Build Big or Build Smart: Examining Scale and Domain Knowledge in Machine Learning for Fundamental Physics

Neural network quantum states and simulation of real-time dynamics of quantum systems

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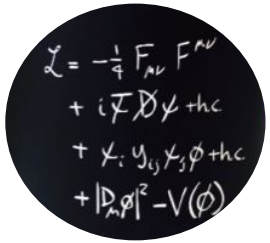
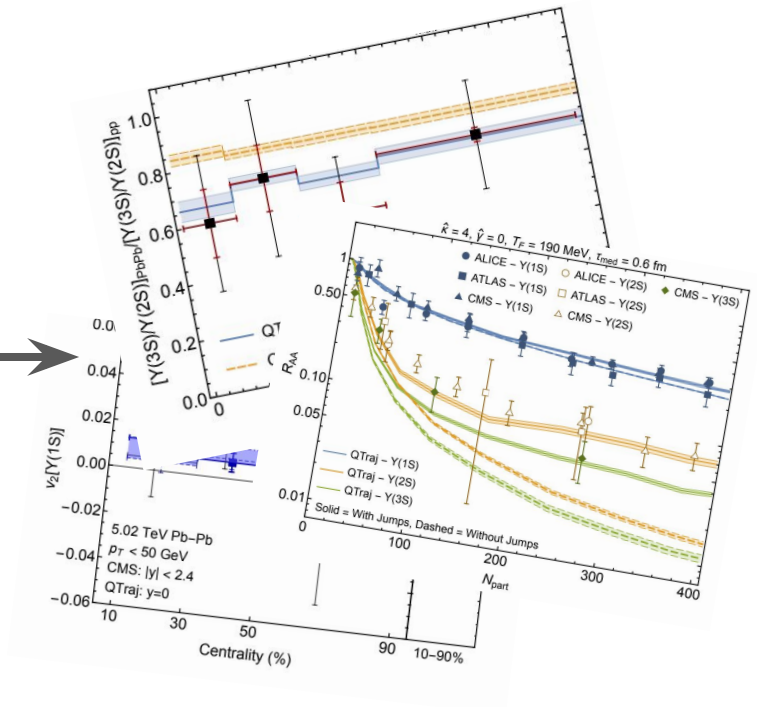
Technical University of Munich

28.08.2025

Predictions from the Standard model





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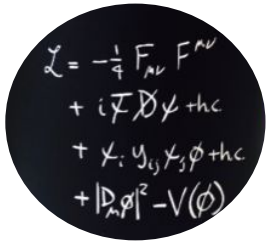

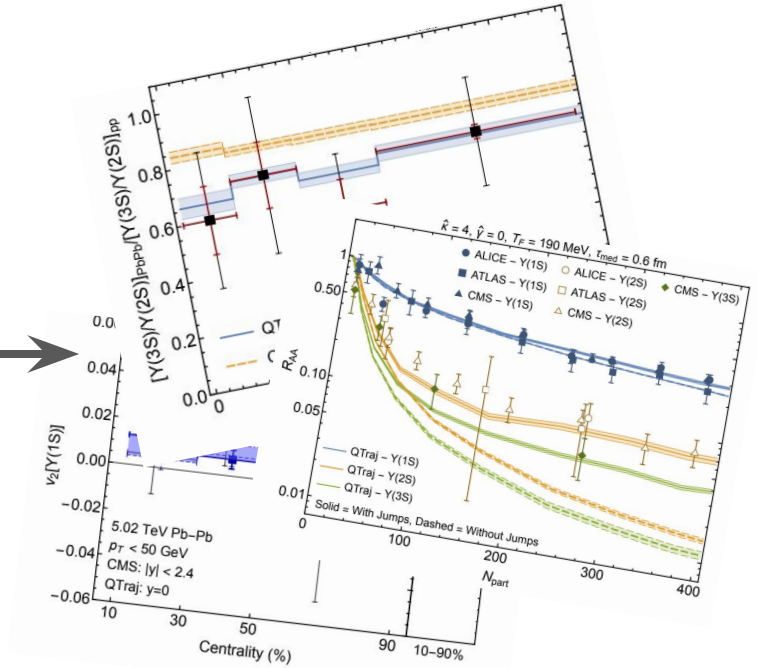

Lattice QCD

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

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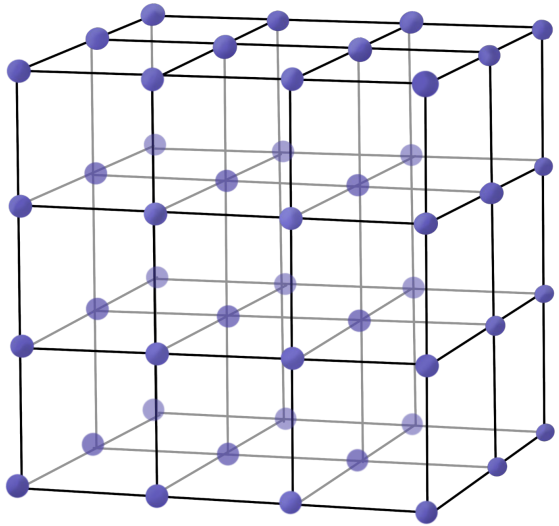
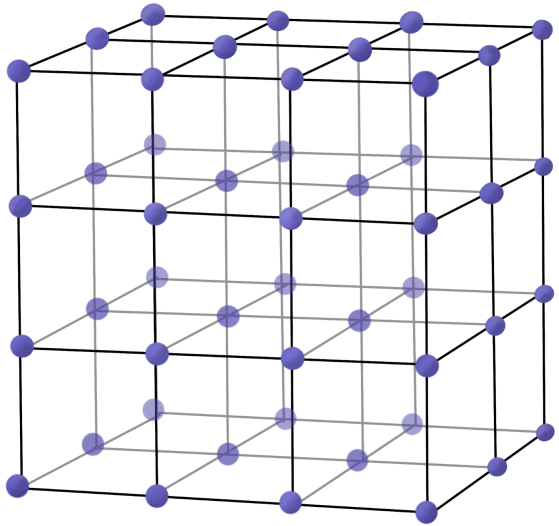


Lattice QCD

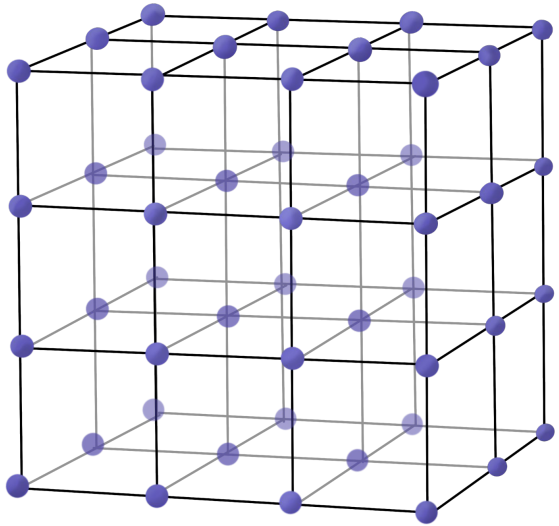
$$\int \prod_x d\phi_x \, e^{iS[\phi]}$$



Lattice QCD

$$\int \prod_x d\phi_x \, e^{iS[\phi]}$$

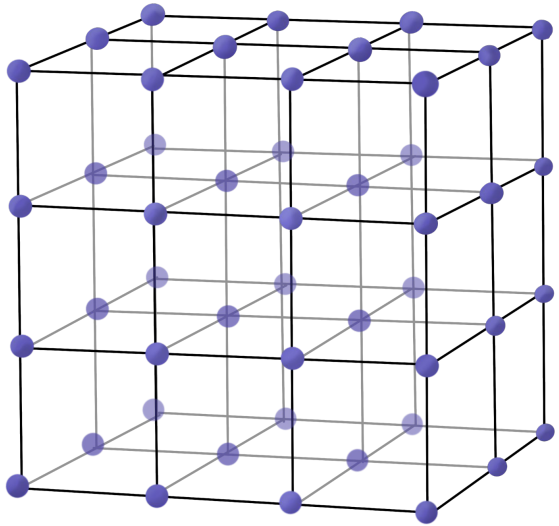
$$24^3 \times 64 \approx 900\text{k}$$



Lattice QCD

$$t \to -i\tau$$

$$\int \prod_x d\phi_x \, e^{-S_E[\phi]}$$

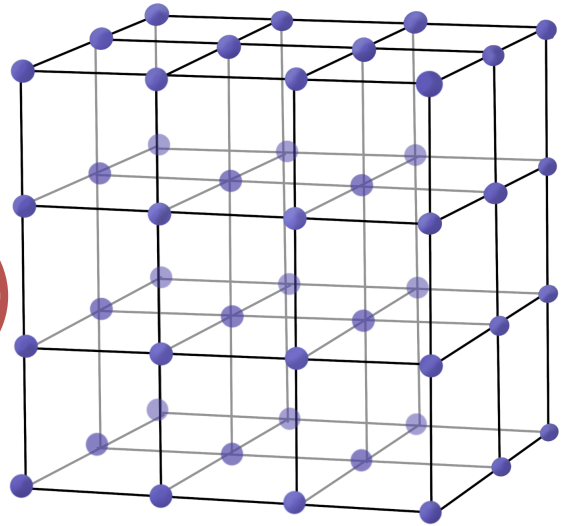


Lattice QCD

$$t \to -i\tau$$

$$\int \prod_x d\phi_x \, e^{-S_E[\phi]}$$

$$p(\phi)$$



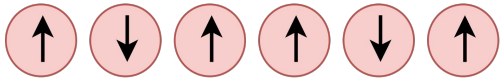
Hamiltonian methods

$$|\phi\rangle \in \mathcal{H}$$

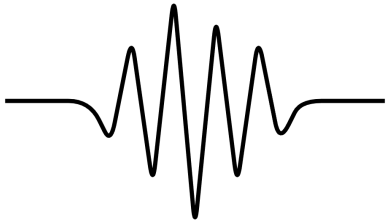
$$i\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle$$

Simulating large Quantum systems

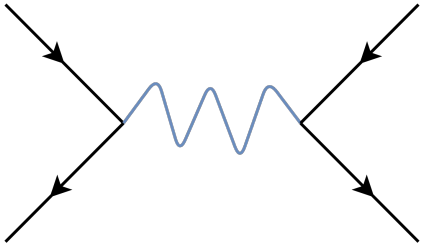
Spin Systems



Non-Rel. Systems



QFTs



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

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

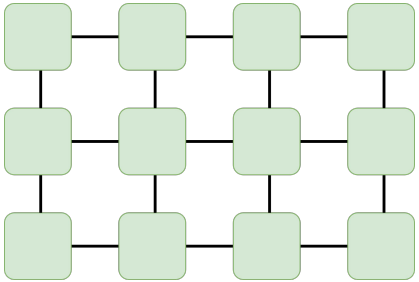
$$\Theta \leftarrow \Theta - \alpha \nabla_\Theta E$$

Variational states

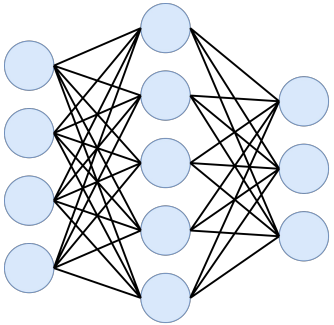
Hartree–Fock

$$\psi_\Theta \propto \begin{vmatrix} \phi_{\Theta_1} & \phi_{\Theta_2} & \cdots \\ \phi_{\Theta_3} & \phi_{\Theta_4} & \cdots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

Tensor Networks



Neural Network



Expressiveness

Variational Monte Carlo

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

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

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

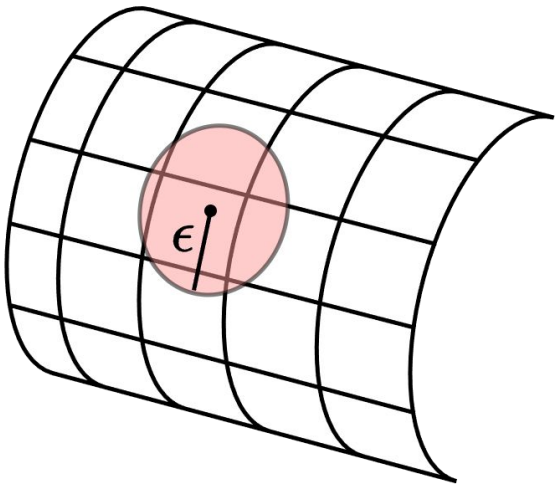
$$= 2\mathrm{Re}\, \mathbb{E}_{p(x|\Theta)} \left[\nabla_\Theta \log \psi_\Theta(x)^* \left(E_{\mathrm{loc}}(x, \Theta) - \langle E_{\mathrm{loc}} \rangle \right) \right]$$

Stochastic reconfiguration

Natural gradient descent:

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

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

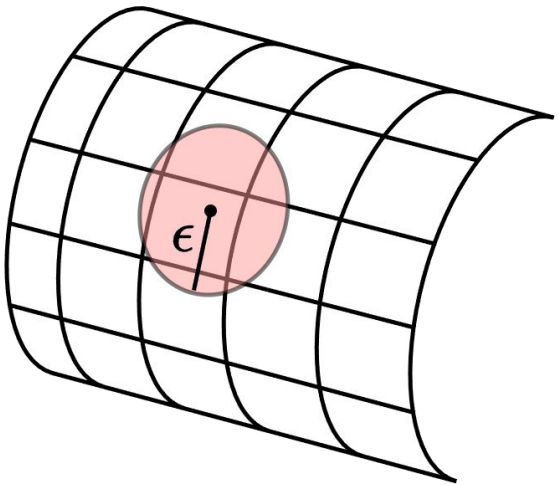


Stochastic reconfiguration

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

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

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



Time evolution: TDVP

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

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

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

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!

Time evolution: TDVP

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

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

solve time evolution of the parameters with an ODE integrator!

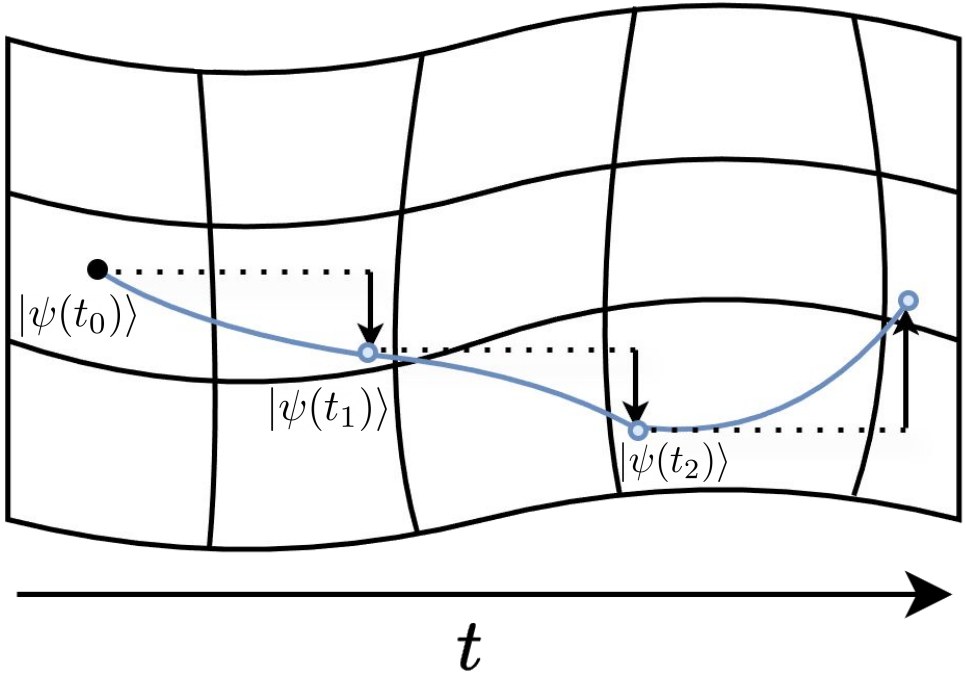
Potential issues:
- Spectrum of S (regularize)
- Expensive for large models

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

Time evolution: p-tVMC

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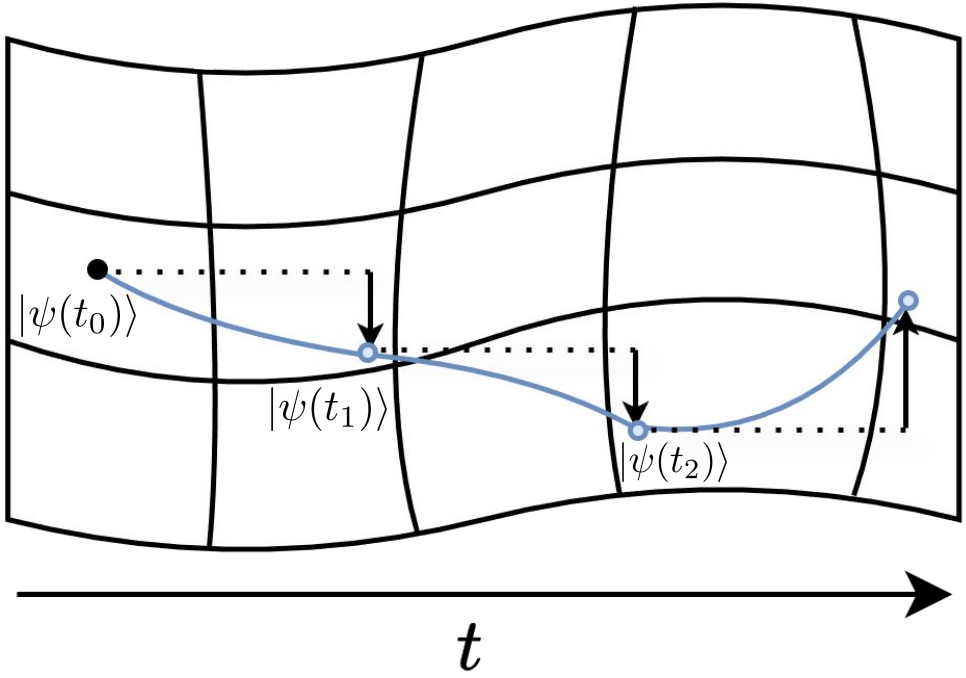
$$|\psi(t)\rangle = e^{-iHt}|\psi(t_0)\rangle$$

