RIKEN
DEEP-IN seminar

Neural Network Quantum State for quarkonium in medium: Real-time Open Quantum System dynamics

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Technical University of Munich

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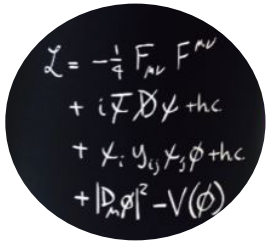
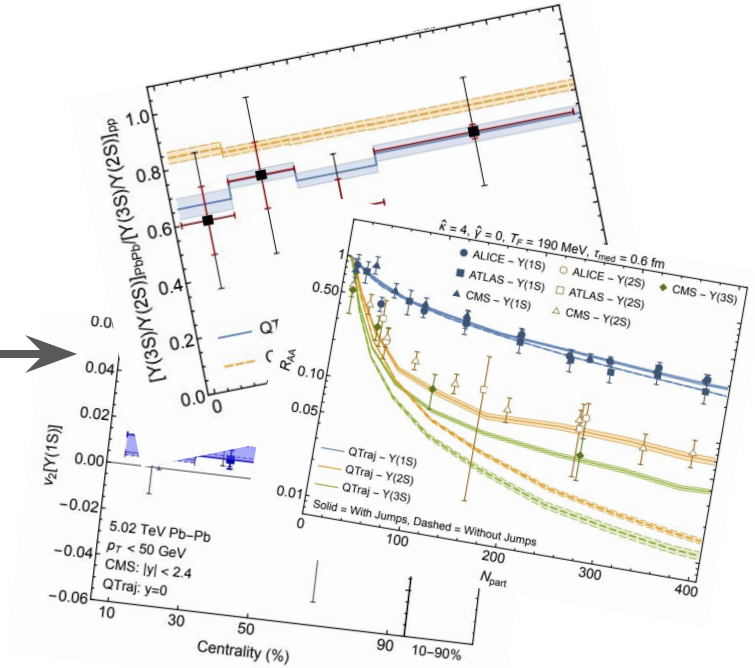
In collaboration with:
Nora Brambilla, Joshua Lin, Phiala Shanahan

We aim to make predictions from the Standard model

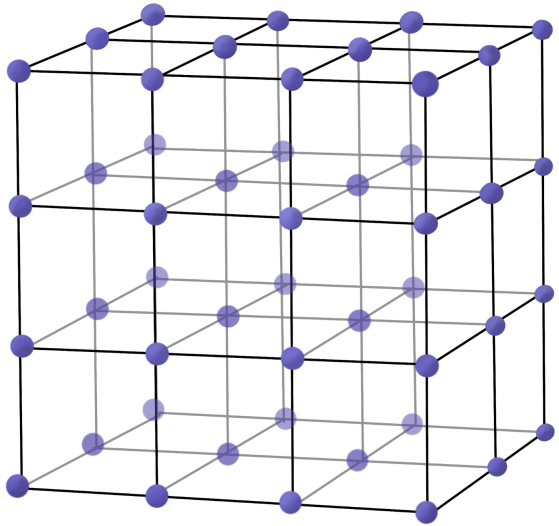




Lattice QCD is well suited for static observables

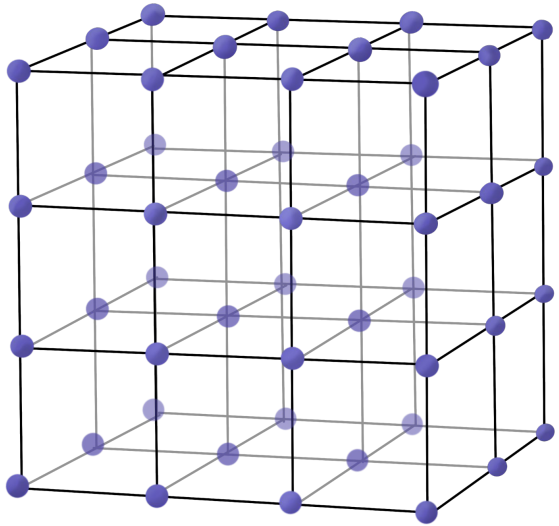
$$t \to -i\tau$$

$$\int \mathcal{D}\phi \, e^{-S_E[\phi]}$$

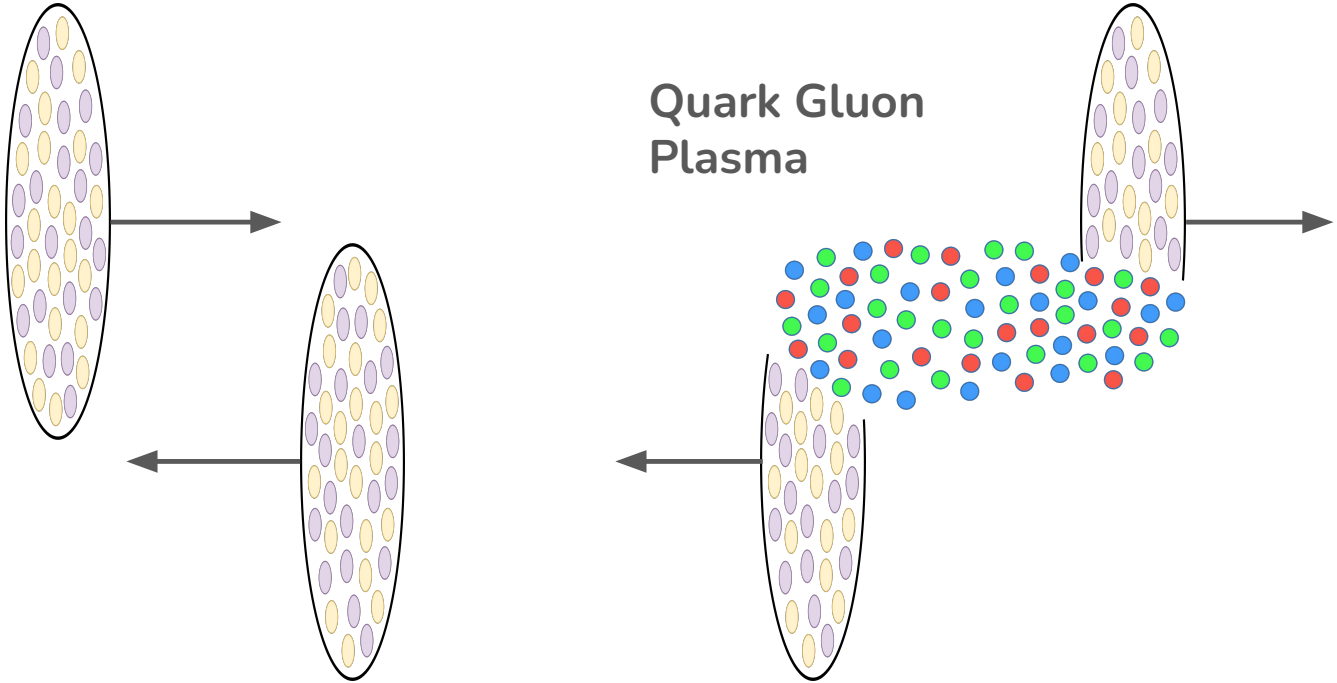


Many observables require real-time or non-equilibrium evolution

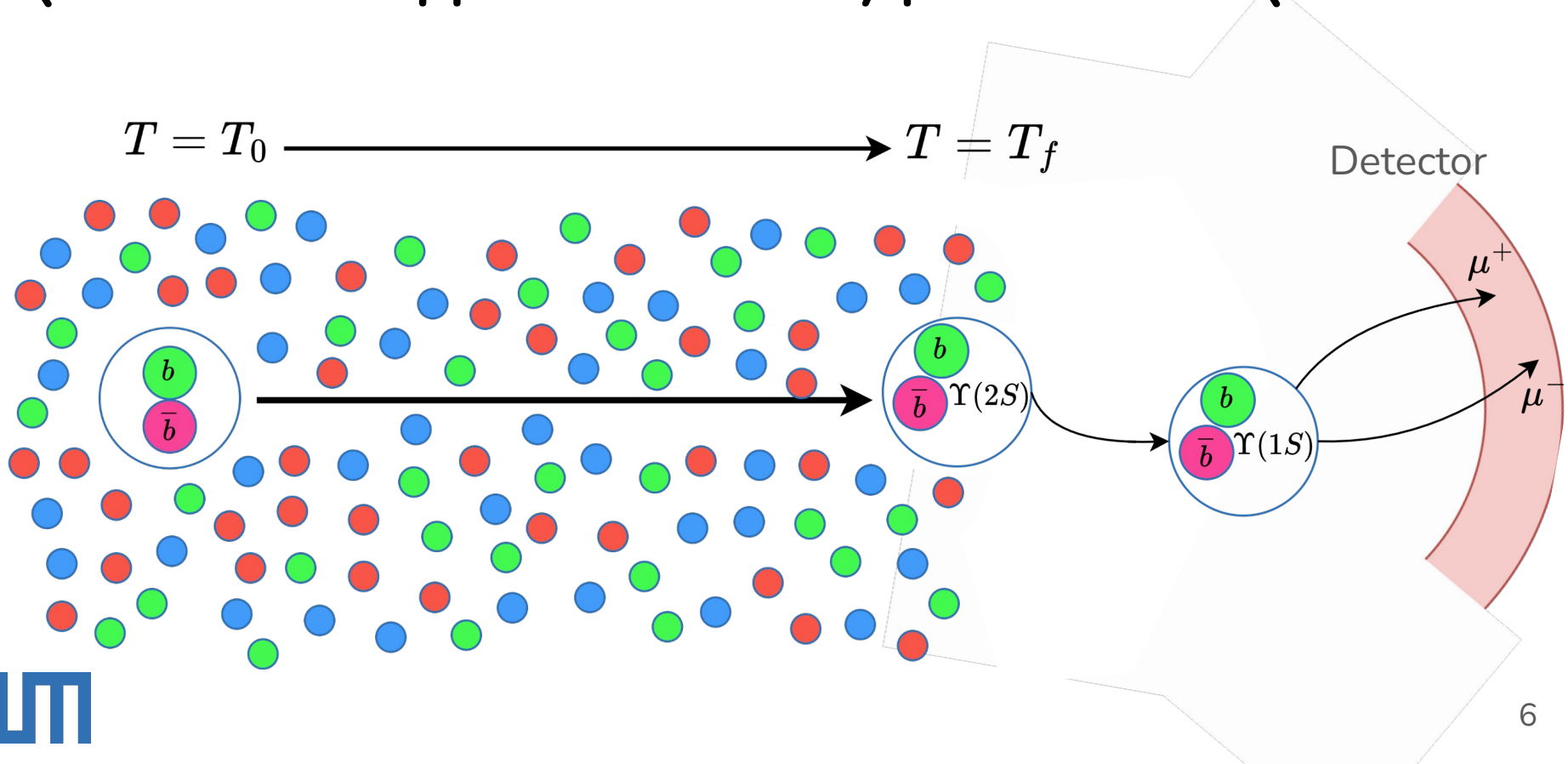
$$\int \mathcal{D}\phi \, e^{iS[\phi]}$$



Heavy-ion collisions involve genuine real-time, non-equilibrium dynamics



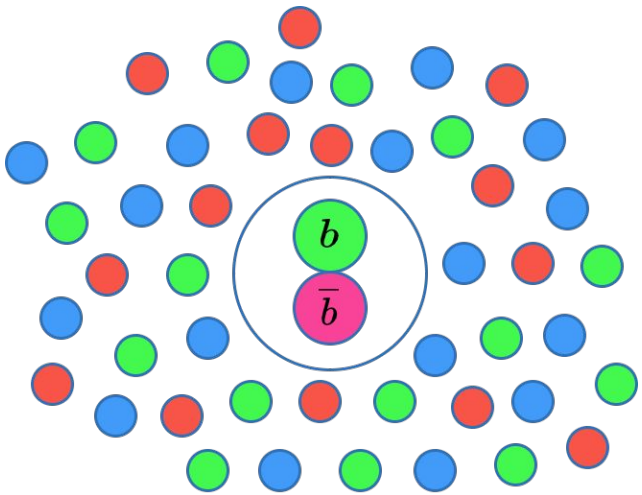
Quarkonium suppression is a key probe of the QGP

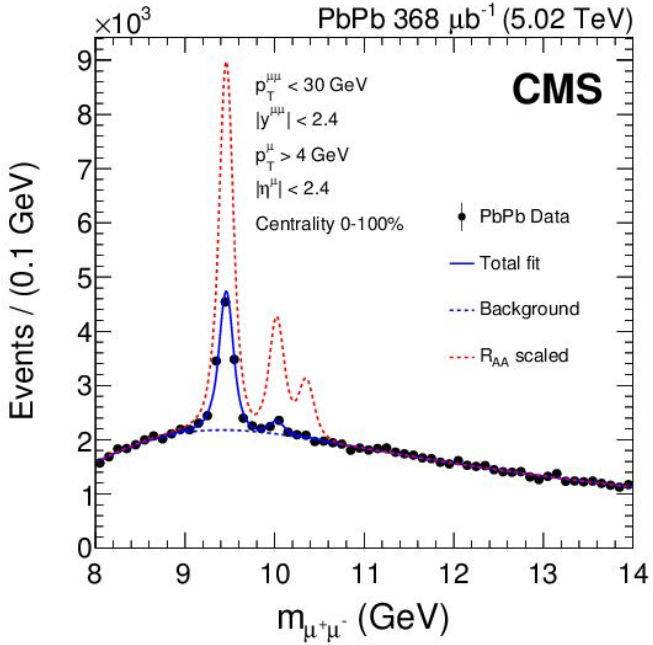


Quarkonium suppression is a key probe of the QGP

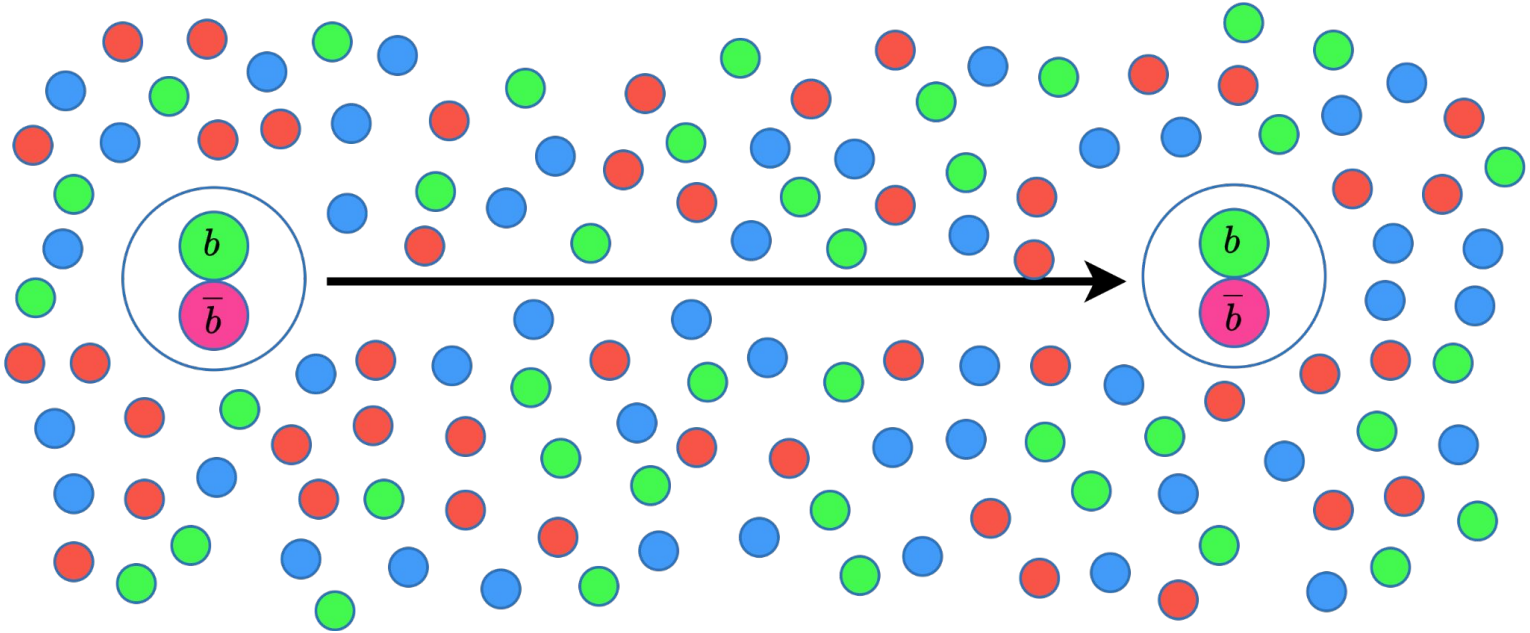
Veres, Gábor I. "Heavy ion physics at CMS and ATLAS: hard probes." *arXiv preprint arXiv:1905.10461* (2019).

Propagation through QGP

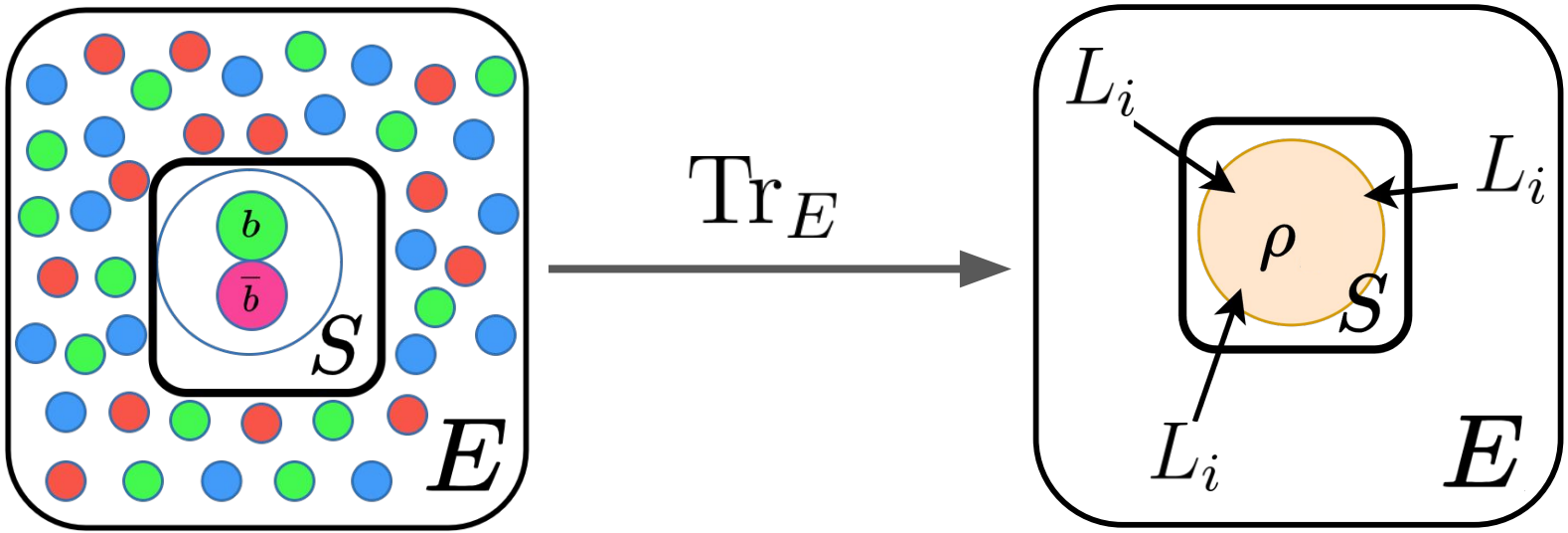




Quarkonium evolution in the QGP is a real-time, non-equilibrium process



We can treat the Quarkonium in medium as an open quantum system

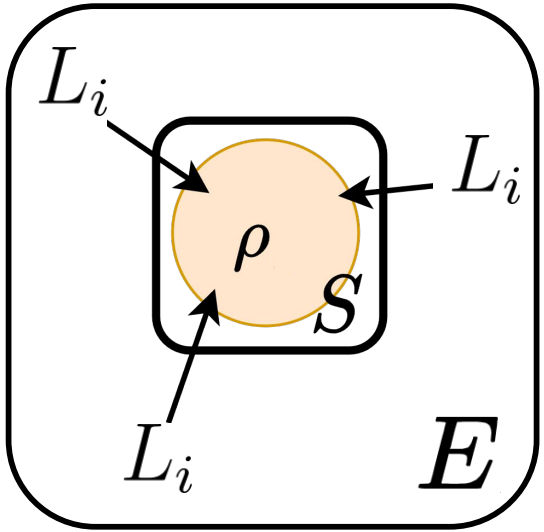


Brambilla, Escobedo, Soto, Vairo: Phys. Rev. D 97 (2018) 7, 074009

Tracing out the environment leads to a Quantum Master Equation for the quarkonium

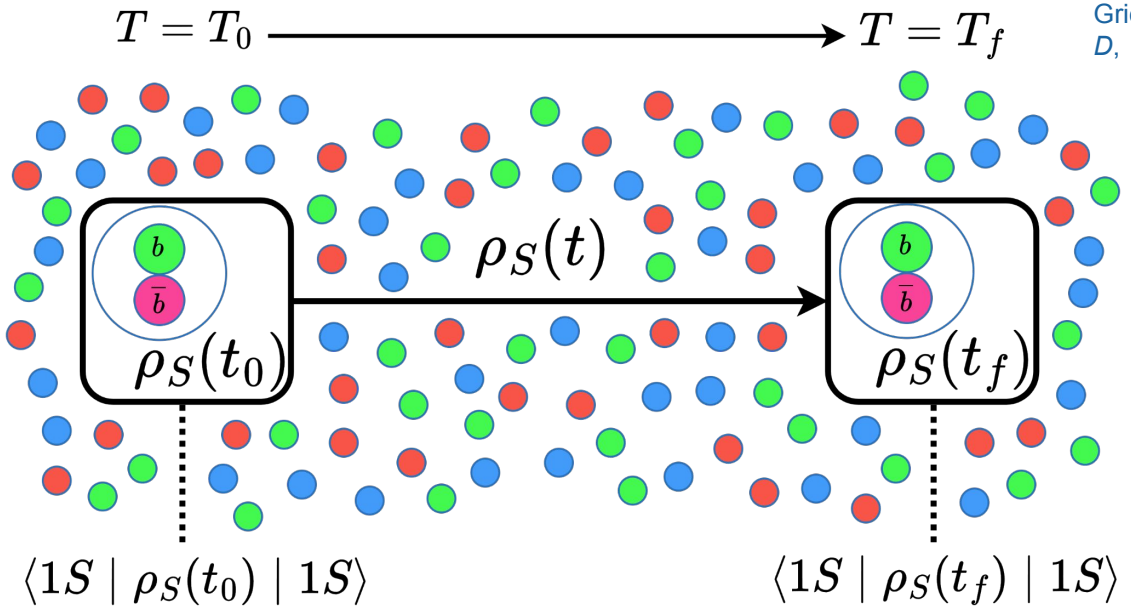
$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right)$$

Very large density matrix



By solving quantum master equation we can make phenomenological predictions

Brambilla, N., Magorsch, T., Strickland, M., Vairo, A., & Vander Griend, P. (2024). *Physical Review D*, *109*(11), 114016.



$$P_{\text{survival}}(1S) = \frac{\langle 1S|\rho(t_f)|1S\rangle}{\langle 1S|\rho(t_0)|1S\rangle}$$

Simulating the real time evolution in challenging

Omar, H. B., Escobedo, M. Á., Islam, A., Strickland, M., Thapa, S., Vander Griend, P., & Weber, J. H. (2022). *Computer Physics Communications*, *273*, 108266.

