Hubbard-Model on C_{60} and C_{20}

Reducing the Sign-Problem

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Hubbard-Model

- The (Fermi-)Hubbard-Model describes the interacting behavior of electrons on a spatial lattice, e.g. a graphene sheet.
- Hamiltonian

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

- Action (derived through Hubbard-Stratonovich transformation)

$$S\left[\phi, \tilde\kappa, \tilde\mu\right] = \frac{1}{2\tilde U}\sum_{t,x} \phi^2_{x,t} - \log\det\left(M\left[+\phi, +\tilde\kappa, +\tilde\mu\right] \cdot M\left[-\phi, -\tilde\kappa, -\tilde\mu\right]\right)$$

Sign-Problem

- expectation values and partition function

$$\left\langle \hat O \right\rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi\, \hat O\left[\phi\right] e^{-S[\phi]} \quad \text{with} \quad \mathcal{Z} = \int \mathcal{D}\phi\, e^{-S[\phi]}$$

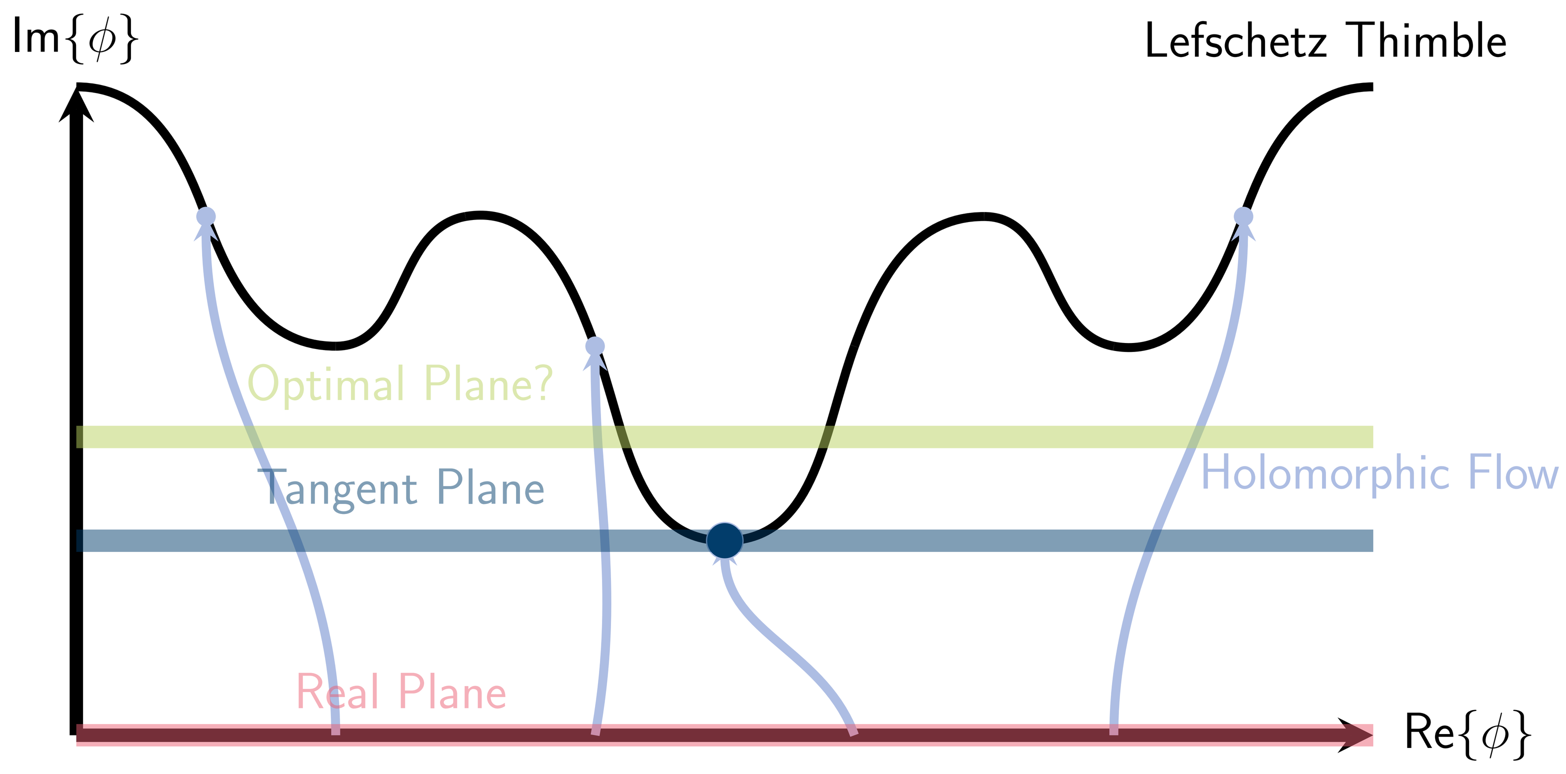
- if $S[\phi] \in \mathbb{C}$ we need reweighting!