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

$$\equiv U$$



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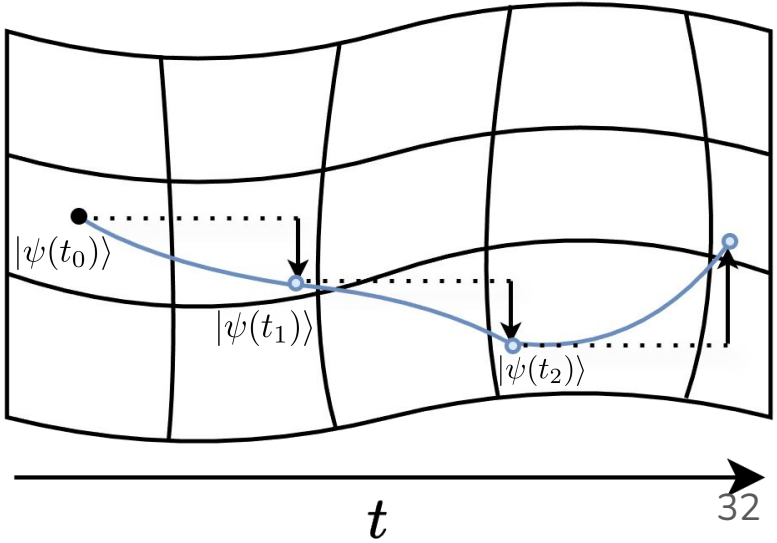
Time evolution: p-tVMC

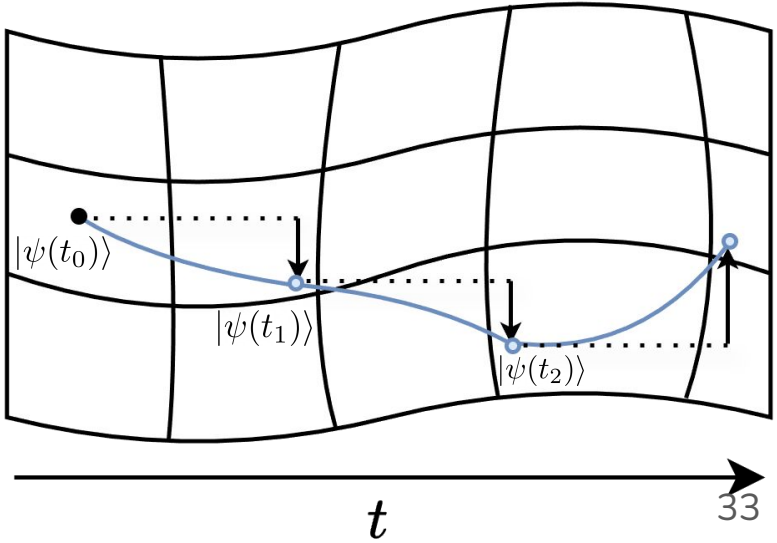
$$I = \mathbb{E}_{\sigma,\eta\sim p(\sigma|\Theta_1)p(\eta|\Theta_0)}\left[1 - \frac{\langle\sigma|U|\psi_{\Theta_0}(t_0)\rangle}{\langle\sigma|\psi_{\Theta_1}(t_1)\rangle}\frac{\langle\eta|U^\dagger|\psi_{\Theta_1}(t_1)\rangle}{\langle\eta|\psi_{\Theta_0}(t_0)\rangle}\right]$$



Time evolution: p-tVMC

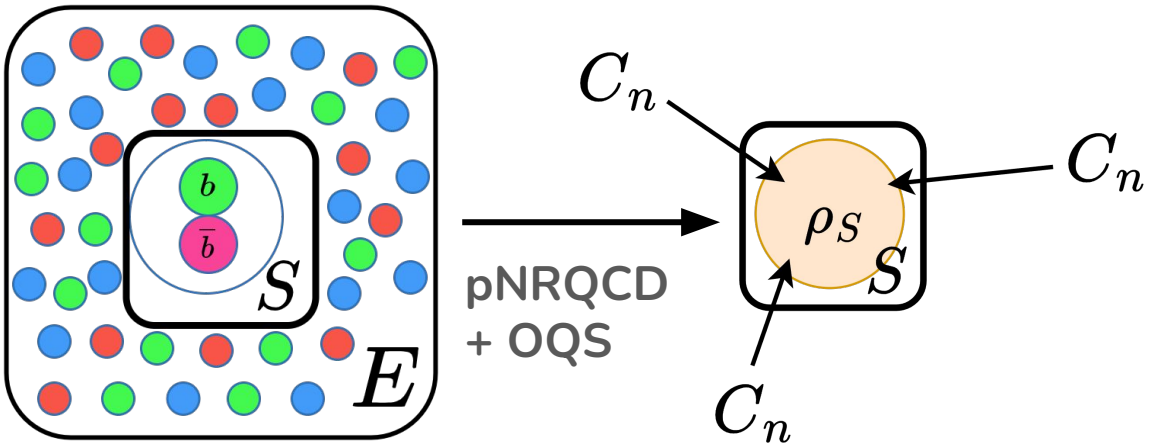
$$I = \mathbb{E}_{\sigma,\eta\sim p(\sigma|\Theta_1)p(\eta|\Theta_0)}\left[1 - \overbrace{\frac{\langle\sigma|U|\psi_{\Theta_0}(t_0)\rangle}{\langle\sigma|\psi_{\Theta_1}(t_1)\rangle}\frac{\langle\eta|U^\dagger|\psi_{\Theta_1}(t_1)\rangle}{\langle\eta|\psi_{\Theta_0}(t_0)\rangle}}^{\mathcal{I}_{\mathrm{loc}}}\right]$$

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



Actually, one can find a Control Variate for this specific estimator, which is important to obtain a good SNR for $\mathcal{I}_{\mathrm{loc}} \to 0$

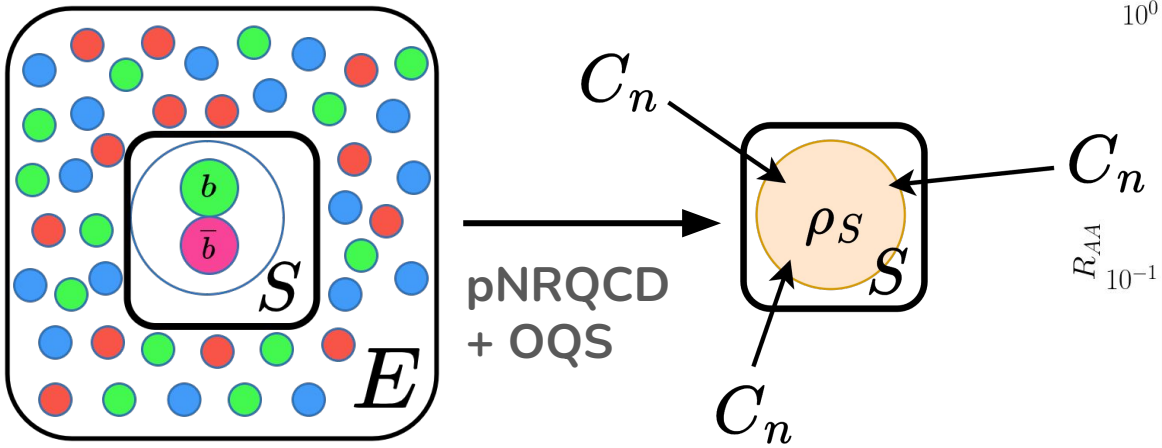
Quarkonium Suppression Simulator

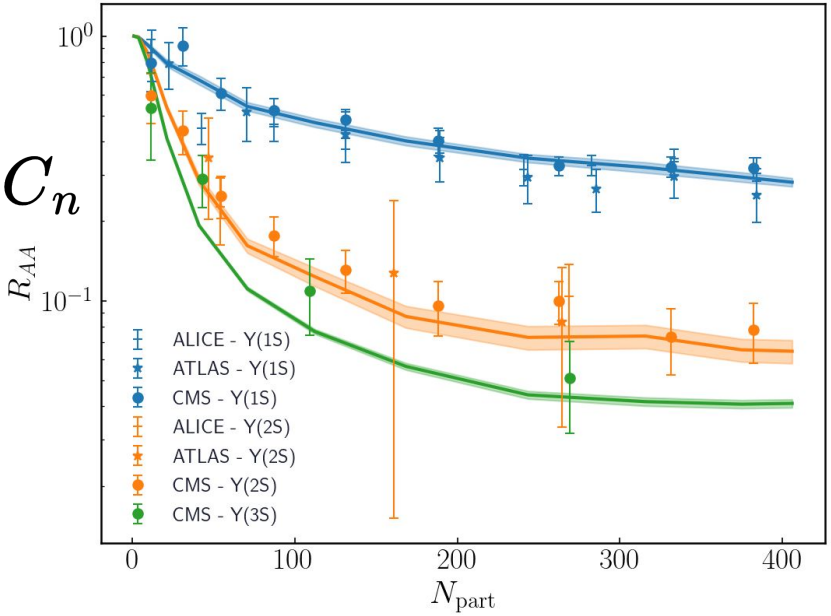


$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2} \left\{ C_n^\dagger C_n, \rho_S \right\} \right)$$

Very large matrix

Quarkonium Suppression Simulator





$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + \sum_n \left(C_n \rho_S C_n^\dagger - \frac{1}{2} \left\{ C_n^\dagger C_n, \rho_S \right\} \right)$$

Very large matrix

Learning the Lindblad equation

Schrödinger equation

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

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

Lindblad equation

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

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

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

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

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

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

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

Density matrices

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

Enforce in a neural network!

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3. $\rho \geq 0$

Enforce in a neural network!

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

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

Density matrices

To evaluate expectation values we have to sample from

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

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

Density matrices

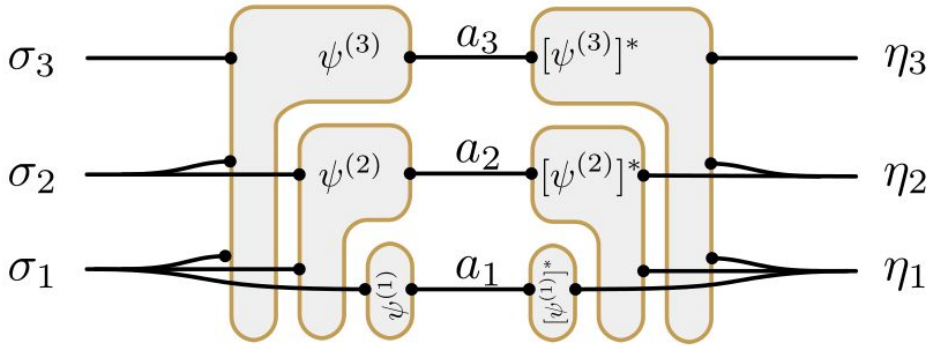
Since we are simulating a particle in position space we implement binary encodings of position basis states

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:

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



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Simulation:

$$H = \frac{p^2}{M} - \frac{\alpha}{x} + \beta\{x, p\} \quad C = x + \gamma i p$$

1. **Initialization:** Learn some ρ_0

2. **Time evolution:**

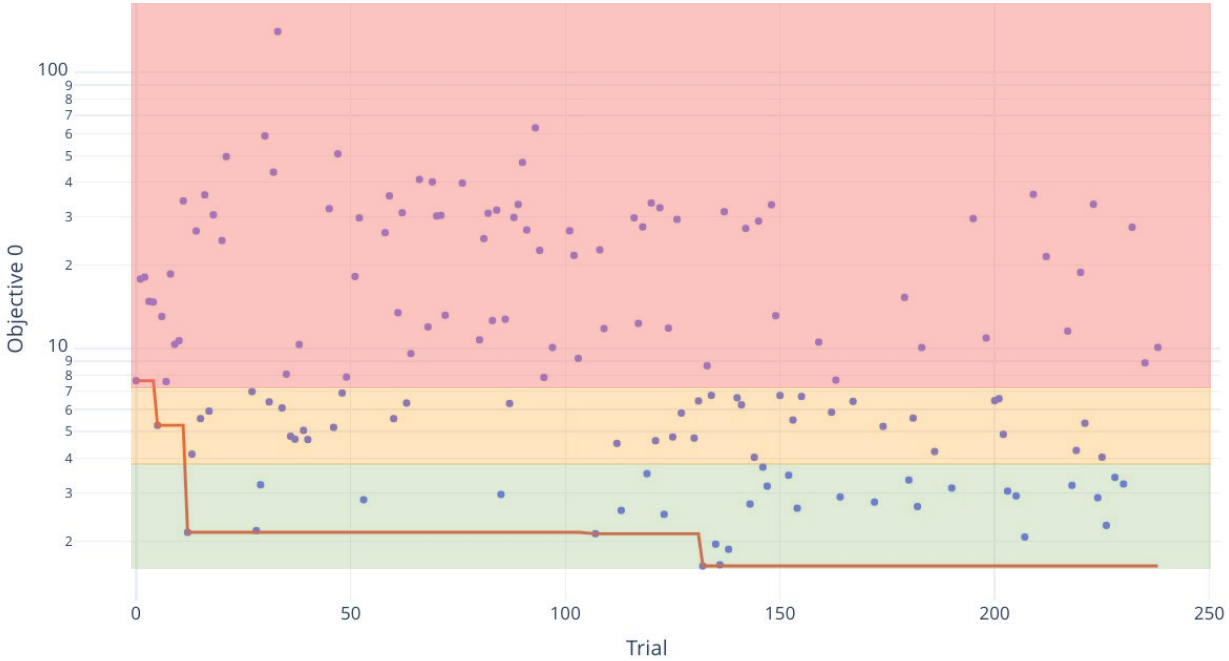
   a. Sample states $\sigma, \eta, \omega, \zeta$ from ρ and $(1 + \delta t \mathcal{L})\rho$

   b. Evaluate $\mathcal{I}_{\text{loc}}(\sigma, \eta, \omega, \zeta) = 1 - \frac{\langle\sigma|(1+\delta t\mathcal{L})\rho_1|\eta\rangle \langle\omega|\rho_2|\zeta\rangle}{\langle\sigma|\rho_2|\eta\rangle \langle\omega|(1+\delta t\mathcal{L})\rho_1|\zeta\rangle}$ and the gradient

   c. Copy model $\rho_1 \leftarrow \rho_2$

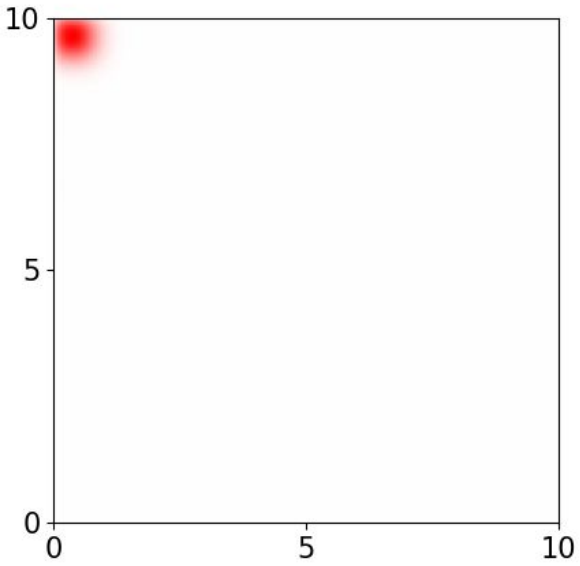
To get better convergence in δt , we designed a special estimator which implements an implicit second order Crank-Nicolson solver, for $e^{\mathcal{L}t}$ including a suitable Control Variate.

