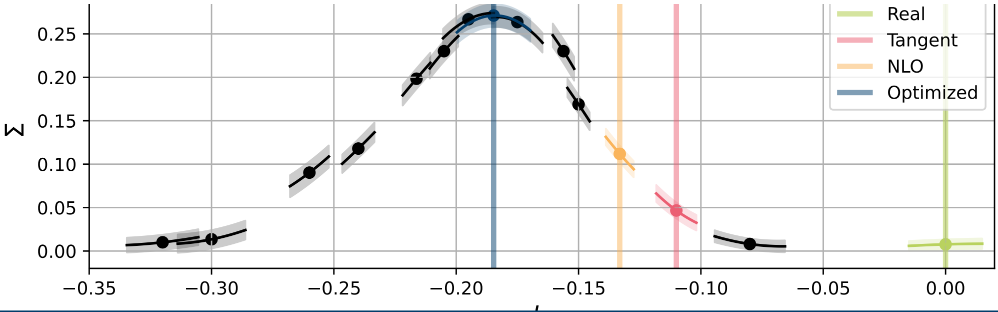

REDUCING THE SIGN PROBLEM

with simple Contour Deformation

August 3, 2023 | Christoph Gäntgen | Forschungszentrum Jülich

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Fermionic Sign Problem Minimization by Constant Path Integral Contour Shifts: arXiv:2307.06785

Hubbard Model

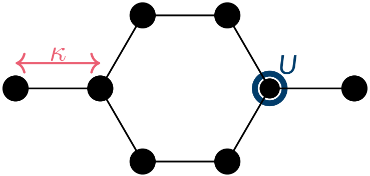
$$H = -\sum_{x,y} \kappa_{x,y} \left(a^\dagger_{x\uparrow} a_{y\uparrow} + a^\dagger_{x\downarrow} a_{y\downarrow} \right) - \frac{U}{2} \sum_x (n_{x\uparrow} - n_{x\downarrow})^2 - \mu \sum_x (n_{x\uparrow} + n_{x\downarrow})$$

- The Hubbard model is used to approximate solid state systems [Hubbard, 1959]

  κ: Nearest-neighbour hopping (tight binding)

  U: On-site interaction

  μ: Chemical potential



The Sign-Problem

Expectation value

$$\langle \hat{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \, \hat{O}[\phi] \, e^{-S[\phi]} , \qquad \mathcal{Z} = \int \mathcal{D}\phi \, e^{-S[\phi]}$$

$$\Rightarrow \quad \langle \hat{O} \rangle = \int \mathcal{D}\phi \, \hat{O}[\phi] \, \rho[\phi] \approx \frac{1}{N} \sum_{n=0}^{N} \hat{O}[\phi_n]$$

with $\phi_n \sim \rho[\phi_n] = \frac{1}{\mathcal{Z}} e^{-S[\phi_n]}$

Action

$$S = \sum_{x,t} \frac{\phi_{x,t}^2}{2\tilde{U}} - \log\det\left(M[\phi, \tilde{\kappa}, \tilde{\mu}] M[-\phi, -\tilde{\kappa}, -\tilde{\mu}]\right)$$

[Duane et al., 1987, Wynen et al., b]

The Sign-Problem

Expectation value

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$$S = \sum_{x,t} \frac{\phi_{x,t}^2}{2\tilde{U}} - \log\det(M[\phi, \tilde{\kappa}, \tilde{\mu}] M[-\phi, -\tilde{\kappa}, -\tilde{\mu}]) \in \mathbb{C}$$

[Duane et al., 1987, Wynen et al., b]

The Sign-Problem

- $S[\phi] \to \mathrm{Re}\{S[\phi]\} + \mathrm{i}\,\mathrm{Im}\{S[\phi]\}$
- $\rho[\phi] \to e^{-\mathrm{Re}\{S[\phi]\}} \in \mathbb{R}$
- $\hat{O}[\phi] \to \hat{O}e^{-\mathrm{i}\,\mathrm{Im}\{S[\phi]\}} \in \mathbb{C}$

$$\Rightarrow \quad \left\langle \hat{O} \right\rangle = \frac{\left\langle \hat{O}e^{-\mathrm{i}S_I} \right\rangle_R}{\left\langle e^{-\mathrm{i}S_I} \right\rangle_R} \approx \frac{\sum_{n=0}^{N} \hat{O}\left[\phi_n\right] e^{-\mathrm{i}S_I[\phi_n]}}{\sum_{n=0}^{N} e^{-\mathrm{i}S_I[\phi_n]}}$$