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right)$$

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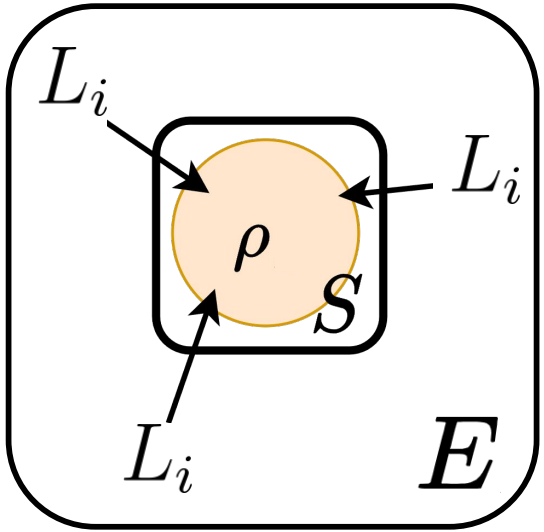
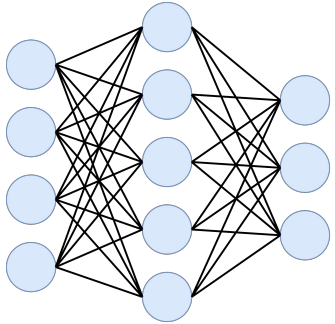


Neural Network Quantum States can represent wavefunctions in large Hilbert spaces

$$|\psi\rangle \in \mathcal{H} \longrightarrow$$



parameters $\sim \dim\mathcal{H}$

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Example: Ground state energy

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

Example: Ground state energy

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

$$H|\psi\rangle = E|\psi\rangle$$

Diagonalize H

Example: Ground state energy

$$E = \frac{\langle \psi_\Theta | H | \psi_\Theta \rangle}{\langle \psi_\Theta | \psi_\Theta \rangle}$$

$$\Theta \leftarrow \Theta - \alpha \nabla_\Theta E$$

Variational Monte Carlo

$$E = \mathbb{E}_{p(x)} \left[\frac{\langle x | H | \psi_\Theta \rangle}{\langle x | \psi_\Theta \rangle} \right]$$

$$p(x) = \frac{|\langle x | \psi_\Theta \rangle|^2}{\sum_x |\langle x | \psi_\Theta \rangle|^2}$$

Variational Monte Carlo

$$E = \mathbb{E}_{p(x)} \left[\overbrace{\frac{\langle x | H | \psi_\Theta \rangle}{\langle x | \psi_\Theta \rangle}}^{E_{\mathrm{loc}}(x)} \right]$$

$$p(x) = \frac{|\langle x | \psi_\Theta \rangle|^2}{\sum_x |\langle x | \psi_\Theta \rangle|^2}$$

Variational Monte Carlo

$$\begin{pmatrix} 0 & 1 & 0 & \dots \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & 1 & \dots \\ 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \psi_\Theta(x_1) \\ \psi_\Theta(x_2) \\ \psi_\Theta(x_3) \\ \vdots \end{pmatrix}$$

$$E_{\mathrm{loc}}(x) = \frac{\langle x | H | \psi_\Theta \rangle}{\langle x | \psi_\Theta \rangle}$$

Variational Monte Carlo

$$\begin{pmatrix} 0 & 1 & 0 & \dots \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & 1 & \dots \\ 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \psi_\Theta(x_1) \\ \psi_\Theta(x_2) \\ \psi_\Theta(x_3) \\ \vdots \end{pmatrix}$$

$$= \psi_\Theta(x_1) + \psi_\Theta(x_3)$$

Variational Monte Carlo

$$\nabla_\Theta \langle H \rangle = \nabla_\Theta \mathbb{E}_{p(x|\Theta)} \left[\frac{\langle x | H | \psi_\Theta \rangle}{\langle x | \psi_\Theta \rangle} \right]$$

Variational Monte Carlo

$$\nabla_\Theta \langle H \rangle = \nabla_\Theta \mathbb{E}_{p(x|\Theta)} \left[\frac{\langle x | H | \psi_\Theta \rangle}{\langle x | \psi_\Theta \rangle} \right]$$

$$= 2\mathrm{Re}\, \mathbb{E}_{p(x|\Theta)} \left[\nabla_\Theta \log \psi_\Theta(x)^* \left(E_{\mathrm{loc}}(x, \Theta) - \langle E_{\mathrm{loc}} \rangle \right) \right]$$

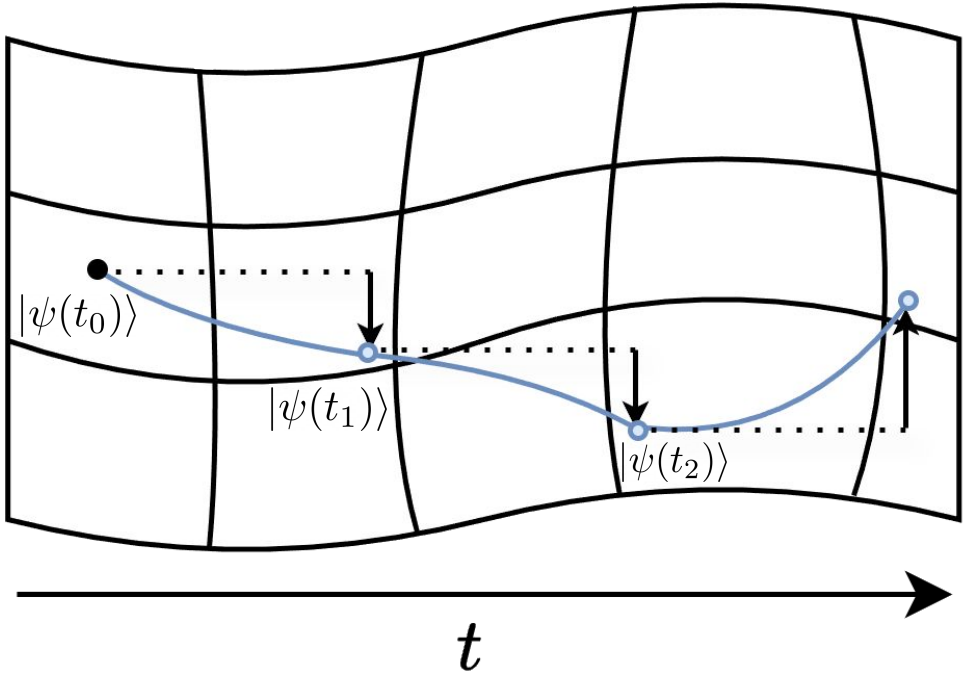
Time evolution: p-tVMC

Sinibaldi, A., Giuliani, C., Carleo, G., & Vicentini, F. (2023). Unbiasing time-dependent Variational Monte Carlo by projected quantum evolution. *Quantum*, *7*, 1131.

Gravina, L., Savona, V., & Vicentini, F. (2025). Neural projected quantum dynamics: a systematic study. *Quantum*, *9*, 1803.

Minimize **Infidelity:**

$$I = 1 - \frac{|\langle\psi(t_1)|\psi(t_0)\rangle|^2}{\langle\psi(t_1)|\psi(t_1)\rangle\langle\psi(t_0)|\psi(t_1)\rangle}$$



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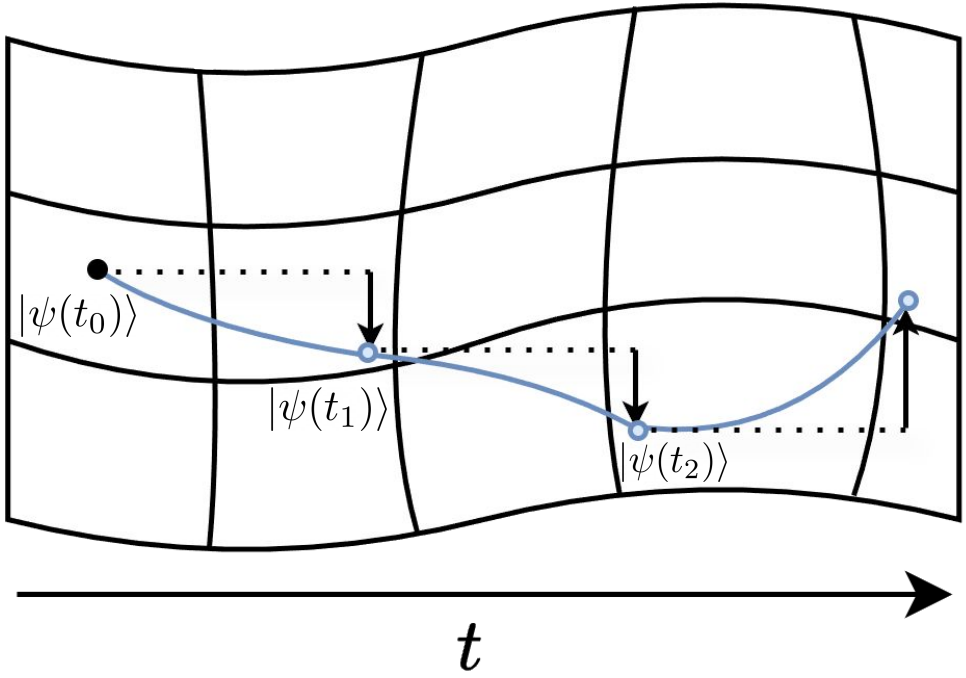
$$I = 1 - \frac{|\langle\psi(t_1)|\psi(t_0)\rangle|^2}{\langle\psi(t_1)|\psi(t_1)\rangle\langle\psi(t_0)|\psi(t_1)\rangle}$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(t_0)\rangle$$

$$|\psi(t_1)\rangle = (1 - iHdt)|\psi(t_0)\rangle$$

$$\equiv U$$



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Gravina, L., Savona, V., & Vicentini, F. (2025). Neural projected quantum dynamics: a systematic study. *Quantum*, *9*, 1803.

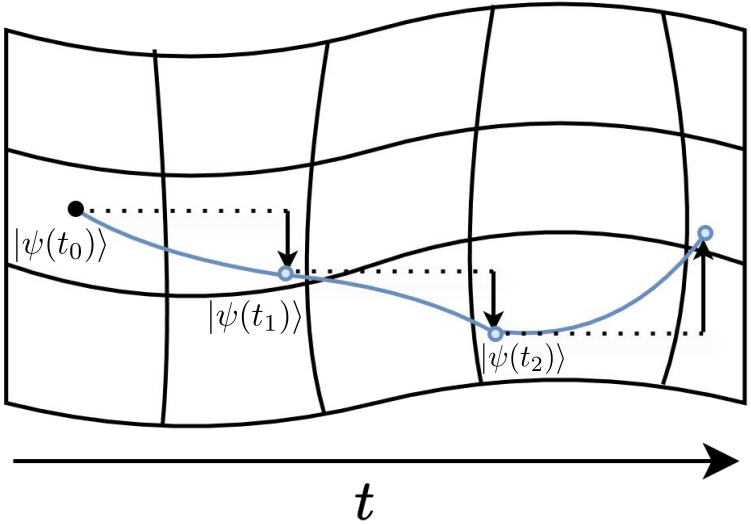
$$U = 1 - iH\delta t$$

Single timestep

$$I = \mathbb{E}_{\sigma,\eta\sim p(\sigma|\Theta_1)p(\eta|\Theta_0)}\left[1 - \frac{\langle\sigma|U|\psi_{\Theta_0}(t_0)\rangle}{\langle\sigma|\psi_{\Theta_1}(t_0)\rangle}\frac{\langle\eta|U^\dagger|\psi_{\Theta_1}(t_0)\rangle}{\langle\eta|\psi_{\Theta_0}(t_0)\rangle}\right]$$

Energy

$$E = \mathbb{E}_{p(\sigma|\Theta)}\left[\frac{\langle\sigma|H|\psi_\Theta\rangle}{\langle\sigma|\psi_\Theta\rangle}\right]$$



Neural Density Operators have to fulfill physical conditions

1. $\mathrm{Tr}\rho = 1$
2. $\rho^\dagger = \rho$
3. $\rho \geq 0$

Enforce in a neural network!

Neural Density Operators have to fulfill physical conditions

1. $\mathrm{Tr}\rho = 1$
2. $\rho^\dagger = \rho$
3. $\rho \geq 0$

$$\langle\sigma|\,\hat{\rho}\,|\eta\rangle = \prod_{h=1}^{K}\sum_{a=1}^{R}\psi^{(h)}_{\sigma,a}\,[\psi^{(h)}_{\eta,a}]^*$$

Vicentini, F., Rossi, R., & Carleo, G. (2022). Positive-definite parametrization of mixed quantum states with deep neural networks. *arXiv:2206.13488*.

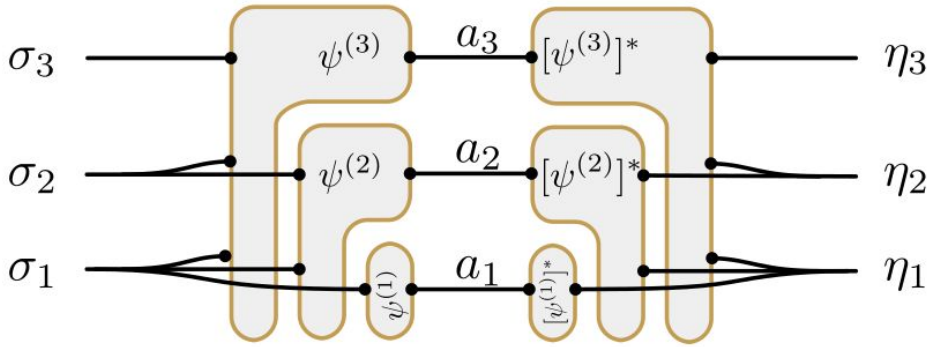
An autoregressive structure enables efficient sampling

To evaluate expectation values we have to sample from

$$p(\sigma, \eta) = \frac{1}{N} |\langle \sigma | \rho | \eta \rangle|^2$$

Restrict to autoregressive structure:

$$\langle \sigma | \hat{\rho} | \eta \rangle = \prod_{h=1}^{N} \sum_{a=1}^{R} \psi_{\sigma_{\leq h}, a} \left[\psi_{\eta_{\leq h}, a} \right]^*$$



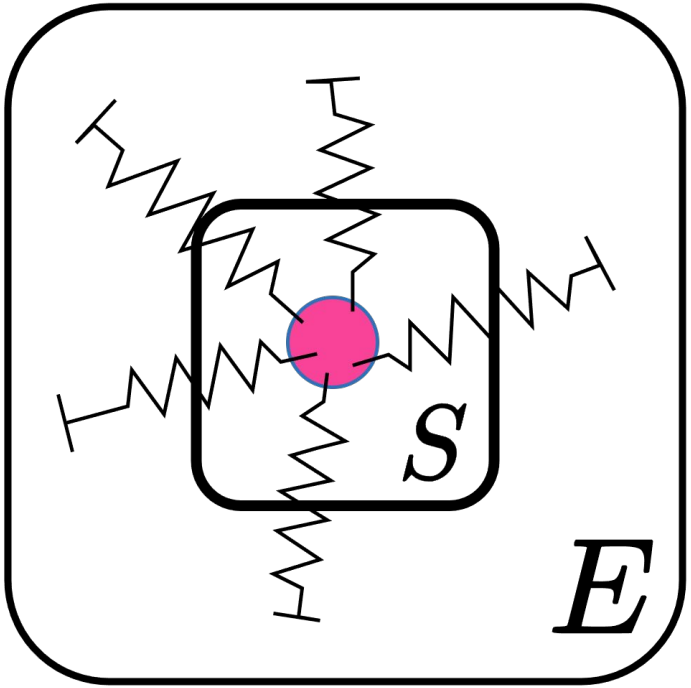
Vicentini, F., Rossi, R., & Carleo, G. (2022). Positive-definite parametrization of mixed quantum states with deep neural networks. *arXiv:2206.13488*.

The Caldeira–Leggett model is the simplest model of quantum Brownian motion

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right)$$

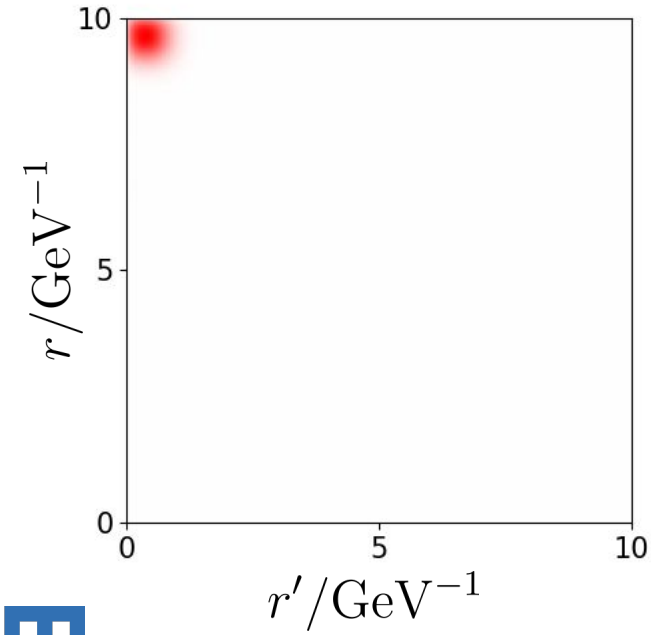
$$H = \frac{p^2}{2M} + V(r) + \frac{\kappa}{4MT}\{r,p\}$$

$$L_i = \kappa \left(r_i + i\frac{p_i}{2MT} \right)$$

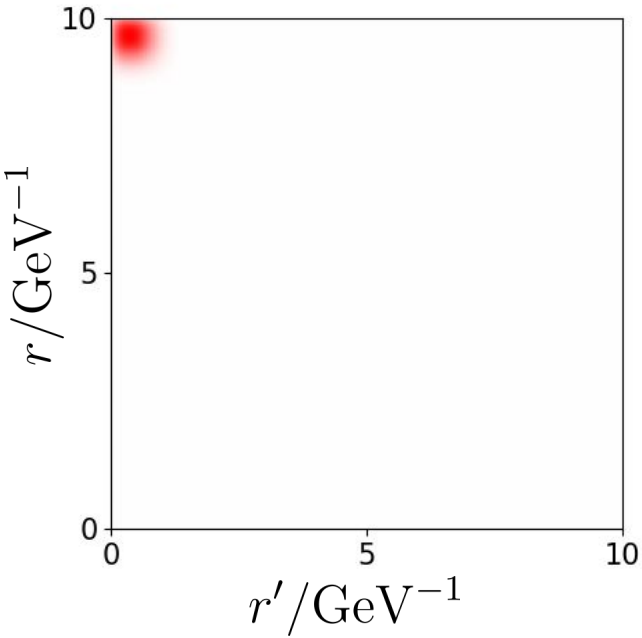


Simulation results

Monte Carlo Wavefunction



Neural Network



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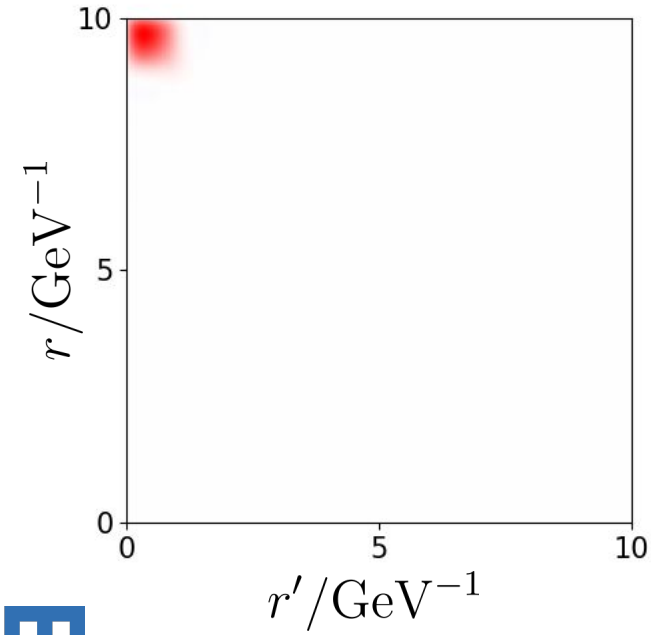

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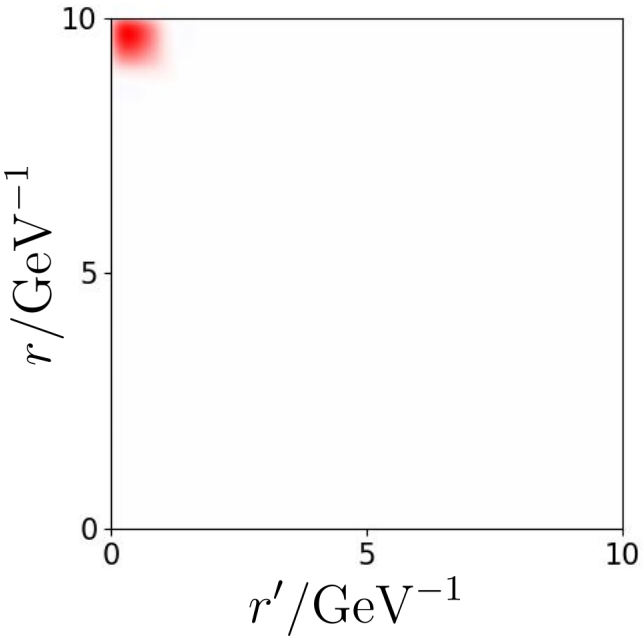