Hyperparameters

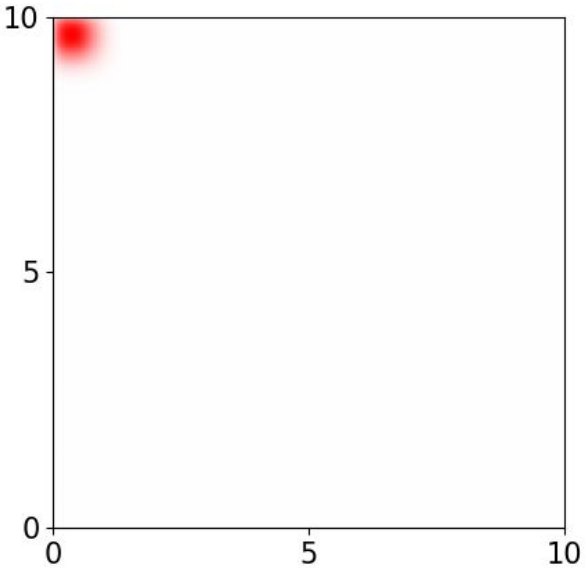


Simulation results

Monte Carlo Wavefunction

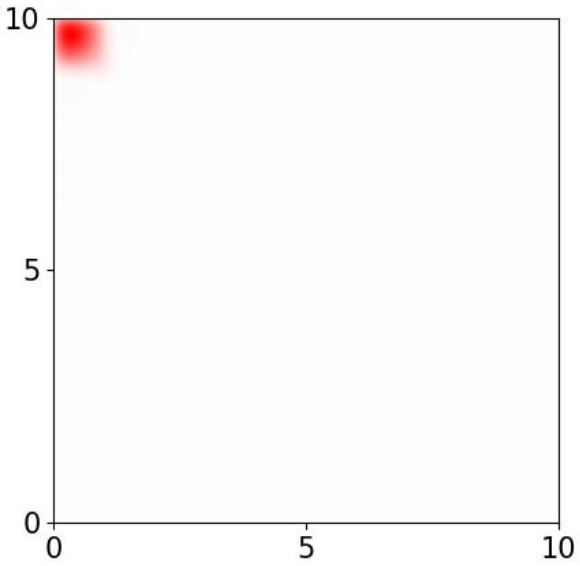


Neural Network

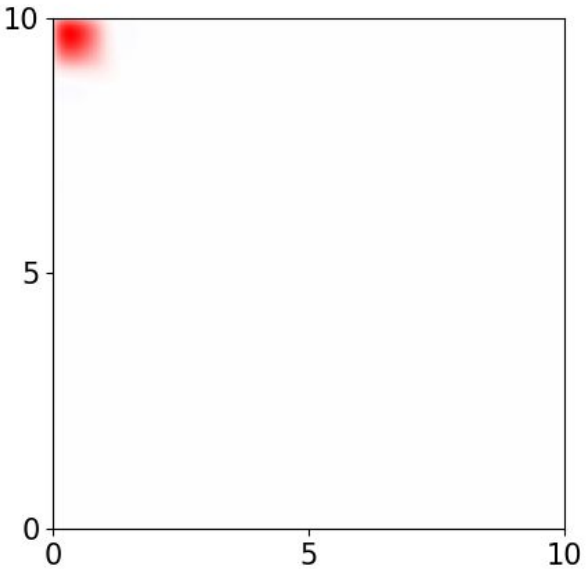


Simulation results

Monte Carlo Wavefunction

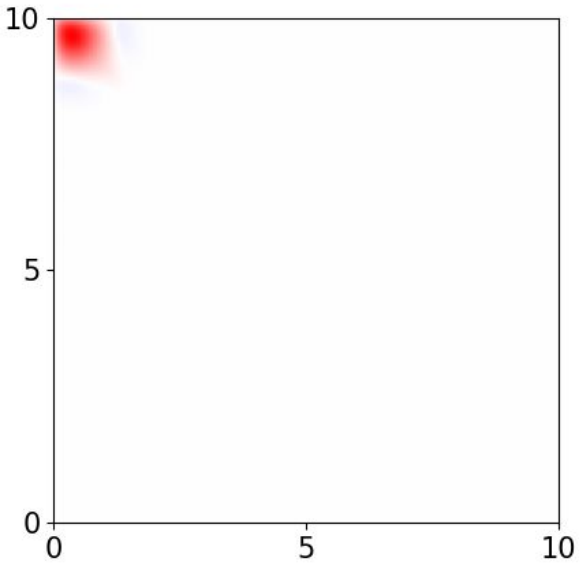


Neural Network



Simulation results

Monte Carlo Wavefunction



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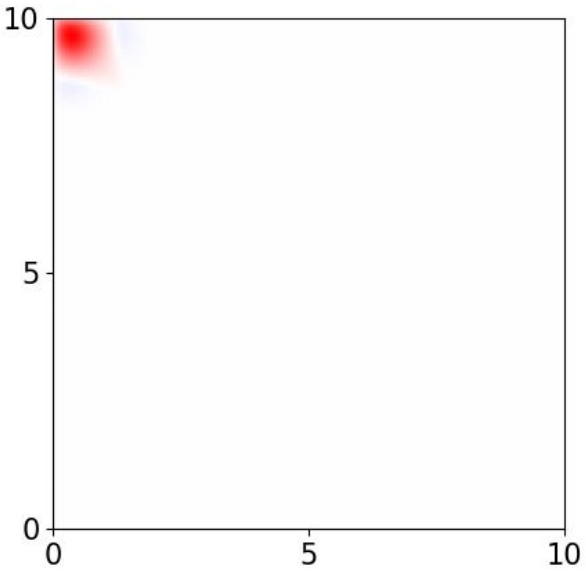
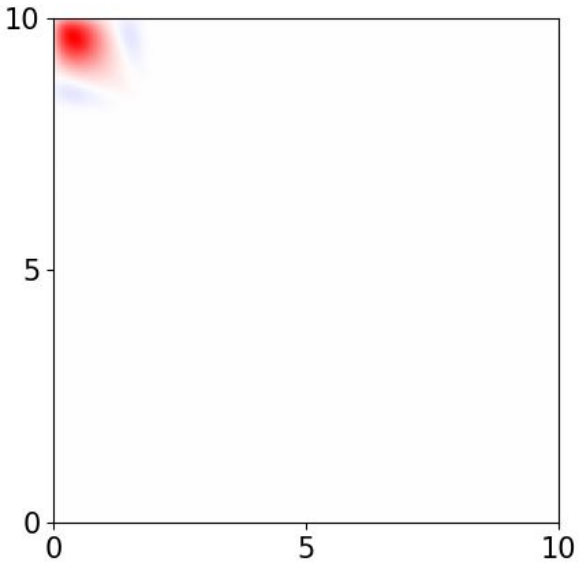


Simulation results

Monte Carlo Wavefunction



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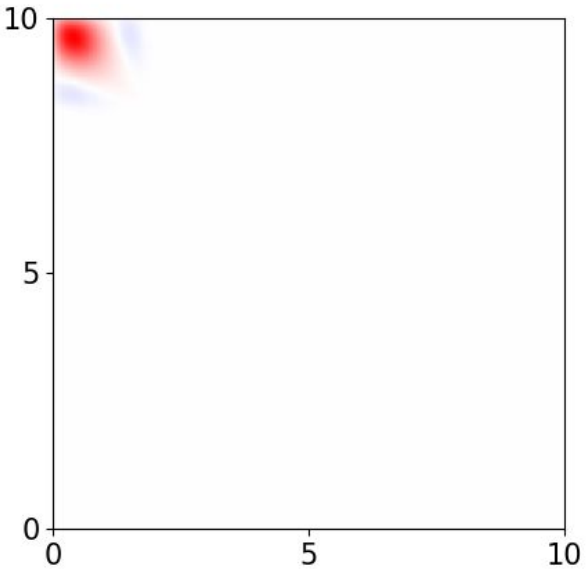
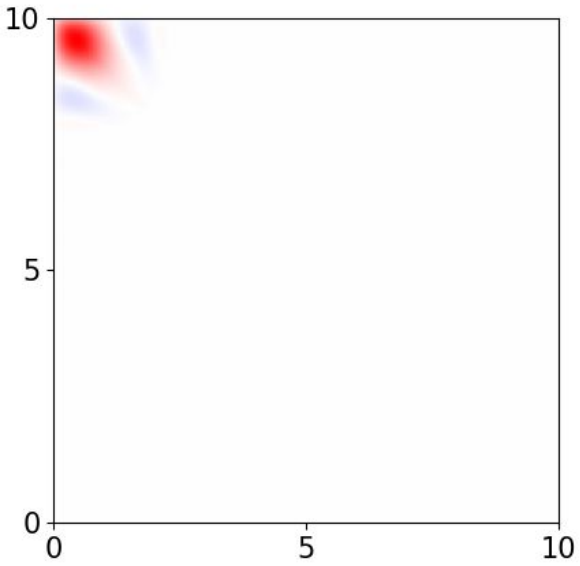


Simulation results

Monte Carlo Wavefunction



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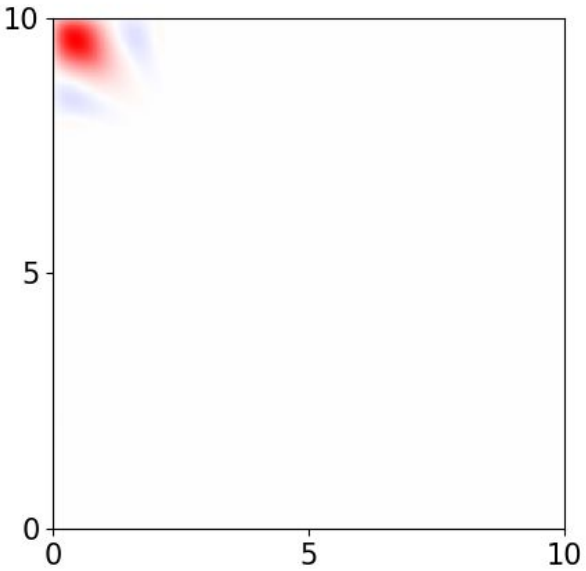
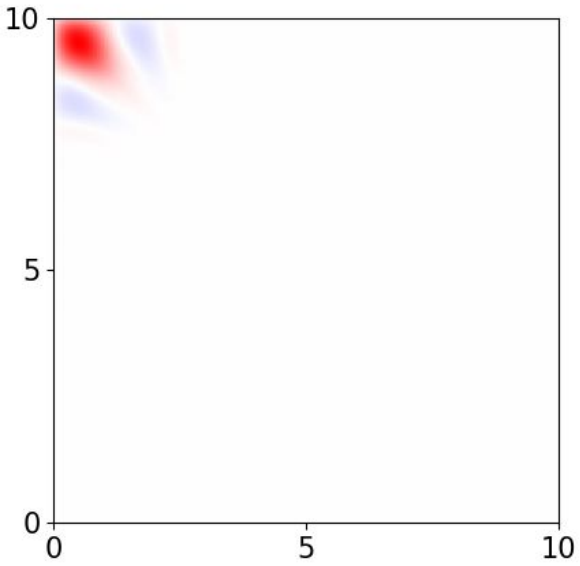


Simulation results

Monte Carlo Wavefunction



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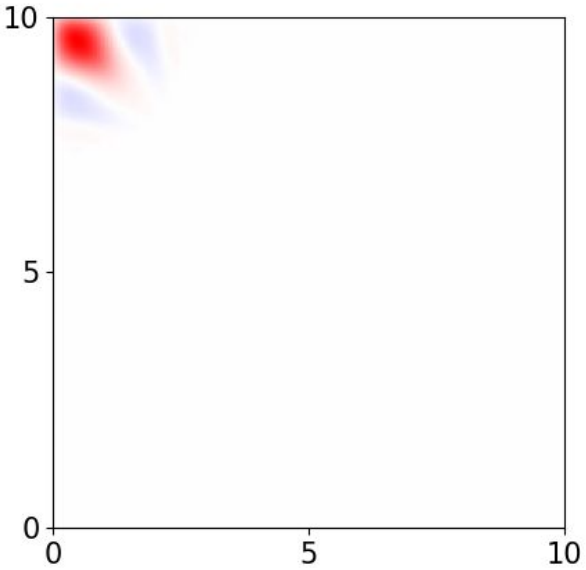
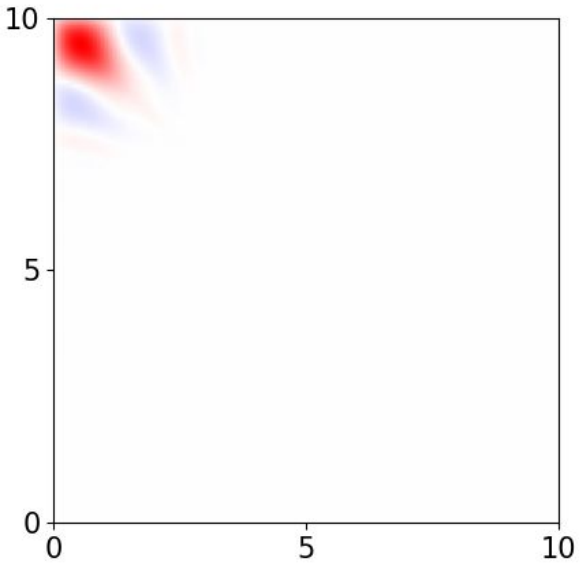


Simulation results

Monte Carlo Wavefunction



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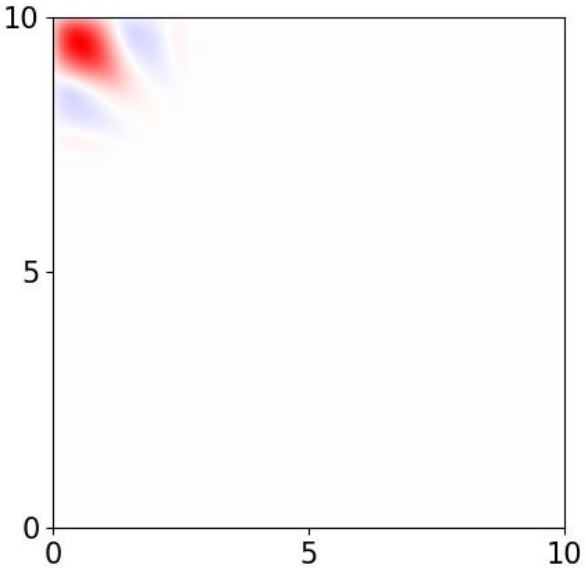
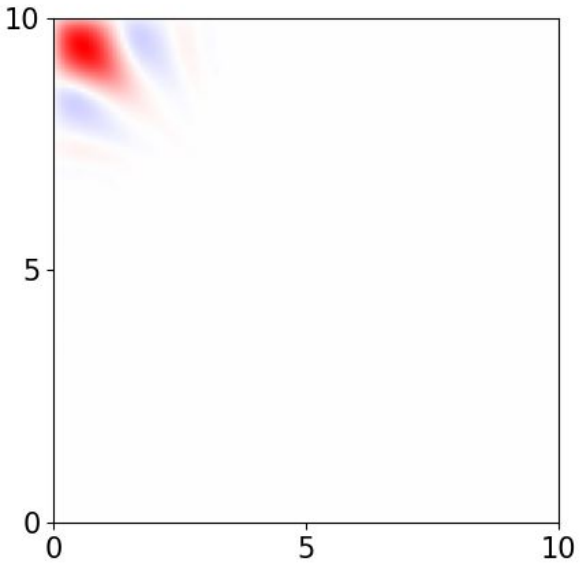


Simulation results

Monte Carlo Wavefunction



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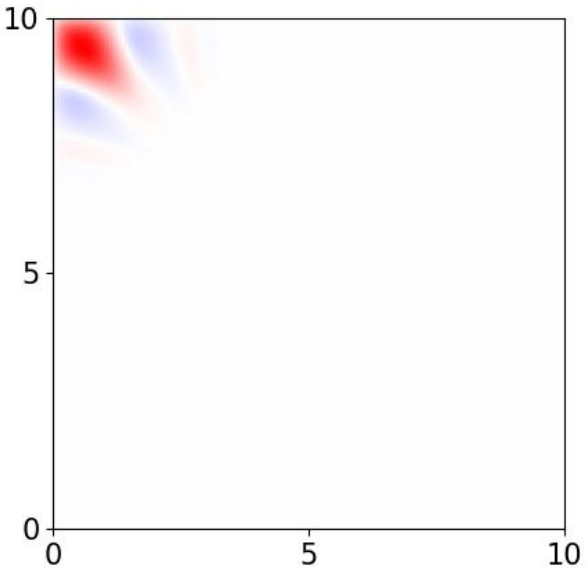
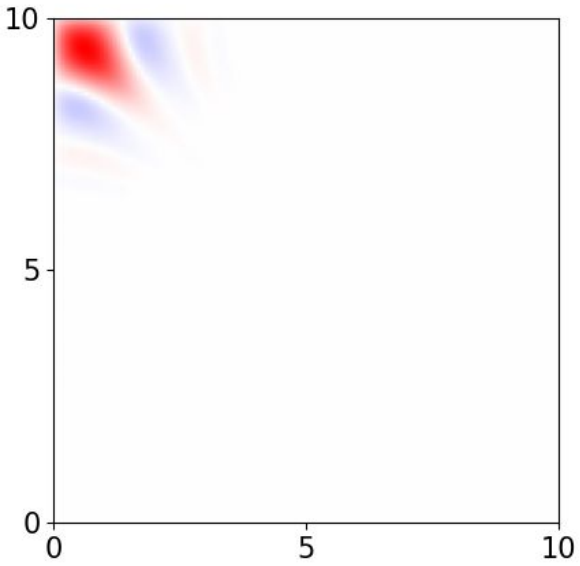


Simulation results

Monte Carlo Wavefunction



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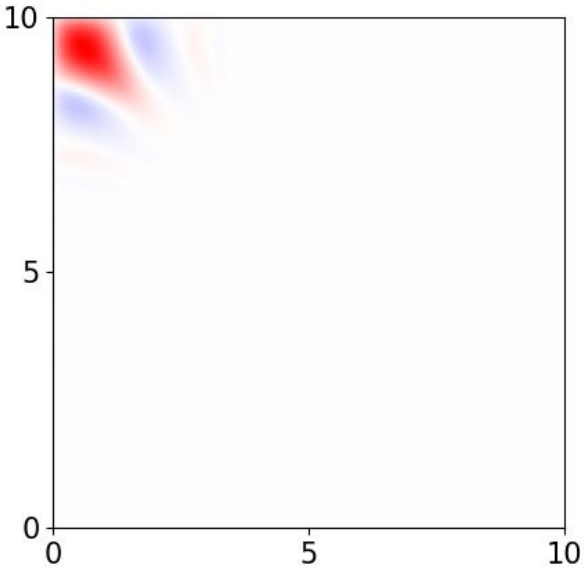
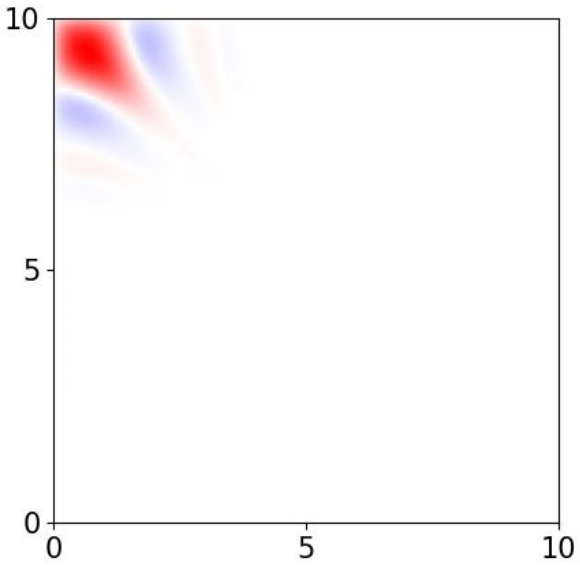


