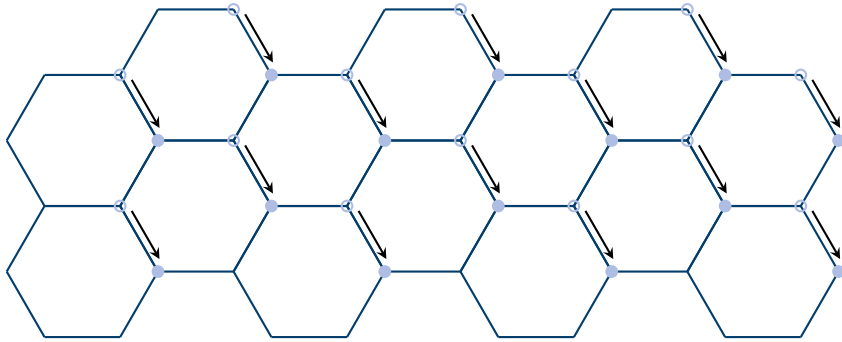


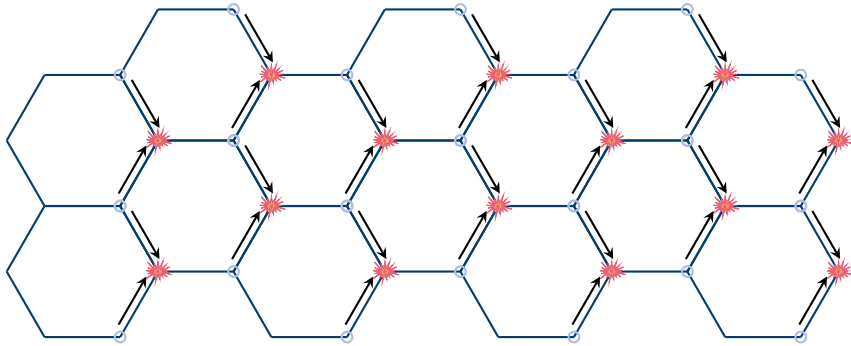
MITIGATING THE HUBBARD SIGN PROBLEM

A Novel Application of Machine Learning

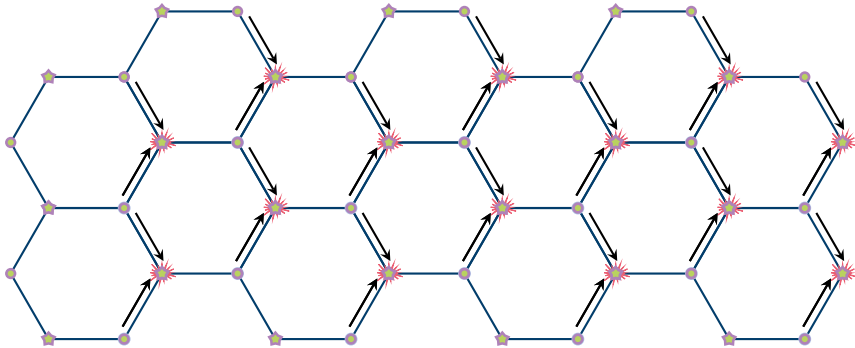
August 9, 2022 | Marcel Rodekamp, Christoph Gántgen | Jülich Supercomputing Center (JSC)



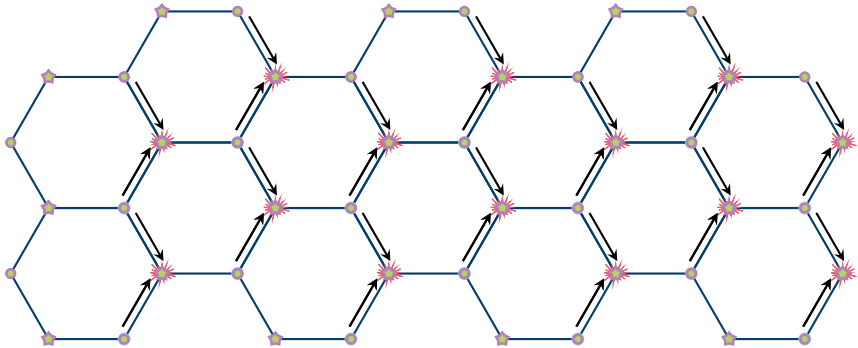
$$\hat{\mathcal{H}} = - \sum_{x,y=0}^{N_x-1} \sum_{\sigma} \left(\hat{a}_{x,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{y,\sigma} + \hat{a}_{y,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{x,\sigma} \right)$$