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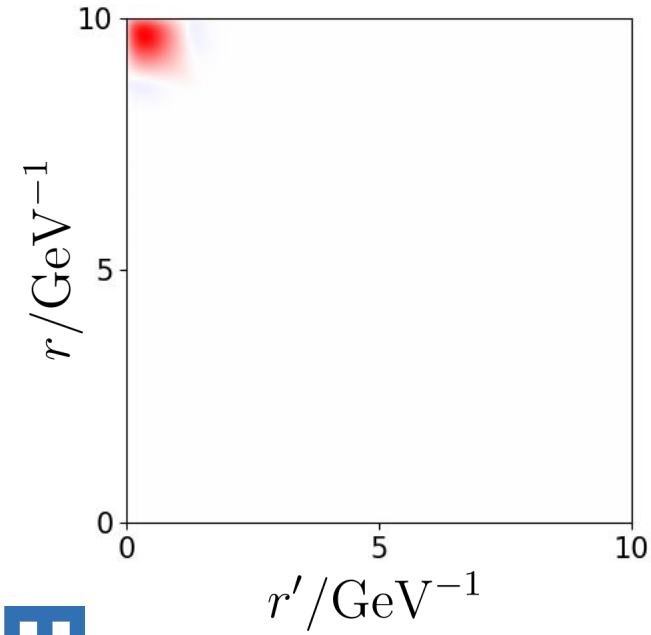

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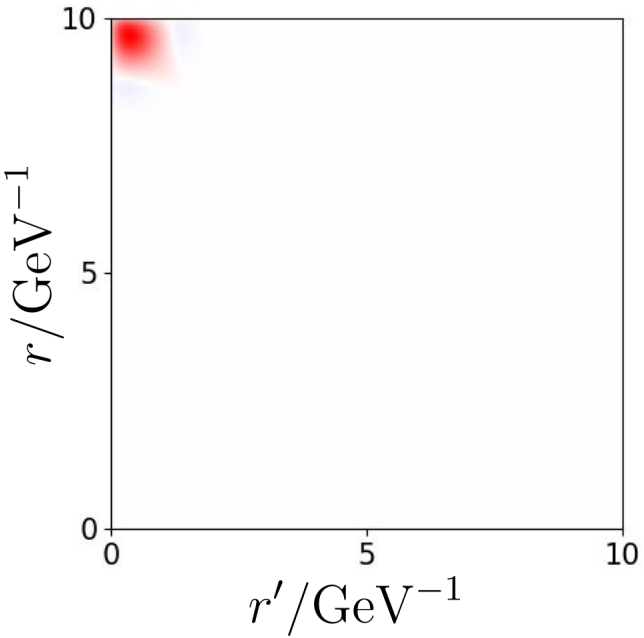

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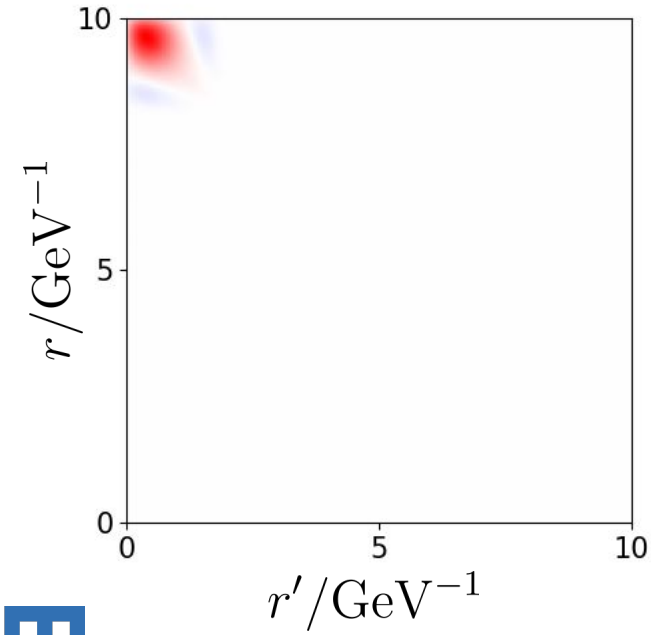

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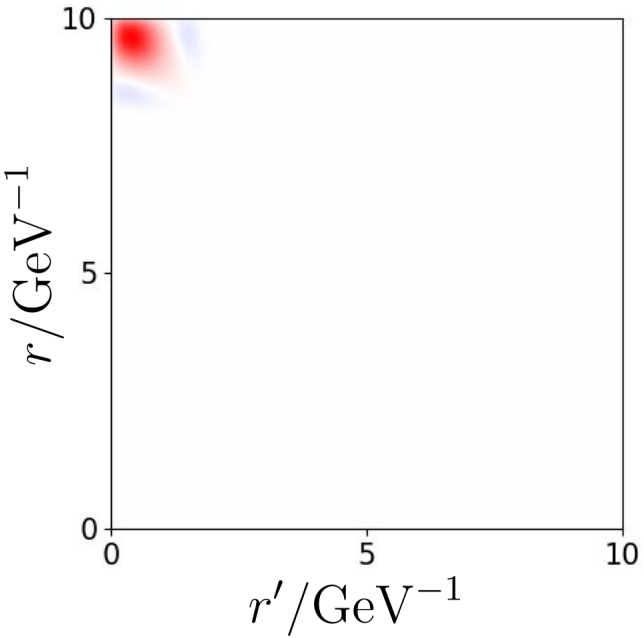

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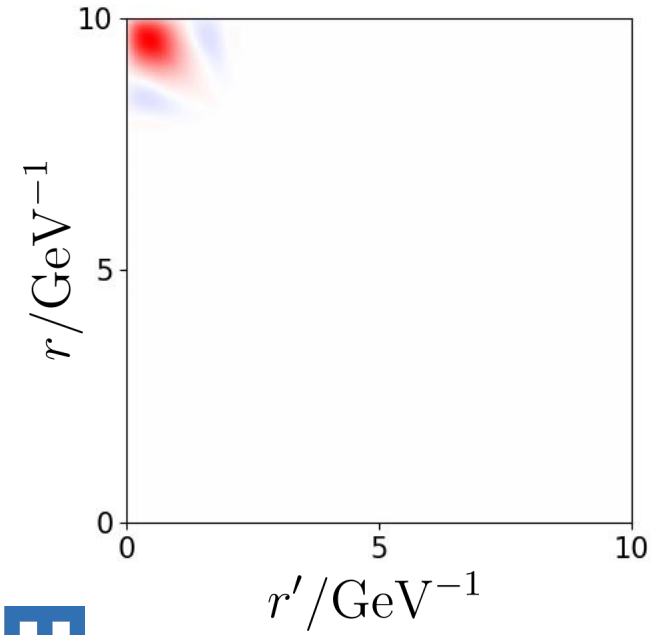

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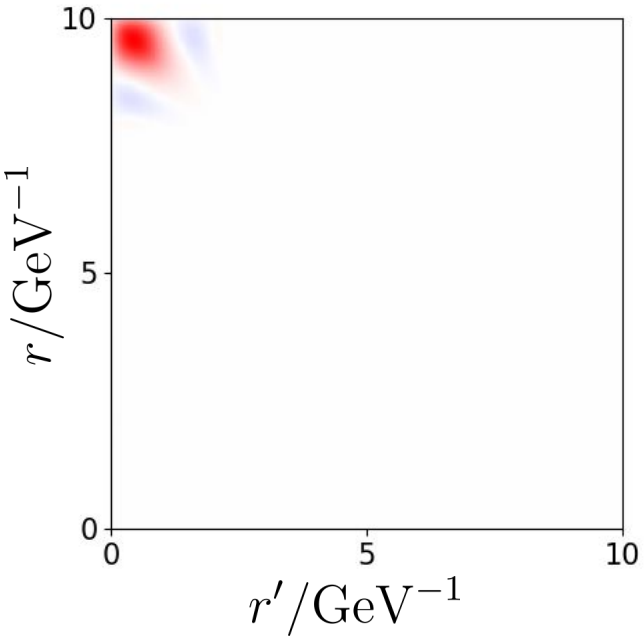

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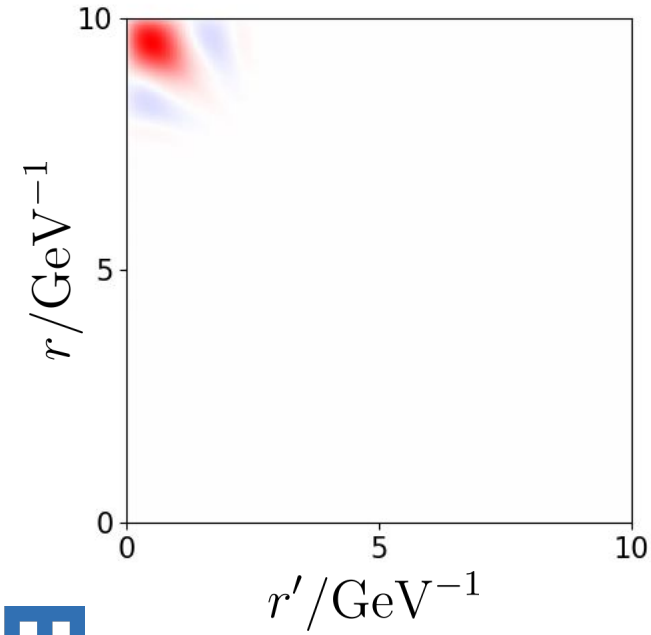

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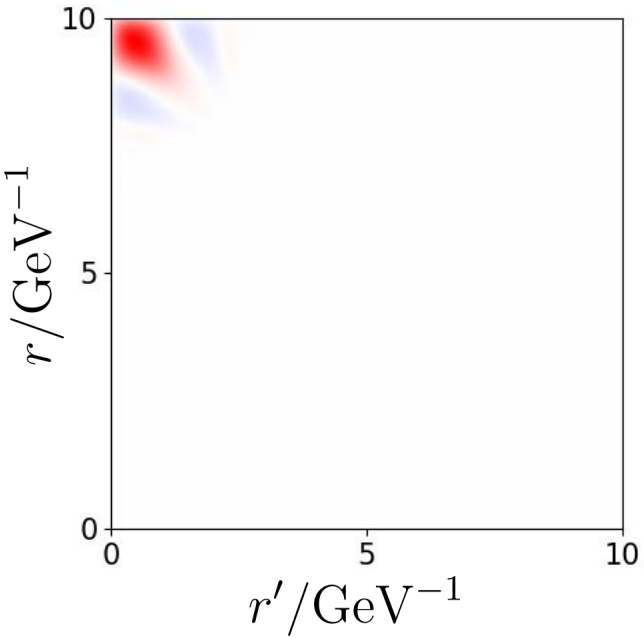

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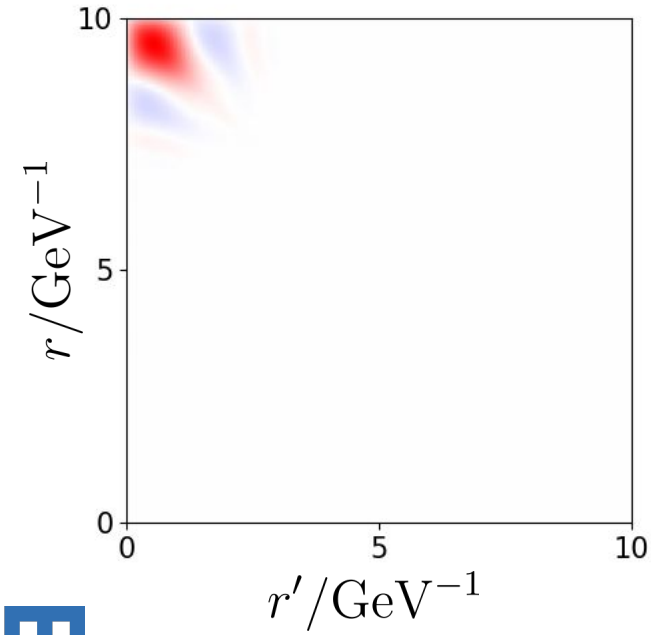

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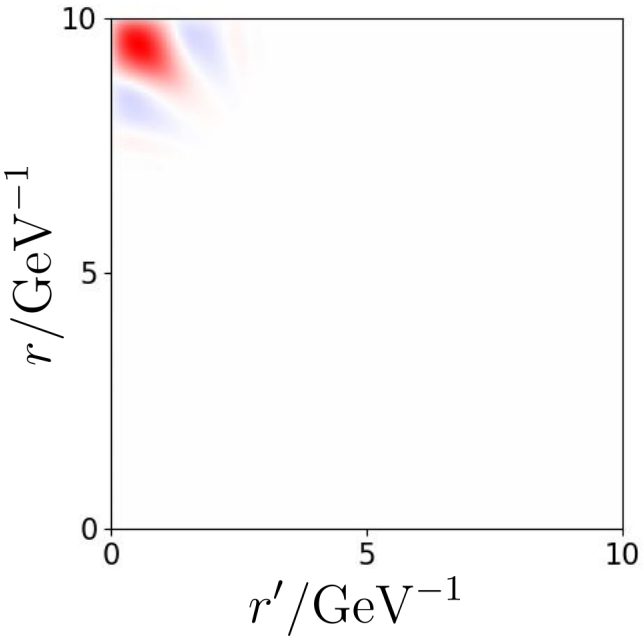

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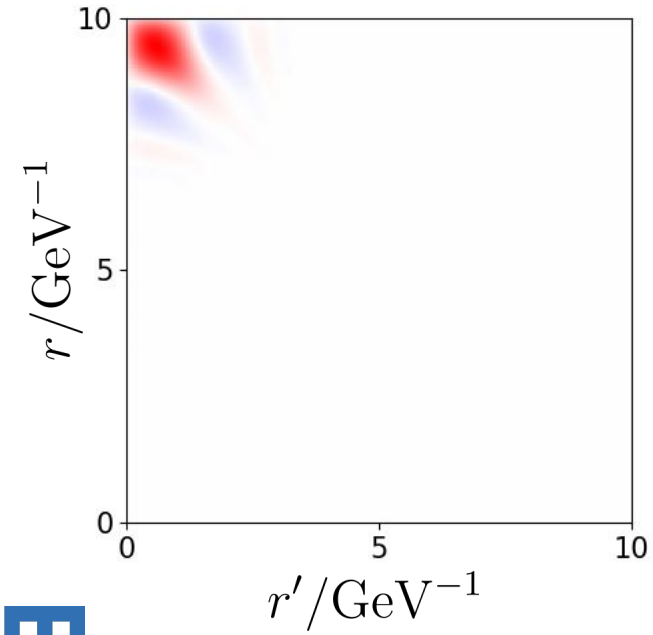

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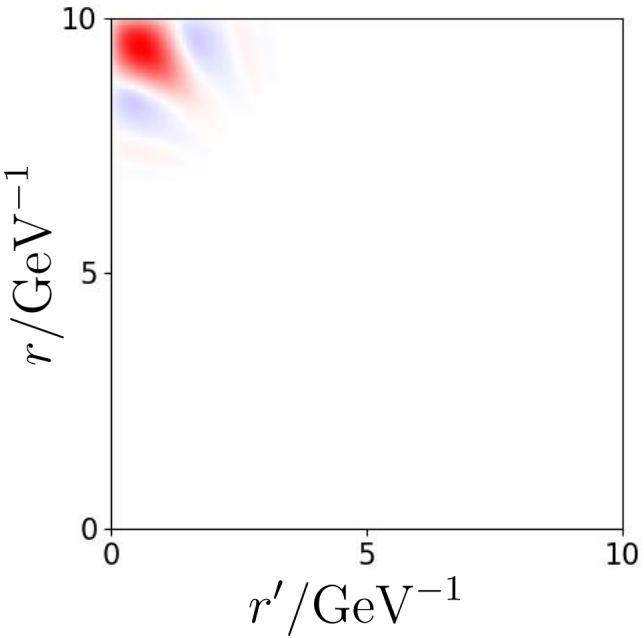

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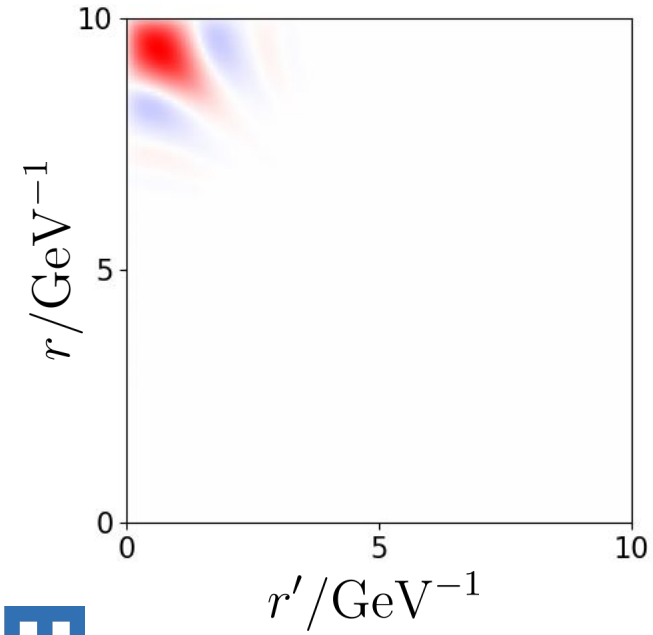

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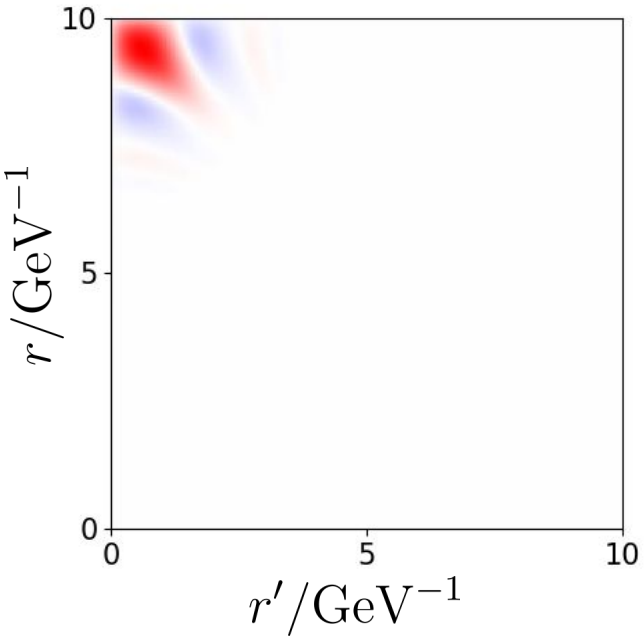
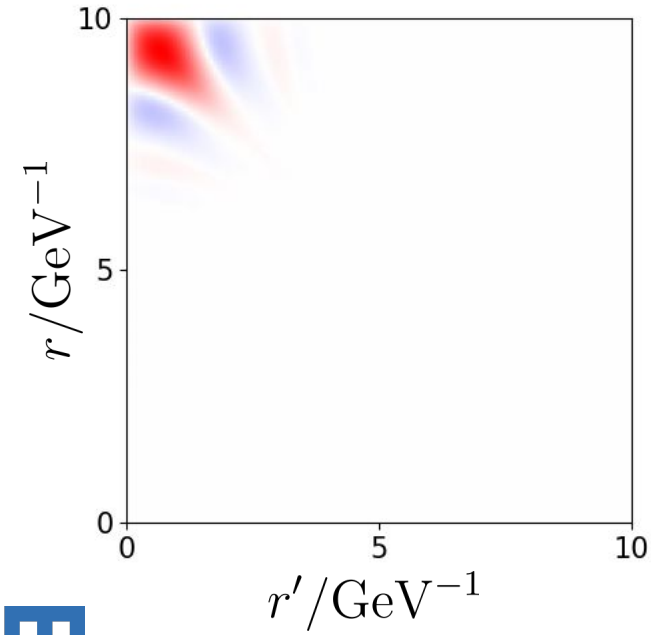
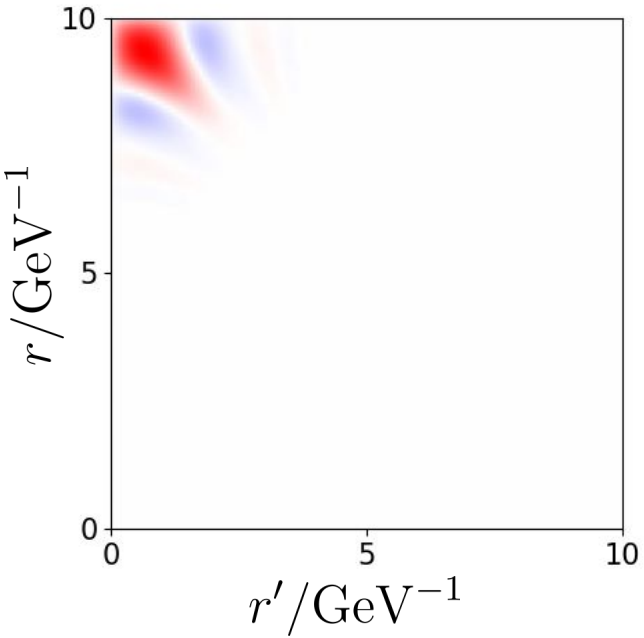