$$\text{with } \phi_n \sim e^{-S_R}$$

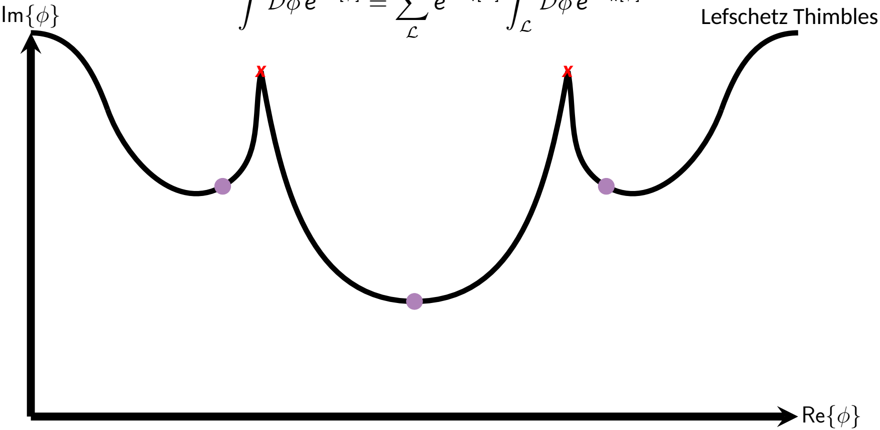
Statistical Power

$$\Sigma = \left| \left\langle e^{-\mathrm{i}S_I} \right\rangle_R \right| \qquad \left(N_{\mathrm{eff}} = \Sigma^2 \times N_{\mathrm{cfg}} \right)$$

Contour Deformation

Lefschetz Thimbles

$$\int \mathcal{D}\phi\, e^{-S[\phi]} = \sum_{\mathcal{L}} e^{-iS_I[\mathcal{L}]} \int_{\mathcal{L}} \mathcal{D}\phi\, e^{-S_R[\phi]}$$

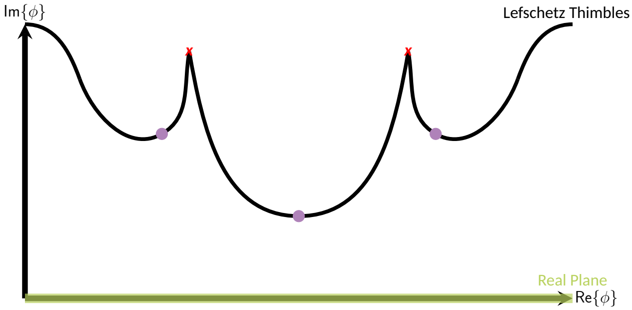


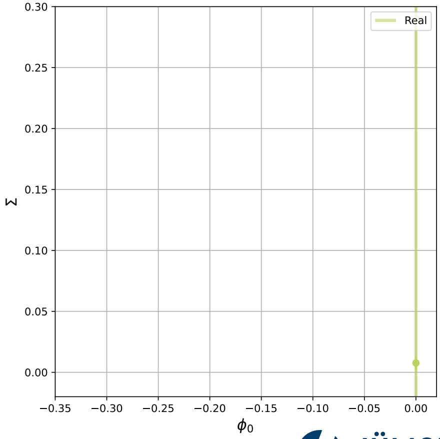
[Alexandru et al., a, Wynen et al., a, Rodekamp et al.,]

Contour Deformation

Constant Offsets

$$\phi = Re(\phi)$$

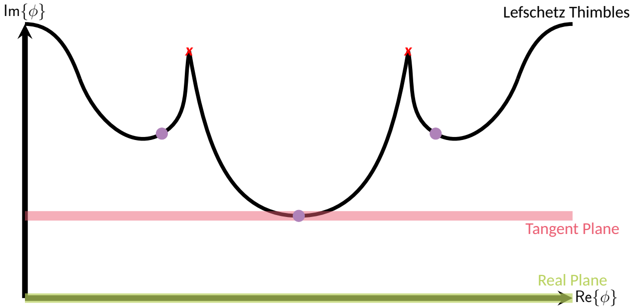


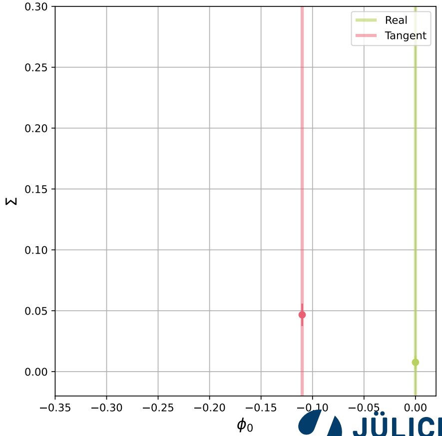


Contour Deformation

Constant Offsets - Tangent Plane

$$\phi_0/\delta = -\frac{U}{N_x}\sum_k \tanh\left(\frac{\beta}{2}\left[\epsilon_k + \mu + \phi_0/\delta\right]\right)$$

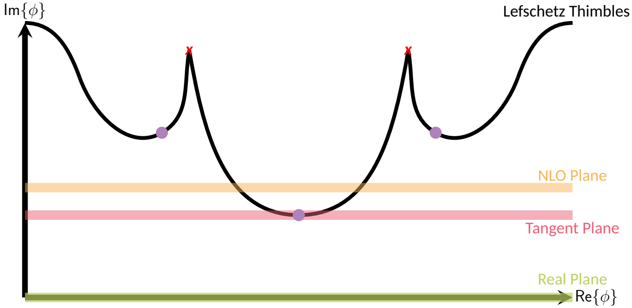


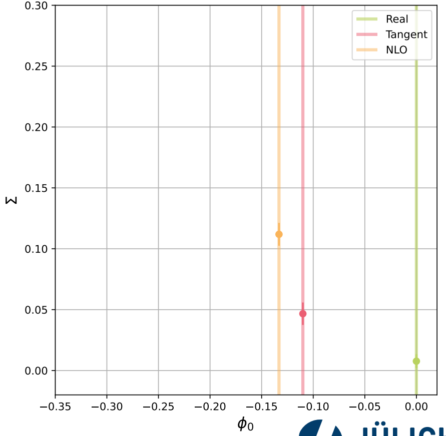


Contour Deformation

Constant Offsets - NLO

$$S_{\text{eff}}[\phi_1] = S[\phi_1] + \frac{1}{2} \log \det \mathbb{H}_{S[\phi_1]}$$