Simulation results

Monte Carlo Wavefunction



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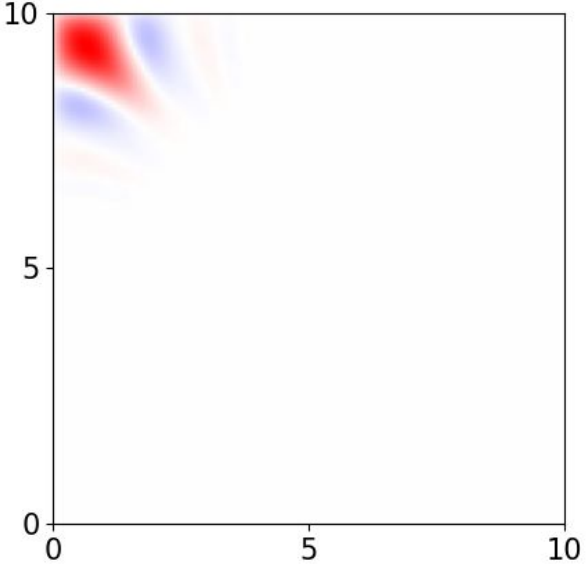
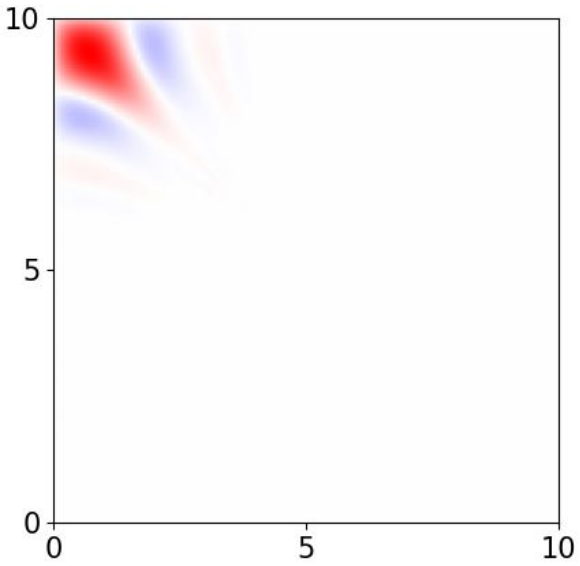


Simulation results

Monte Carlo Wavefunction



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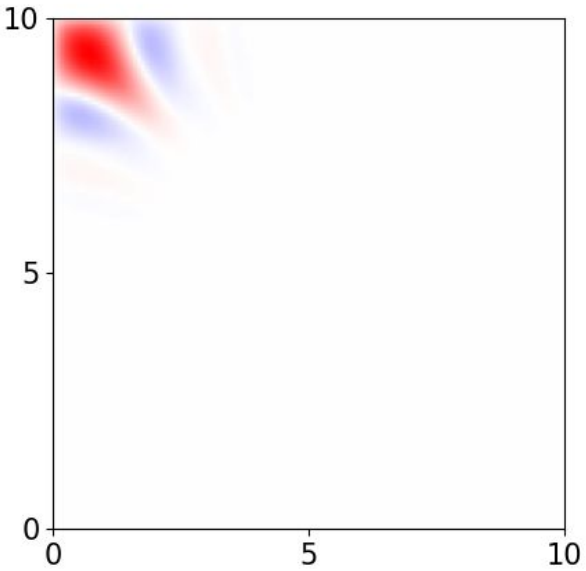
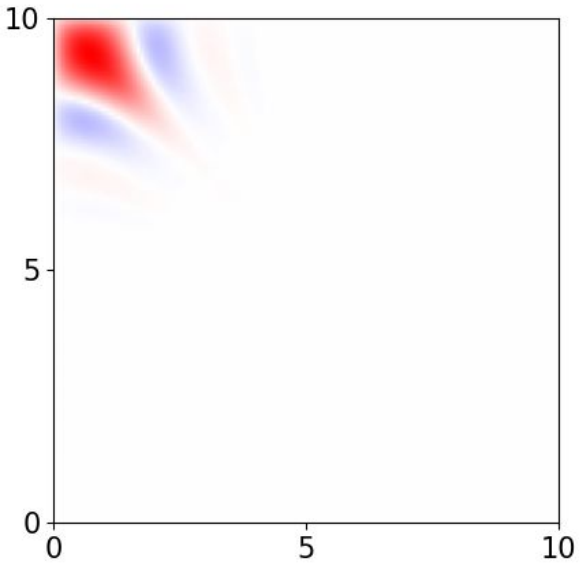


Simulation results

Monte Carlo Wavefunction



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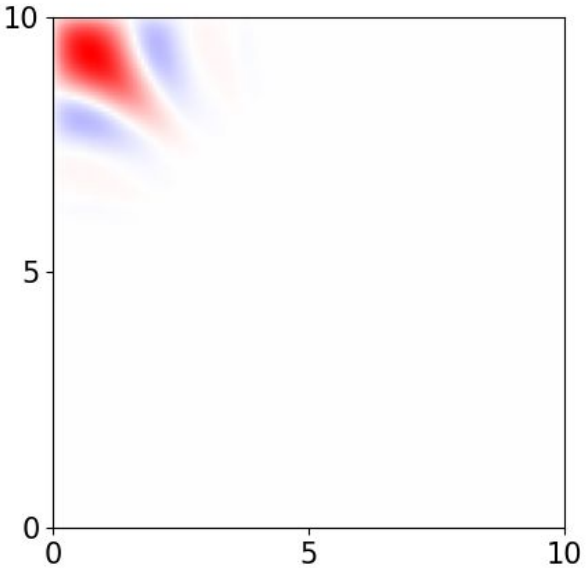
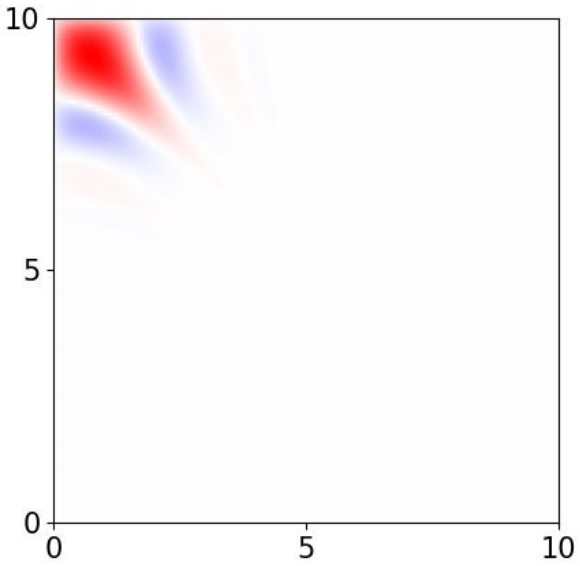


Simulation results

Monte Carlo Wavefunction



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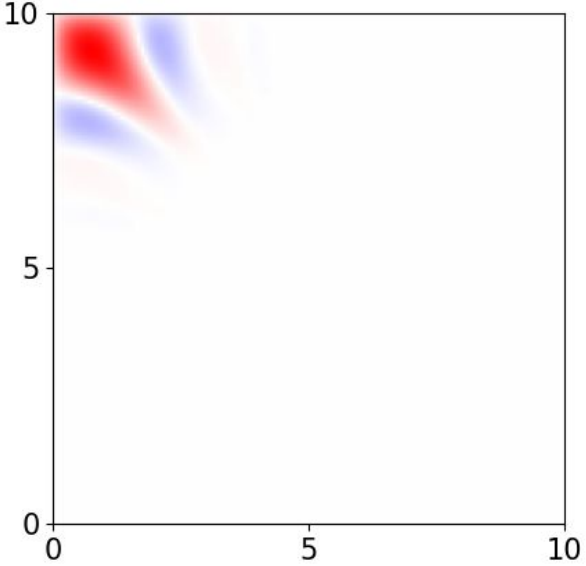
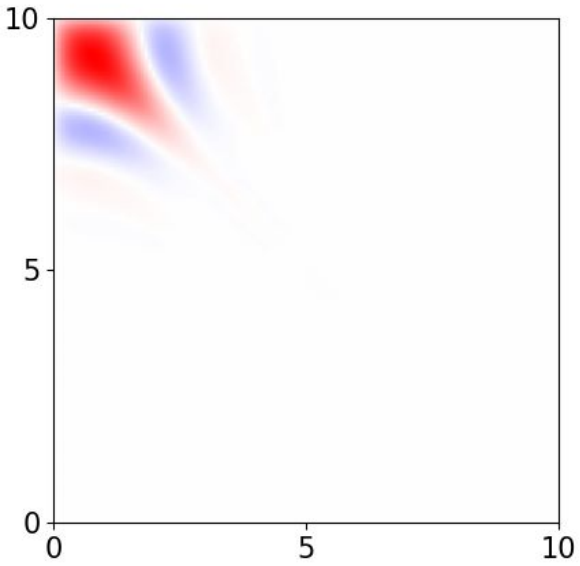


Simulation results

Monte Carlo Wavefunction



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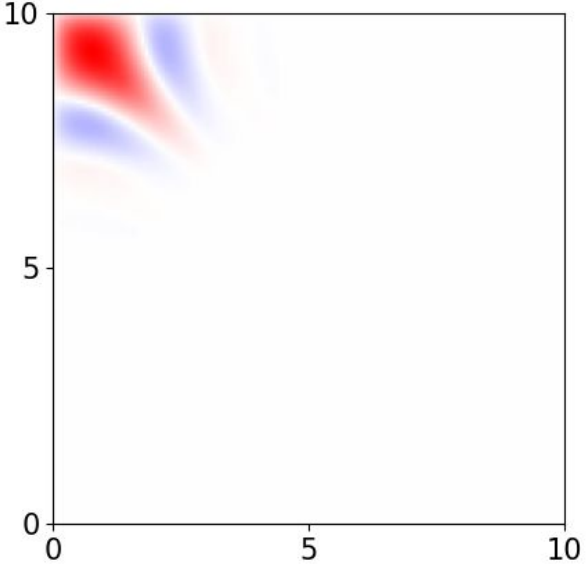
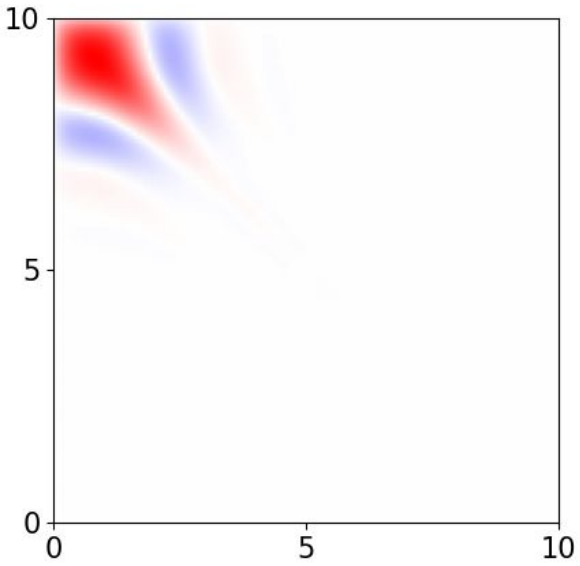


Simulation results

Monte Carlo Wavefunction



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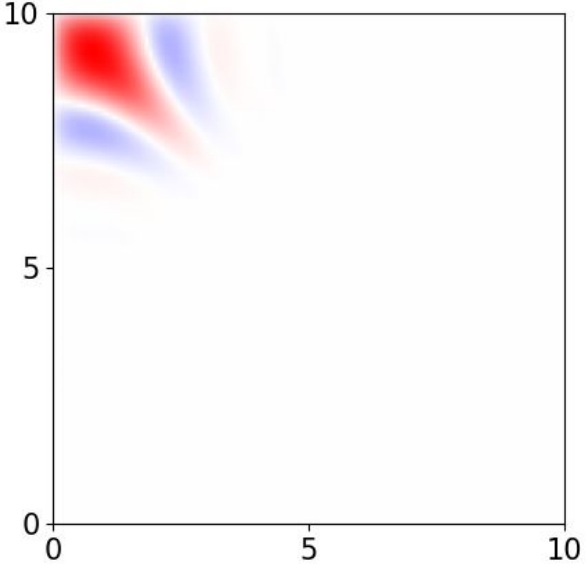
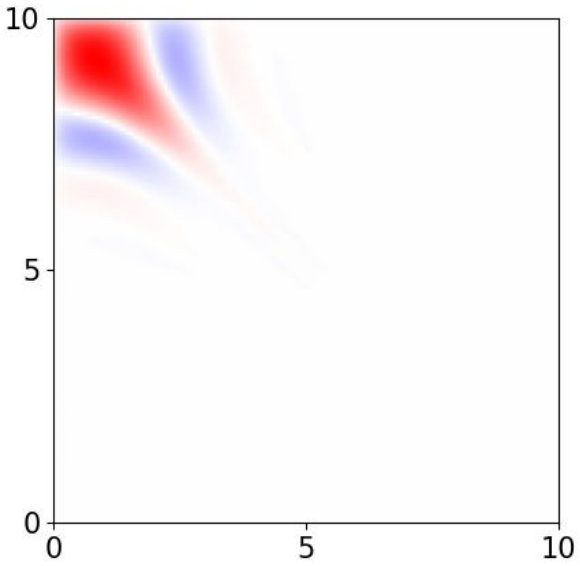


Simulation results

Monte Carlo Wavefunction



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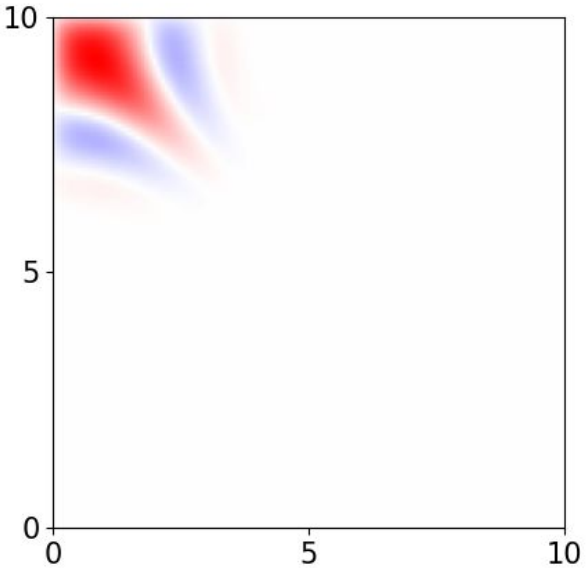
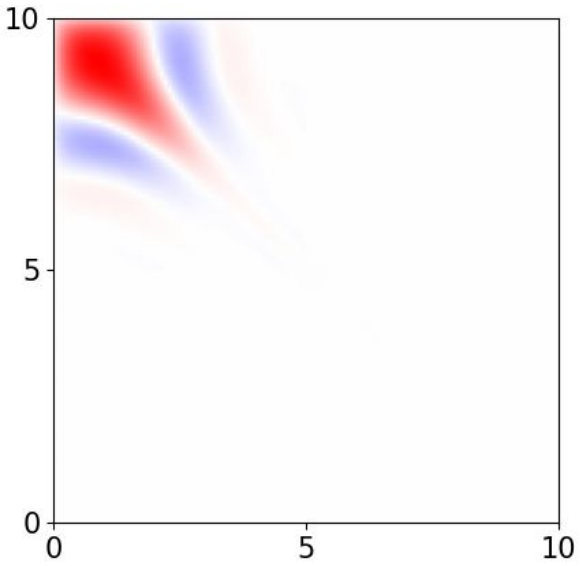


Simulation results

Monte Carlo Wavefunction



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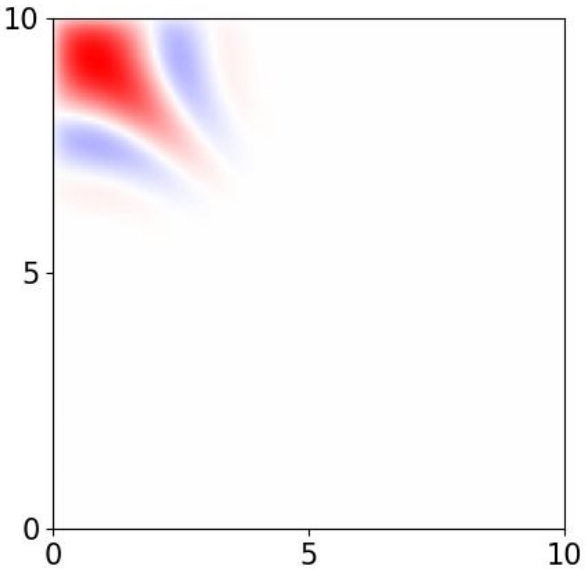
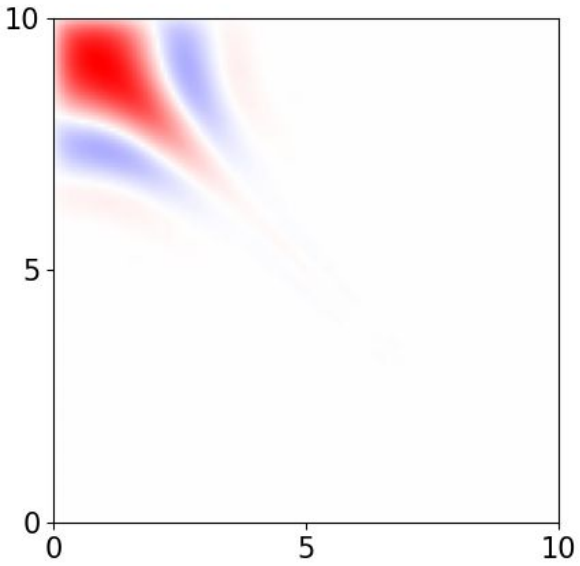


Simulation results

Monte Carlo Wavefunction



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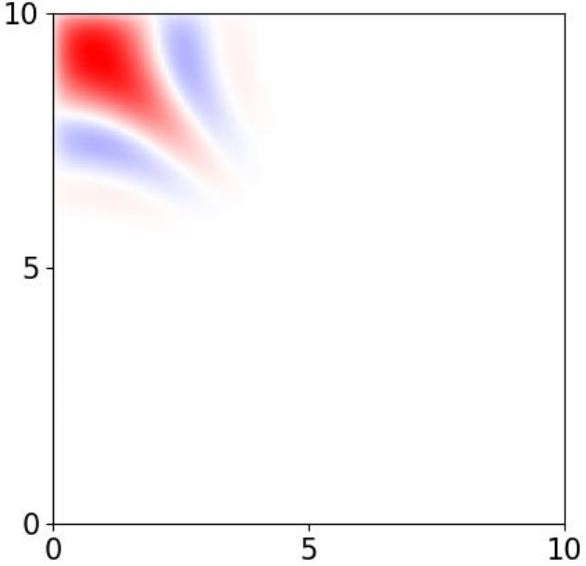
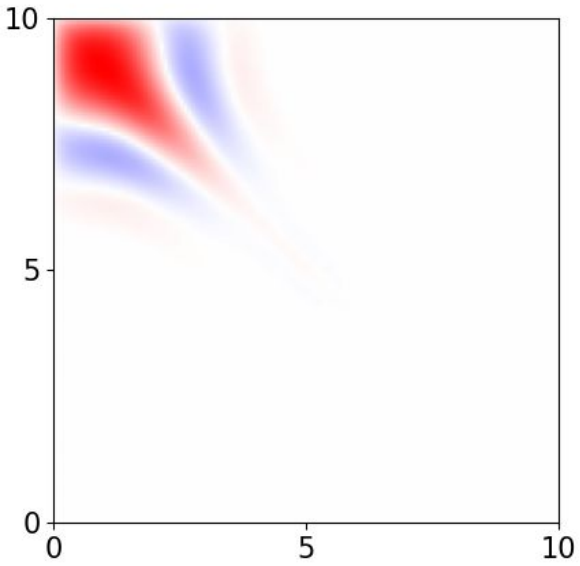