$$\left\langle \hat O \right\rangle = \frac{\int \mathcal{D}\phi\, \hat O\left[\phi\right] e^{-i\,\mathrm{Im}\{S[\phi]\}} e^{-\mathrm{Re}\{S[\phi]\}}}{\int \mathcal{D}\phi\, e^{-i\,\mathrm{Im}\{S[\phi]\}} e^{-\mathrm{Re}\{S[\phi]\}}} = \frac{\left\langle \hat O e^{-iS_I} \right\rangle_R}{\left\langle e^{-iS_I}\right\rangle_R}$$

- In Markov-Chain Monte Carlo calculations the denominator slows down convergence of the expectation value, thus we need more random samples for the desired precision. This phenomenon is called Sign-Problem and prevents the calculation of numerous physical problems.
- the Statistical-Power $\left|\left\langle e^{-iS_I}\right\rangle_R\right|$ is a measure for the severity of the Sign-Problem.

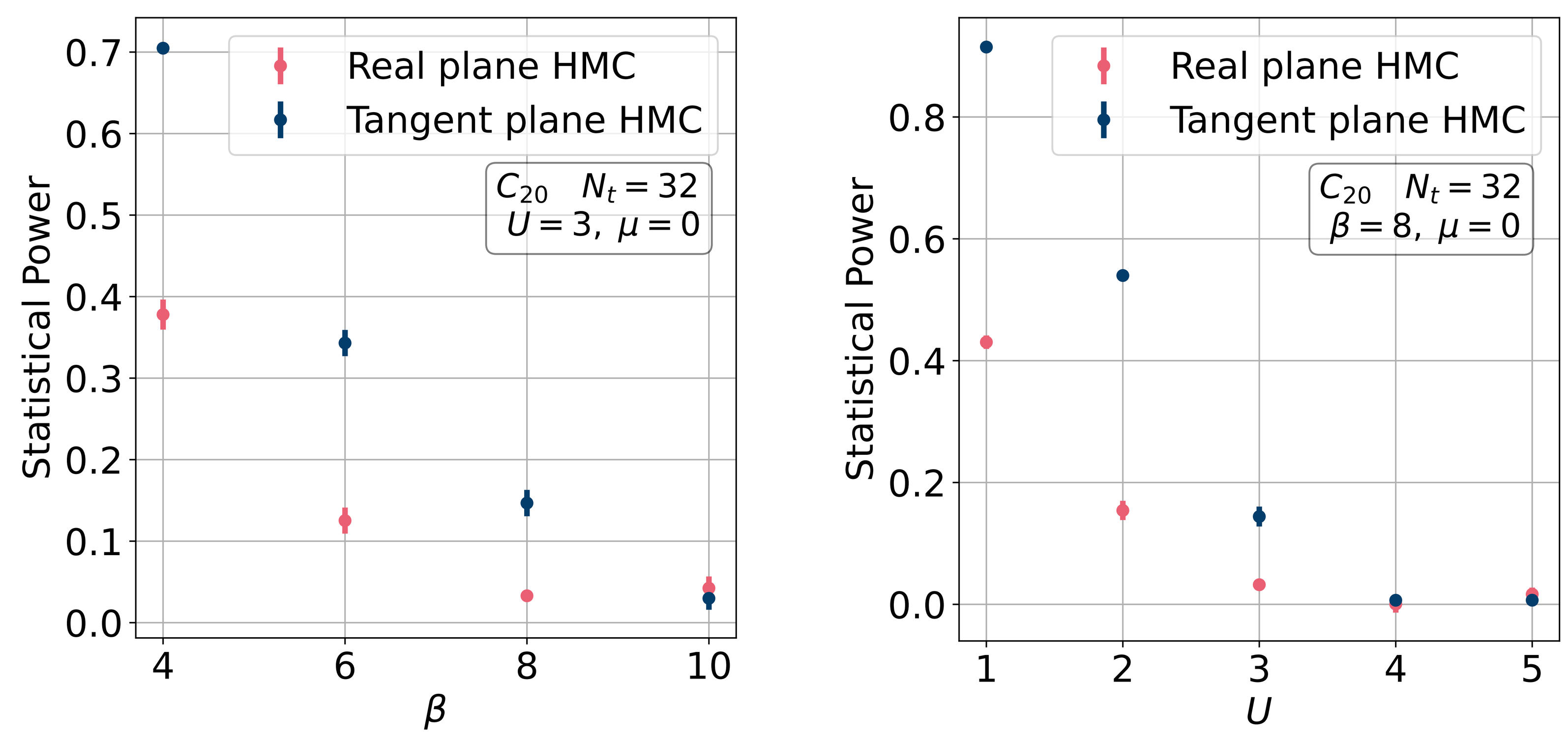
Method

- The Statistical-Power depends on the integration domain and the Sign-Problem can be completely lifted by contour deformation, thanks to Cauchy's theorem and Lefschetz thimbles.
- We use neural networks to approximate these favorable manifolds cheaply.
- However, the simplest and cheapest contour deformation, a constant imaginary shift, is often sufficient to reduce the Sign-Problem significantly.