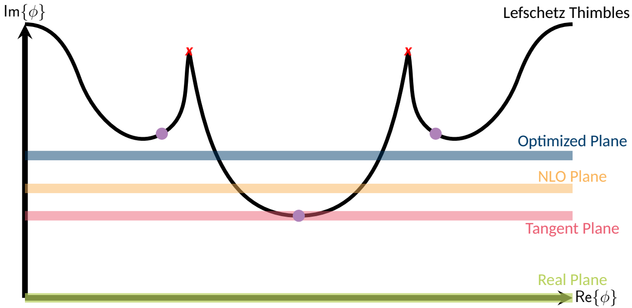


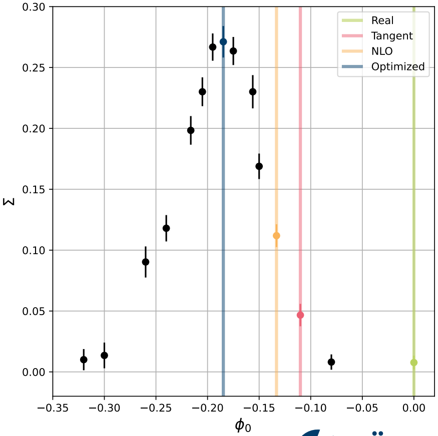


Contour Deformation

Constant Offsets - Optimized Offset

$$\Sigma[\phi_{\text{opt}}] = max\left(\Sigma[\phi]\right)$$

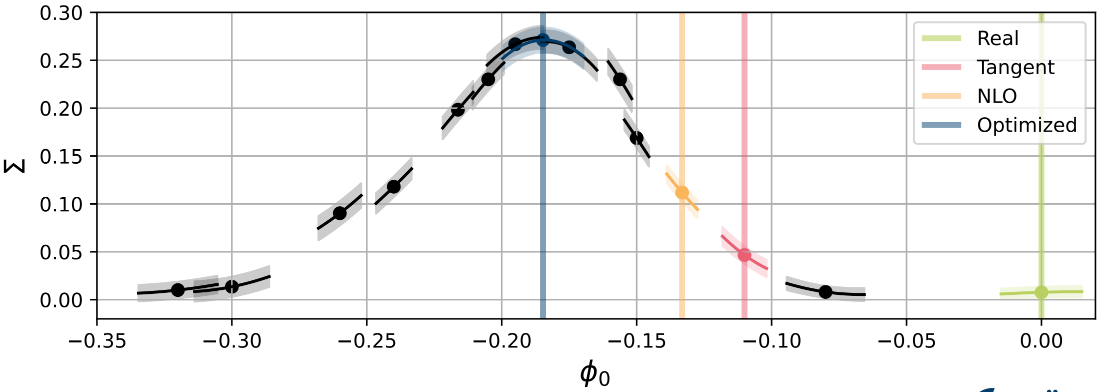




Optimizing Statistical Power

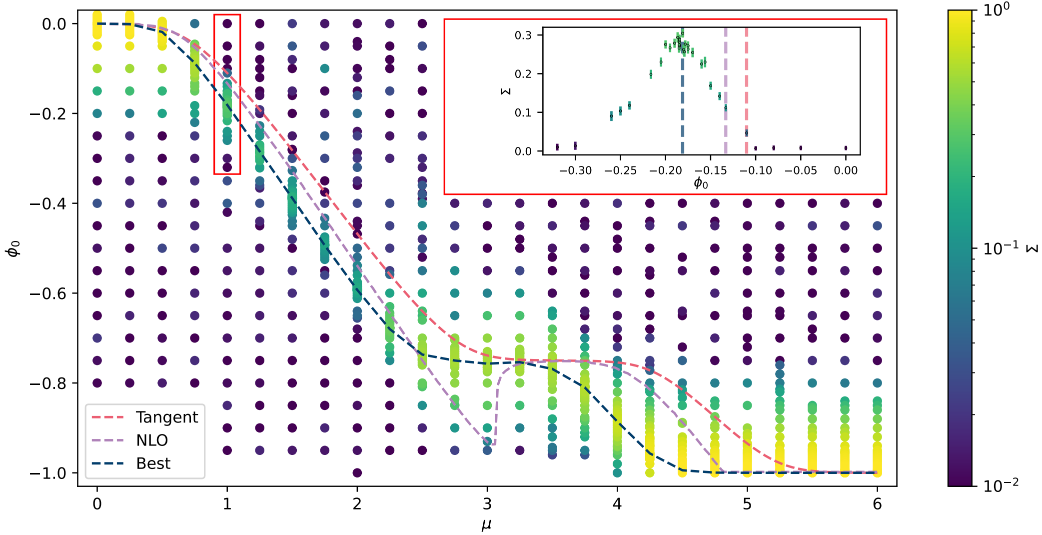
with Derivatives

$$\frac{\mathrm{d}\Sigma[\phi_0]}{\mathrm{d}\phi_0} \quad \text{and} \quad \frac{\mathrm{d}^2\Sigma[\phi_0]}{\mathrm{d}\phi_0^2}$$ [Alexandru et al., b]