Simulation results

Monte Carlo Wavefunction



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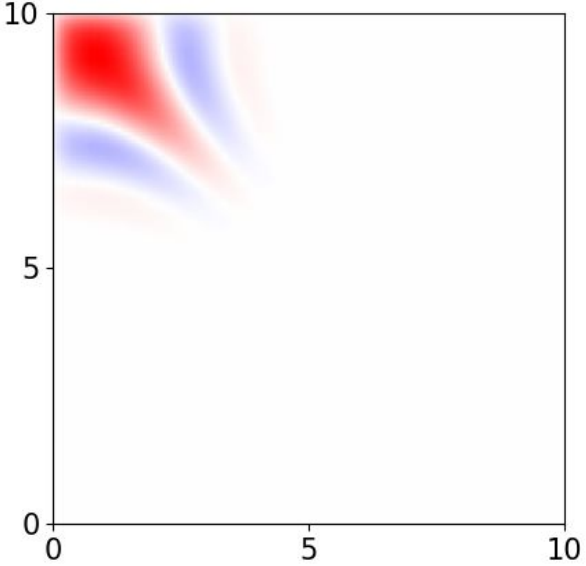
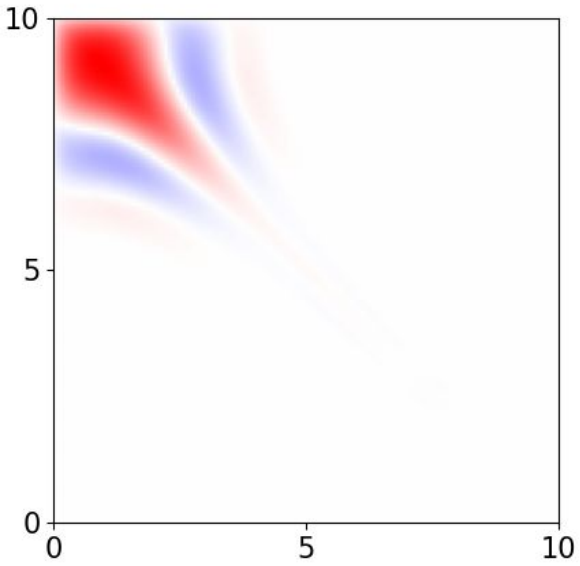


Simulation results

Monte Carlo Wavefunction



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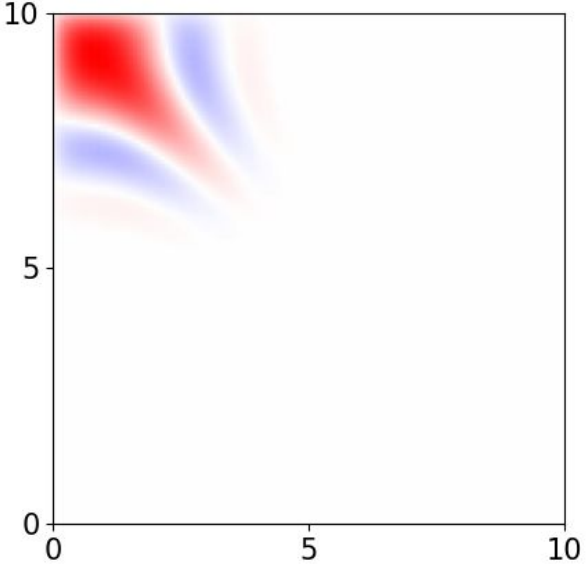
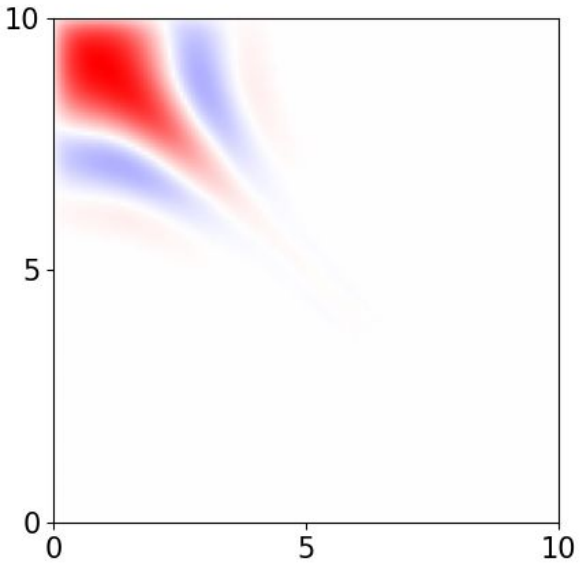


Simulation results

Monte Carlo Wavefunction



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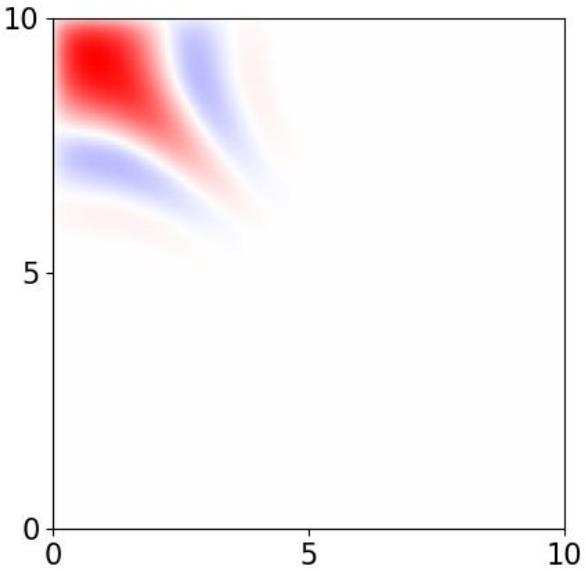
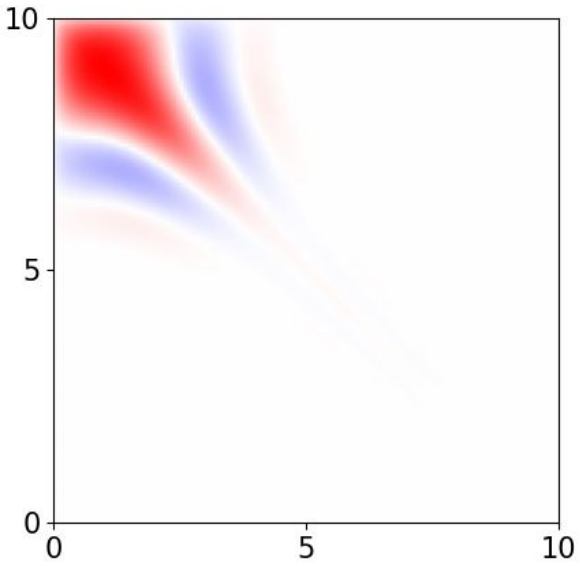


Simulation results

Monte Carlo Wavefunction



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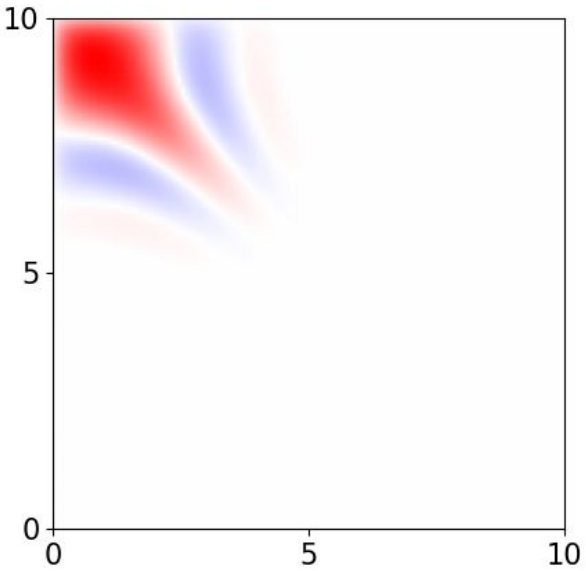
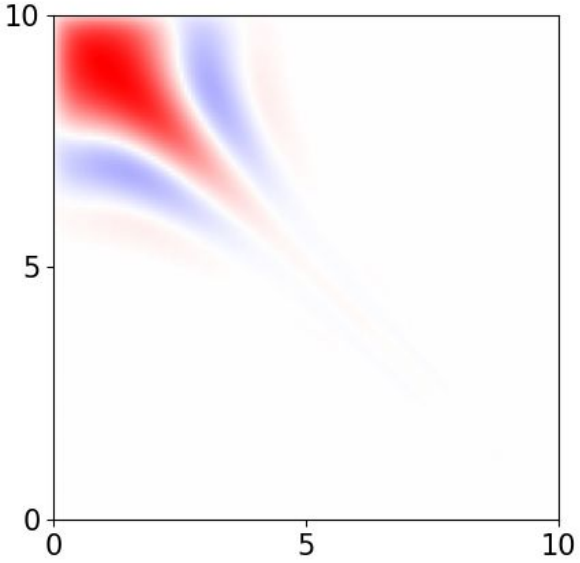


Simulation results

Monte Carlo Wavefunction



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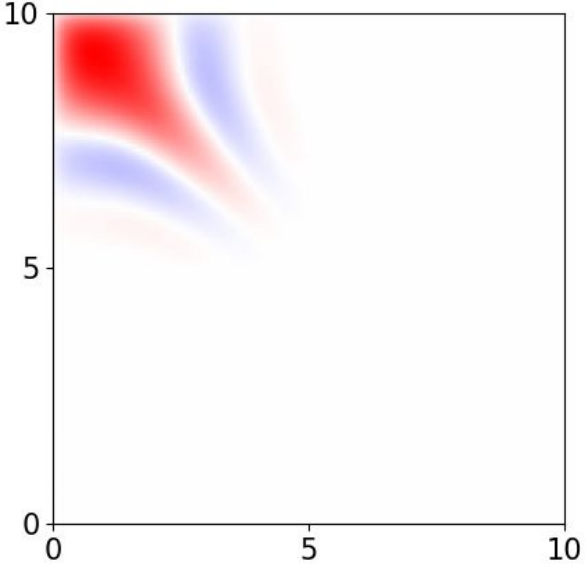
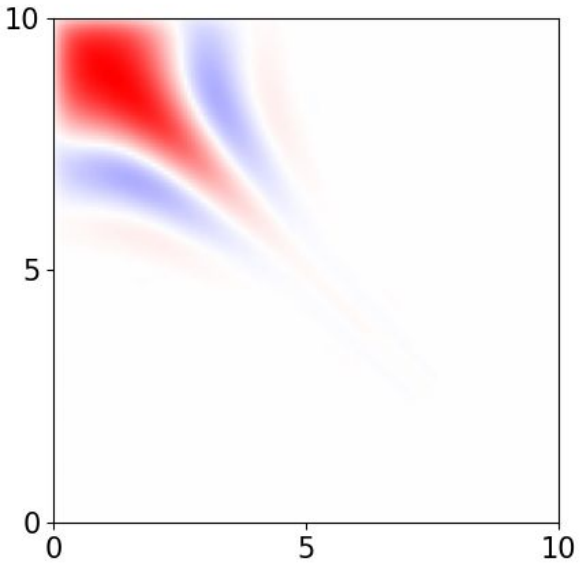


Simulation results

Monte Carlo Wavefunction



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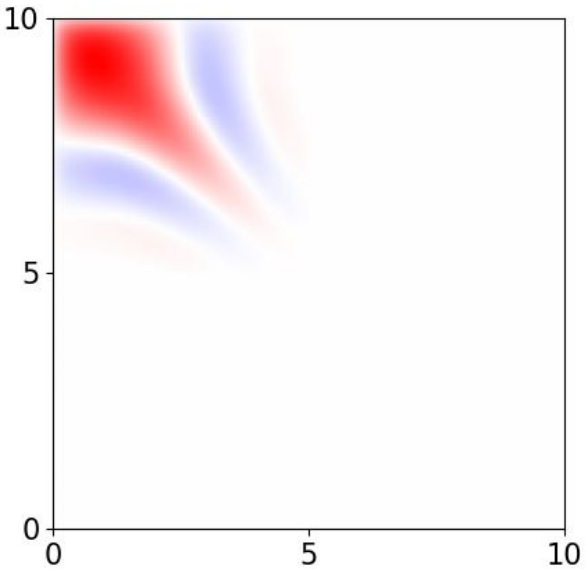
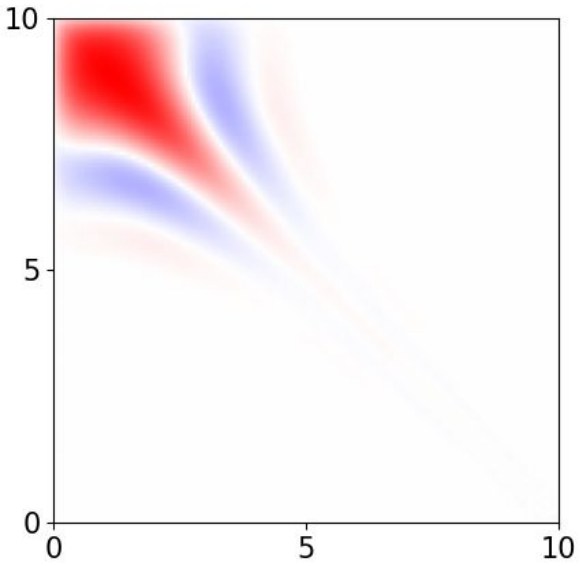
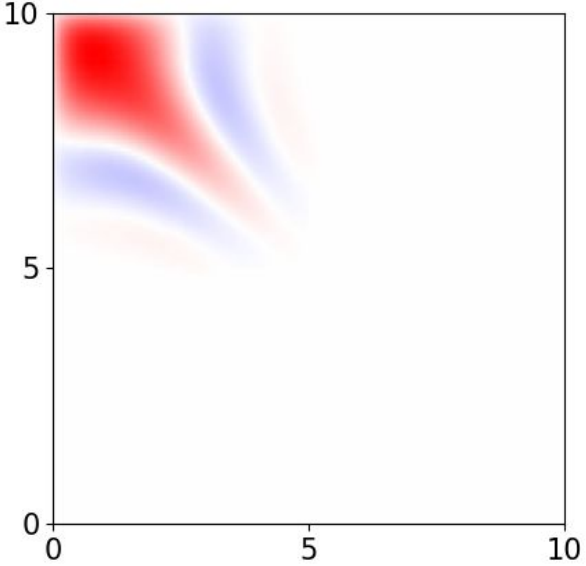


Simulation results

Monte Carlo Wavefunction

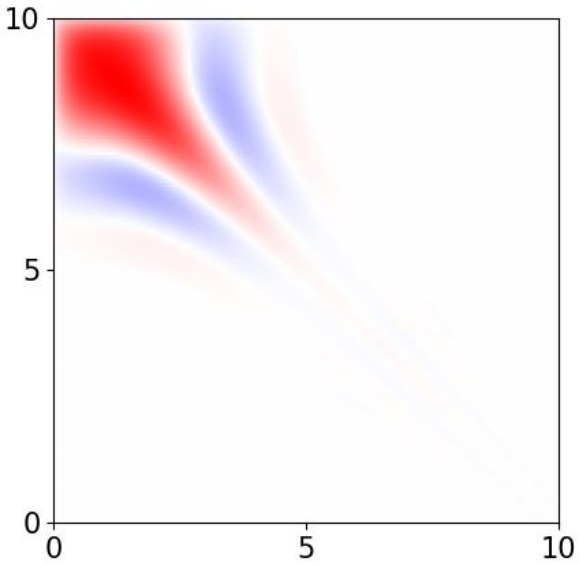


Neural Network



Simulation results

Monte Carlo Wavefunction



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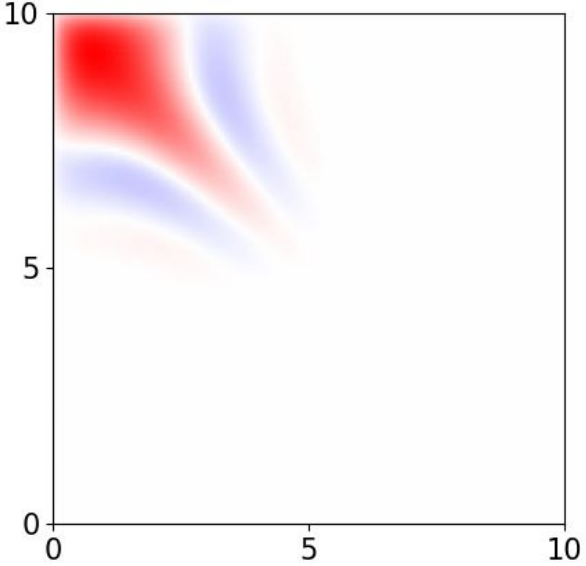
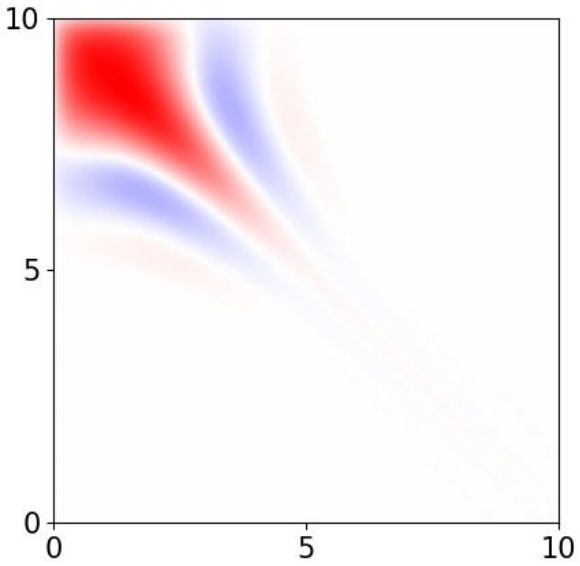