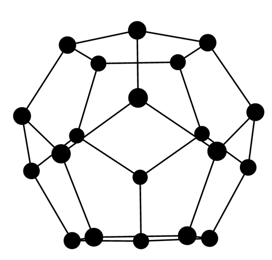


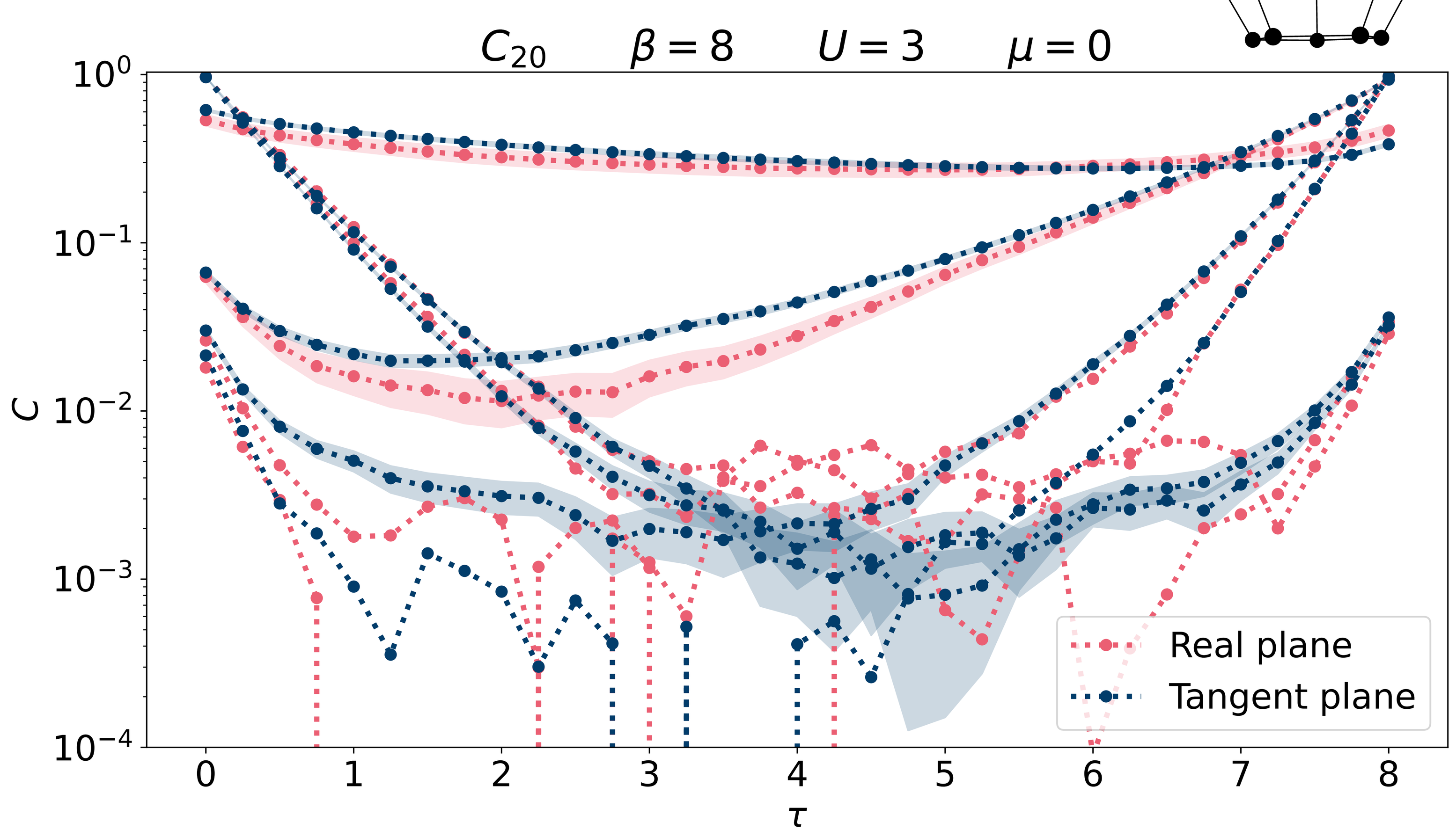
Statistical Power

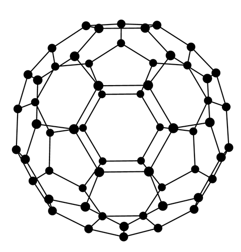
These plots show how the Sign-Problem scales with the physical parameters and demonstrate the benefit of a simple imaginary offset.