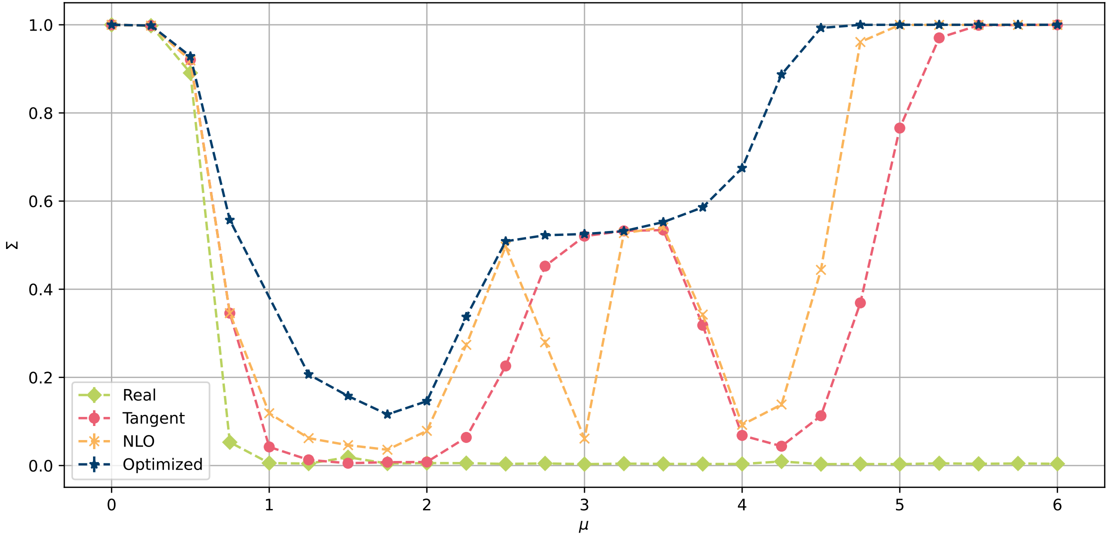
Optimizing Statistical Power

μ-Offset Heatmap



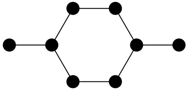
Optimizing Statistical Power

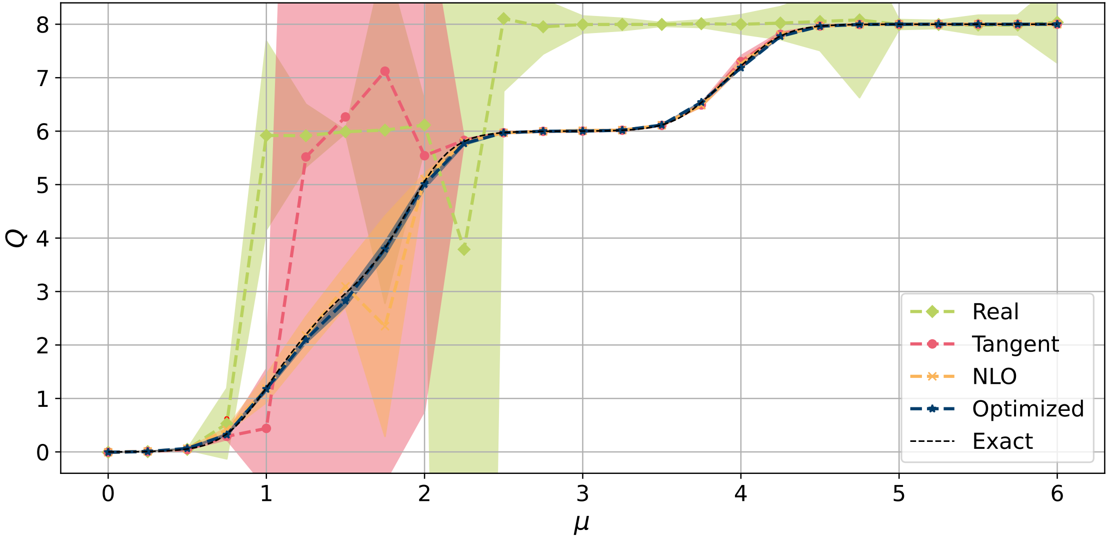
for varying μ



Results

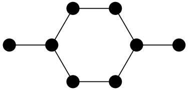
8-Sites Charge

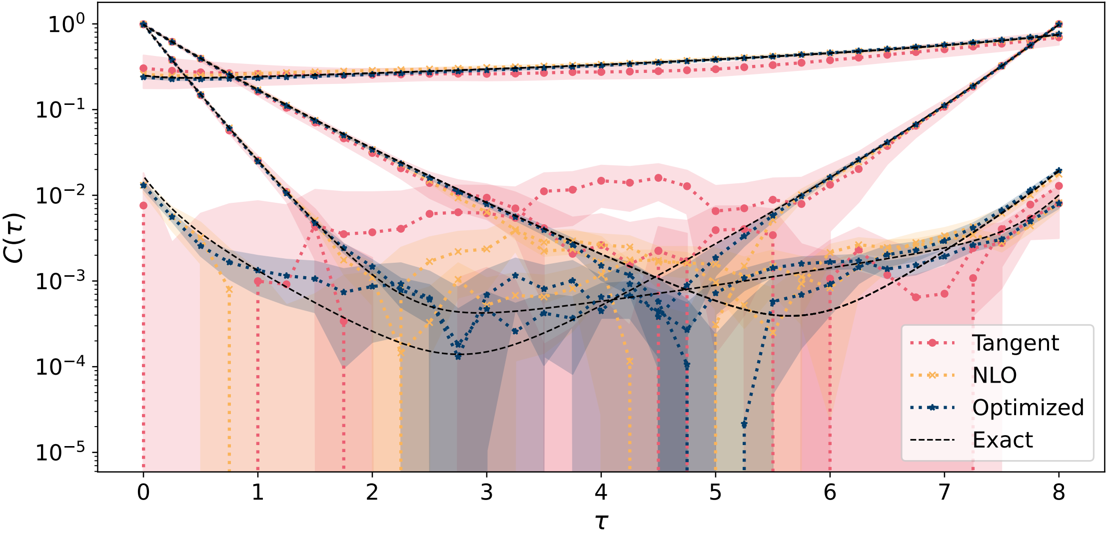




Results

