Neural Wavefunctions in Quantum Field Theory

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Variational Monte Carlo

- Variational principle: Trial wavefunction Ψ_θ has minimum energy at the ground state

$$E_\theta = \frac{\langle \Psi_\theta | H | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \geq E_0$$

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- Minimize with gradient descent

VMC for lattice field theories

- Parameterize the wavefunctional $\Psi[\phi_x]$ on a spatial lattice

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$$m = E_1 - E_0$$

UV finite
IR finite

UV divergent
IR divergent

Nonlinear sigma model

The 1+1d nonlinear O(3) sigma model is defined by

$$S = \frac{1}{2g^2} \int d^2x \, (\partial_\mu n)^2 \qquad\qquad n(x) \cdot n(x) = 1$$

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We use the discretized Hamiltonian on a 1d spatial lattice with PBCs

$$H = -\frac{\sqrt{\eta}g^2}{2}\sum_{x=1}^{L}\nabla_x^2 - \frac{\sqrt{\eta}}{g^2}\sum_{x}^{L}\boldsymbol{n}_x\cdot\boldsymbol{n}_{x+1}$$

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Asymptotically free, with the continuum limit at $g^2 \rightarrow 0$

Variational Ansatz – Ground state

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$$\Psi^0_\theta[\mathbf{n}] = \frac{1}{L}\sum_{i=1}^{L} \exp[-\mathrm{MLP}_\theta(\mathbf{G}^{(i)})] \qquad G^{(i)}_{xy} = \mathbf{n}_{x+i} \cdot \mathbf{n}_{y+i}$$

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Translational invariance

$$G_{xy}^{(i)} = \mathbf{n}_{x+i} \cdot \mathbf{n}_{y+i}$$

O(3) invariance

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Translational invariance

O(3) invariance

- Universal ansatz for vacuum wavefunction

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$$\Psi_\theta^1[\boldsymbol{n}] = O_1 \Psi_\theta^0[\boldsymbol{n}]$$

Has k=0, I=1, I^z=0 quantum numbers

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$$\Psi^1_\theta[\boldsymbol{n}] = O_1 \Psi^0_\theta[\boldsymbol{n}] = \sum_x \boldsymbol{n}_x^{(z)} \Psi^0_\theta[\boldsymbol{n}]$$

Gets 99% of the energy right but
is not universal!

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$$\Psi^1_\theta[\boldsymbol{n}] = O_1 \Psi^0_\theta[\boldsymbol{n}] = \sum_x f_{\theta x}[\boldsymbol{n}] \boldsymbol{n}^{(z)}_x \Psi^0_\theta[\boldsymbol{n}]$$

Arbitrary function of the fields, has site index

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$$f_{\theta x}[T^k \boldsymbol{n}] = f_{\theta x+k}[\boldsymbol{n}] \longleftarrow$$ For translational invariance

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$$\Psi^1_\theta[\boldsymbol{n}] = O_1 \Psi^0_\theta[\boldsymbol{n}] = \sum_x f_{\theta x}[\boldsymbol{n}]\boldsymbol{n}^{(z)}_x \Psi^0_\theta[\boldsymbol{n}] = \sum_x \exp[-\mathrm{MLP}_\theta(\mathbf{G}^{(x)})]\boldsymbol{n}^{(z)}_x \Psi^0_\theta[\boldsymbol{n}]$$

Shifted matrix of pair products of fields

Variational Ansatz – Excited State

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$$\Psi^1_\theta[\mathbf{n}] = \frac{1}{L}\sum_{x=1}^{L} \exp[-\mathrm{MLP}_\theta(\mathbf{G}^{(x)})] n_x^{(z)} \Psi^0_{\bar{\theta}}[\mathbf{n}]$$

