal to noise ratio as a function of the number of stochastic sources N_ξ in N_{src} sources stochastic locations for the nucleon 2pt correlator at $t/a^2 = 1$.



As a consequence, we have determined that with $N_\xi \simeq 10$ and $N_{src} \simeq 20$, the signal to noise ratio is saturated.

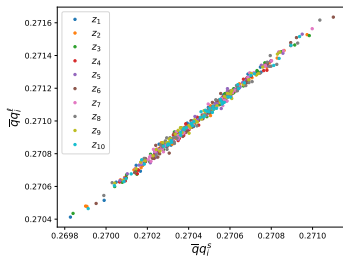
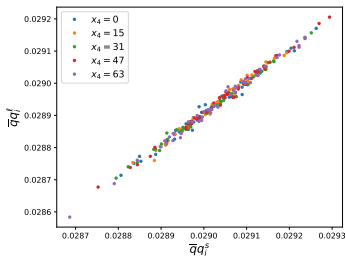
Quark Condensate $S^f(t) = \bar{\chi}^f(t, x)\chi^f(t, x)$

- Light and strange quark condensates at $t/a^2 = 0$.



- Euclidean time independent quantity.
- A huge number of inversions is required: $N_{\text{src}} \times N_{\text{conf}} \times N_{\text{flow}} \times N_{\text{flavors}}$
- Since they are strongly correlated, we developed a ML method which uses subset of the ensemble and predict the remains.

Correlations in the Training Set



This correlation provides a non-trivial mapping from $S^s(t/a^2 = 0)$ to $S^l(t/a^2 = 0)$.

Lattice Ensemble and ML Sets

Ens	β	κ_l	κ_s	V	m_π [MeV]	m_N [GeV]	N_{conf}	a [fm]
M_1	1.90	0.13700	0.1364	$32^3 \times 64$	699.0(3)	1.585(2)	399	0.0907(13)

- light quark condensate $S^\ell(t)$

$t/a^2 \backslash i_{\text{src}}$	1	2	3	4	5	6	7	8	9	10
0.0	50	399	399	399	399	399	399	399	399	399
0.5	50	399	399	399	399	399	399	399	399	399
1.0	50	399	399	399	399	399	399	399	399	399

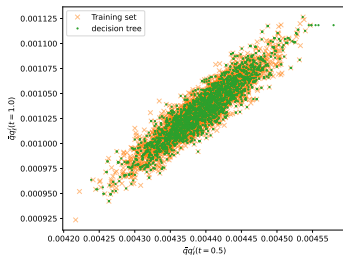
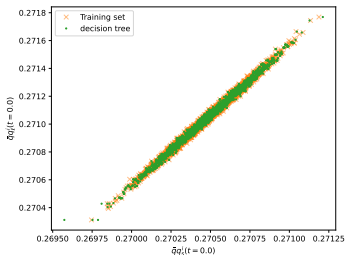
- strange quark condensate $S^s(t)$

$t/a^2 \backslash i_{\text{src}}$	1	2	3	4	5	6	7	8	9	10
0.0	50	399	399	399	399	399	399	399	399	399

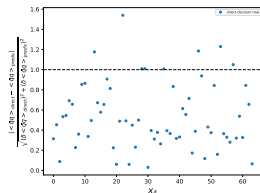
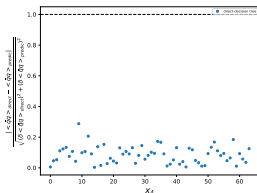
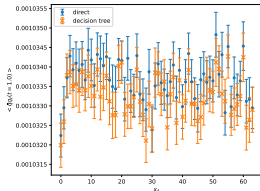
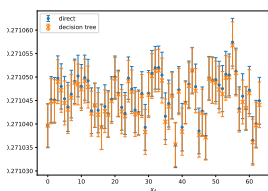
- $i_{\text{src}} = 1$ are used for training set.
- test ML method for two cases:
 - Between quark flavors: $S^s(t/a^2 = 0)$ and $S^\ell(t/a^2 = 0)$
 - For different flow time: $S^\ell(t/a^2 = 0.5)$ and $S^\ell(t/a^2 = 1)$

Decision Tree Results

- We used Decision Trees with infinite depth for the regression problem, flexible and easy to train (using scikit-learn)
- We make use of translation invariance in order to increase the sample of training data in the ML model.
- The number of training points : $N_{\text{src}} \times N_{\text{conf}} = 50 \times 64 = 3200$



Quark Condensate Results



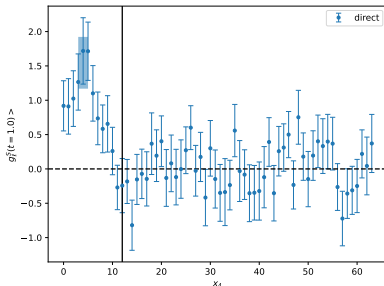
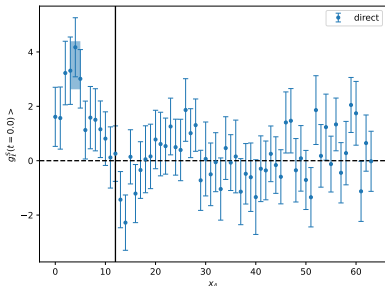
■ Deviation: $\Delta S = \frac{|S^{\text{direct}} - S^{\text{DT}}|}{\sqrt{(\delta S^{\text{direct}})^2 + (\delta S^{\text{DT}})^2}}$