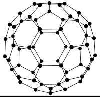
8-Sites Single Particle Correlator

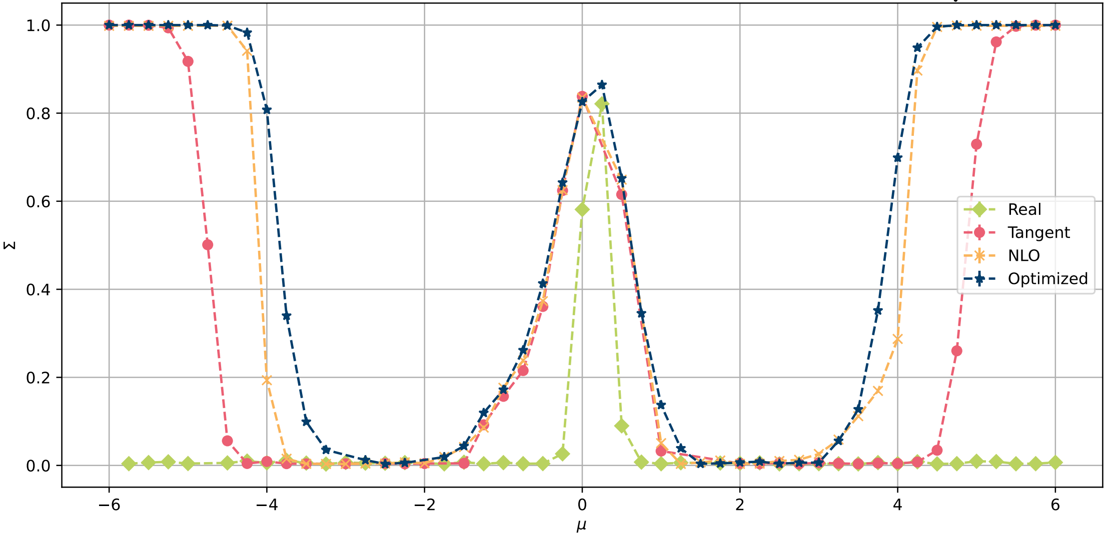




Results

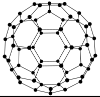
Statistical power C_{60}

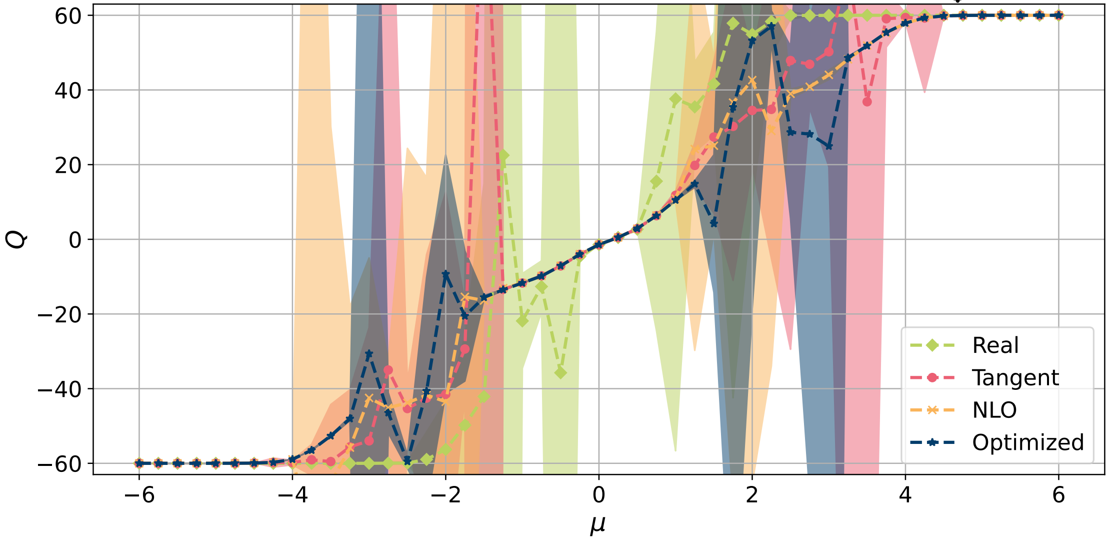




Results

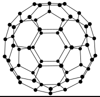
C_{60} Charge

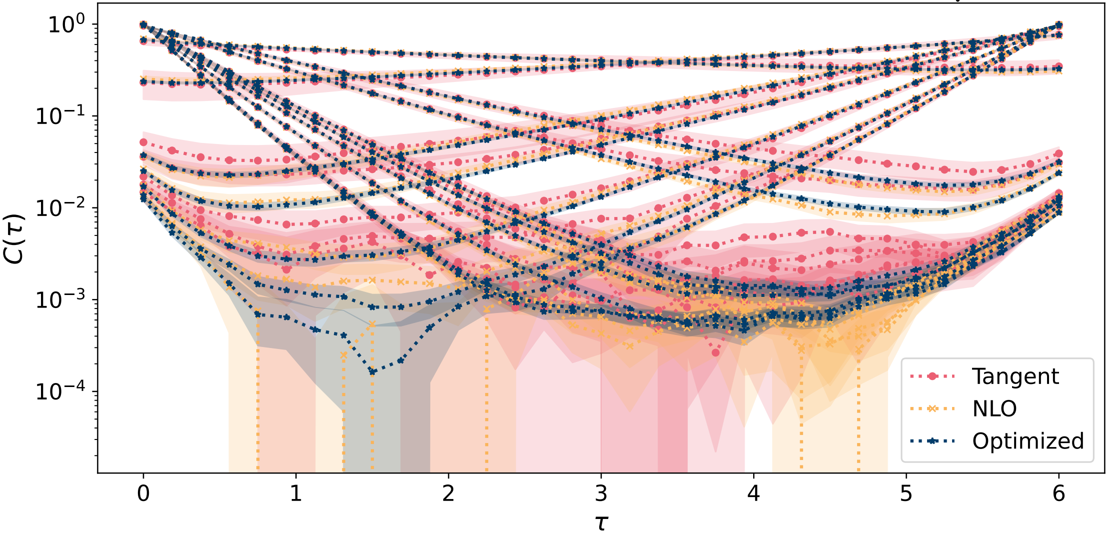