Simulation results

Monte Carlo Wavefunction

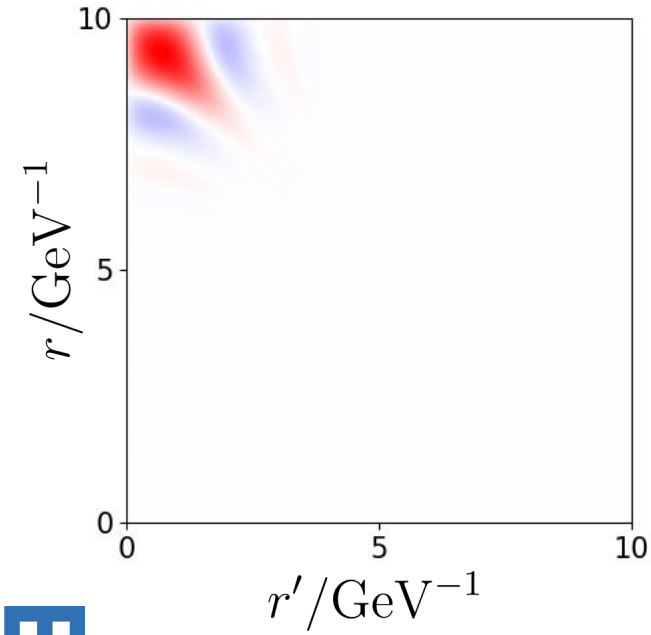


Neural Network



Simulation results

Monte Carlo Wavefunction



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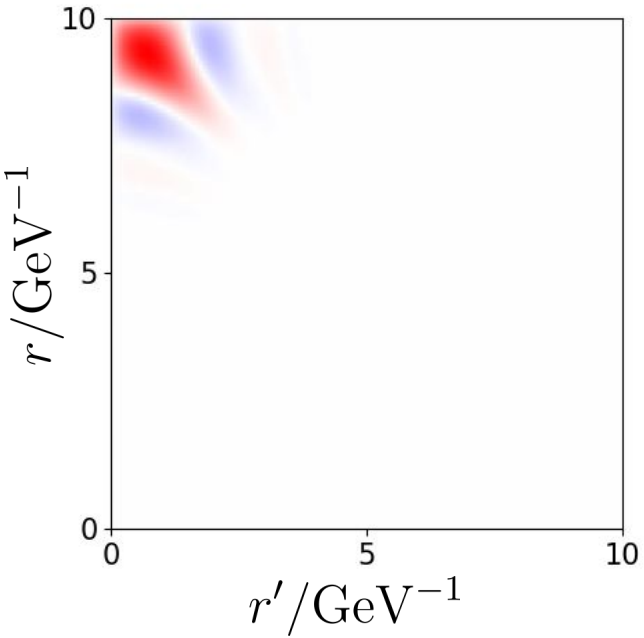
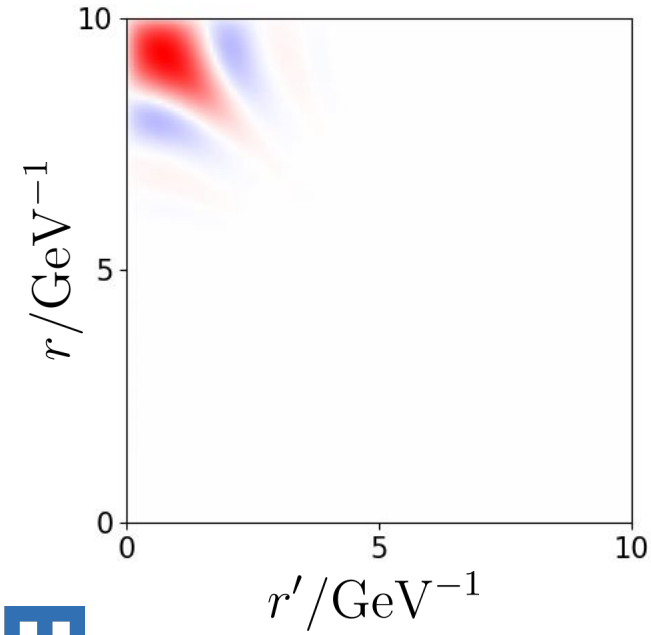


Simulation results

Monte Carlo Wavefunction



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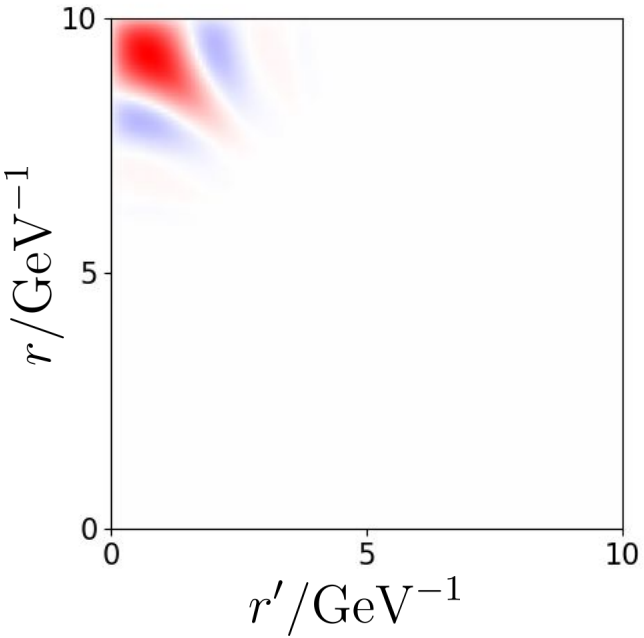
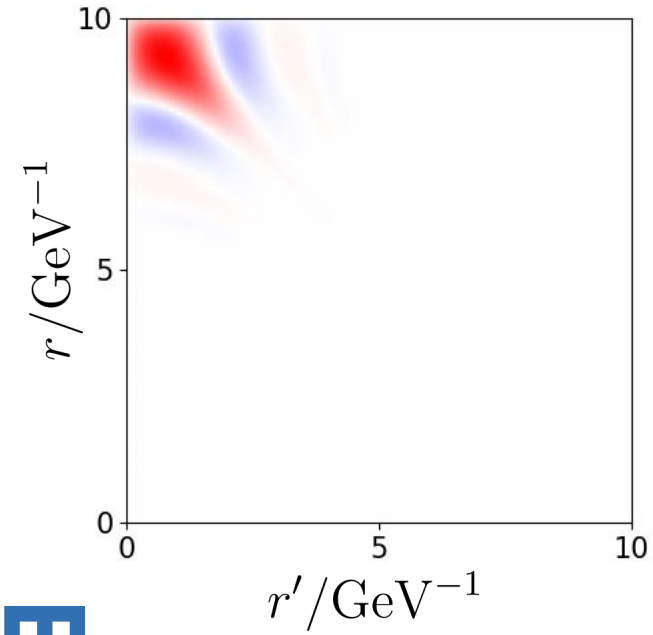


Simulation results

Monte Carlo Wavefunction



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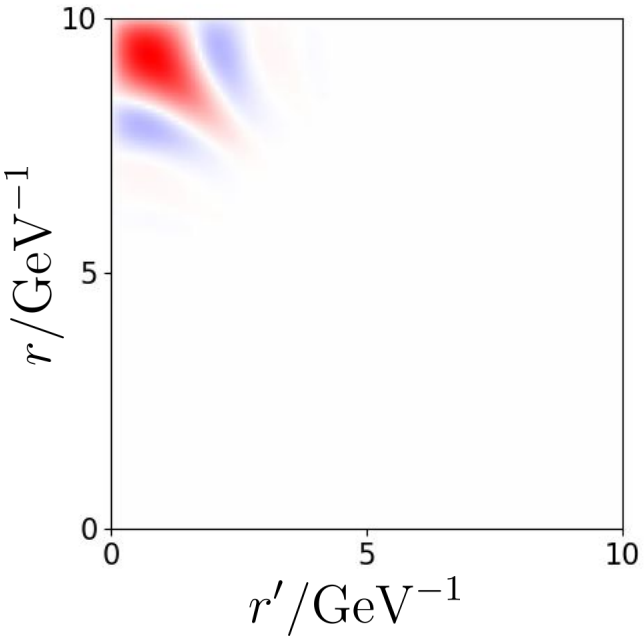
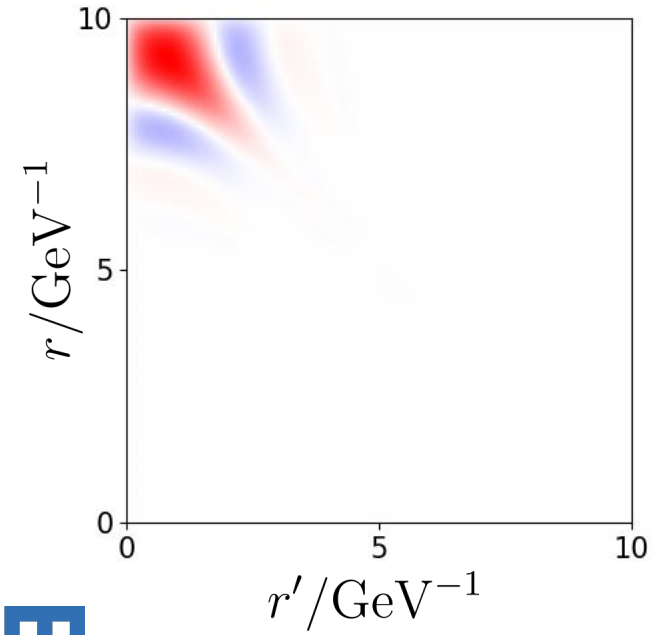


Simulation results

Monte Carlo Wavefunction



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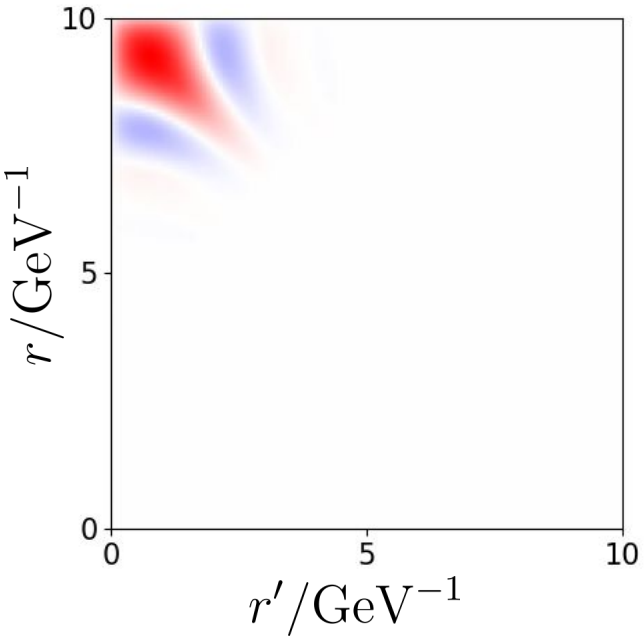
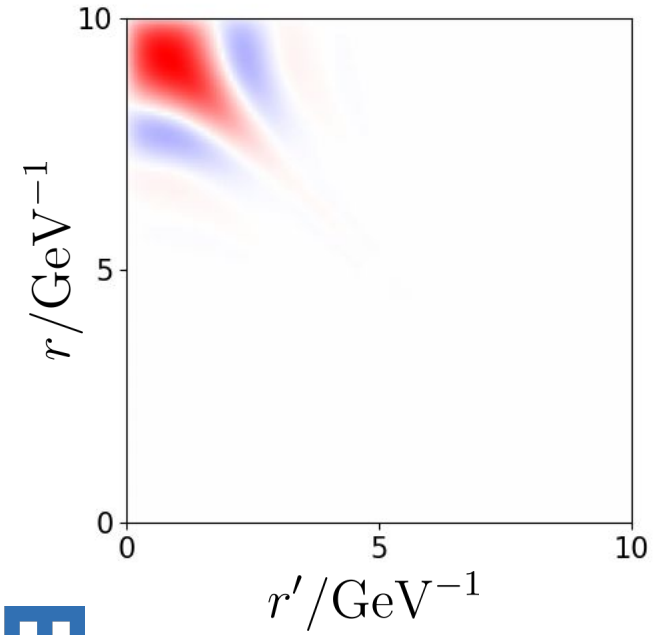


Simulation results

Monte Carlo Wavefunction



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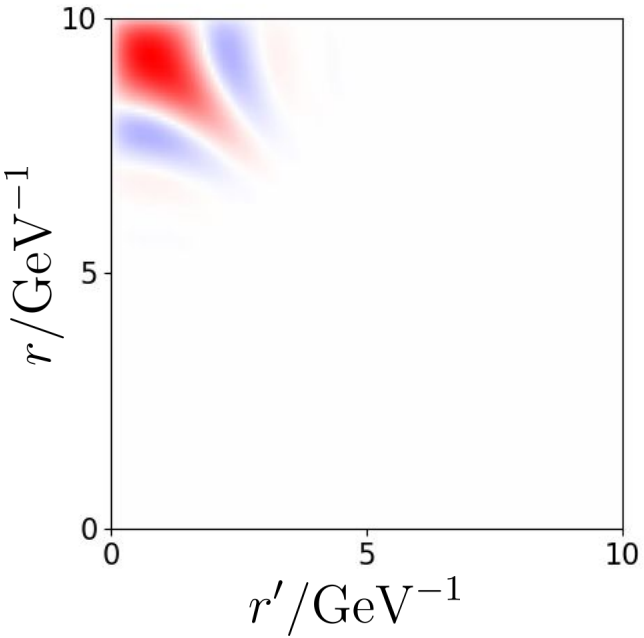
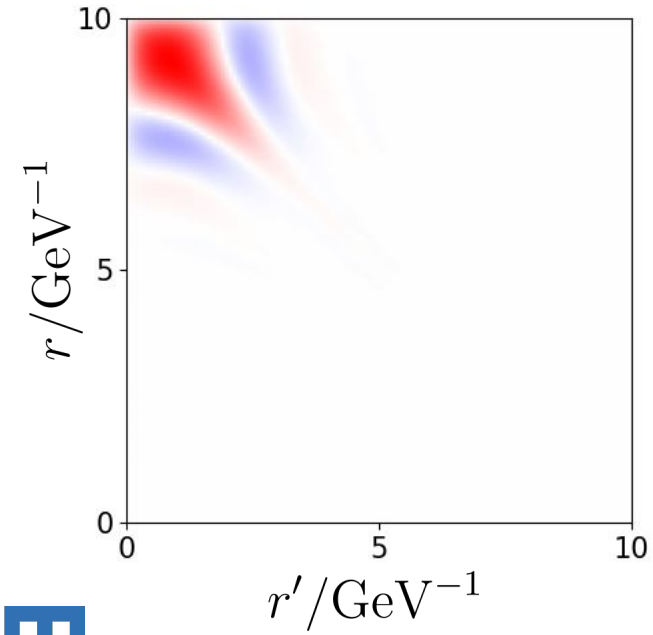


Simulation results

Monte Carlo Wavefunction



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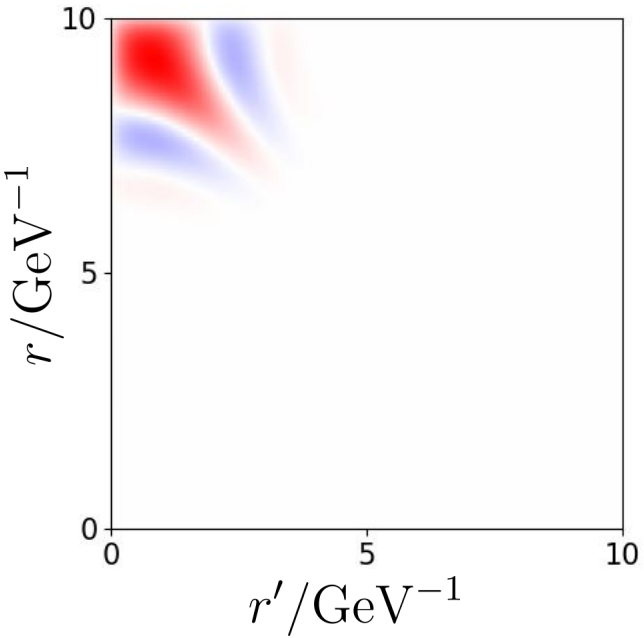
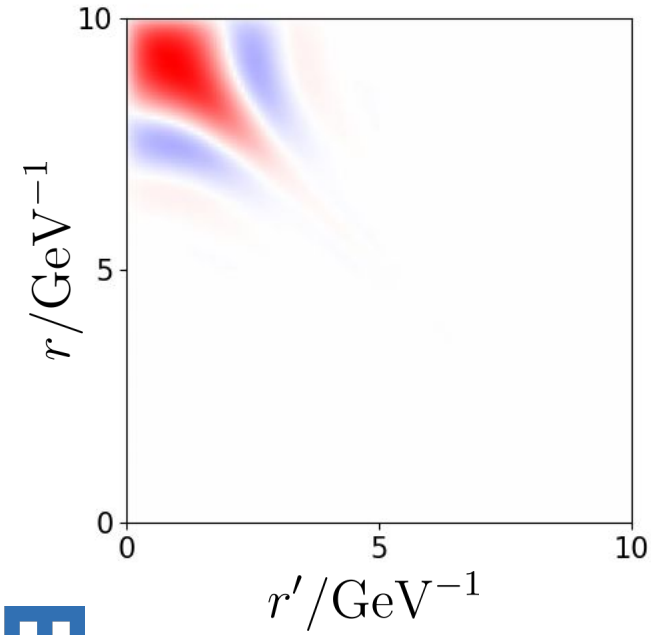


Simulation results

Monte Carlo Wavefunction



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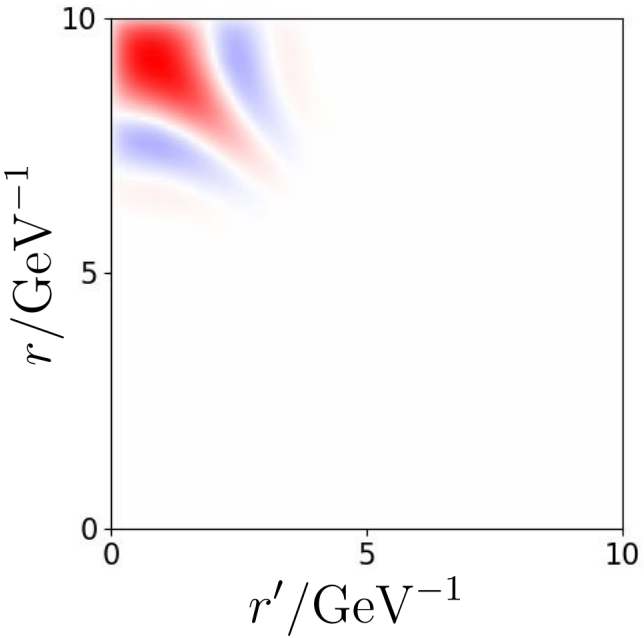
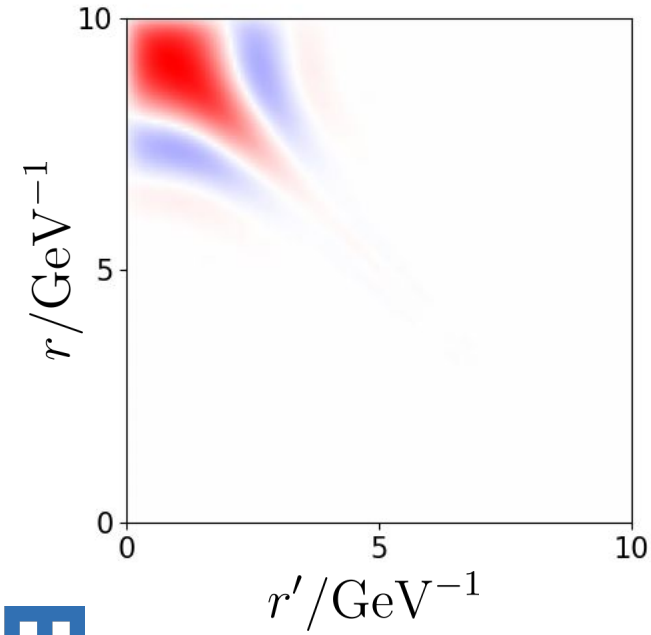


Simulation results

Monte Carlo Wavefunction



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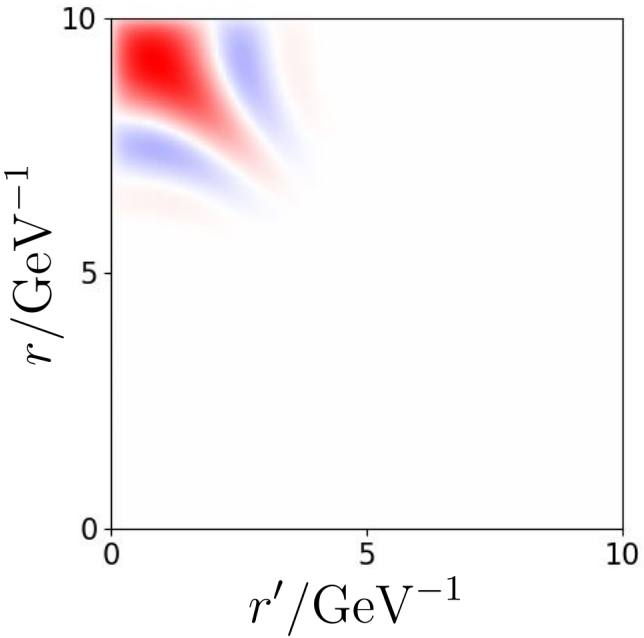
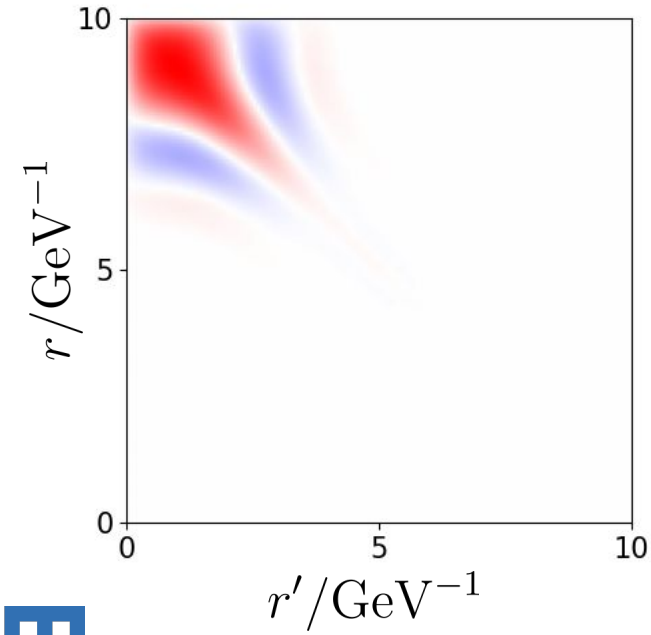