Fix the parameters of this wavefunction

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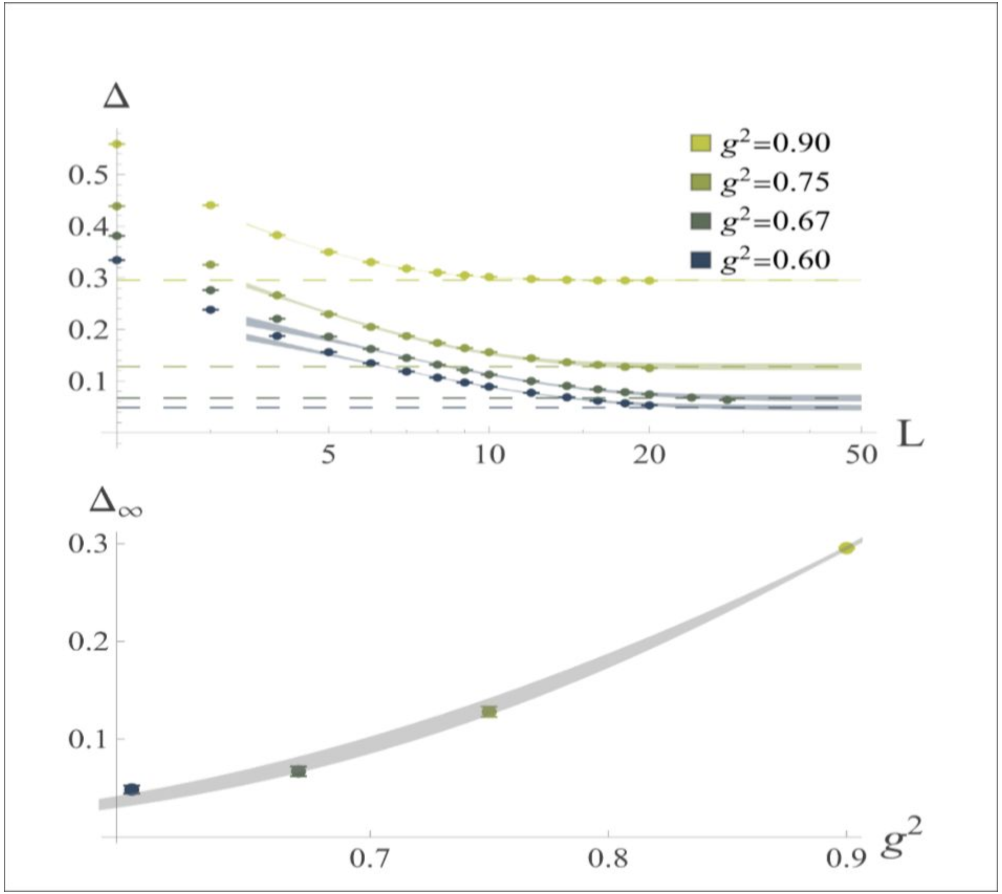
$$\Psi_\theta^1[\mathbf{n}] = \frac{1}{L}\sum_{x=1}^{L} \exp[-\mathrm{MLP}_\theta(\mathbf{G}^{(x)})] n_x^{(z)} \Psi_{\bar{\theta}}^0[\mathbf{n}]$$

Fix the parameters of this wavefunction

- Shared UV systematic error cancels in $E_1 - E_0$
- Compute E_0 and E_1 with reweighting