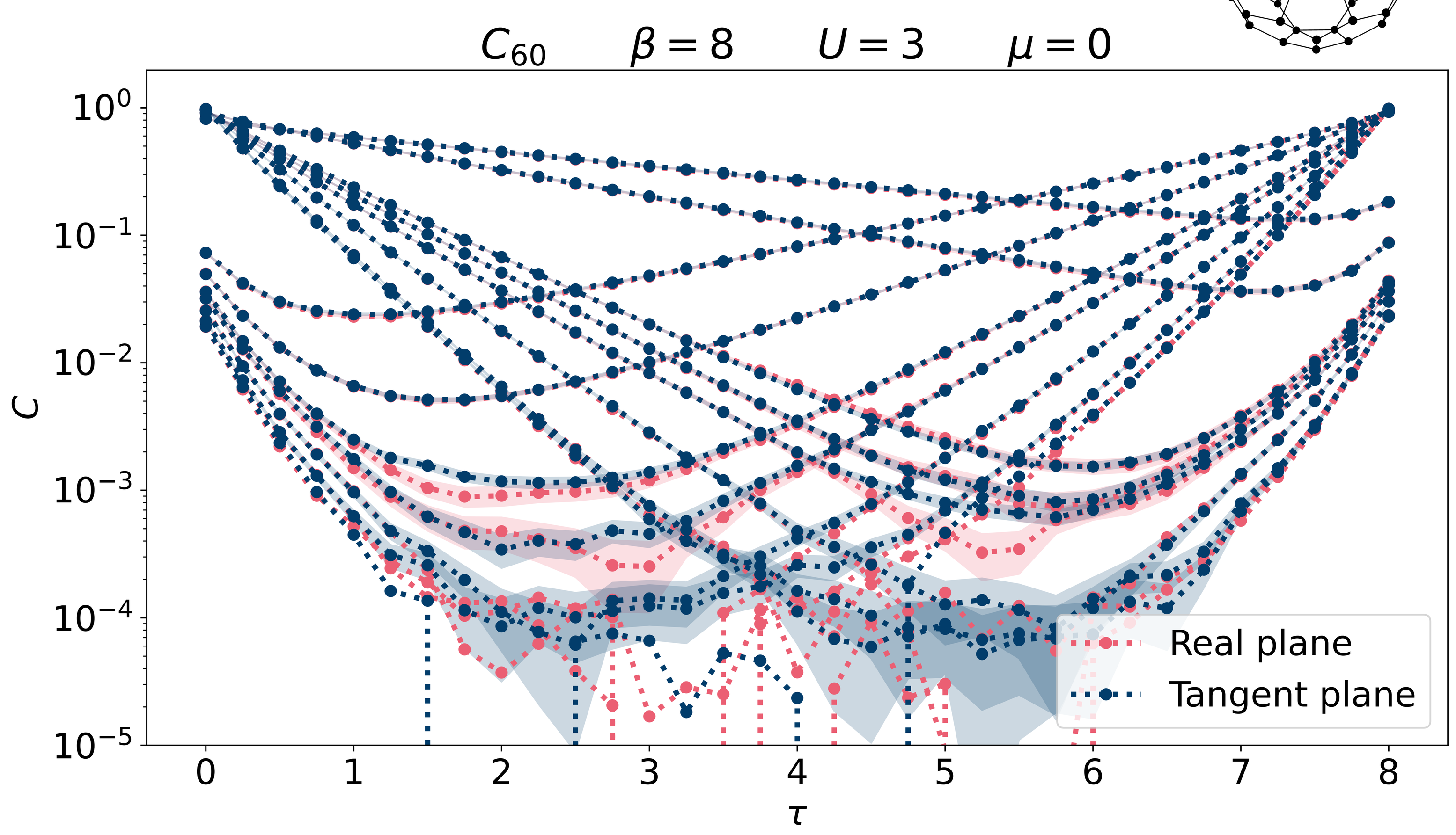


Single Particle Correlation Function



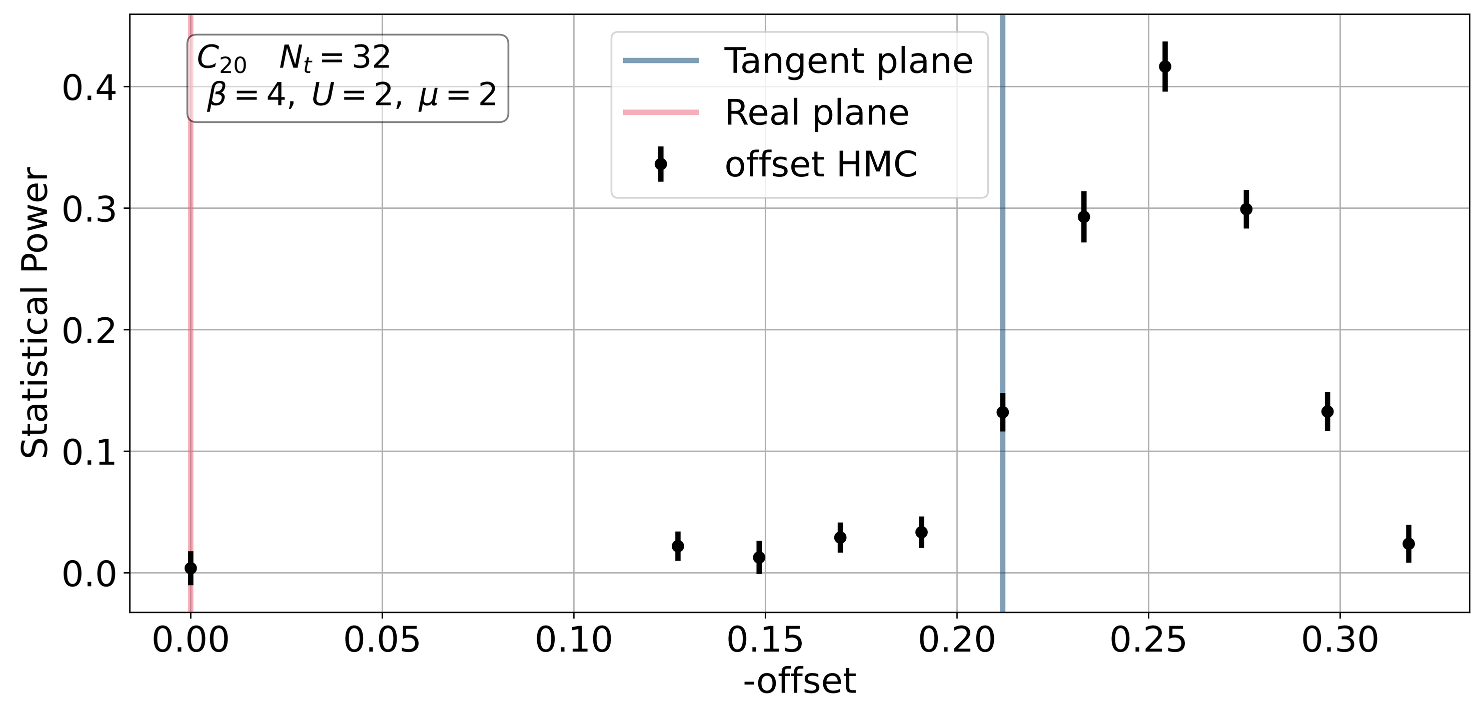






Outlook

- Find a cheap way to determine the optimal imaginary offset
  The benefit of the optimal offset over the easily determined tangent plane varies strongly, but it has the potential to increase the Statistical-Power by an order of magnitude in some cases.



- Complex valued neural networks
  In our latest paper Marcel Rodekamp introduced complex valued neural networks for a better volume scaling of the Jacobian (PhysRevB.106.125139, arXiv:2203.00390v2).
- Investigate the fullerenes with varying chemical potential
  We look forward to calculate the charge density of these systems and compare it with our graphene sheet results.
- Iterative learning approach for neural network contour deformation
  As the Lefschetz thimbles presumably vary smoothly with the physical parameters, we can retrain a network stepwise for more efficient parameter parsing.

Acknowledgements

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