Simulation results

Monte Carlo Wavefunction



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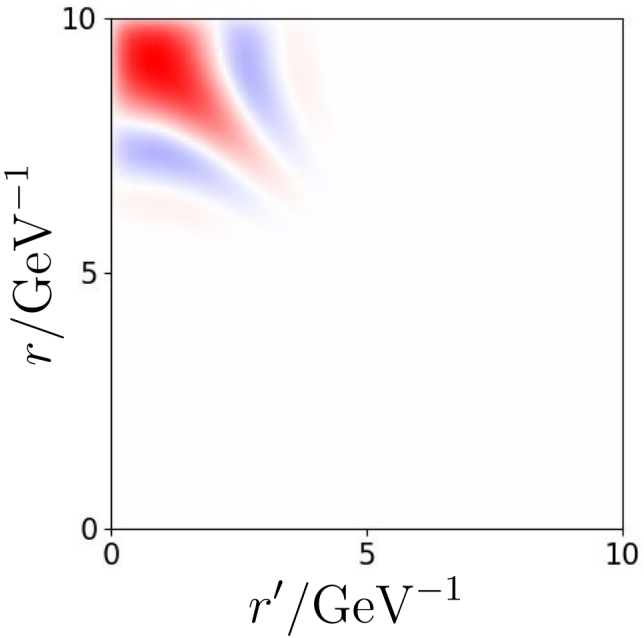
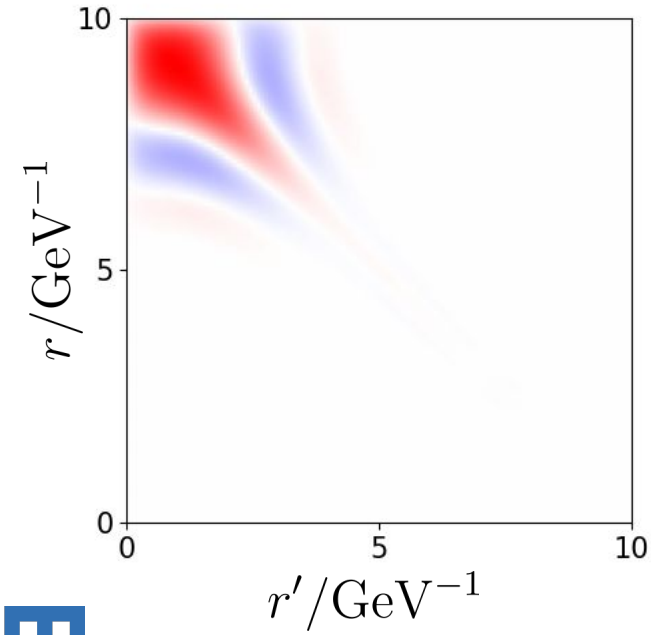


Simulation results

Monte Carlo Wavefunction



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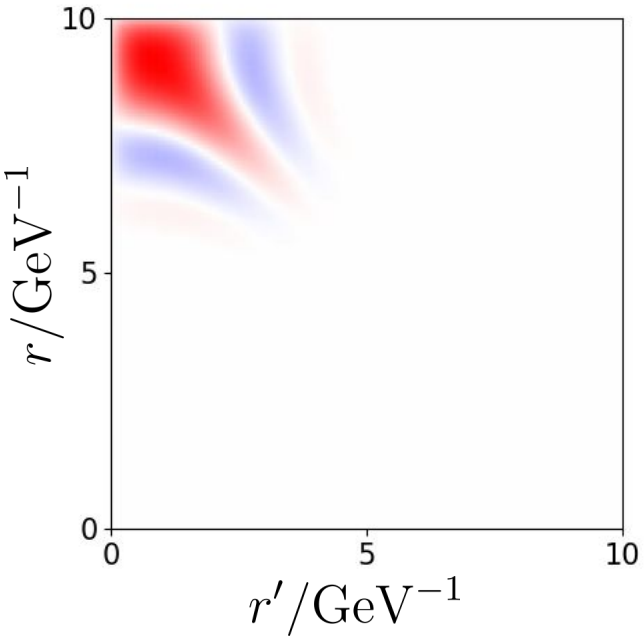
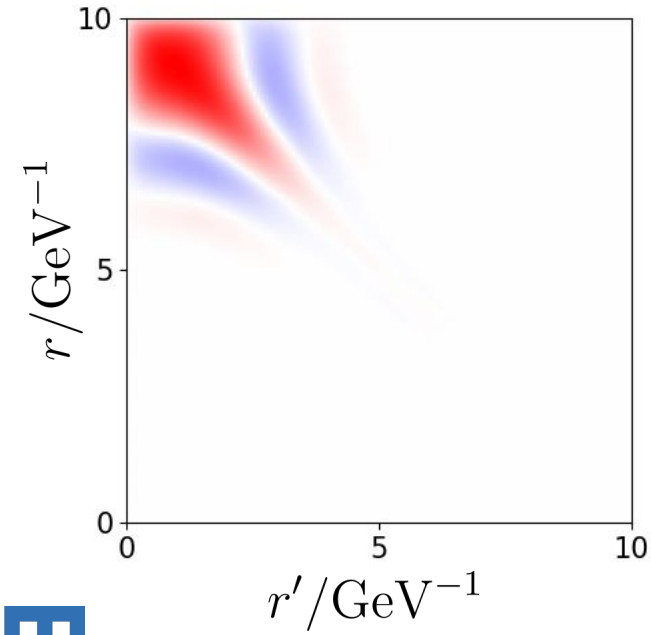


Simulation results

Monte Carlo Wavefunction



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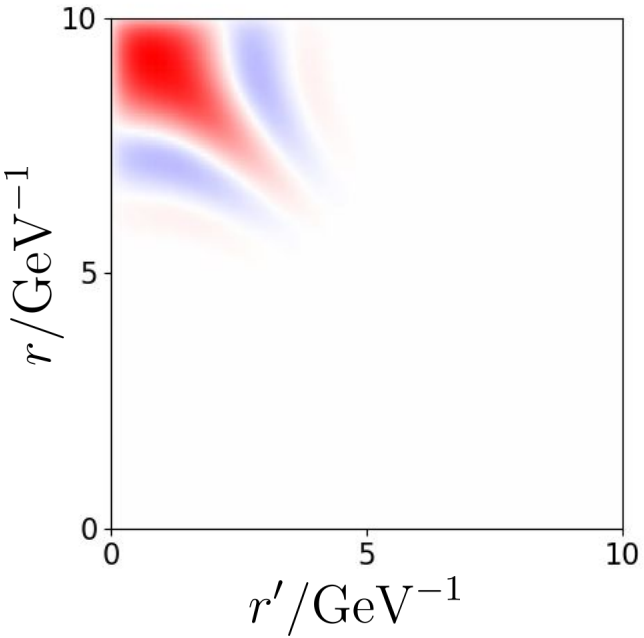
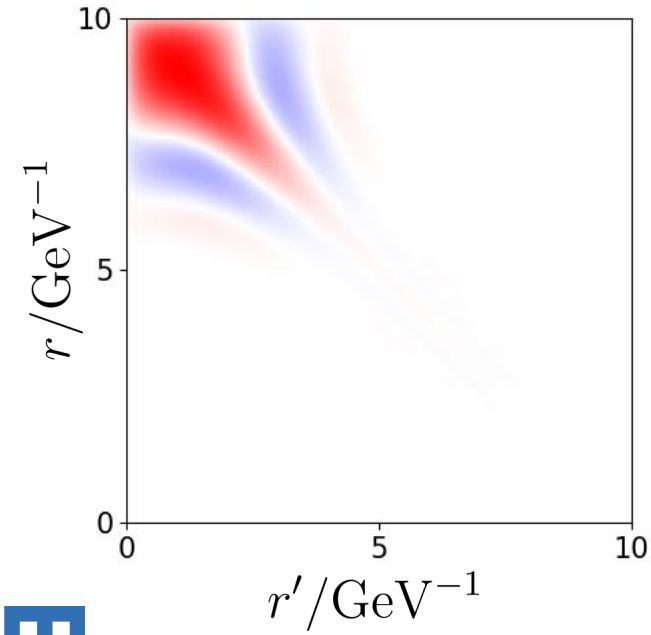


Simulation results

Monte Carlo Wavefunction



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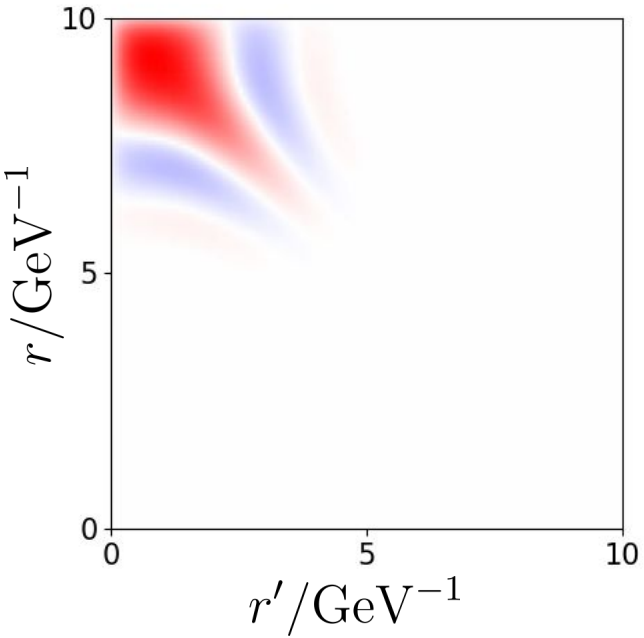
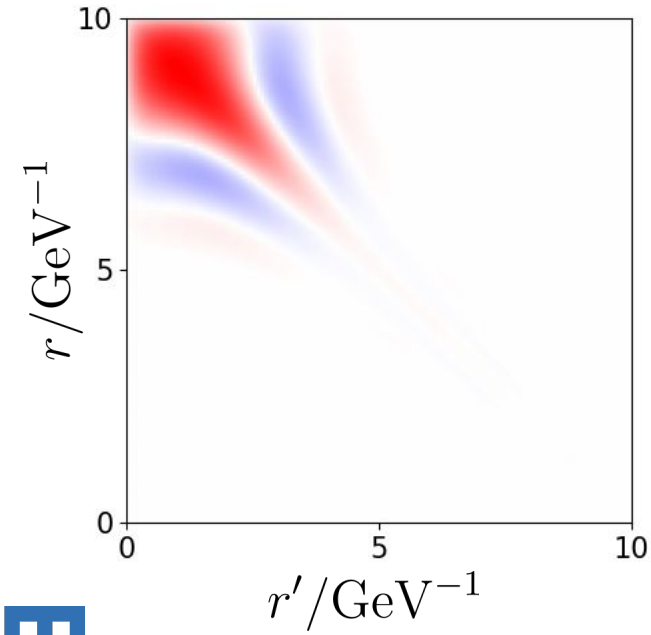


Simulation results

Monte Carlo Wavefunction



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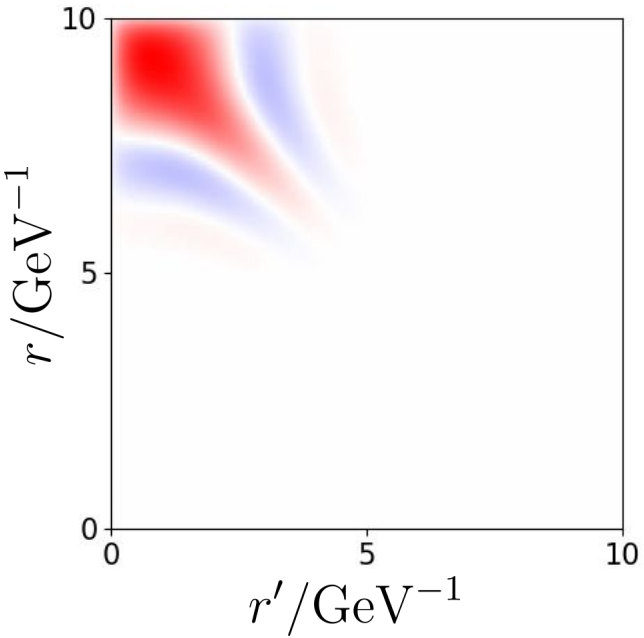
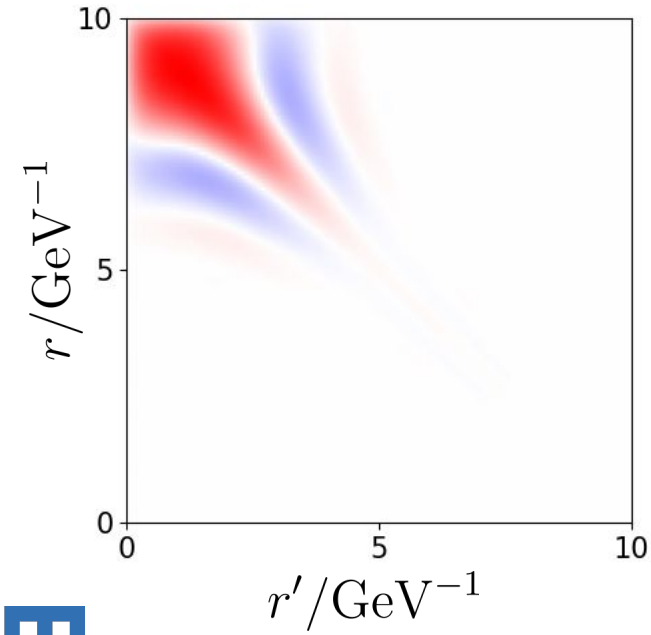


Simulation results

Monte Carlo Wavefunction



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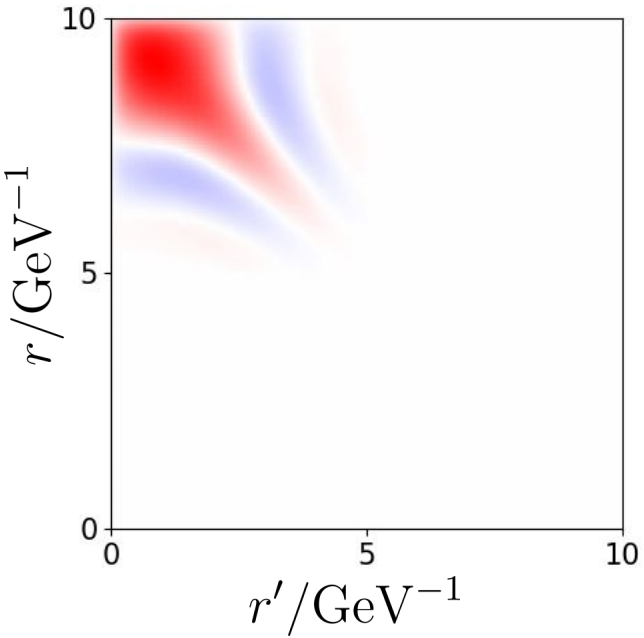
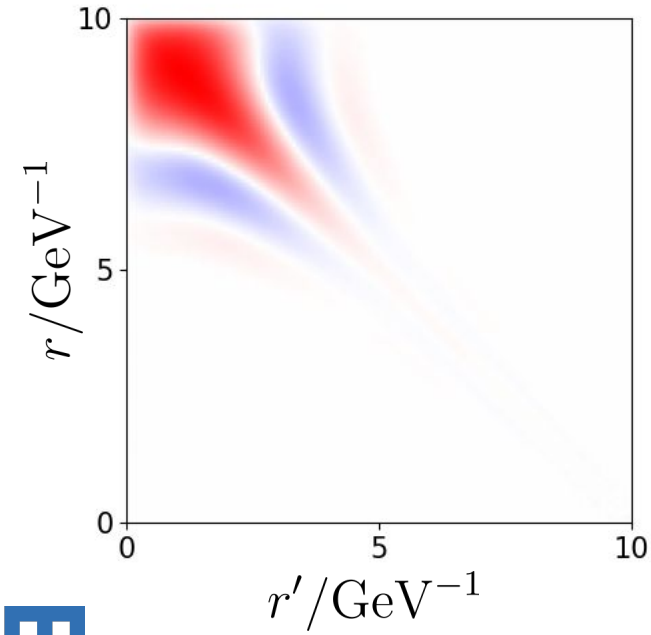


Simulation results

Monte Carlo Wavefunction



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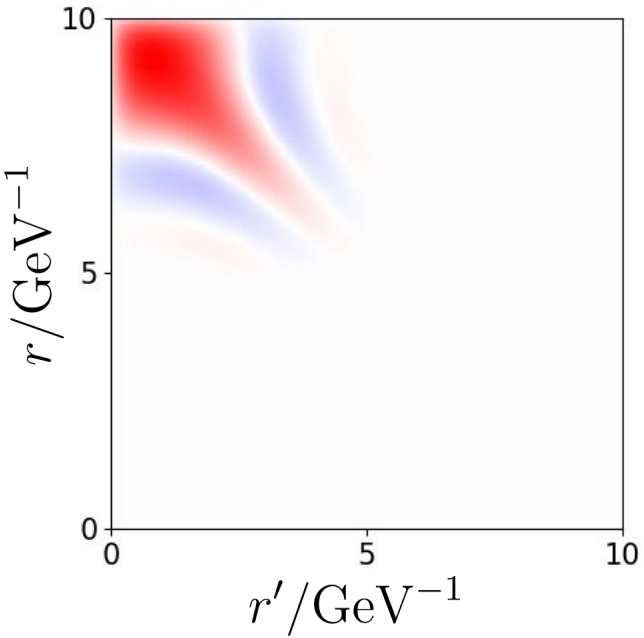
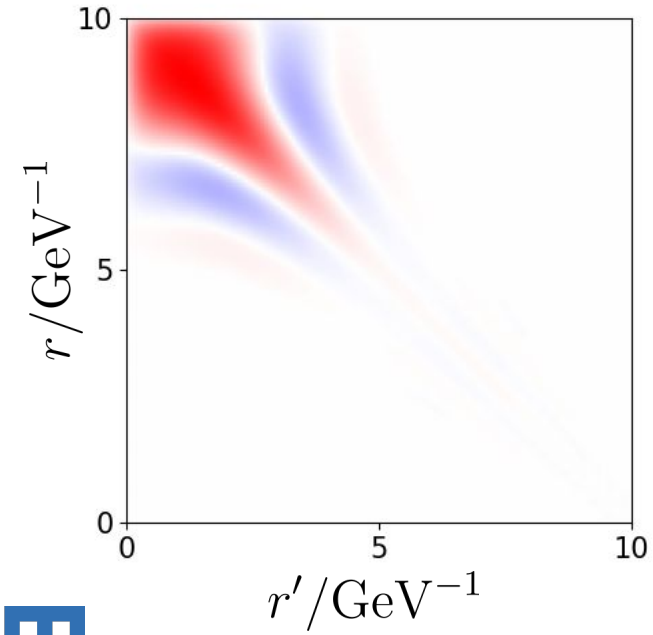


Simulation results

Monte Carlo Wavefunction



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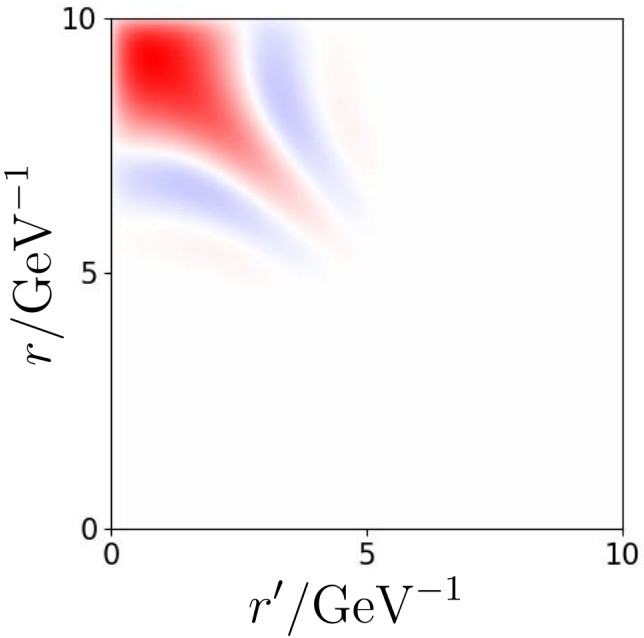
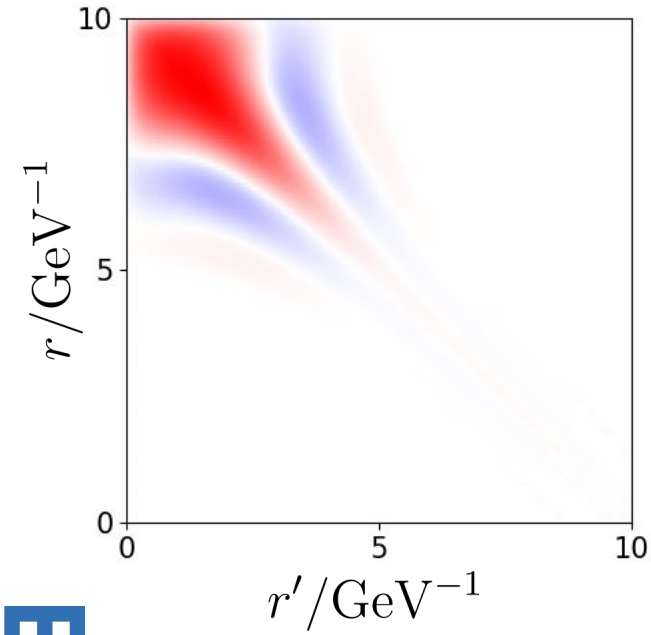