Combining with Nucleon 2-point Function

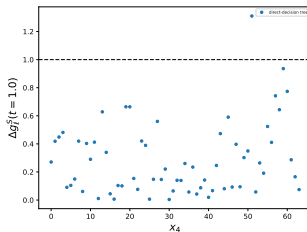
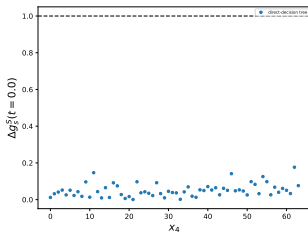
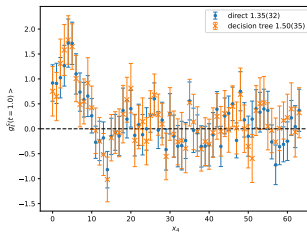
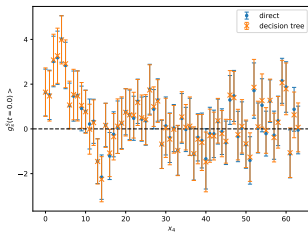
$$R(y_4, x_4, t) \tag{6}$$

$$\equiv \frac{\langle N(y_4, 0) | qq^f(x_4, t) | \bar{N}(0, 0) \rangle - \langle qq^f(x_4, t) \rangle \langle N(y_4, 0) \bar{N}(0, 0) \rangle}{\langle N(y_4, 0) \bar{N}(0, 0) \rangle} \frac{G_\pi(0)}{G_\pi(t)} \tag{7}$$

$$= g_S^f + O(e^{-\Delta E|x_4|}) + O(e^{-\Delta E|y_4-x_4|}) \tag{8}$$



Comparison with Direct Calculation



Computing time saving

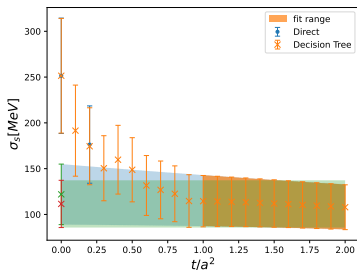
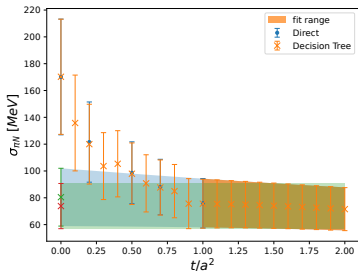
Calculation of light quark condensate.

$t/a^2 \backslash i_{\text{src}}$	1	2	3	4	5	6	7	8	9	10
0.0	50	399	399	399	399	399	399	399	399	399
0.1	50	0	0	0	0	0	0	0	0	0
0.2	50	399	399	399	399	399	399	399	399	399
0.3	50	0	0	0	0	0	0	0	0	0
0.4	50	0	0	0	0	0	0	0	0	0
0.5	50	399	399	399	399	399	399	399	399	399
0.6	50	0	0	0	0	0	0	0	0	0
0.7	50	399	399	399	399	399	399	399	399	399
0.8	50	0	0	0	0	0	0	0	0	0
0.9	50	0	0	0	0	0	0	0	0	0
1.0	50	399	399	399	399	399	399	399	399	399

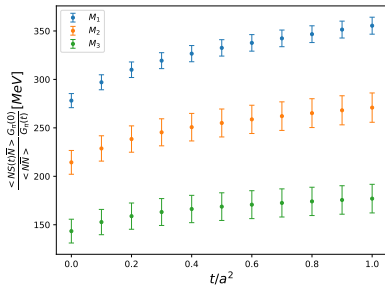
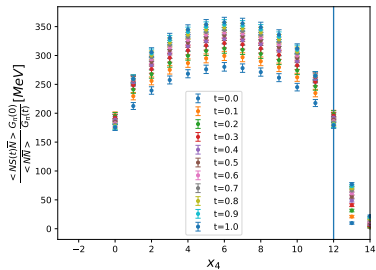
- full calculation : $399 \times 9 \times 11 \times 2 = 79002$ data points
- Training and input set : $50 \times 11 \times 2 + 399 \times 9 = 4691$ confs
- 5.94% of full calculation is needed for both light and strange quark condensates.

Results of $\sigma_f(t)$ (Preliminary)

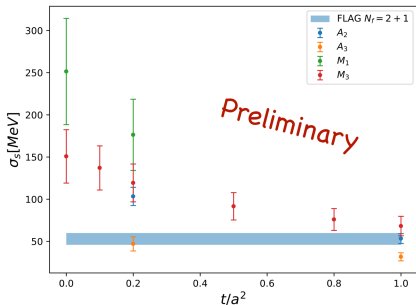
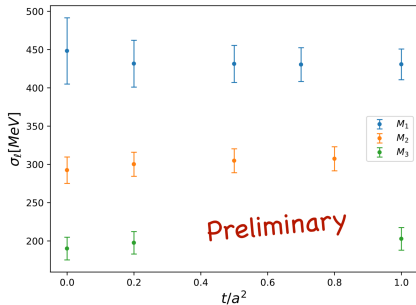
- $\sigma_f = m_f g_S^f$
- Input is $g_S^\ell(t = 0.5)$ with 9 stochastic sources.



Light quark connected diagram



Adding light quark connected and disconnected diagrams



Summary and Outlook

- ML can help us reduce the computational cost of computing observables in case of strong correlations
- We computed σ_s terms from disconnected diagram calculations and $\sigma_{\pi N}$ from connected and disconnected contributions.
- Using a machine learning method we achieves similar precision using about 5% of the computing resources compare to direct calculations.
- Need to analyze other ensembles for the continuum limit
- Other observables (vector, Dslash, tensor) currents instead of scalar are available with the same machine learning method.