Results

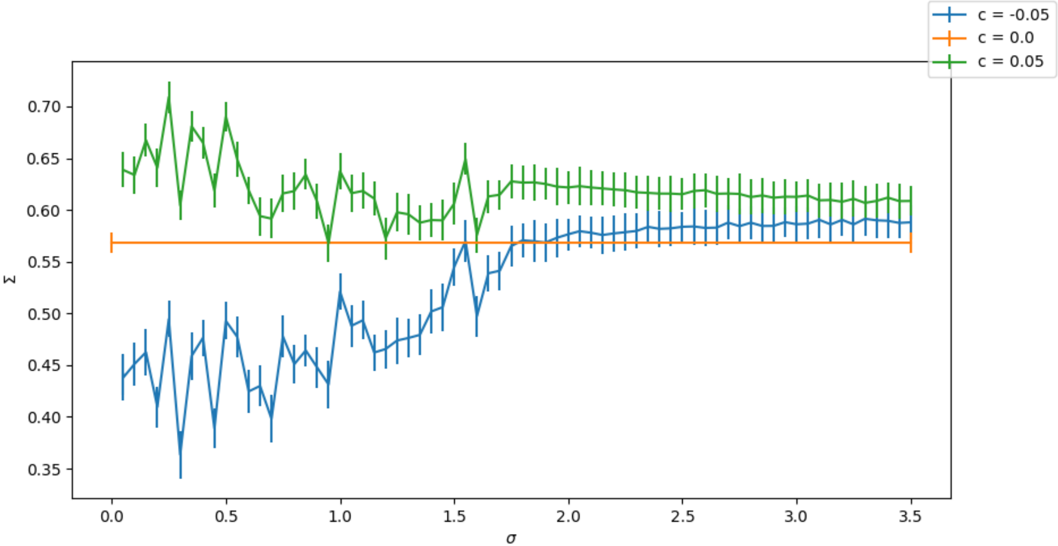
C_{60} Single Particle Correlator





Work in Progress

Offset + Gaussian - Preliminary results



Conclusion

- the Sign-problem can be reduced without slowing down the HMC
- the Sign-problem vanishes for $\mu \to \pm\infty$
- the best imaginary offset can be determined efficiently