Simulation results

Monte Carlo Wavefunction



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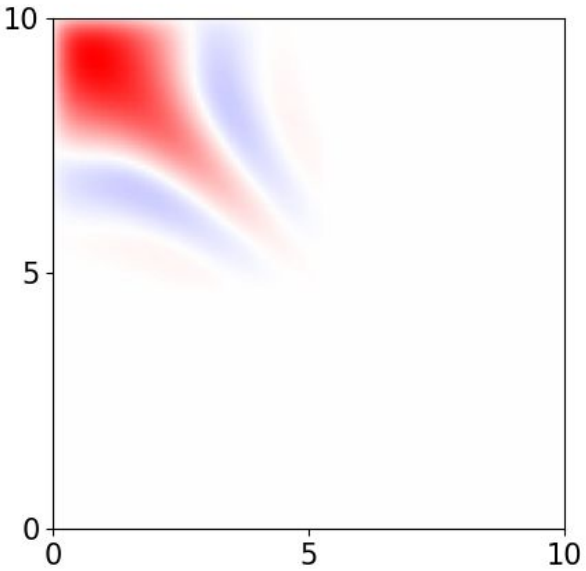
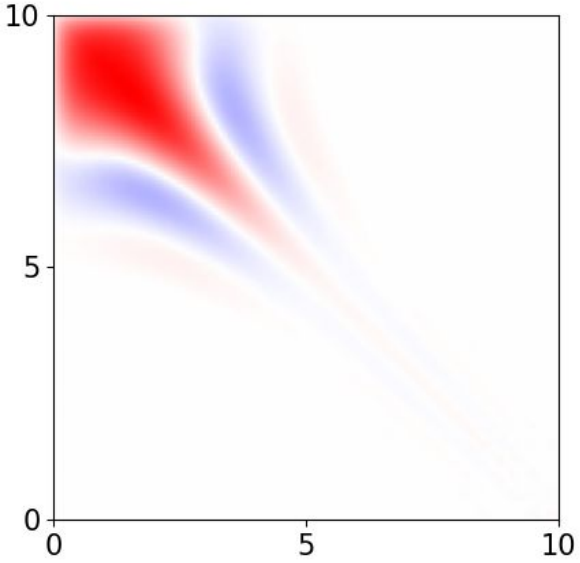
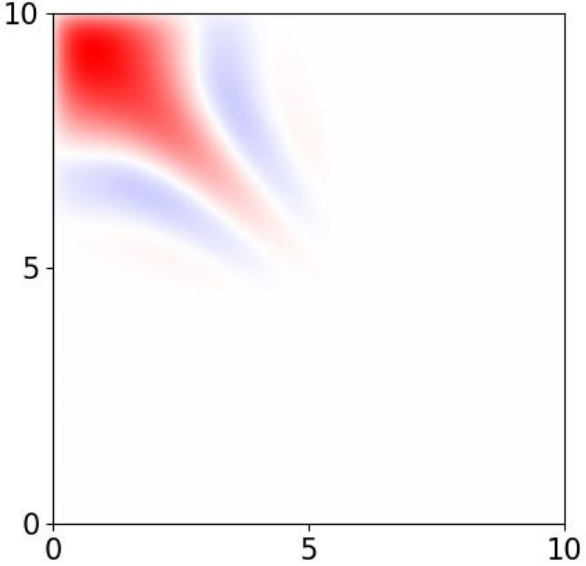


Simulation results

Monte Carlo Wavefunction

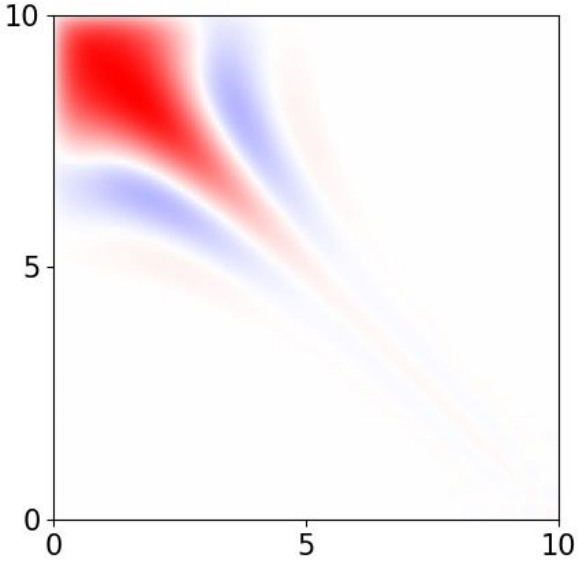


Neural Network

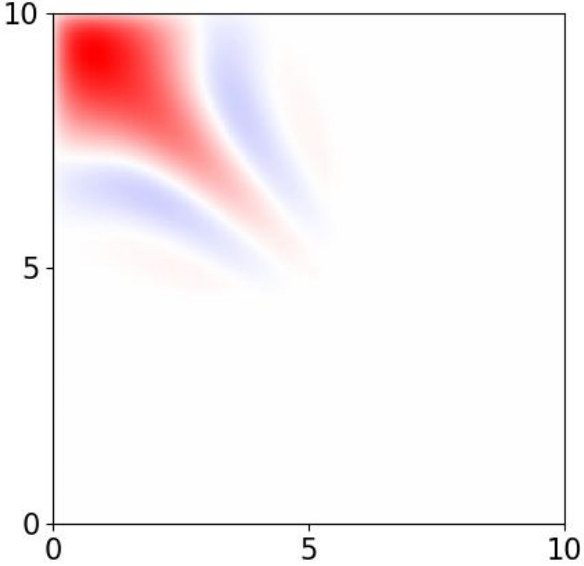


Simulation results

Monte Carlo Wavefunction

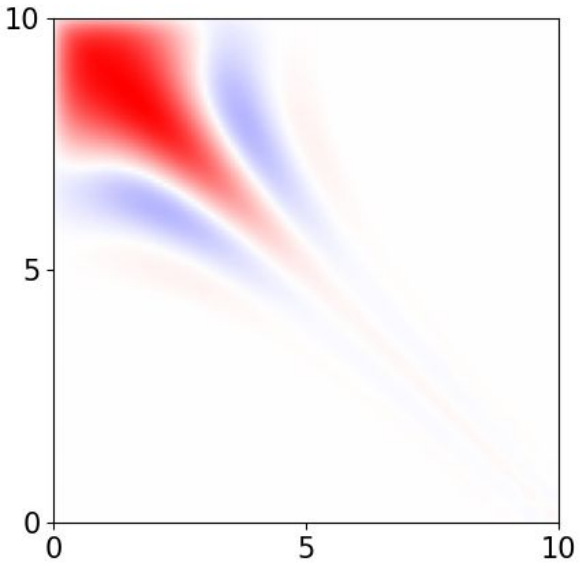


Neural Network

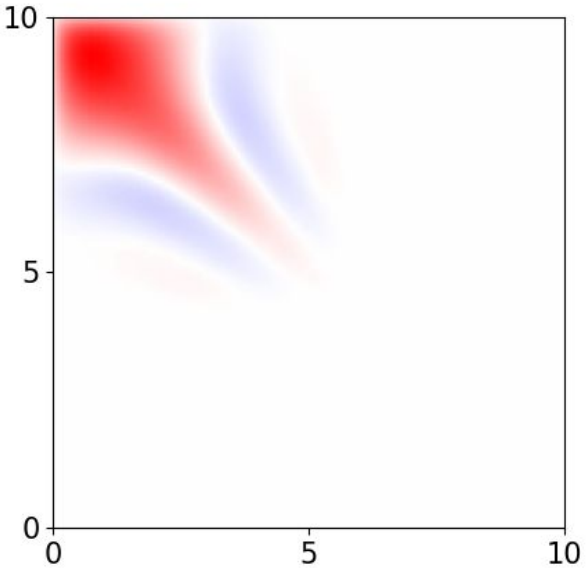


Simulation results

Monte Carlo Wavefunction



Neural Network



Simulation results

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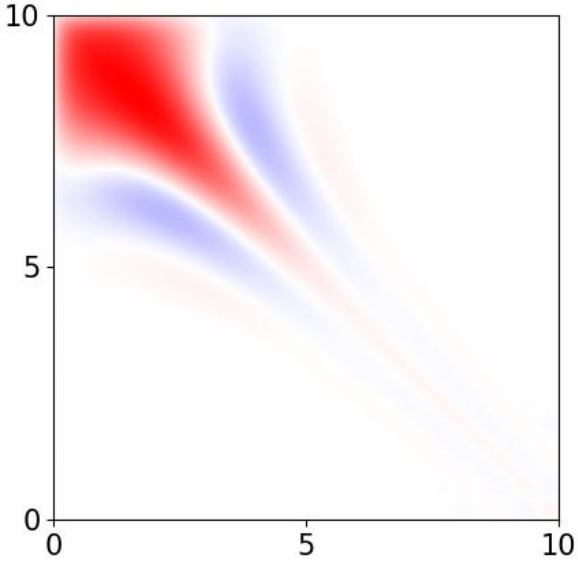

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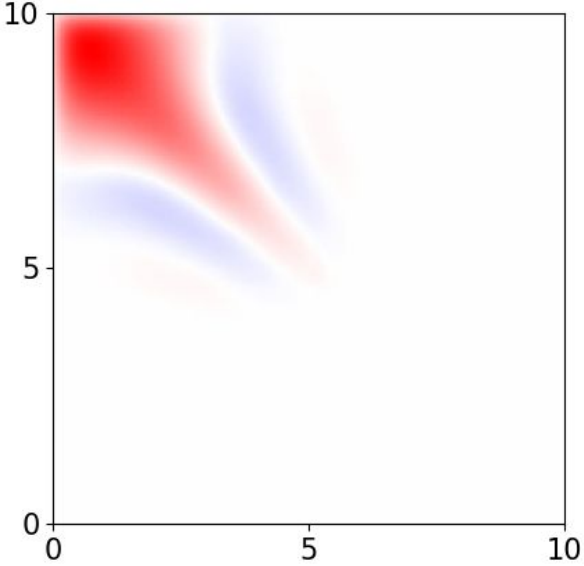
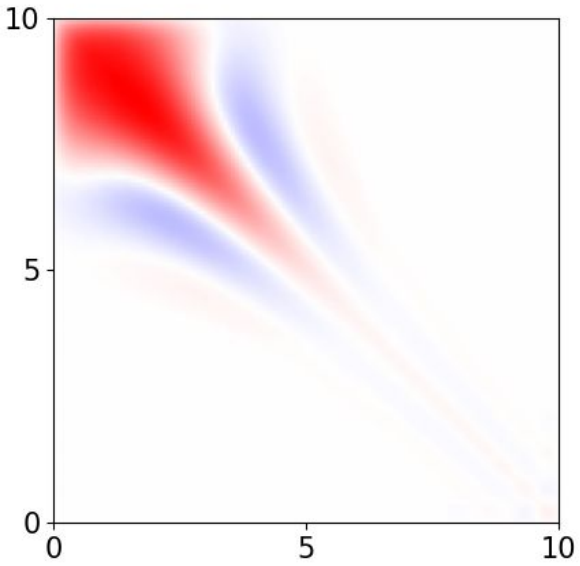


Simulation results

Monte Carlo Wavefunction



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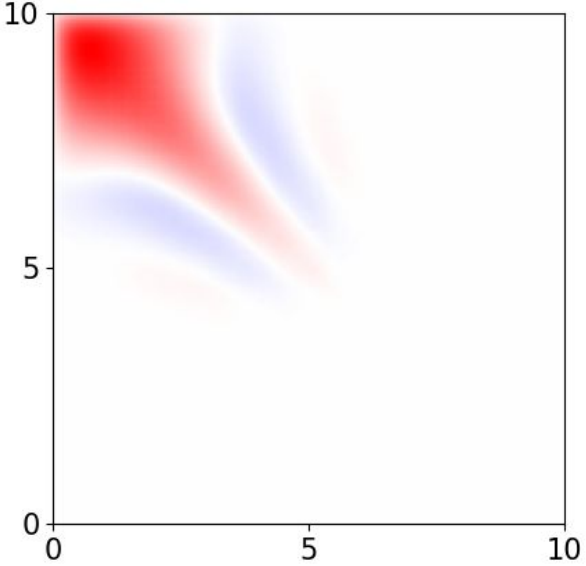
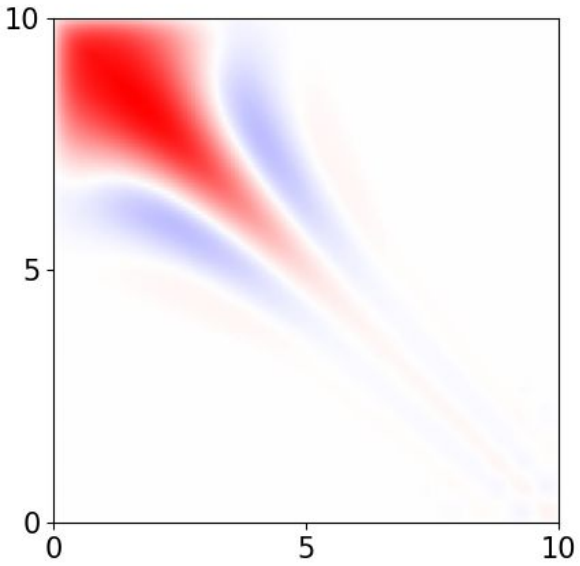
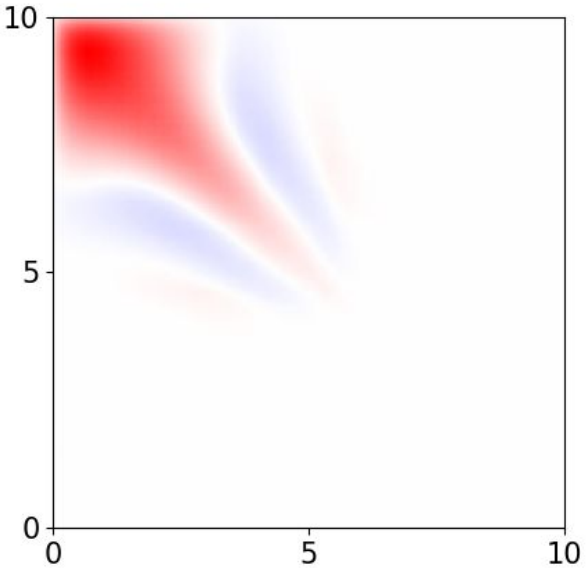


Simulation results

Monte Carlo Wavefunction

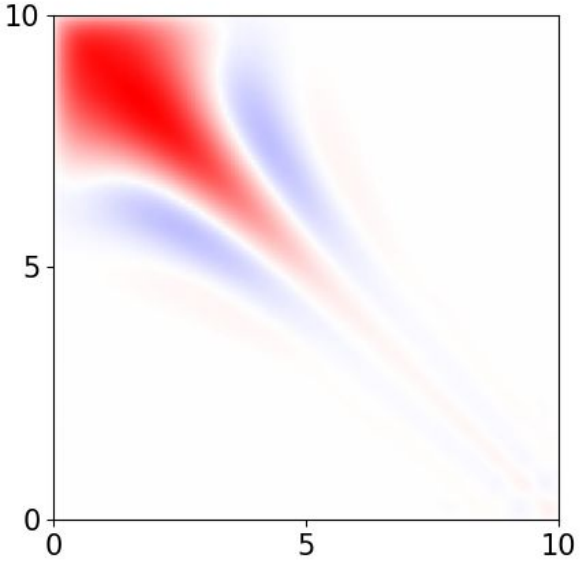


Neural Network

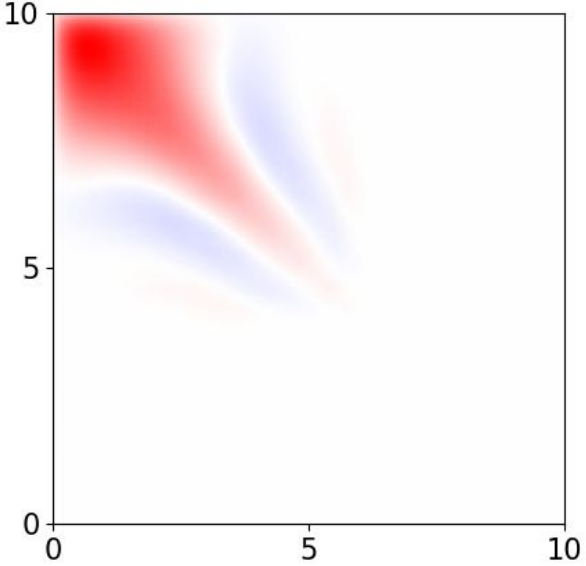


Simulation results

Monte Carlo Wavefunction



Neural Network



Simulation results

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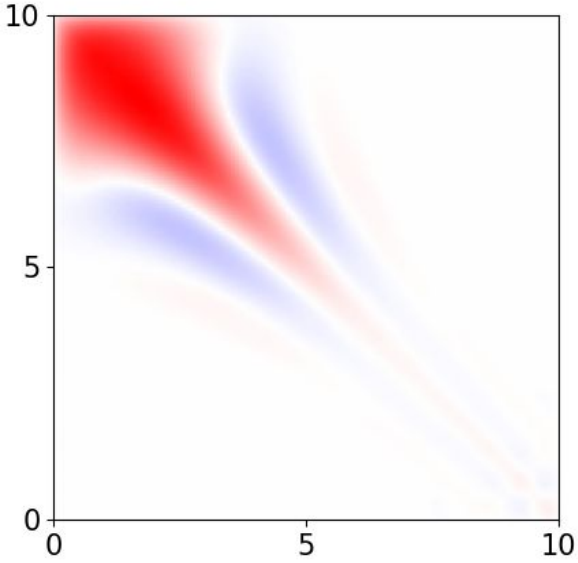