Simulation results

Monte Carlo Wavefunction



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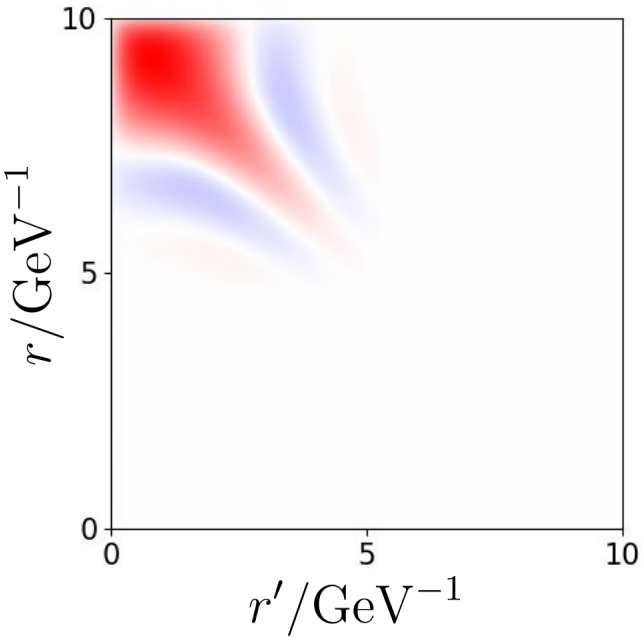
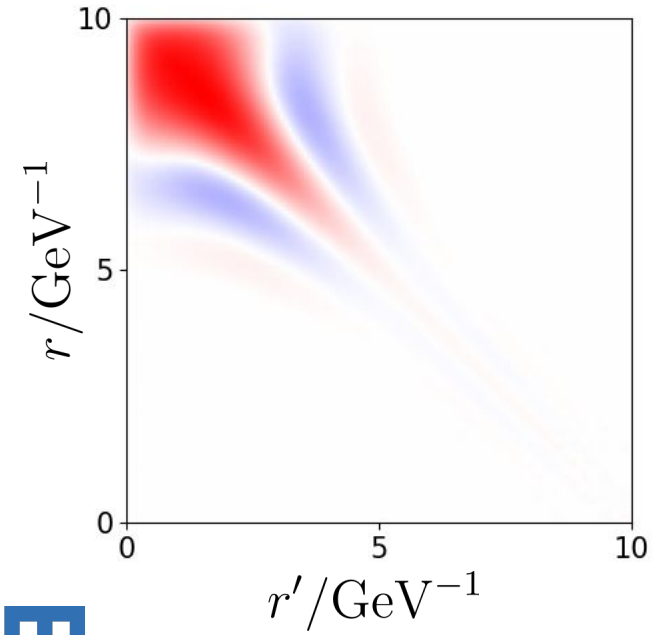


Simulation results

Monte Carlo Wavefunction



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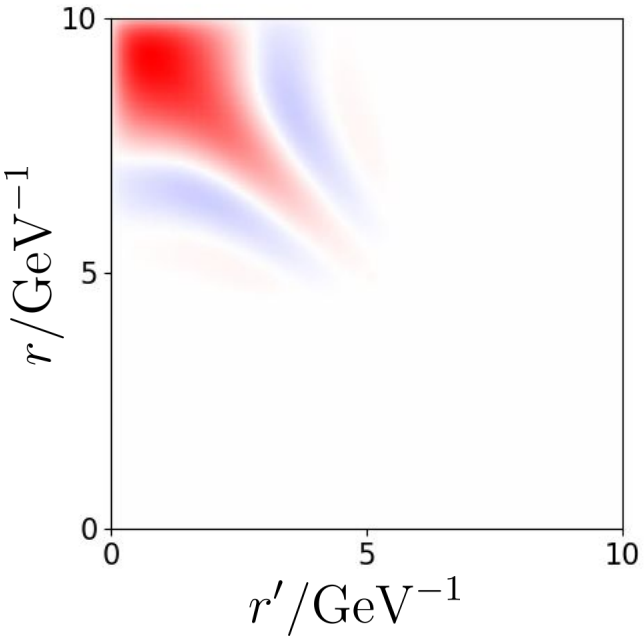
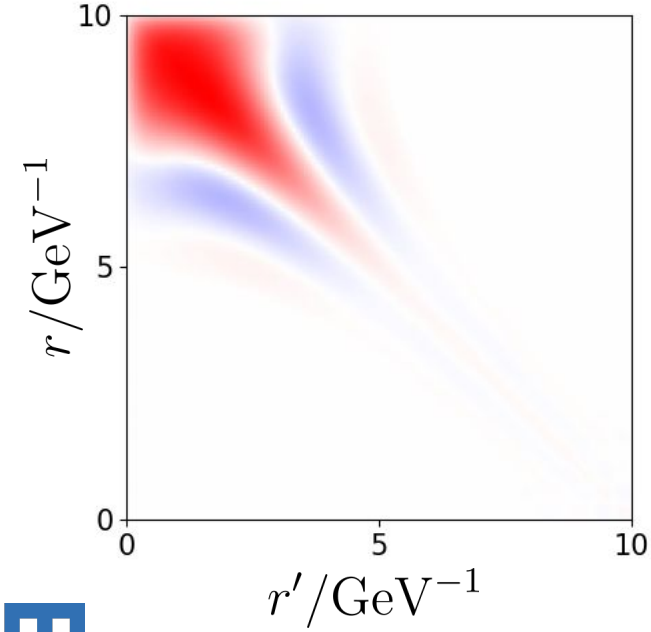


Simulation results

Monte Carlo Wavefunction



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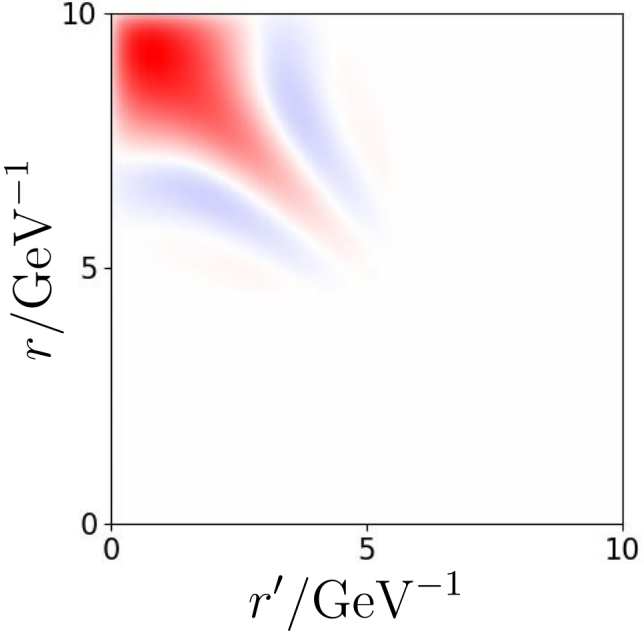
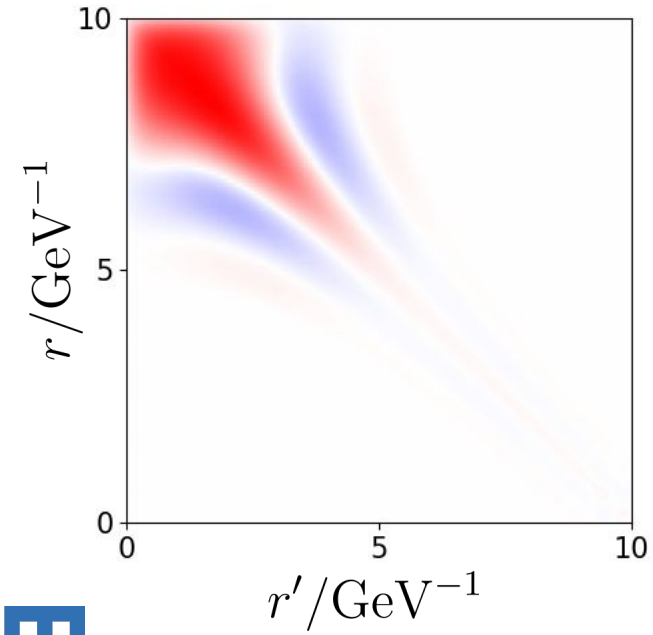


Simulation results

Monte Carlo Wavefunction



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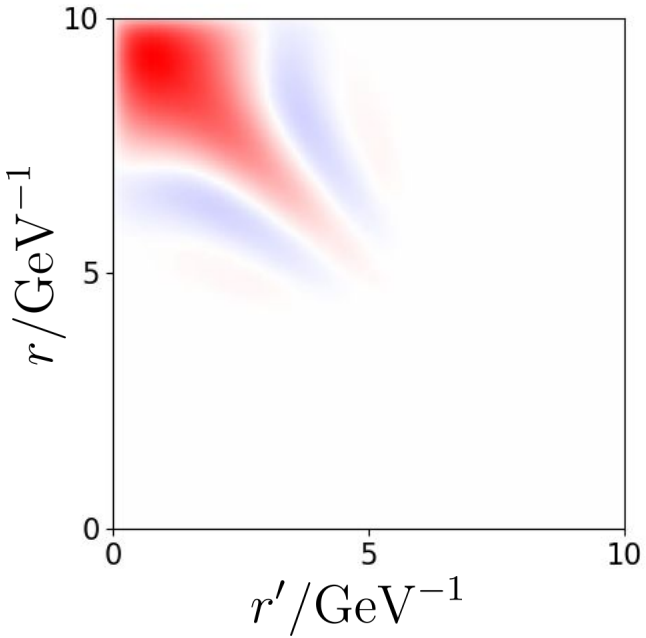
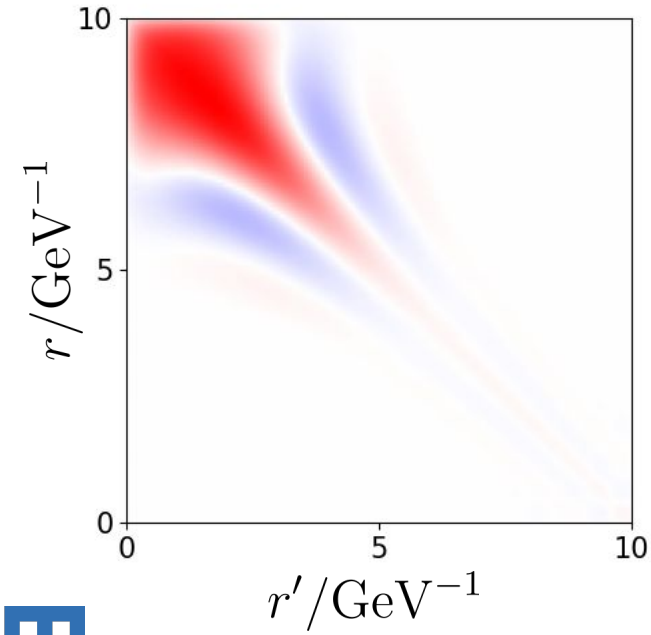


Simulation results

Monte Carlo Wavefunction



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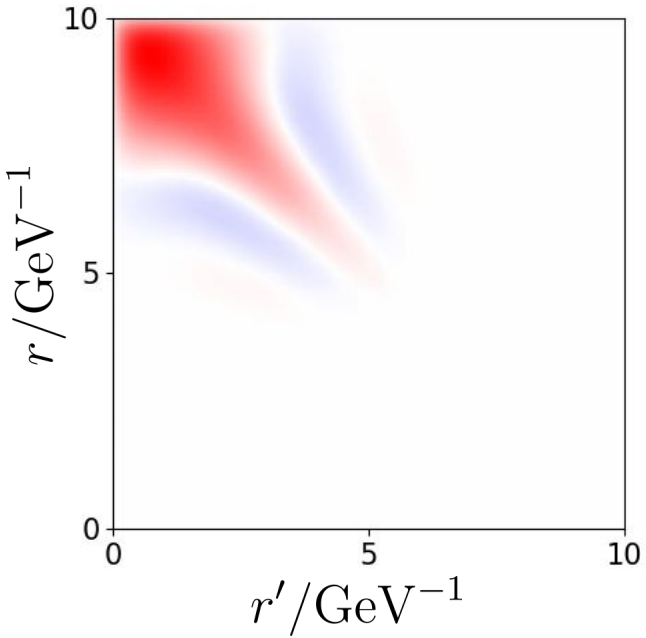
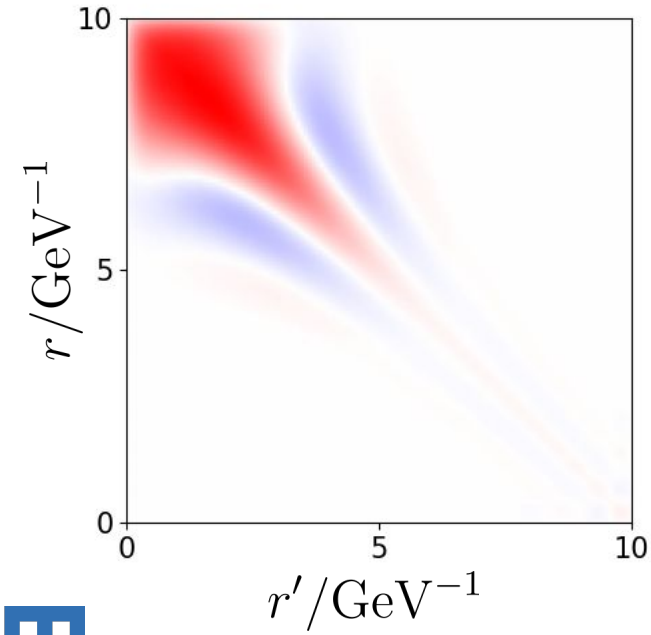


Simulation results

Monte Carlo Wavefunction



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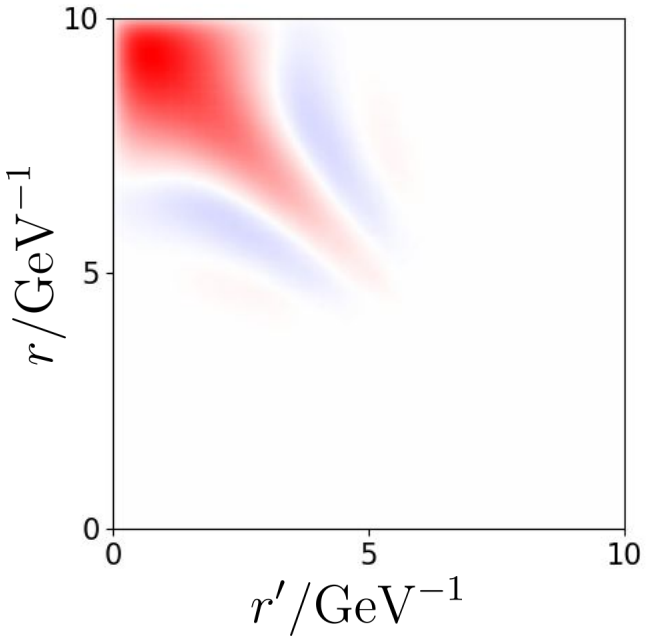
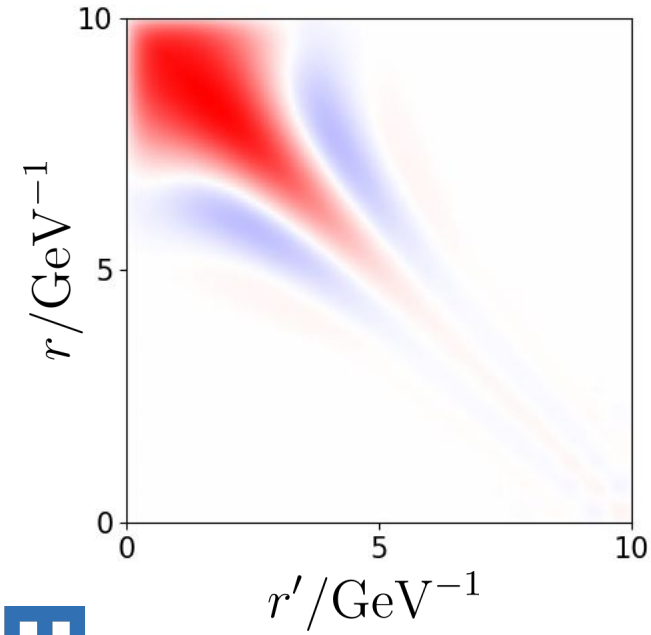
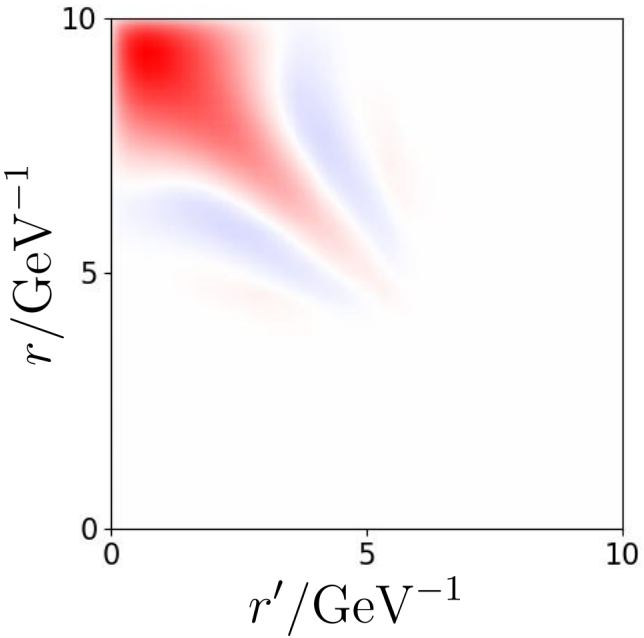


Simulation results

Monte Carlo Wavefunction

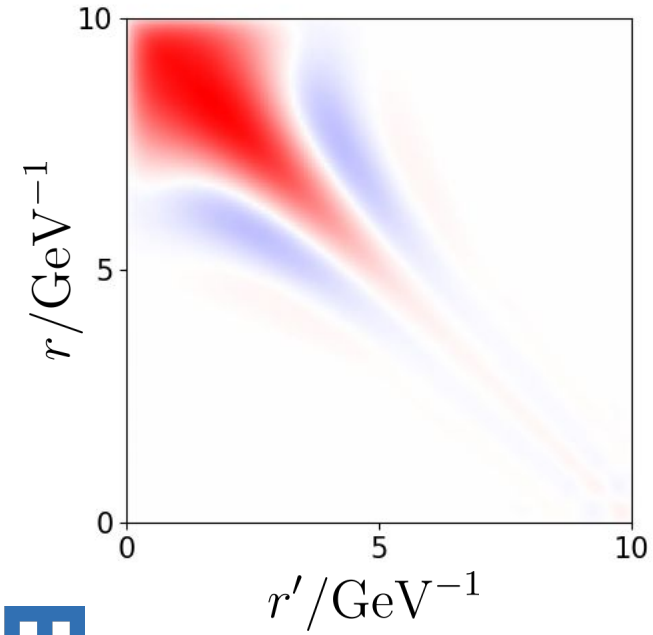


Neural Network

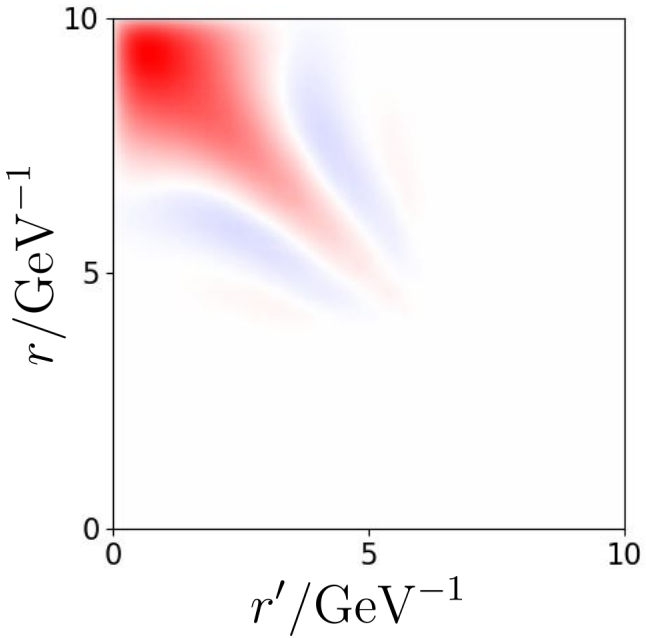


Simulation results

Monte Carlo Wavefunction

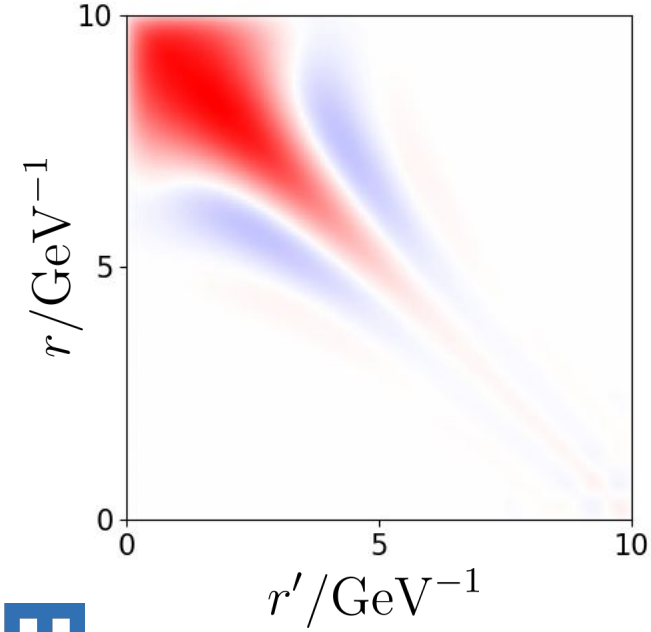


Neural Network



Simulation results

Monte Carlo Wavefunction



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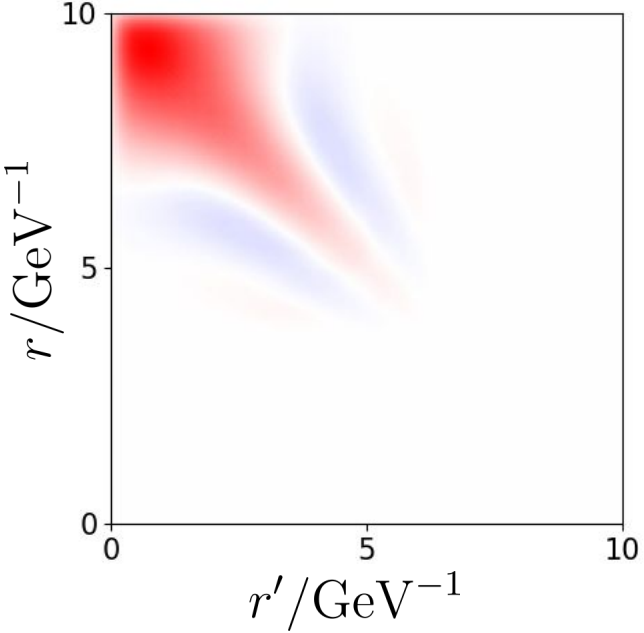
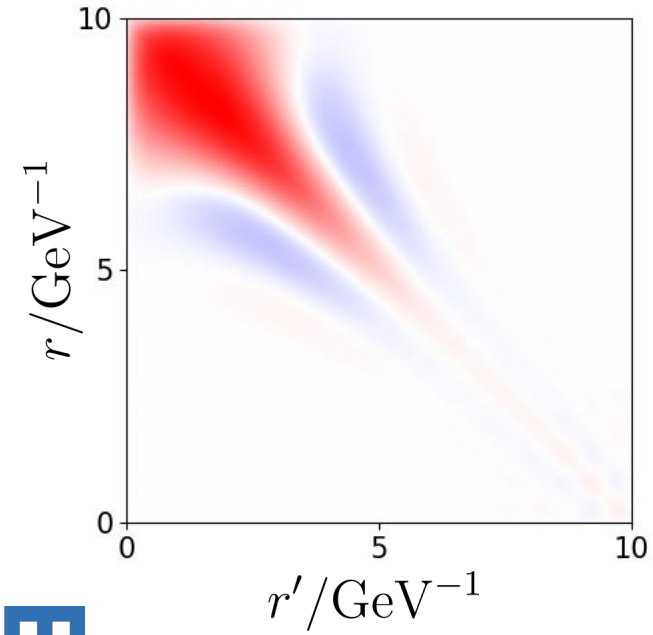