References I

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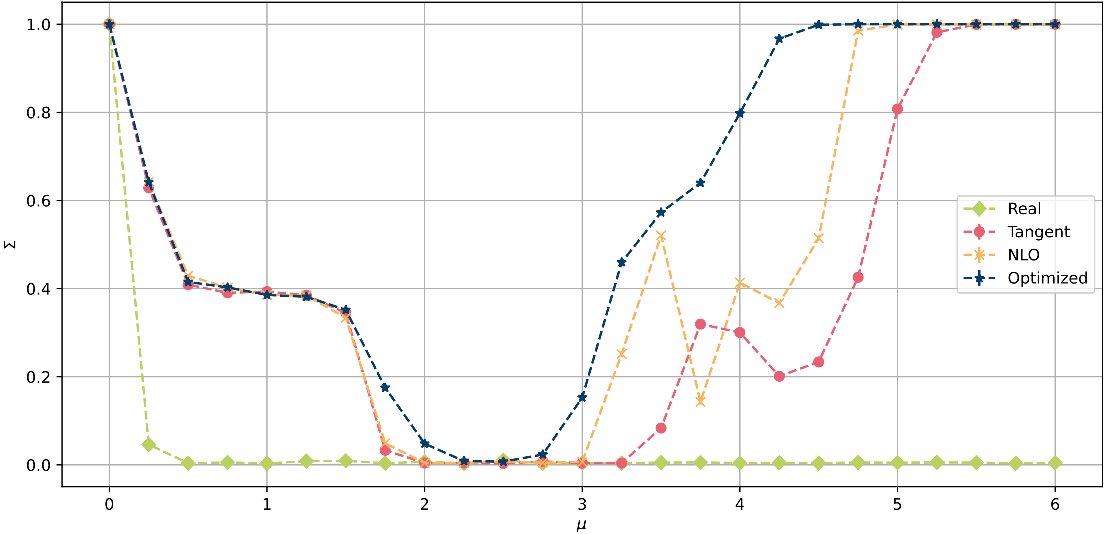
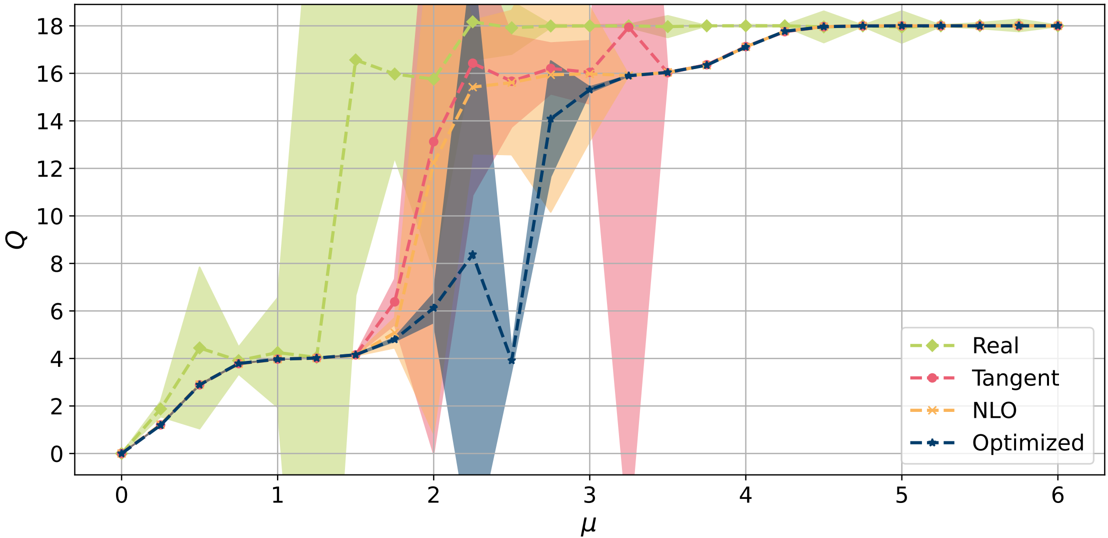
Backup

