# Density of States for Observables. A derivative method

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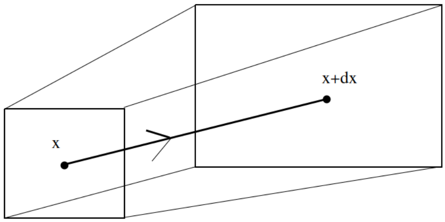
# Motivation

- Improve precision of lattice measurements by using smooth behavior of observable $O$ and action $S$

$$\langle f(O)\rangle \quad = \quad \frac{1}{Z}\int f(O(x))\exp(-S(x))dx = \frac{\int f(O)\rho(O)dO}{\int \rho(O)dO} \qquad (1)$$

- We will look at the change to the volume at $O(x) = O$ to find the derivative of the density $\rho$



# Change to observable

- In an D dimensional space there is at each local point only 1 direction in which an observable is changing.

$$\frac{\partial O(x)}{\partial x_j} \equiv O_j(x) \tag{2}$$

- All directions orthogonal to this direction gives 0 change to the observable
- The relative change to the total volume with $O$ is directly related to the relative density

$$\frac{1}{\epsilon}\log(V(O+\epsilon)/V(O)) = \frac{1}{\epsilon}\log(\rho(O+\epsilon)/\rho(O)) = \frac{d\log(\rho(O))}{dO} + R(\epsilon) \tag{3}$$

# Change to volume

- To get an infinitesimal change that does a change of 1 to our variable we have to normalize by $O_i^2$

$$O(x_i + \epsilon O_i) \quad = \quad O(x_i) + \epsilon O_i^2 + R(\epsilon^2) \tag{4}$$

- sum when index appears twice, square included
- The change to the relative volume along a direction can be calculated as [arxiv:2205.02257]

$$dV(x) \quad \equiv \quad \partial_{x_i}(\frac{O_i}{O_j^2}) = \frac{O_{i,i}}{O_j^2} - \frac{2O_iO_{i,j}O_j}{(O_k^2)^2} \tag{5}$$

# Average change

- We look for how the total volume changes from $O$ to $O+\epsilon$
- We assume that each $O(x)$ was sampled in a Monte-Carlo sampling of $\exp(-S)$

$$\begin{aligned} V(O+\epsilon) &= V_{norm}(\sum_{O(x)=O} \exp(\epsilon dV(x) - [S(x_i + \epsilon dO_i/O_j^2) - S(x_i)])) \\ &= V_{norm} N(1+\epsilon(\langle dV\rangle - \langle \frac{S_i O_i}{O_j^2}\rangle) + R(\epsilon^2)) \qquad (6) \\ \log(V(O+\epsilon)/V(O)) &= \log((1+\epsilon(\langle dV\rangle - \langle \frac{S_i O_i}{O_j^2}\rangle) + R(\epsilon^2))) \qquad (7) \\ &= \epsilon(\langle dV\rangle - \langle \frac{S_i O_i}{O_j^2}\rangle) + R(\epsilon^2) \\ d_O \log(\rho(O)) &= \langle dV\rangle - \langle \frac{S_i O_i}{O_j^2}\rangle \qquad (8) \\ &= \langle \frac{O_{i,i}}{O_j^2} - \frac{2O_i O_{i,j} O_j}{(O_k^2)^2} - \frac{S_i O_i}{O_j^2}\rangle \qquad (9) \end{aligned}$$

- Average is for all x where $O(x) = O$

# Simple Example

- $S = O = x_i^2$
- $\langle O \rangle = \frac{1}{Z} \int x_i^2 \exp(-x_j^2) d^D x$

$$\begin{aligned} O_i &= \partial_{x_i}(x_j^2) = 2x_i & (10) \\ O_{i,i} &= \partial^2_{x_i}(x_j^2) = 2D & (11) \\ O_i^2 &= 4x_i^2 = 4S & (12) \\ O_i O_{i,j} O_j &= 2x_i 2\delta_{i,j} 2x_j = 8x_i^2 = 8S & (13) \\ d_S \log(\rho(S)) &= \frac{2D}{4S} - \frac{2*8S}{(4S)^2} - 1 = \frac{1}{S}(D/2-1) - 1 & (14) \end{aligned}$$

- The last differential equation can then be solved which gives

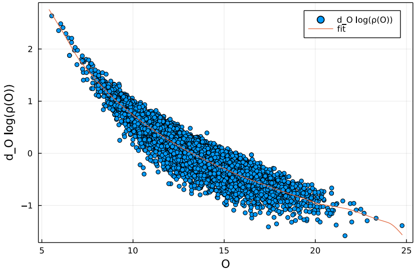
$$\rho(S) = Constant * \exp(\log(S)(D/2-1) - S) = Constant * S^{D/2-1} \exp(-S)$$

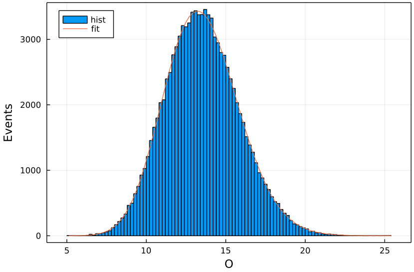
# Less Simple Example

- $S = x_j^4$
- $O = x_j^2$
- $D = 40$
- Fitted with spline of order 25

| N | Observable | Re | Im |
|---|---|---|---|
| $10^5$ | O | $13.515 \pm 0.018$ | 0 |
| $10^6$ | O | $13.512 \pm 0.005$ | 0 |
| $10^7$ | O | $13.521 \pm 0.001$ | 0 |
| $10^5$ | dV | $13.523 \pm 0.007$ | 0 |

Table: Exact result is $13.5196$.