$$\hat{\mathcal{H}} = - \sum_{x,y=0}^{N_x-1} \sum_{\sigma} \left(\hat{a}_{x,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{y,\sigma} + \hat{a}_{y,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{x,\sigma} \right) + \frac{U}{2} \sum_{x=0}^{N_x-1} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow})^2$$

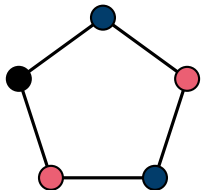
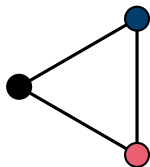


$$\hat{\mathcal{H}} = - \sum_{x,y=0}^{N_x-1} \sum_{\sigma} \left(\hat{a}_{x,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{y,\sigma} + \hat{a}_{y,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{x,\sigma} \right) + \frac{U}{2} \sum_{x=0}^{N_x-1} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow})^2 + \mu \sum_{x=0}^{N_x-1} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow})$$



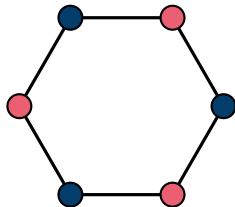
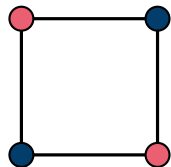
$$\hat{\mathcal{H}} \xrightarrow[\text{Stratonovich}]{\text{Hubbard}} S[\Phi] \quad \wedge \quad \Phi \in \mathbb{R}^{N_t \cdot N_x}$$