18-Sites Statistical Power



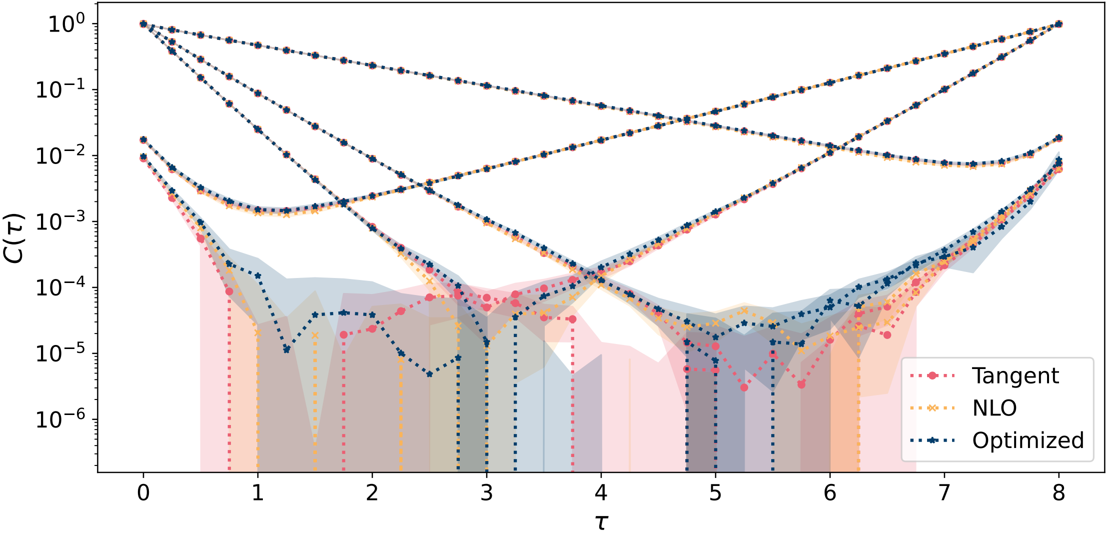
Backup

18-Sites Charge



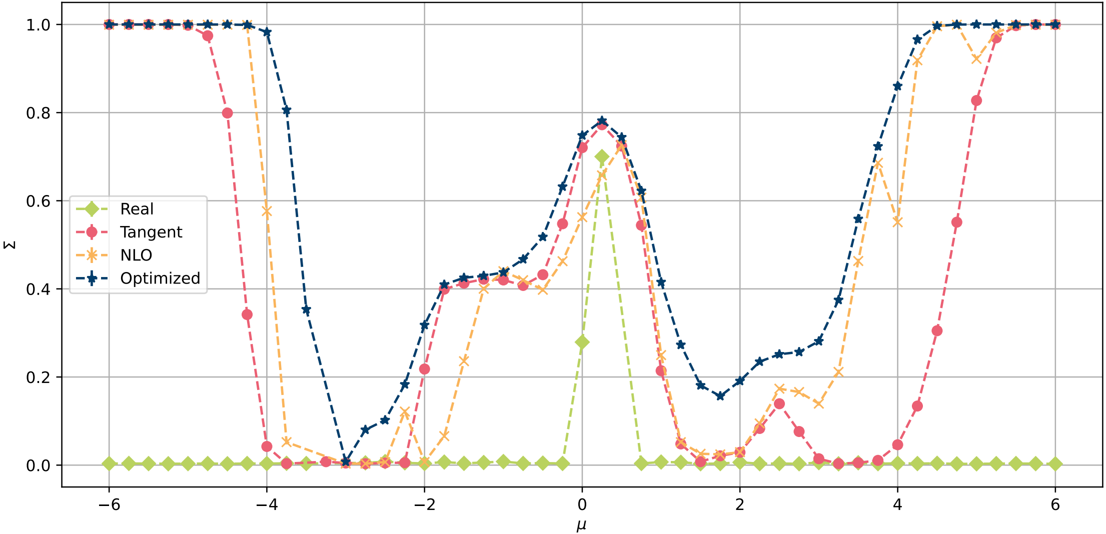
Backup

18-Sites Single Particle Correlators



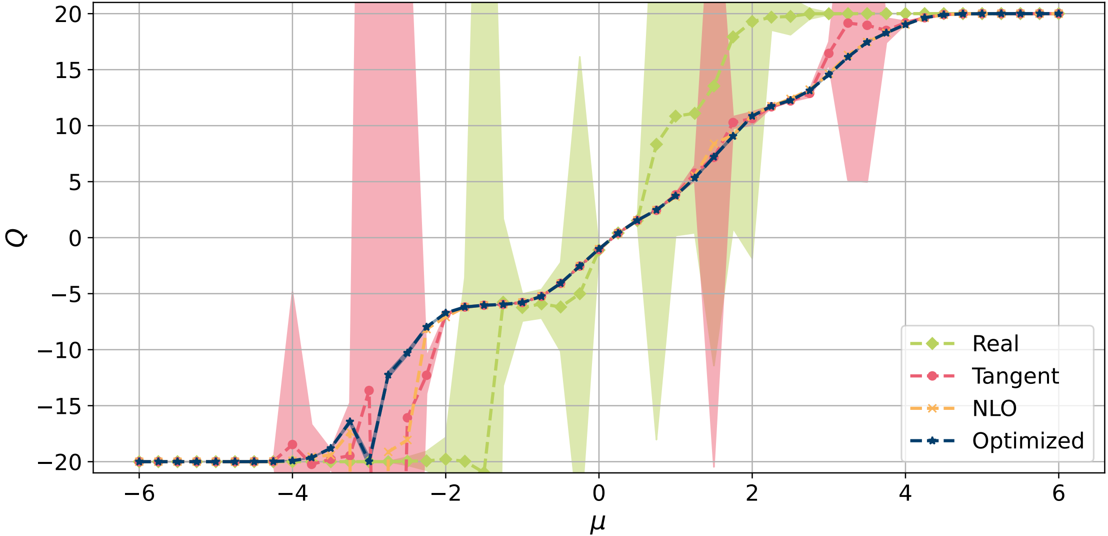
Backup

C_{20} Statistical Power



Backup

C_{20} Charge



Backup

C_{20} Single Particle Correlators