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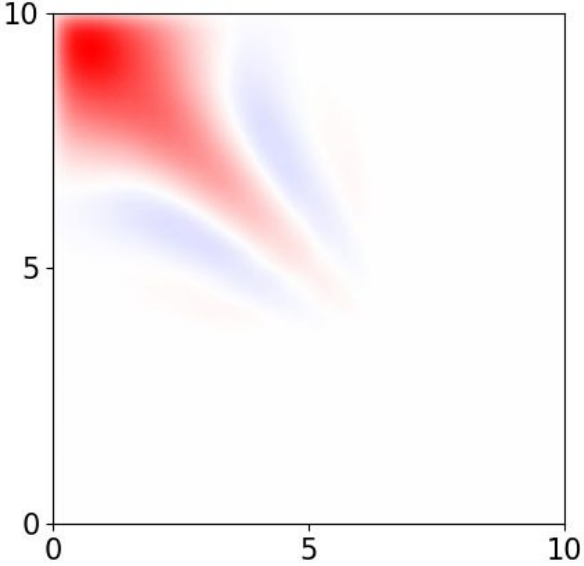
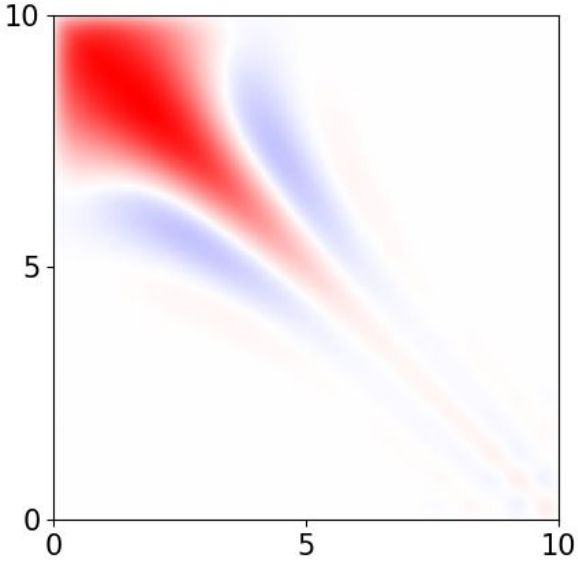
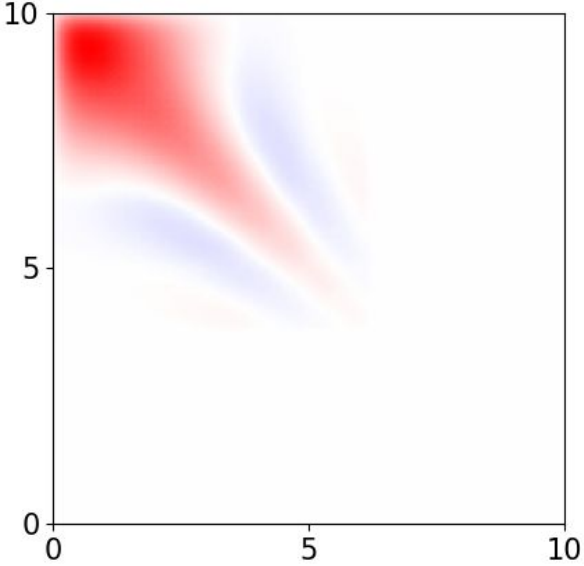


Simulation results

Monte Carlo Wavefunction

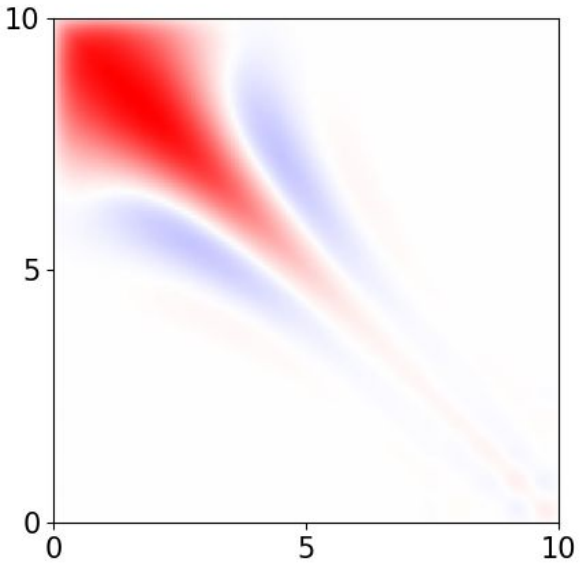


Neural Network

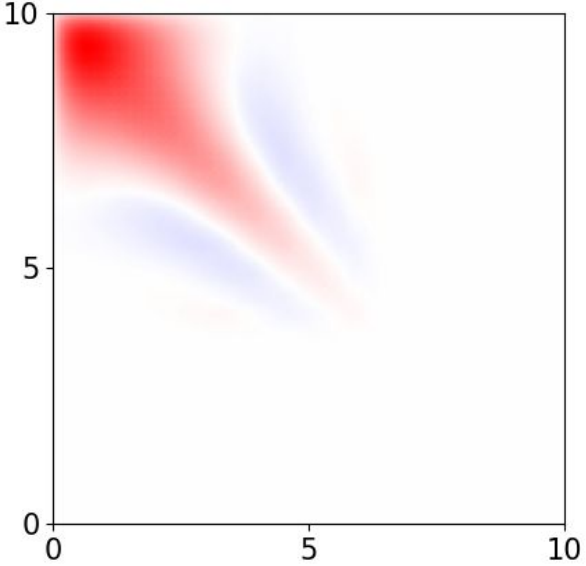


Simulation results

Monte Carlo Wavefunction

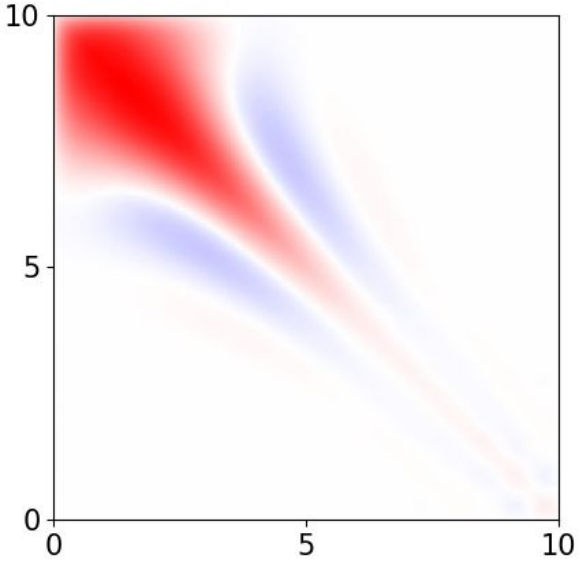


Neural Network



Simulation results

Monte Carlo Wavefunction



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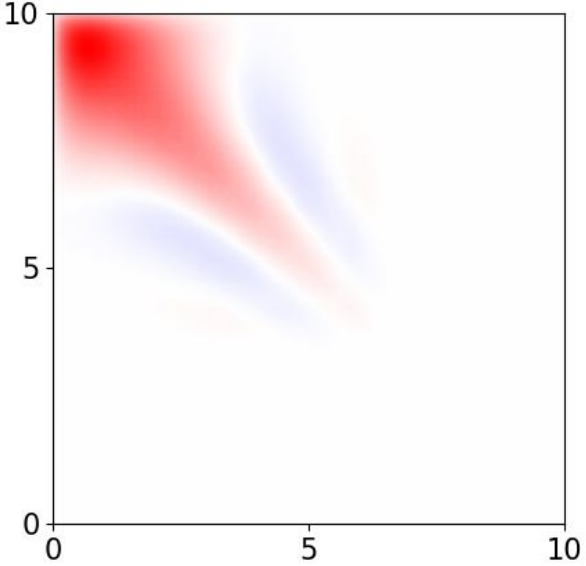
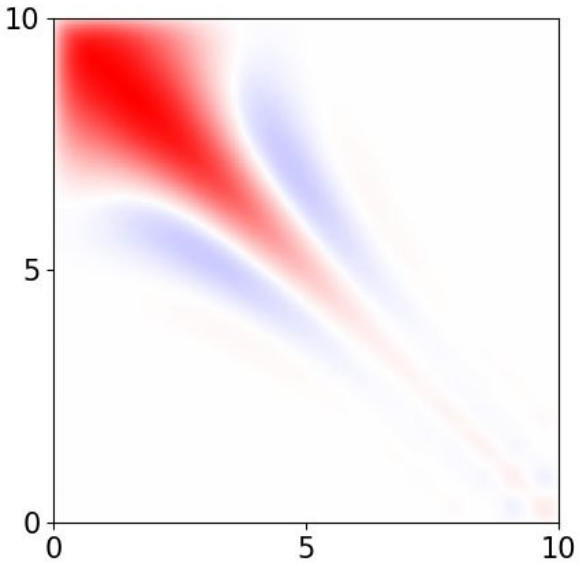
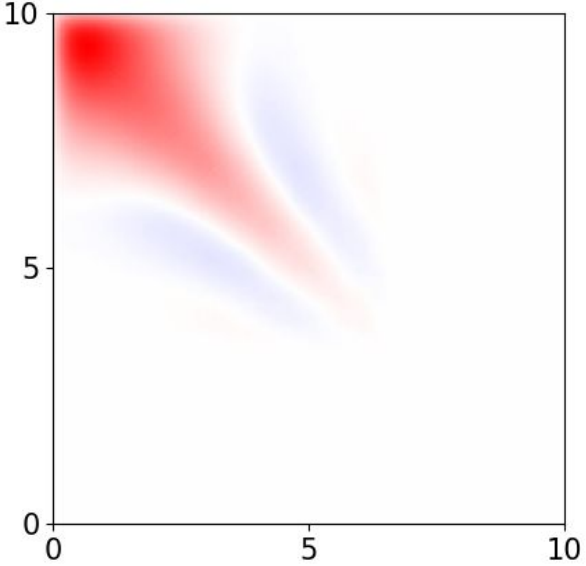


Simulation results

Monte Carlo Wavefunction

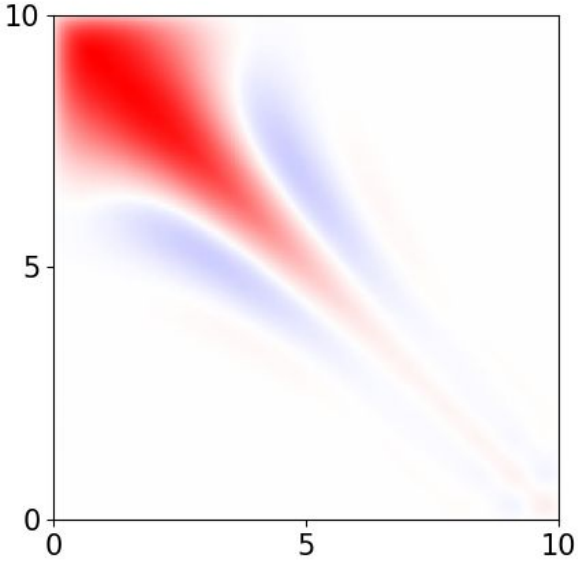


Neural Network



Simulation results

Monte Carlo Wavefunction



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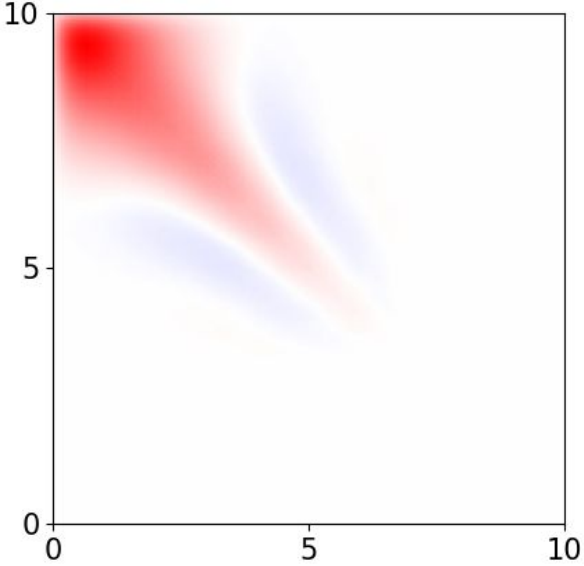
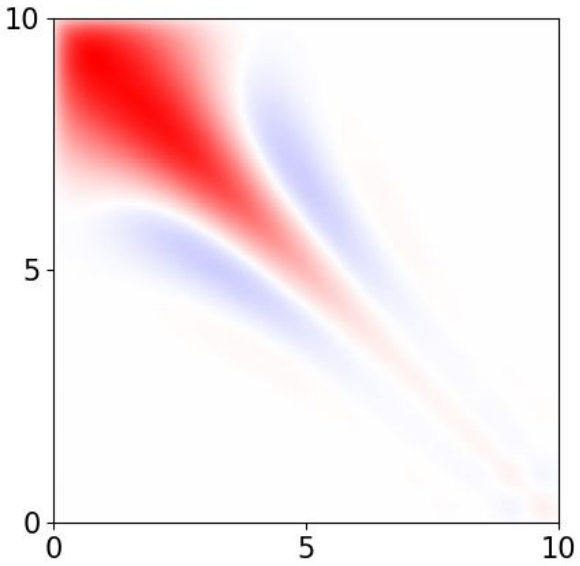


Simulation results

Monte Carlo Wavefunction



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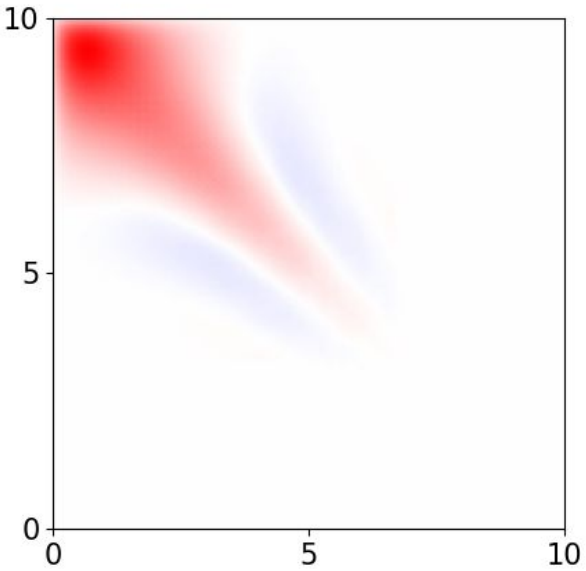
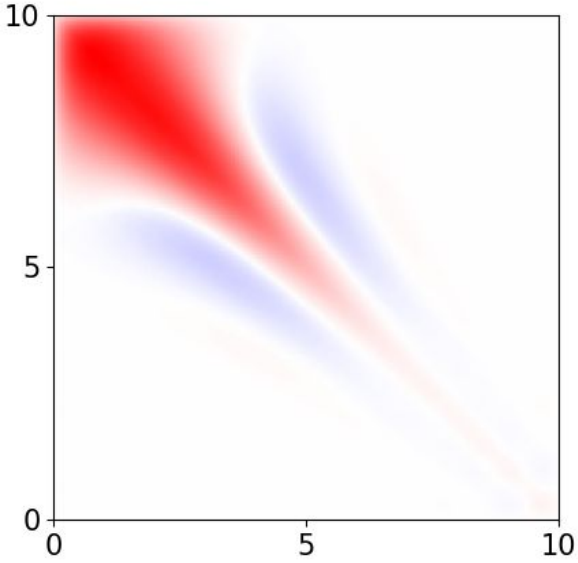


Simulation results

Monte Carlo Wavefunction



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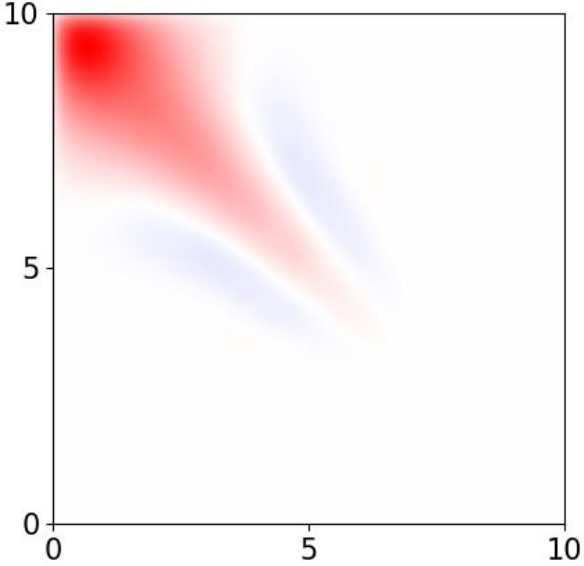
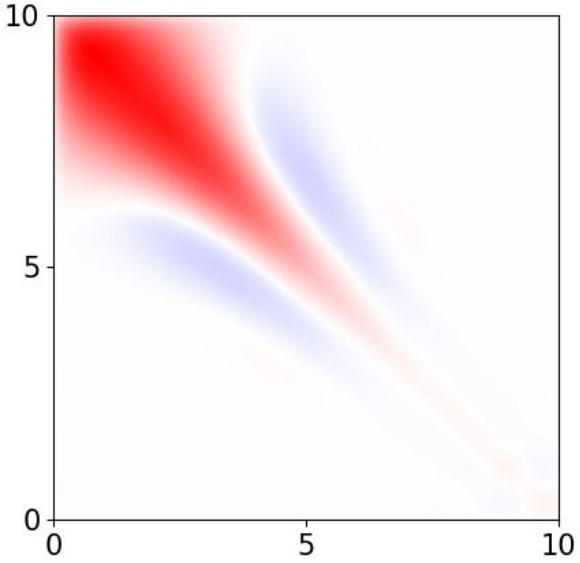