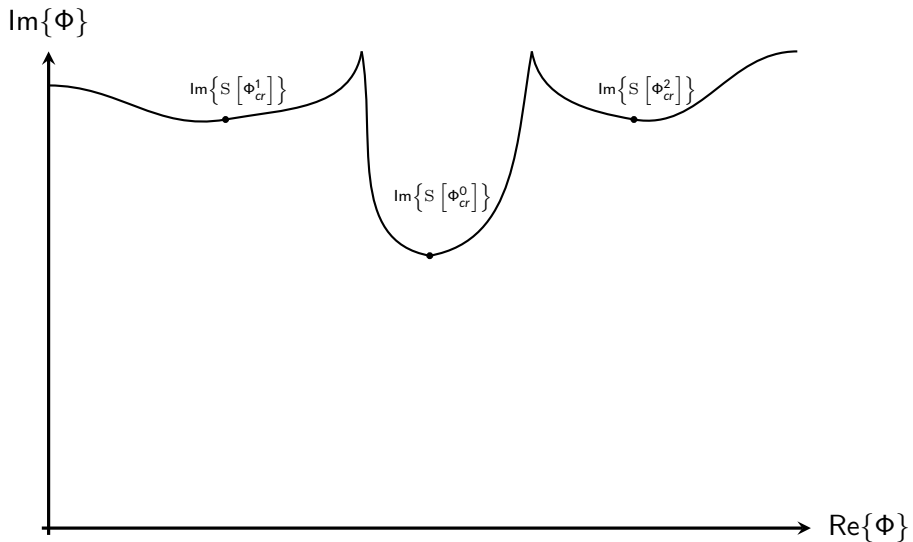
Non-Bipartite

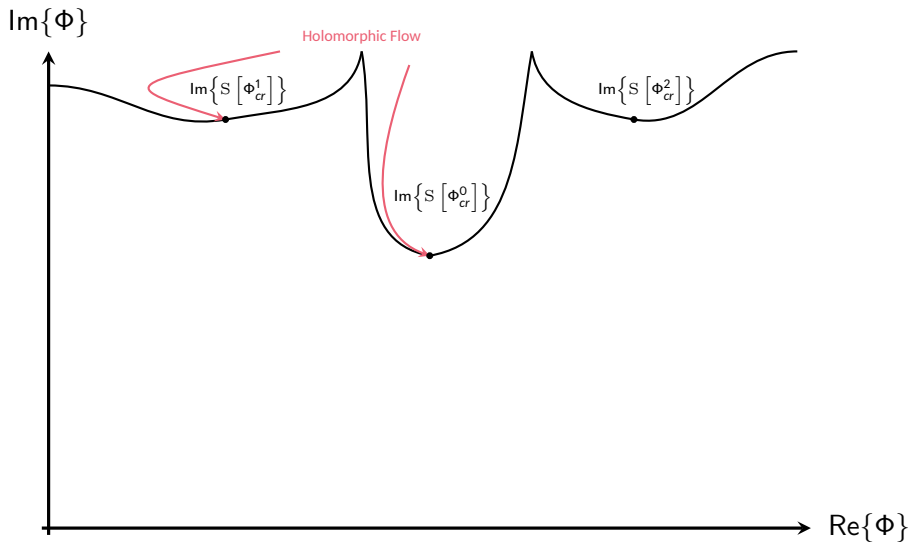


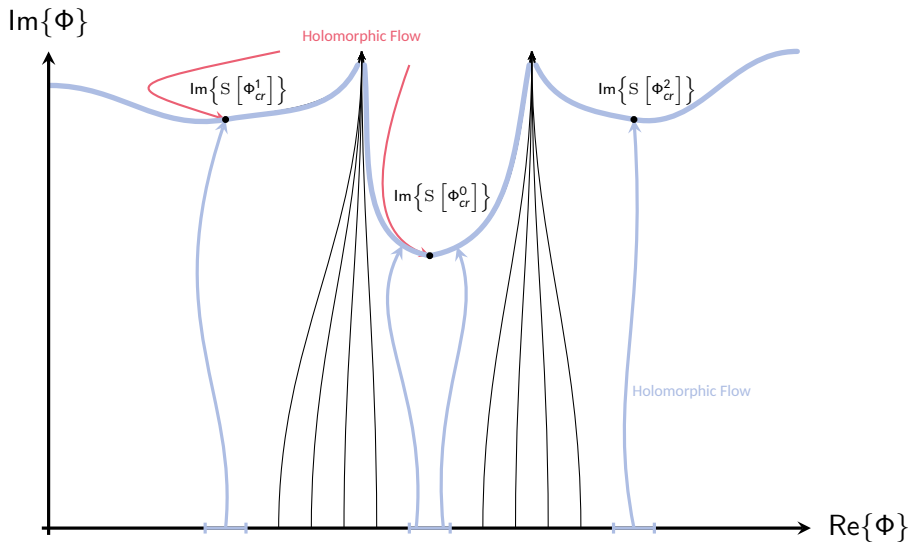
$$\mu \neq 0$$

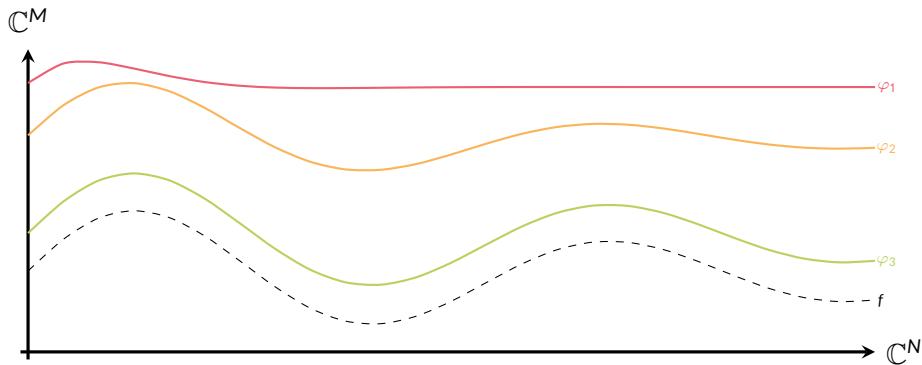
Bipartite





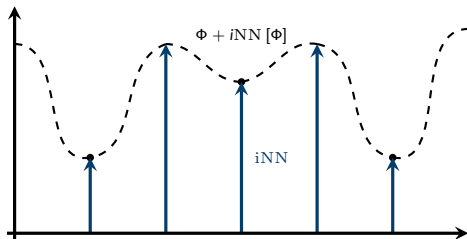






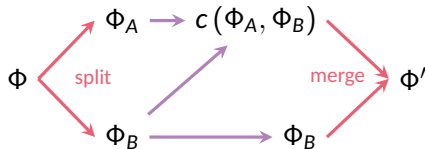
$$\mathcal{F}_\varphi = \{\varphi_i : \mathbb{C}^N \rightarrow \mathbb{C}^M\} \xleftrightarrow[\text{Approximation}]{\text{Universal}} \sup_z |f(z) - \varphi_i(z)| < \varepsilon$$

$\mathbb{R}$ -Valued Neural Network

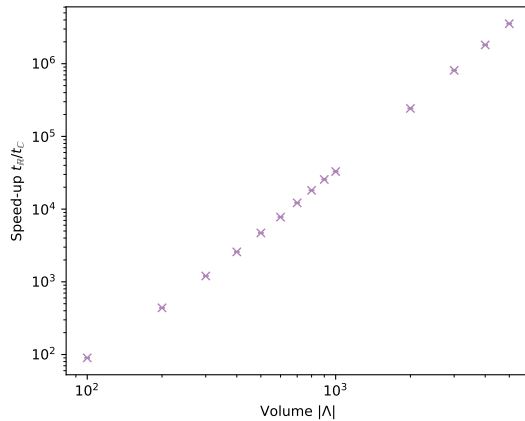