Simulation results

Monte Carlo Wavefunction



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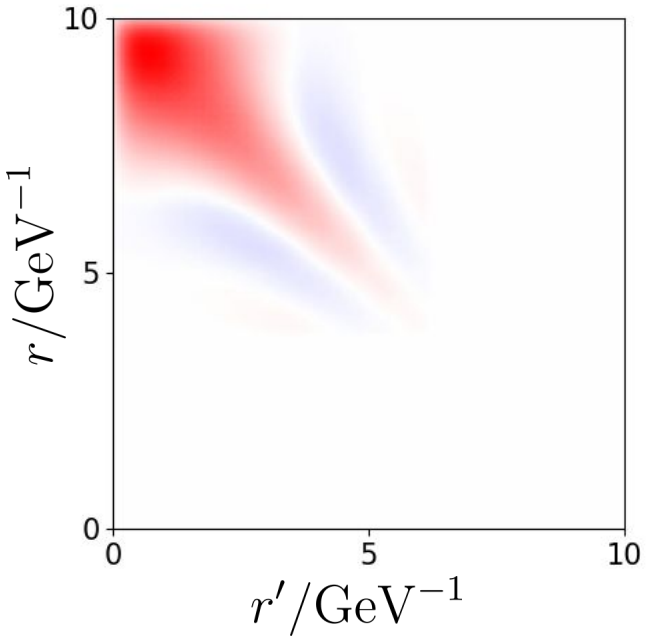
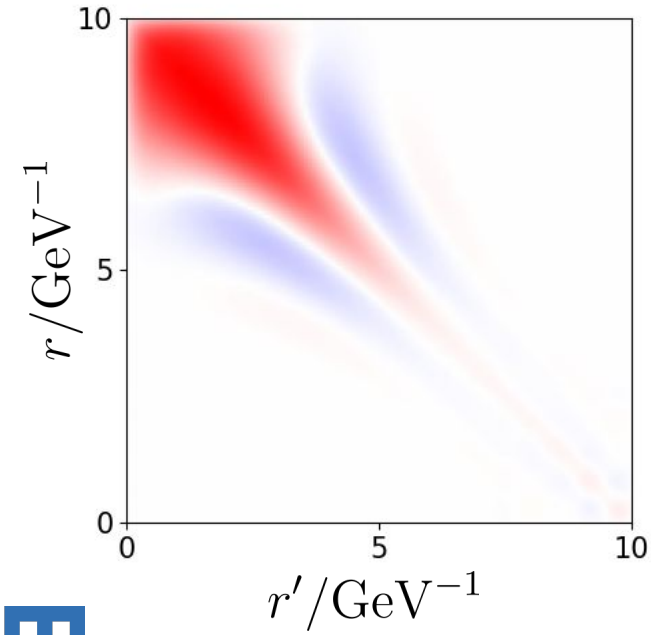
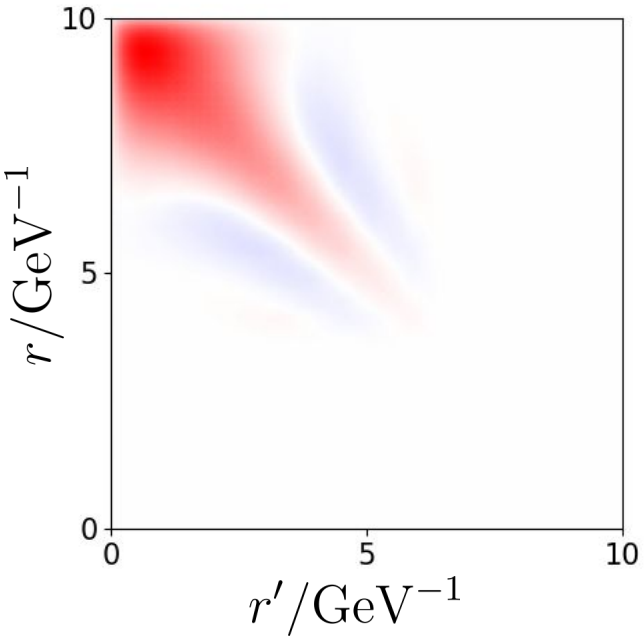