Simulation results

Monte Carlo Wavefunction



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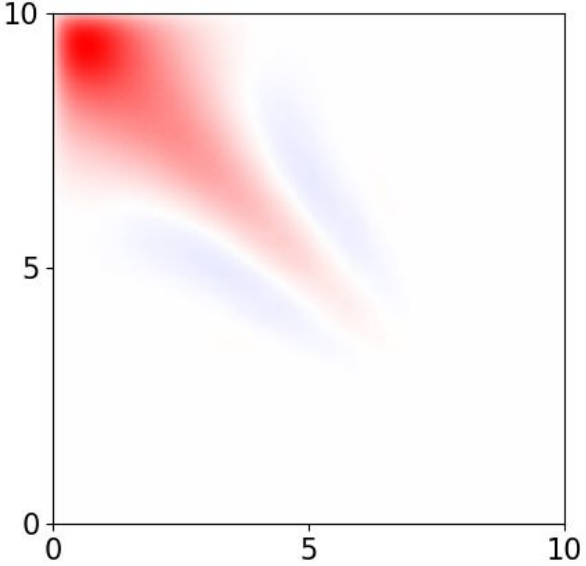
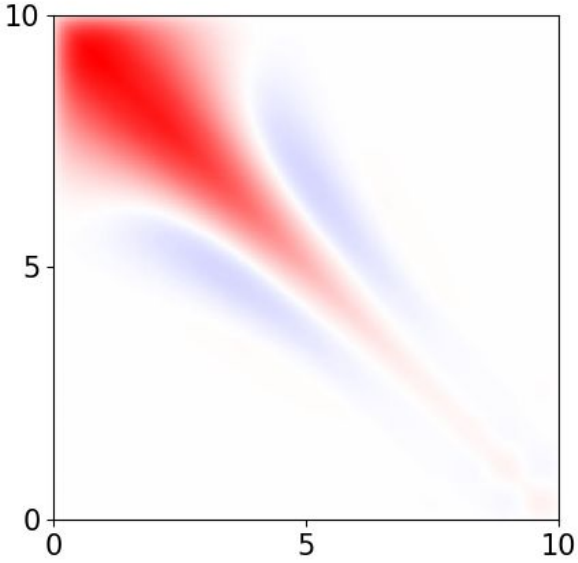


Simulation results

Monte Carlo Wavefunction



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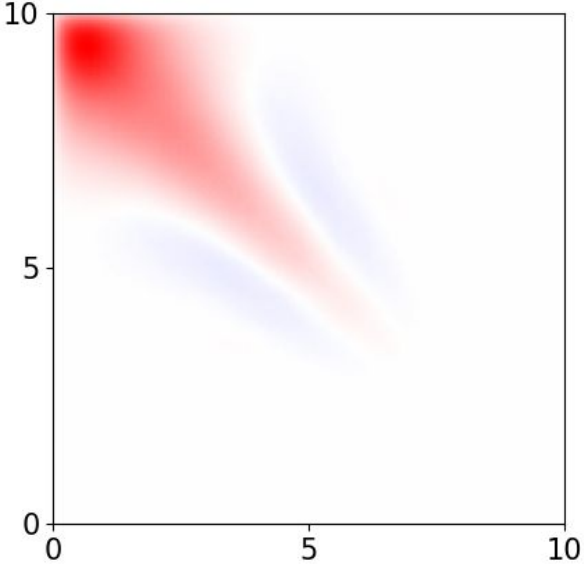
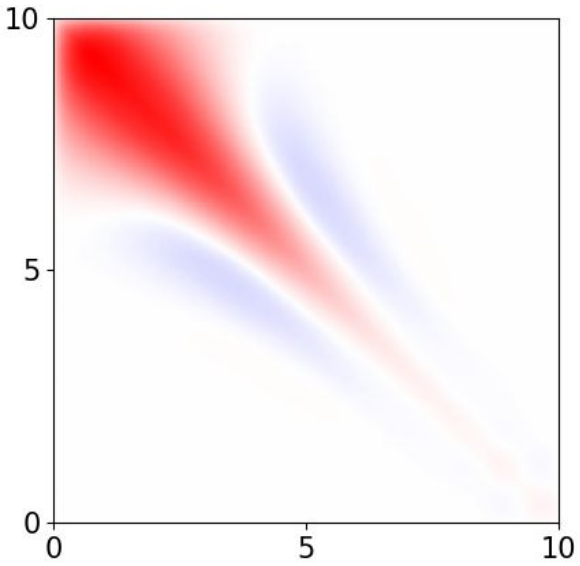


Simulation results

Monte Carlo Wavefunction



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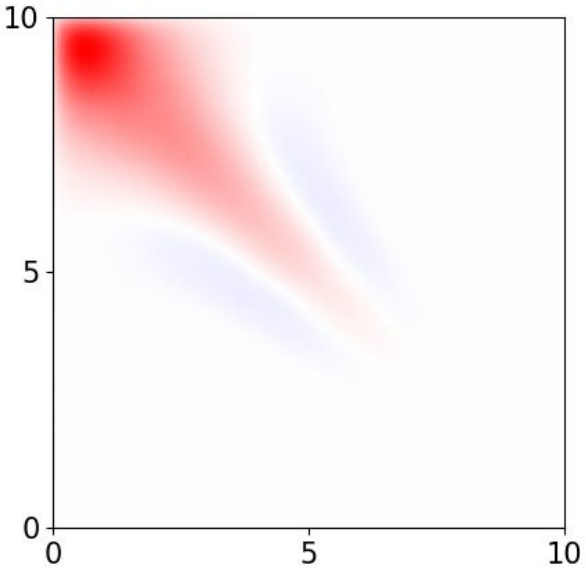

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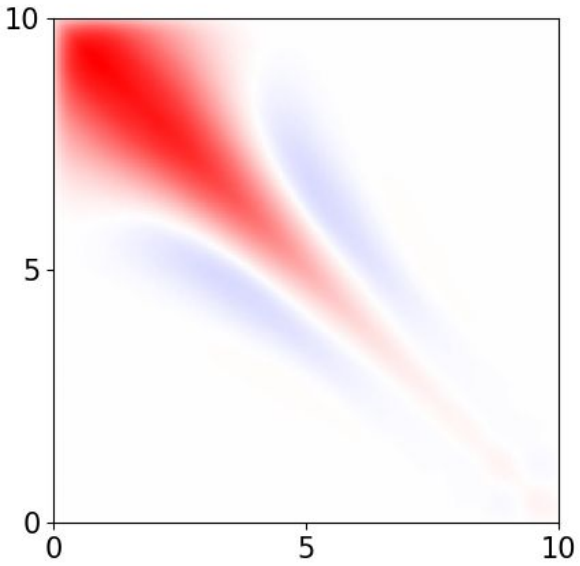

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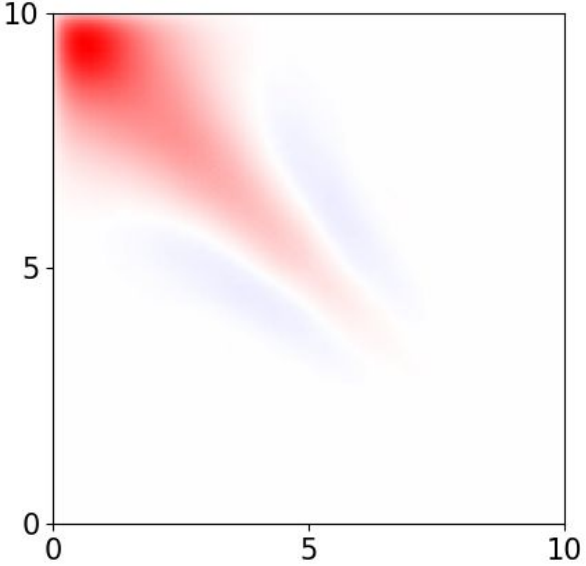

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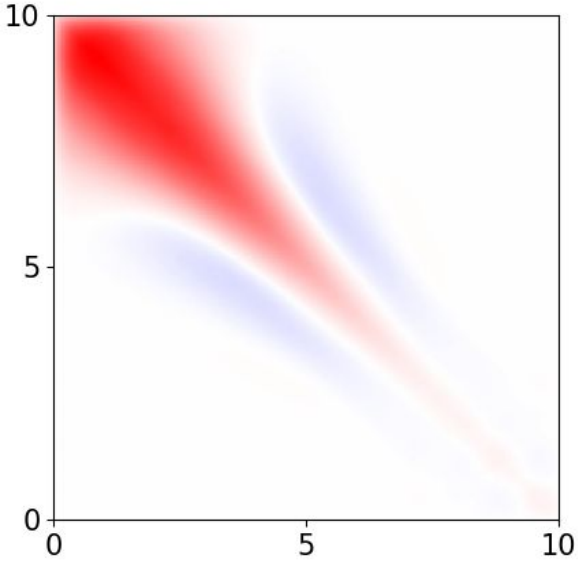

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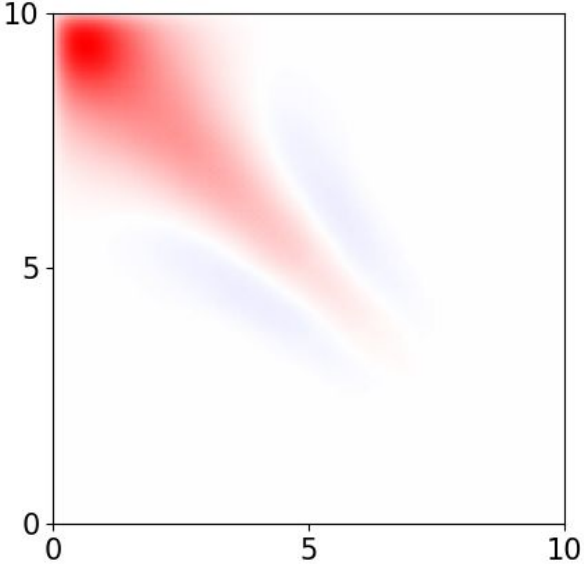
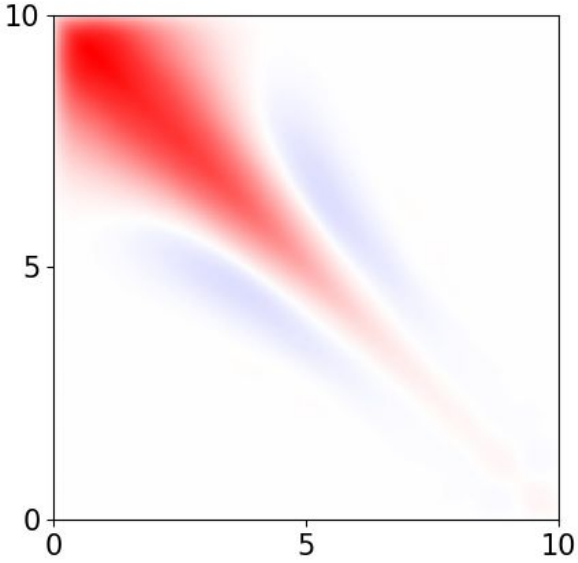


Simulation results

Monte Carlo Wavefunction



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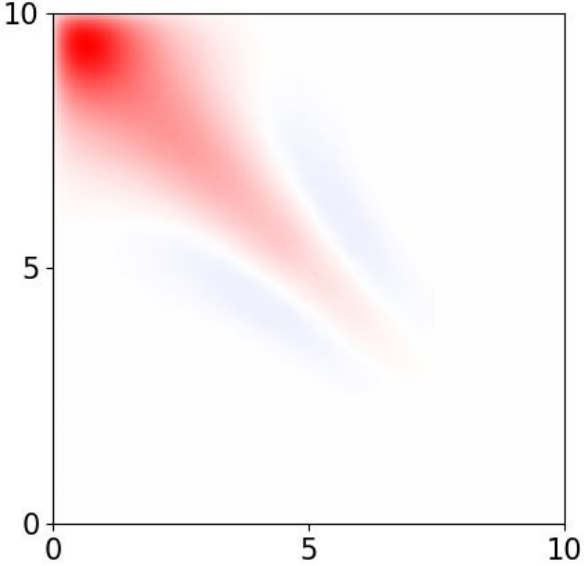
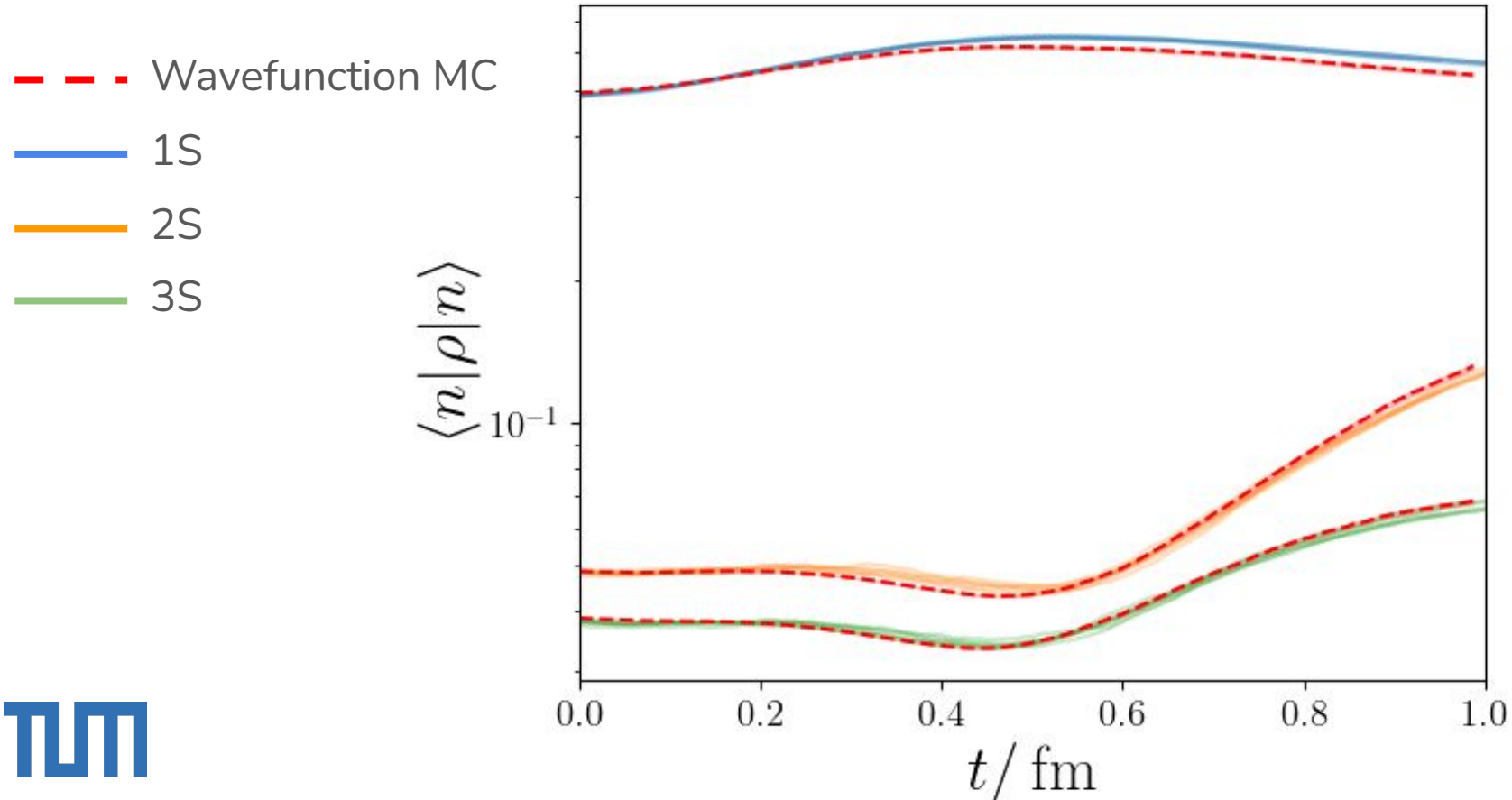


Simulation results



✓

- Time evolution works
- Scaling to larger systems seems to work
- Reasonable stability around certain parameters spots

?

- Optimization still seems very hard ? (use something geometry aware?)
- How far can we scale ?

Outlook

How far is this scalable ?

larger hilbert spaces ?

Scalar field theory?

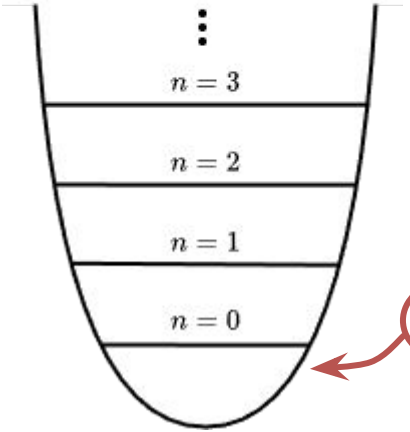
Many body dynamics?

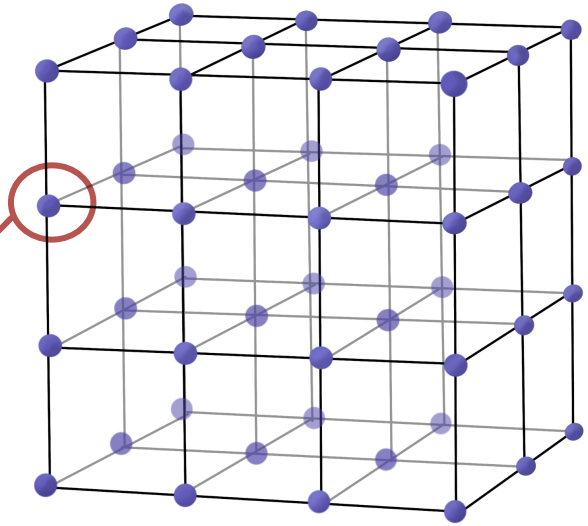
Gauge theories?

- **Guarantees of correctness**
- **What do we really need for scale ?**

Backup

Hamiltonian methods





$$|\phi\rangle \in \mathcal{H}$$

$$i\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle$$

Caldeira leggett

$$\frac{d\rho}{dt} = -i[H,\rho] + C\rho C^\dagger - \frac{1}{2}\{C^\dagger C, \rho\}$$

$$H = \frac{p^2}{M} - \frac{\alpha}{x} + \beta\{x,p\}$$

$$C = x + \gamma i p$$

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 $c = -\frac{1}{2}$

Cranck Nicholoson

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

$$U_- = 1 - \frac{dt}{2}L$$

$$U_+ = 1 + \frac{dt}{2}L$$

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