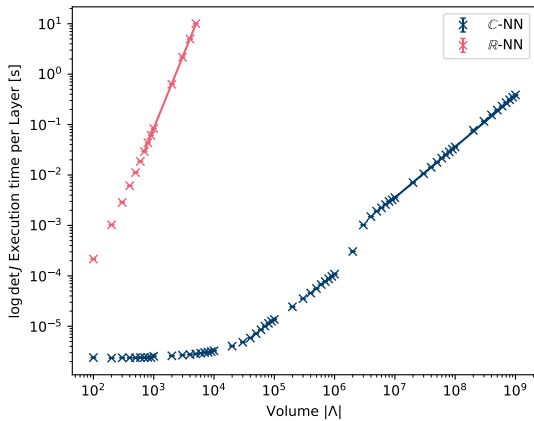


$$\mathbb{1} + i \begin{pmatrix} \frac{\partial NN[\Phi]_0}{\partial \Phi_0} & \dots & \frac{\partial NN[\Phi]_{|\Lambda|}}{\partial \Phi_0} \\ \vdots & \ddots & \vdots \\ \frac{\partial NN[\Phi]_0}{\partial \Phi_{|\Lambda|}} & \dots & \frac{\partial NN[\Phi]_{|\Lambda|}}{\partial \Phi_{|\Lambda|}} \end{pmatrix}$$

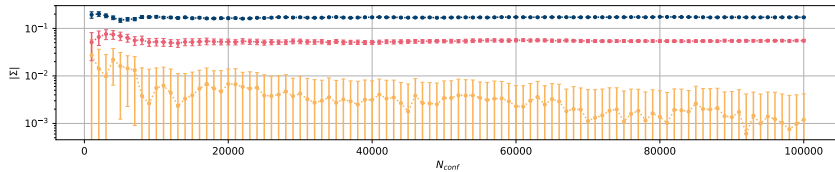
$\mathbb{C}$ -Valued Neural Network



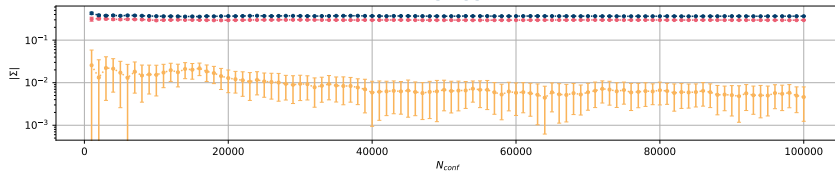
$$\begin{pmatrix} \frac{\partial c(\Phi_A, \Phi_B)}{\partial \Phi_A} & 0 \\ \star & \mathbb{1} \end{pmatrix}$$