Simulation results

Monte Carlo Wavefunction

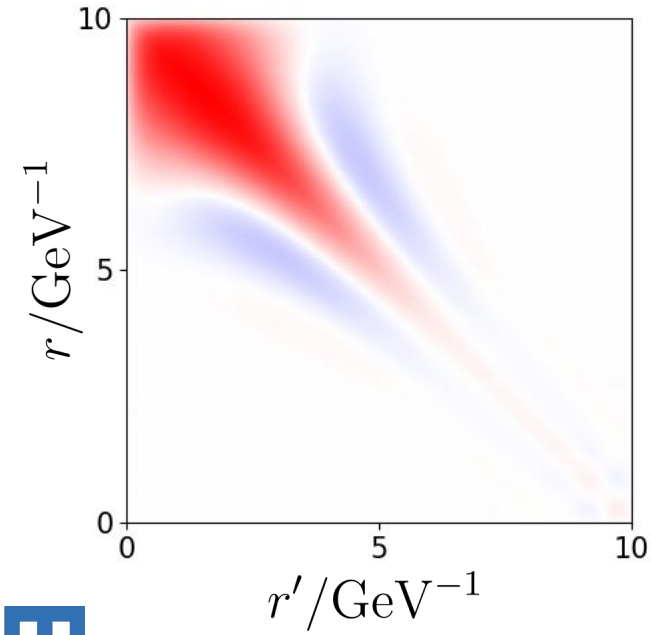


Neural Network

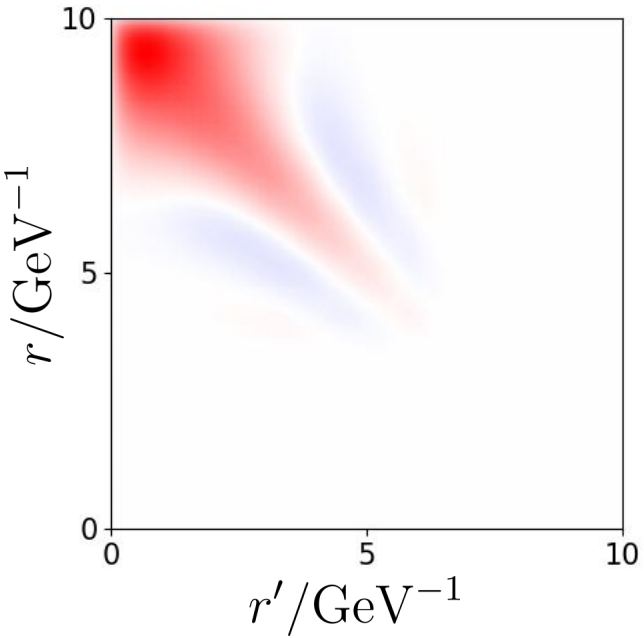


Simulation results

Monte Carlo Wavefunction

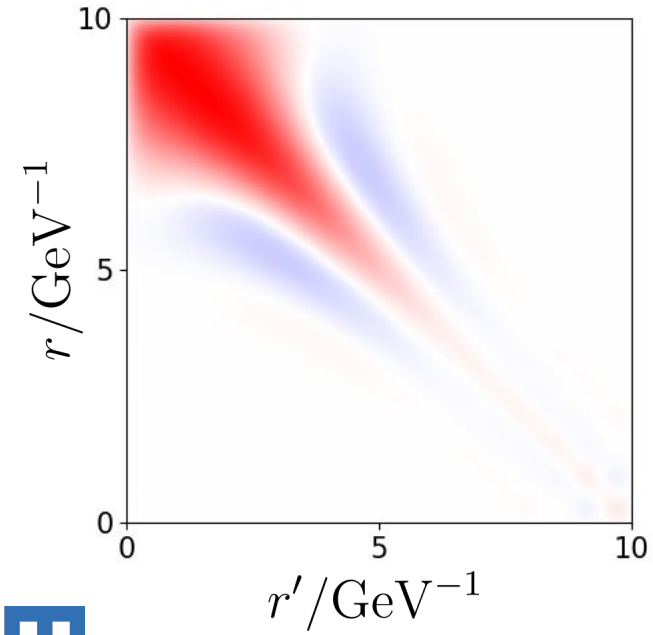


Neural Network

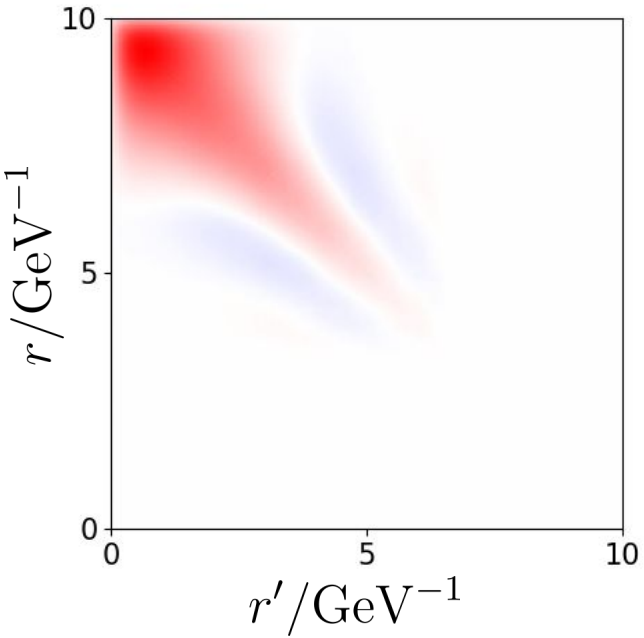


Simulation results

Monte Carlo Wavefunction

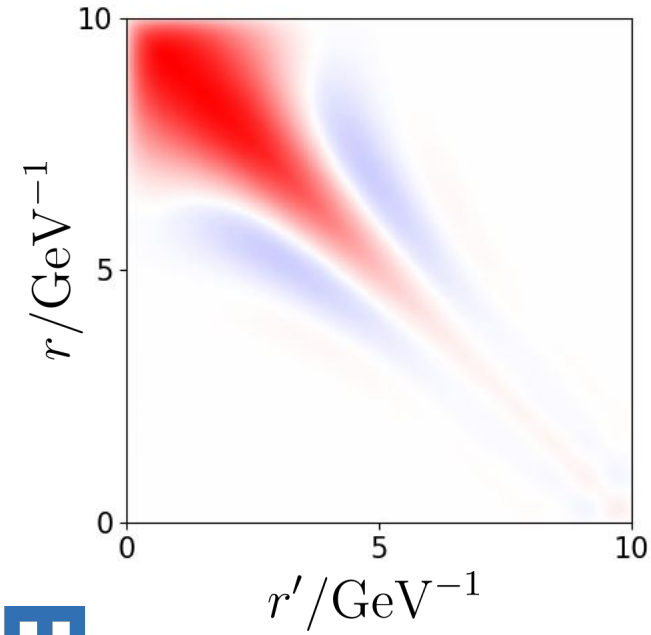


Neural Network

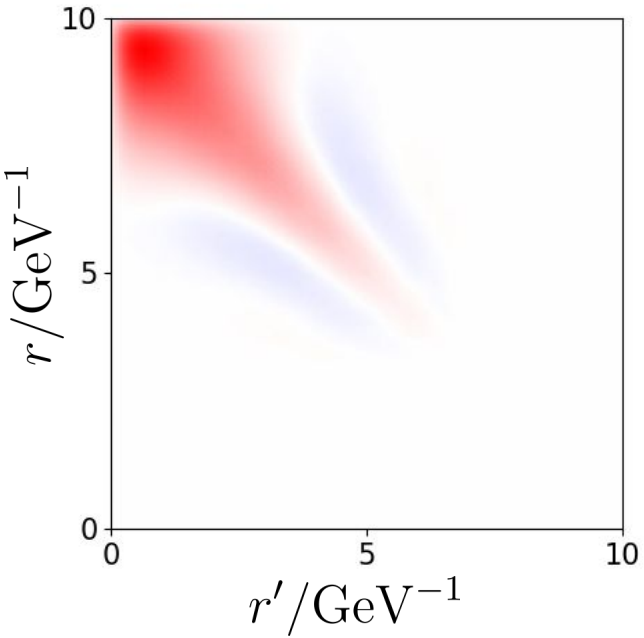


Simulation results

Monte Carlo Wavefunction

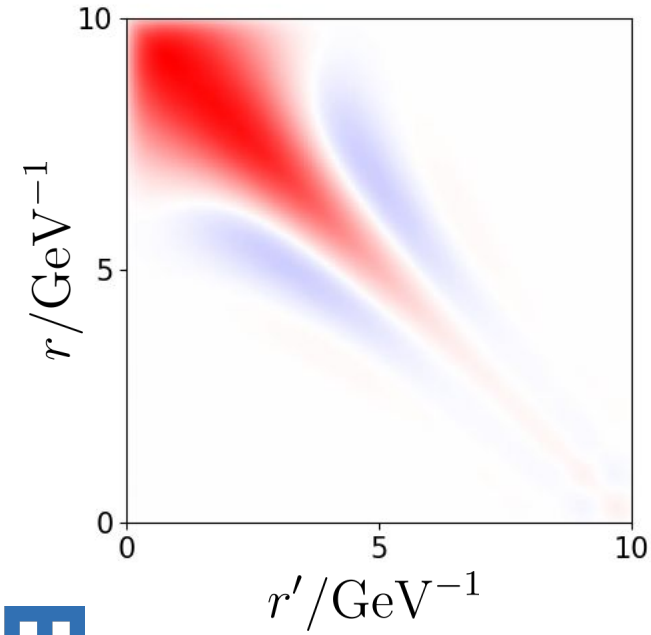


Neural Network

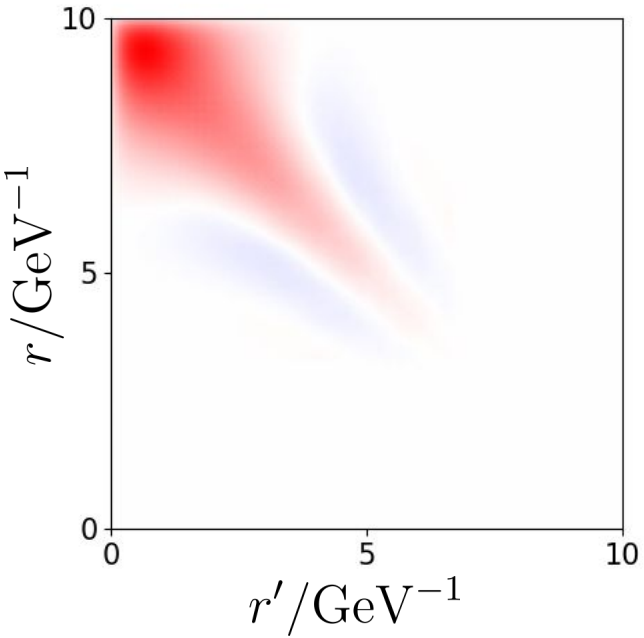


Simulation results

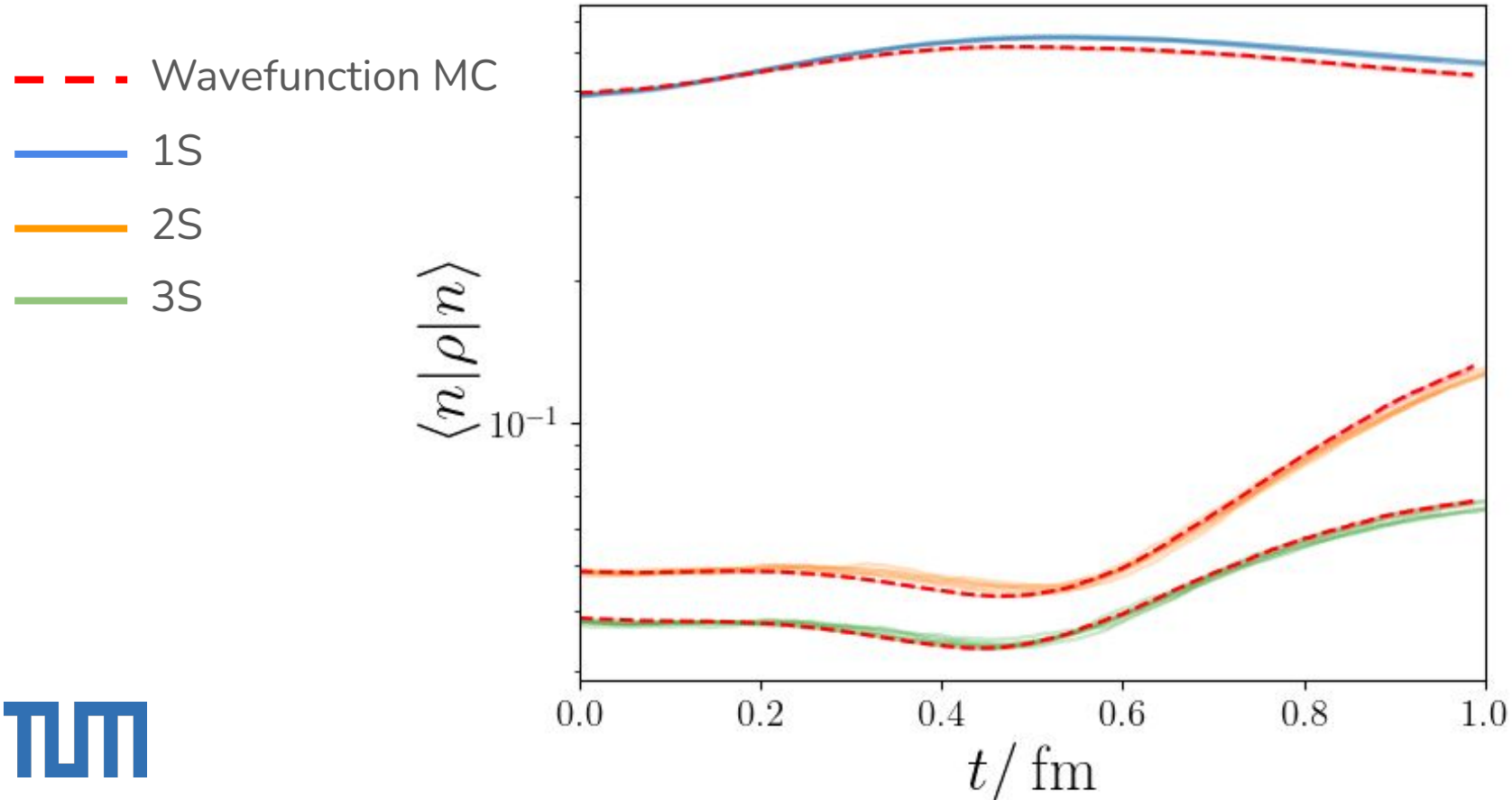
Monte Carlo Wavefunction



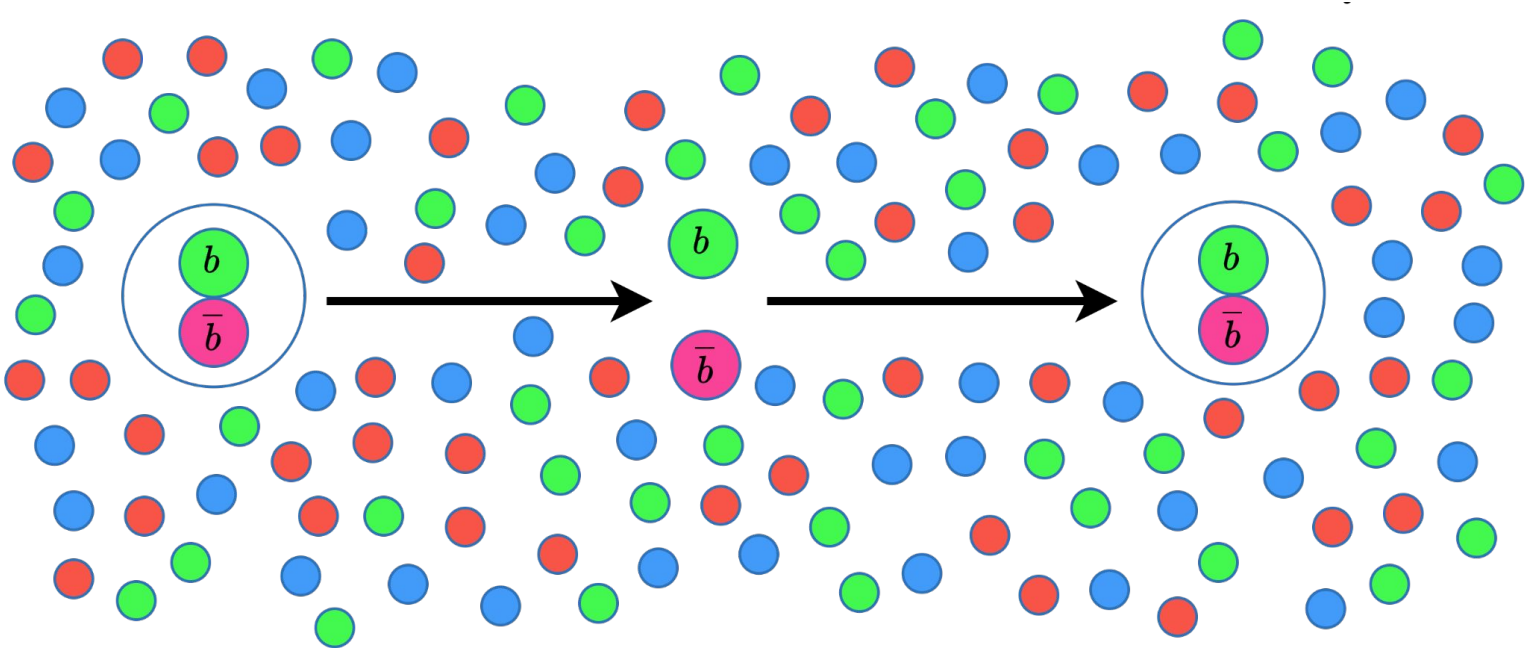
Neural Network



Simulation results

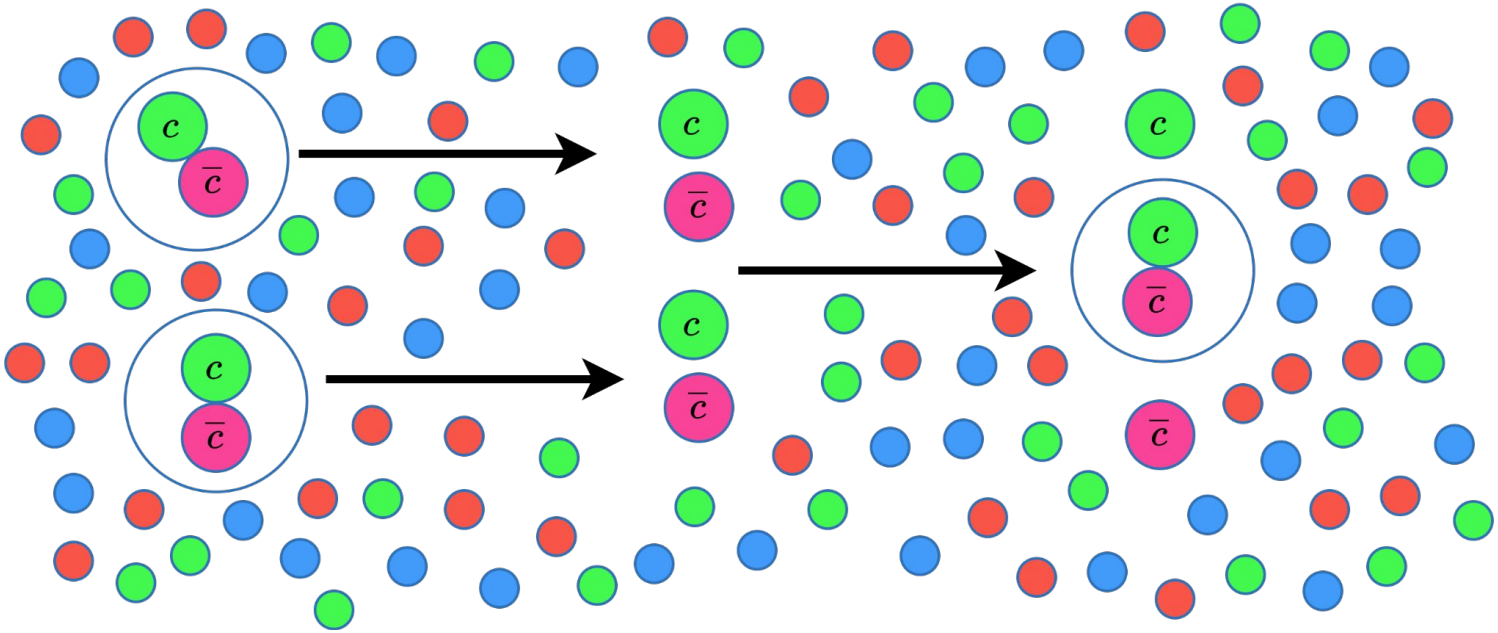


Outlook: Only few bottomonium states are produced per event



$< 10 \quad b\bar{b}$ pairs in the plasma

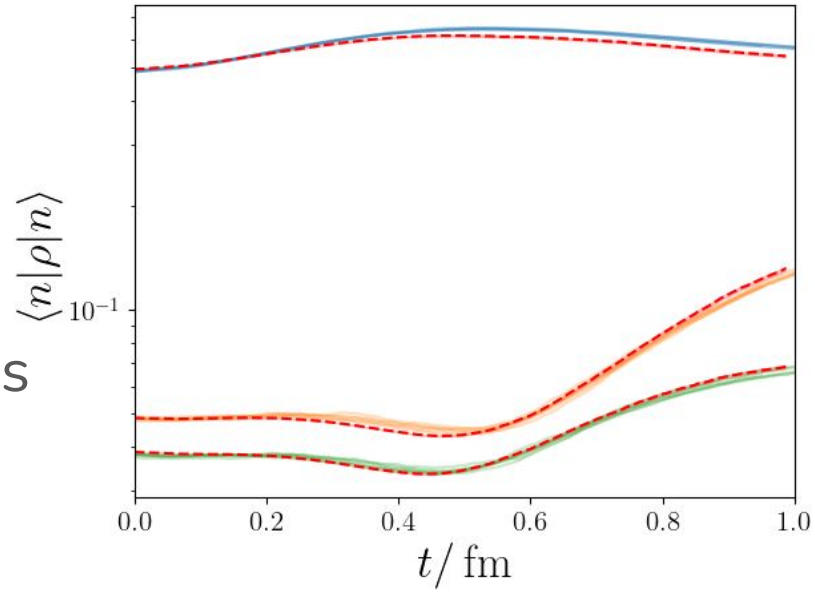
Outlook: A large number of charmonia leads to a many-body problem



$\sim 100\ c\bar{c}$ in the plasma

Summary

- Non-equilibrium, real-time evolution needed to describe phenomena in heavy-ion collisions
- NNQS for the simulation of open quantum systems
- Application to brownian motion for quarkonium in medium

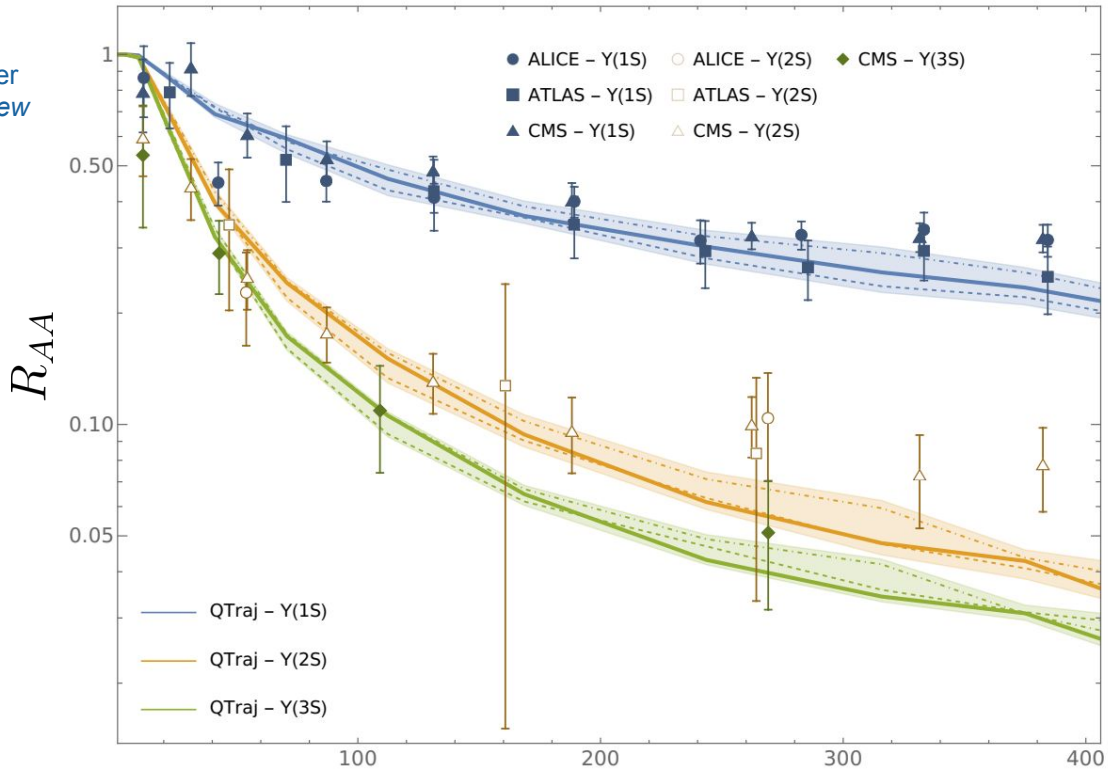


Outlook: Application to the many body problem!

Backup

Overlaps lead to phenomenological predictions

Brambilla, N., Magorsch, T., Strickland, M., Vairo, A., & Vander Griend, P. (2024). *Physical Review D*, *109*(11), 114016.

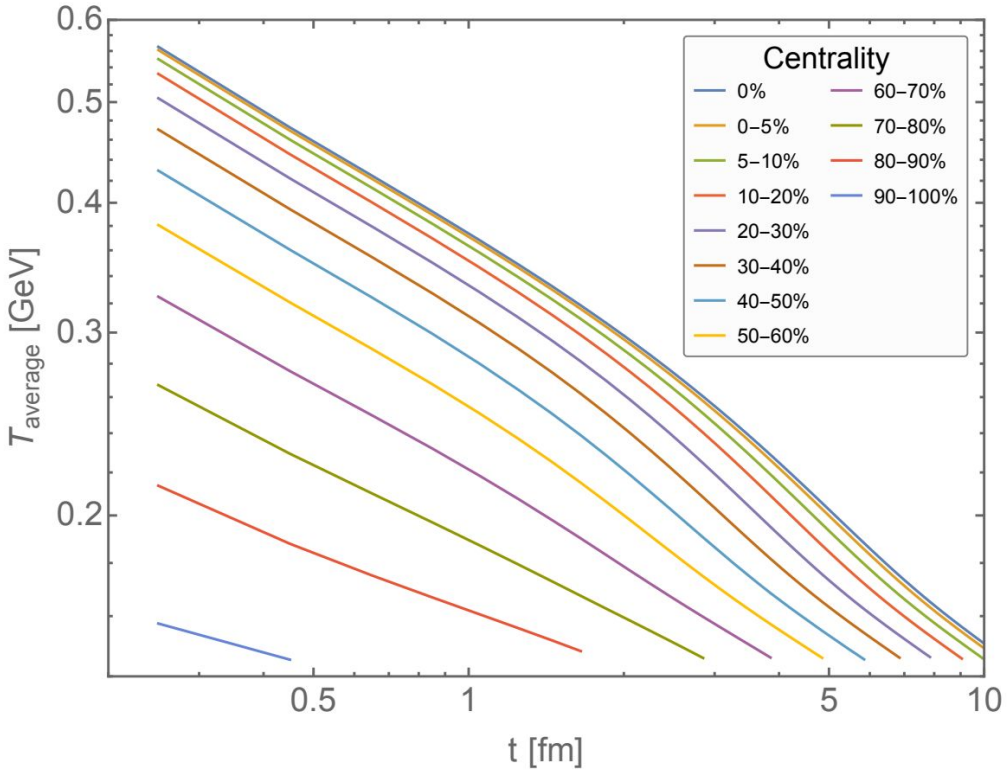


Connecting to phenomenology

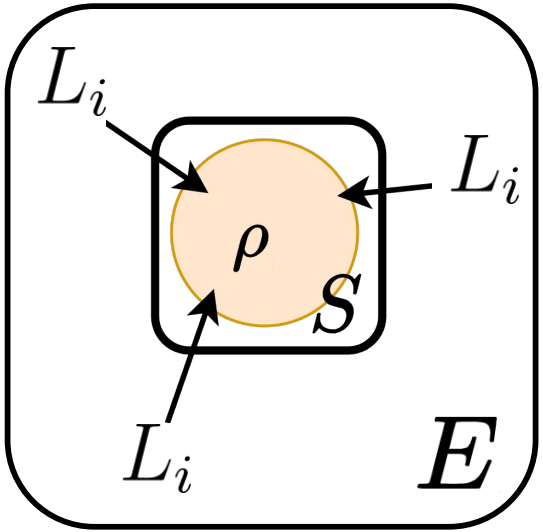
Brambilla, Nora, et al. *Journal of High Energy Physics* 2021.5 (2021): 1-47.

centrality

$$R^i_{AA}(c) = \frac{(F \cdot S(c) \cdot \vec{\sigma}_{\text{direct}})^i}{\sigma^i_{\text{exp}}}$$



Quarkonium suppression



$$\frac{d\rho(t)}{dt} = -i\left[H, \rho(t)\right] + \sum_{nm} h_{nm}\left(L_i^n \rho(t) L_i^{m\dagger} - \frac{1}{2}\left\{L_i^{m\dagger} L_i^n, \rho(t)\right\}\right)$$

$$h = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$L_i^0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} r_i, \quad L_i^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{N_c^2-4}{2(N_c^2-1)} A_i^{oo\dagger} \end{pmatrix}$$

$$L_i^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} r_i, \quad L_i^3 = \begin{pmatrix} 0 & \frac{1}{N_c^2-1} A_i^{os\dagger} \\ A_i^{so\dagger} & 0 \end{pmatrix}$$

$$A_i^{uv} = \frac{g^2}{6N_c} \int_0^\infty \mathrm{d}s e^{-ih_u s} r_i e^{ih_v s} \langle E_j^a(s) \Omega(s,0)^{ab} E_j^b(0) \rangle$$

$$h_u = \frac{p^2}{M} + V_u(r)$$

To simplify the equation one can expand in E/T

Transport coefficients

$$A_i^{uv} = \frac{r_i}{2}(\kappa - i\gamma) + \kappa\left(-\frac{ip_i}{2MT} + \frac{\Delta V_{uv}}{4T} r_i\right)$$

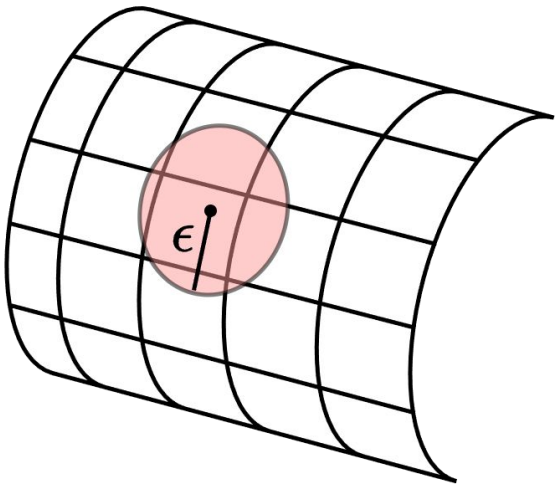
Brambilla, N., Escobedo, M. Á., Islam, A., Strickland, M., Tiwari, A., Vairo, A., & Vander Griend, P. (2022). *Journal of High Energy Physics*, *2022*(8), 1-39.

Stochastic reconfiguration

Natural gradient descent:

$$F_{ij} = \mathbb{E}[\partial_i \log p_\Theta(x) \partial_j \log p_\Theta(x)]$$

$$\Theta \leftarrow \Theta - \alpha F^{-1} \nabla_\Theta L$$

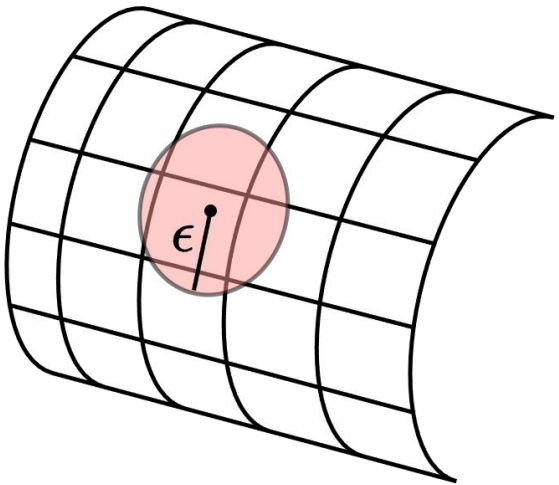


Stochastic reconfiguration

$$S_{ij} = \mathrm{Re}\left[\langle \partial_i \log \psi^* \partial_j \log \psi \rangle - \langle \partial_i \log \psi^* \rangle \langle \partial \log \psi \rangle\right]$$

$$g = 2\mathrm{Re}\,\mathbb{E}_{p(x|\Theta)}\left[\nabla_\Theta \log \psi_\Theta(x)^* \left(E_{\mathrm{loc}}(x,\Theta) - \langle E_{\mathrm{loc}} \rangle\right)\right]$$

$$\Theta \leftarrow \Theta - \alpha S^{-1} g$$



Time evolution: TDVP

$$\frac{d}{dt}|\psi_\Theta\rangle = -iH|\psi_\Theta\rangle$$

$$\frac{d}{dt}|\psi_\Theta\rangle = \sum_i \frac{d\Theta_i}{dt}\frac{d}{d\Theta_i}|\psi_\Theta\rangle$$

Time evolution: TDVP

Variational principle:

$$\min \left\| \sum_i \frac{d\Theta_i}{dt} \frac{d}{d\Theta_i} |\psi_\Theta\rangle - iH|\psi_\Theta\rangle \right\|^2$$

Time evolution: TDVP

$$S_{ij} = \mathrm{Re}\left[\langle \partial_i \log \psi^* \partial_j \log \psi \rangle - \langle \partial_i \log \psi^* \rangle \langle \partial \log \psi \rangle\right]$$

$$F_i = 2\mathrm{Re}\left[\langle \partial_i \log \psi^* E_{\mathrm{loc}} \rangle - \langle \partial_i \log \psi^* \rangle \langle E_{\mathrm{loc}} \rangle\right]$$

$$\frac{d\Theta}{dt} = S^{-1} F$$

solve time evolution of the parameters with an ODE integrator!

Potential issues:
- Spectrum of S (regularize)
- Expensive for large models

Time evolution: p-tVMC Control variate

- Instead of the local infidelity estimator

$$\mathcal{I}_{\mathrm{loc}}(\sigma,\eta) = 1 - \frac{\langle\sigma|U|\phi\rangle\,\langle\eta|U^\dagger|\psi\rangle}{\langle\sigma|\psi\rangle\,\langle\eta|\phi\rangle}$$

- We can subtract a Control Variate

$$\mathcal{I}_{\mathrm{loc}}^{CV} = \mathrm{Re}\mathcal{I}_{\mathrm{loc}} - c(|1-\mathcal{I}_{\mathrm{loc}}|^2) - 1).$$

- Want to improve the signal to noise ratio when $\mathcal{I}_{\mathrm{loc}} \to 0$
- In this limit one can proof the optimal $c = -\frac{1}{2}$

Learning the Lindblad equation

Since $e^{\mathcal{L}t}$ is non unitary the actual time evolution requires to sample from a different distribution which we do by reweighting

Schrödinger equation

$$\frac{d}{dt}|\psi\rangle = -iH|\psi\rangle$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

$$\mathcal{I}_{\text{loc}} = 1 - \frac{\langle\sigma|\psi_0\rangle}{\langle\sigma|\psi_1\rangle}\frac{\langle\eta|\psi_1\rangle}{\langle\eta|\psi_0\rangle}$$

$$p(\sigma|\Theta_1)p(\eta|\Theta_0) = \frac{|\langle\sigma|\psi_{\Theta_1}\rangle|^2|\langle\eta|\psi_{\Theta_0}\rangle|^2}{\langle\psi_{\Theta_1}|\psi_{\Theta_1}\rangle\langle\psi_{\Theta_0}|\psi_{\Theta_0}\rangle}$$

Lindblad equation

$$\frac{d}{dt}\rho = \mathcal{L}\rho$$

$$\rho(t) = e^{\mathcal{L}t}\rho(0)$$

$$\mathcal{I}_{\text{loc}} = 1 - \frac{\langle\sigma|\rho_0|\eta\rangle}{\langle\sigma|\rho_1|\eta\rangle}\frac{\langle\omega|\rho_1|\zeta\rangle}{\langle\omega|\rho_0|\zeta\rangle}$$

$$p(\sigma,\eta)p(\omega,\zeta) = \frac{|\langle\sigma|\rho_2|\eta\rangle|^2}{\sum_{\eta\sigma}|\langle\sigma|\rho_2|\eta\rangle|^2}\frac{|\langle\omega|\rho_1|\zeta\rangle|^2}{\sum_{\omega\zeta}|\langle\omega|\rho_1|\zeta\rangle|^2}$$

Cranck Nicholoson

$$\left(1 - \frac{dt}{2}L\right)\psi_\Theta(t+dt) = \left(1 + \frac{dt}{2}L\right)\psi(t),$$

$$U_- = 1 - \frac{dt}{2}L \qquad F_{loc} = \frac{\langle\sigma|U_+|\phi\rangle\,\langle\eta|U_-|\psi_\Theta\rangle}{\langle\sigma|U_-|\psi_\Theta\rangle\,\langle\eta|U_+|\phi\rangle}$$

$$U_+ = 1 + \frac{dt}{2}L \qquad I_{loc} = 1 - F_{loc}$$

$$
\begin{aligned}
E_{\sigma,\eta\sim\chi}[\mathcal{I}_{\mathrm{loc}}] &= 1 - \sum_{\sigma,\eta} \frac{|\langle\sigma|\psi\rangle|^2 |\langle\eta|\phi\rangle|^2}{\langle\psi|\psi\rangle\langle\phi|\phi\rangle} \frac{\langle\sigma|U|\phi\rangle\langle\eta|U^\dagger|\psi\rangle}{\langle\sigma|\psi\rangle\langle\eta|\phi\rangle} \\
&= 1 - \frac{1}{\langle\psi|\psi\rangle\langle\phi|\phi\rangle} \left(\sum_{\sigma} \langle\sigma|\psi\rangle^* \langle\sigma|U|\phi\rangle\right) \left(\sum_{\eta} \langle\eta|\phi\rangle^* \langle\eta|U^\dagger|\psi\rangle\right) \\
&= 1 - \frac{|\langle\psi|U|\phi\rangle|^2}{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}.
\end{aligned}
$$