- Changes to SU3 is done by the 8 generators $\tau_i$ of the su3 algebra

$$U \rightarrow \exp(i\epsilon_i\tau_i)U \tag{15}$$

- We find that there is no change to the volume of the group elements from this change

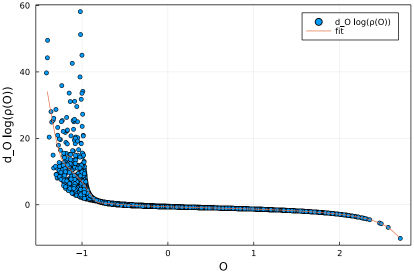
$$\det(Tr[\frac{\partial U}{\partial \tau_i}\frac{\partial U^\dagger}{\partial \tau_j}]) = 1 \tag{16}$$

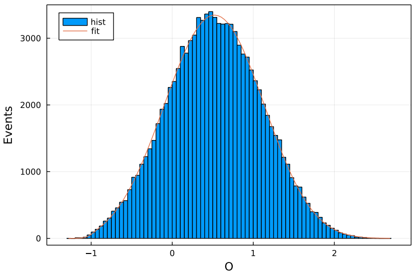
# SU3 example

- $S = Re[Tr(U) - 1]^2$
- $O = Re[Tr(U)]$
- $D = 1$
- Fitted with spline of order 20, but too smooth, due to pole at $O = -1$
- Table Shows results from extrapolating with 3rd order polynomial in small area around O

| N | Observable | Re | Im |
|---|---|---|---|
| $10^5$ | O | $0.5313 \pm 0.0094$ | 0 |
| $10^6$ | O | $0.5194 \pm 0.0037$ | 0 |
| $10^5$ | dV | $0.5244 \pm 0.0002$ | 0 |
| $10^6$ | dV | $0.5242 \pm 0.00009$ | 0 |

Table: Results for different amount of samples.



- The wilson line correlator is defined as

$$C(\tau, r) \quad = \quad \sum_x Tr[(\Pi_{t=1}^{\tau} U_4(t,x))(\Pi_{t=1}^{\tau} U_4(t,x+r))^{\dagger}] \tag{17}$$

- multiplications starts to the left and then move to the right.
- We have

$$C(\tau, r) = C(\tau, -r)^{\dagger} \tag{18}$$

- The average over r is therefore completely real
- $O_i(x)$ found by inserting $\tau_i$ in front of $U_4(x)$
- The double derivative becomes $O_{i,i} = -(16/3)2\tau O$ since $\exp(i\epsilon_i\tau_i) = 1 + i\epsilon_i\tau_i - (\epsilon_i\tau_i)^2/2$ and we use that $\tau_i^2 = 16/3$. We get this contribution for every link in the product, which is $2\tau$.

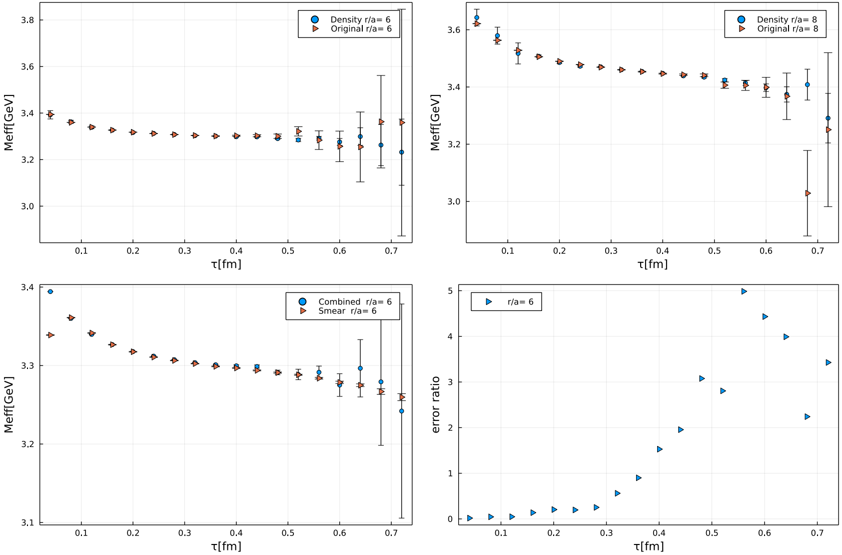
# Setup

- $\partial_{x_i} S$ is taken from the Hybrid-Monte-Carlo simulation code from which the configurations were generated. In this case it is SIMULATeQCD.
- HISQ configurations of size $64^3 20$ for $\beta = 7.825$, $T = 244 MeV$ and $m_s/m_l = 20$, $N_{conf} = 4400$.
- Distribution close to gaussian since each observable average over entire volume
- Fitted with second order polynomial to $d_O \log(\rho)$
- Third order checked, but not significant
- From the found correlation functions we plot the effective mass

$$M_{eff}(\tau) = \frac{1}{a} \log(C(\tau)/C(\tau+1)) \tag{19}$$

- Configurations needs to be gauge fixed
- Might be a derivative on gauge fixing which is not taken into account

# Wilson Lines Results



# Conclusion

- Derived formula for change to density of observable

$$\frac{d\log(\rho(O))}{dO} = \langle \frac{O_{i,i}}{O_j^2} - \frac{2O_iO_{i,j}O_j}{(O_k^2)^2} - \frac{S_iO_i}{O_j^2} \rangle \tag{20}$$

- Showed results from using the formula in a range of different examples
- Improvements found in many cases, though not always and can be expensive to calculate for some observables