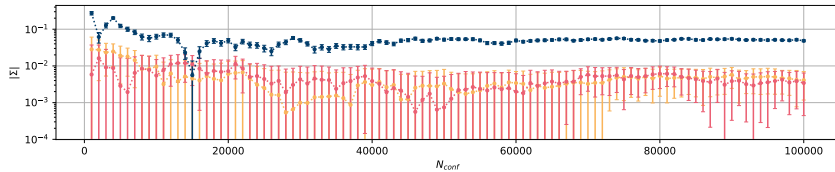
2 Sites



4 Sites



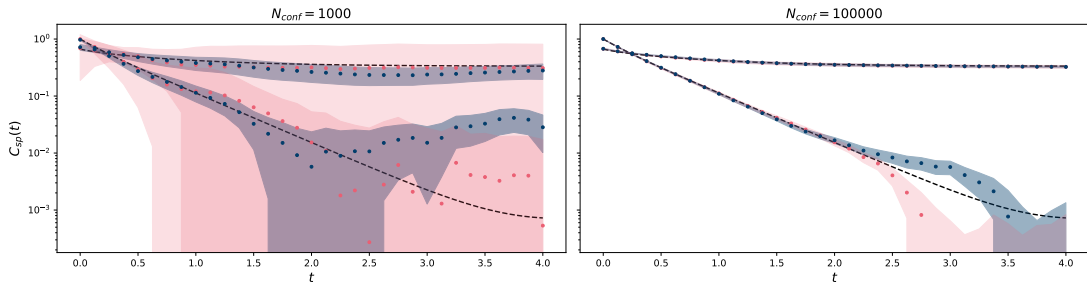
8 Sites



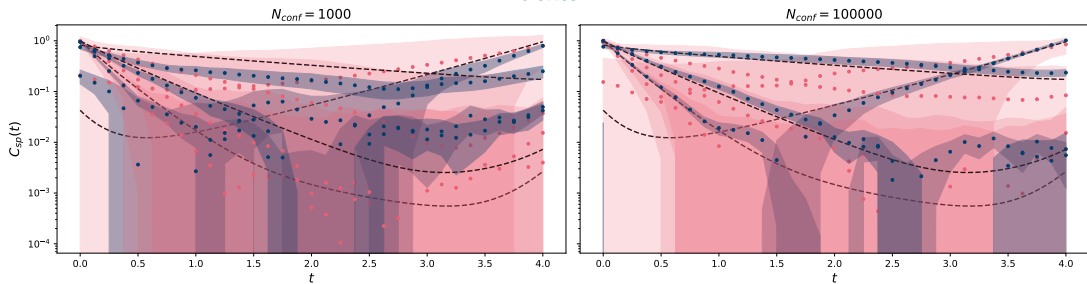
Real Plane HMC Tangent Plane HMC ML HMC

$N_t = 32, \beta = 4, U = 4, \mu = 3$

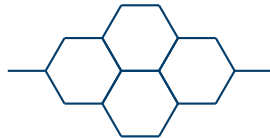
2 Sites



8 Sites



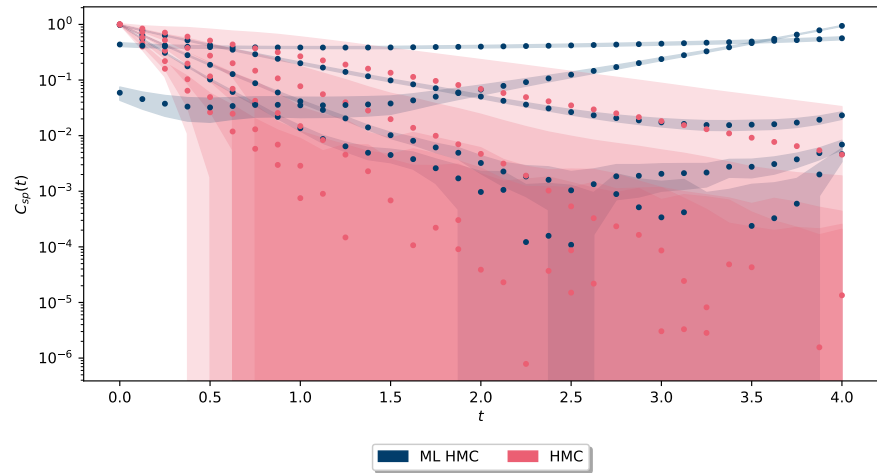
ML HMC HMC Exact Diagonalization

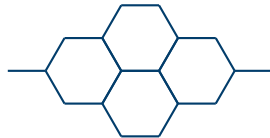


18 Sites

$$N_t = 32, \beta = 4, U = 3$$

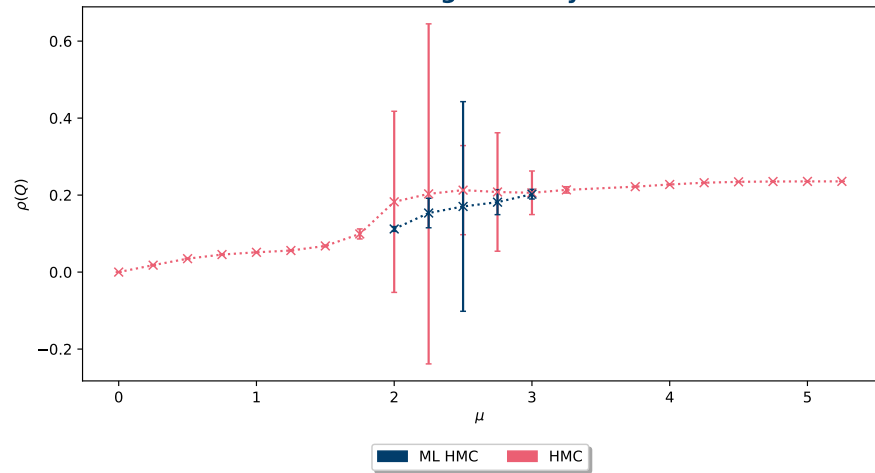
$$\mu = 3$$

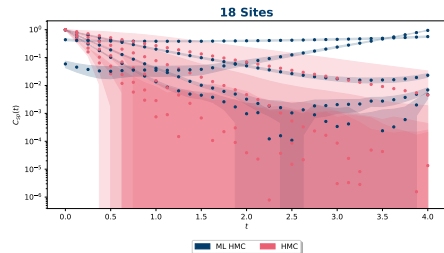
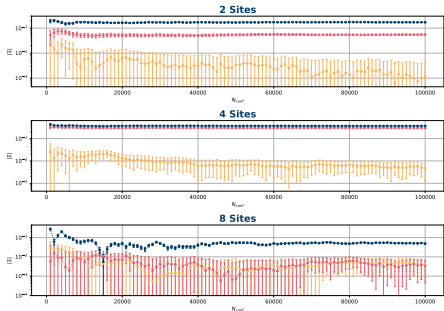




$N_t = 32, \beta = 5, U = 2$

Charge Density





The Team: arXiv 2203.00390



Evan
Berkowitz



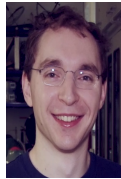
Christoph
Gäntgen



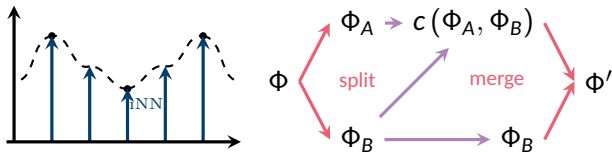
Stefan
Krieg



Tom Luu



Johann
Ostmeyer



$$\hat{\mathcal{H}} = - \sum_{x,y=0}^{N_x-1} \sum_{\sigma} \left(\hat{a}_{x,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{y,\sigma} + \hat{a}_{y,\sigma}^{\dagger} \kappa_{x,y} \hat{a}_{x,\sigma} \right) + \frac{U}{2} \sum_{x=0}^{N_x-1} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow})^2 + \mu \sum_{x=0}^{N_x-1} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow}) \quad (1)$$

■ Electron creation-/annihilation operator

$$\hat{a}_{x,\sigma}^{\dagger} \wedge \hat{a}_{x,\sigma} \quad (2)$$

- Lattice site $x \in [0, N_x - 1]$
- Spin $\sigma \in \{\uparrow, \downarrow\}$

■ Number operator

$$\hat{n}_{x,\sigma} = \hat{a}_{x,\sigma}^{\dagger} \hat{a}_{x,\sigma} \quad (3)$$

Particle-Hole Basis

$$\hat{p}_x^{\dagger} = \hat{a}_{x,\uparrow}^{\dagger}, \hat{p}_x = \hat{a}_{x,\uparrow} \quad \wedge \quad \hat{h}_x^{\dagger} = \hat{a}_{x,\downarrow}, \hat{h} = \hat{a}_{x,\downarrow}^{\dagger} \quad (4)$$

$$\hat{n}_x^p = \hat{p}_x^{\dagger} \hat{p}_x \quad \wedge \quad \hat{n}_x^h = \hat{h}_x^{\dagger} \hat{h}_x \quad (5)$$

■ Hopping Matrix $\kappa_{x,y}$

- Geometry of the Lattice (nearest neighbours)
- Hopping amplitude

■ On-Site Interaction U

■ Chemical Potential μ

- Trotterize $e^{-\beta\hat{\mathcal{H}}}$

$$e^{-\beta\hat{\mathcal{H}}} = e^{-\delta\hat{\mathcal{H}}} \dots e^{-\delta\hat{\mathcal{H}}} \Big|_{\delta=\beta/N_t} \quad (6)$$

- Introduce set of coherent states $\Psi_{x,t}, \Psi_{x,t}^\dagger$
- Hubbard-Stratonovich transformation $\rightarrow \Phi_{t,x} \in \mathbb{R}$
- Integrate out fermionic dof. $M[\Phi \mid \kappa, \mu]$

$$S[\Phi] = \frac{1}{\delta U} \sum_{t=0}^{N_t-1} \sum_{x=0}^{N_x-1} \Phi_{t,x}^2 - \log \det \{ M[\Phi \mid \kappa, \mu] \cdot M[-\Phi \mid -\kappa, -\mu] \} \quad (7)$$

$$S[\Phi] \in \mathbb{C} \Rightarrow \frac{1}{Z} e^{-\text{Re}\{S\} + i \text{Im}\{S\}} \in \mathbb{C}$$

Reweightings

$$\langle O \rangle = \frac{\langle O e^{-i \text{Im}\{S\}} \rangle_{\text{Re}}}{\langle e^{-i \text{Im}\{S\}} \rangle_{\text{Re}}}$$

- Real Boltzmann weight
- $\langle e^{-i \text{Im}\{S\}} \rangle$ hard to estimate

Lefschetz Thimbles

$$\frac{d\Phi}{d\tau_f} = \pm \left(\frac{\partial S[\Phi]}{\partial \Phi} \right)^*$$

- Critical Points

$$\left. \frac{\partial S[\Phi]}{\partial \Phi} \right|_{\Phi = \Phi_{cr}^\sigma} = 0$$

■ Single Particle Correlator

$$C_{sp}^{xy}(t) = \langle \hat{p}(t) \hat{p}^\dagger(0) \rangle = \left\langle \sum_{\tau=0}^{N_t-1} M_{x,t+\tau;y,\tau}^p(\Phi)^{-1} \right\rangle \quad (8)$$

■ Charge Density

$$\rho(Q) = \frac{1}{N_x} \sum_{x=0}^{N_x-1} \langle \hat{\eta}_x^p - \hat{\eta}_x^h \rangle \quad (9)$$