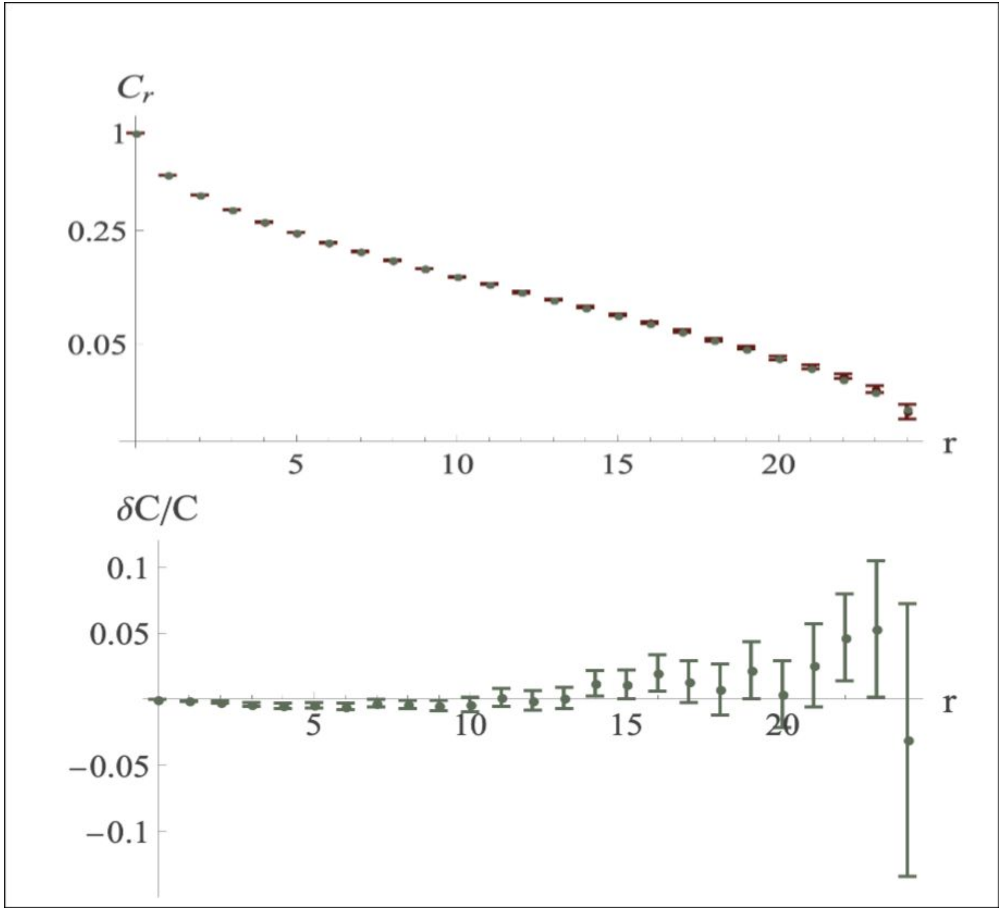
Computing the gap

- Infinite volume + continuum extrapolation of the gap



Computing correlators

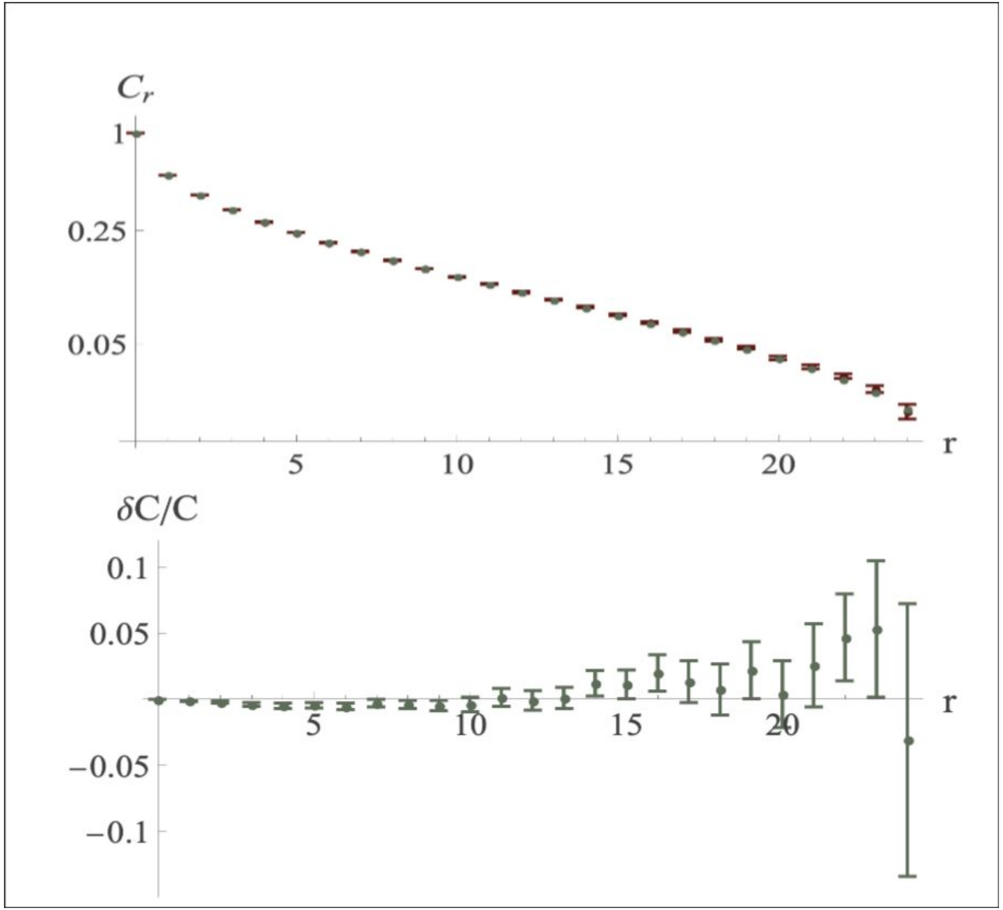
- Comparison with MPS of spatial correlators



Computing correlators

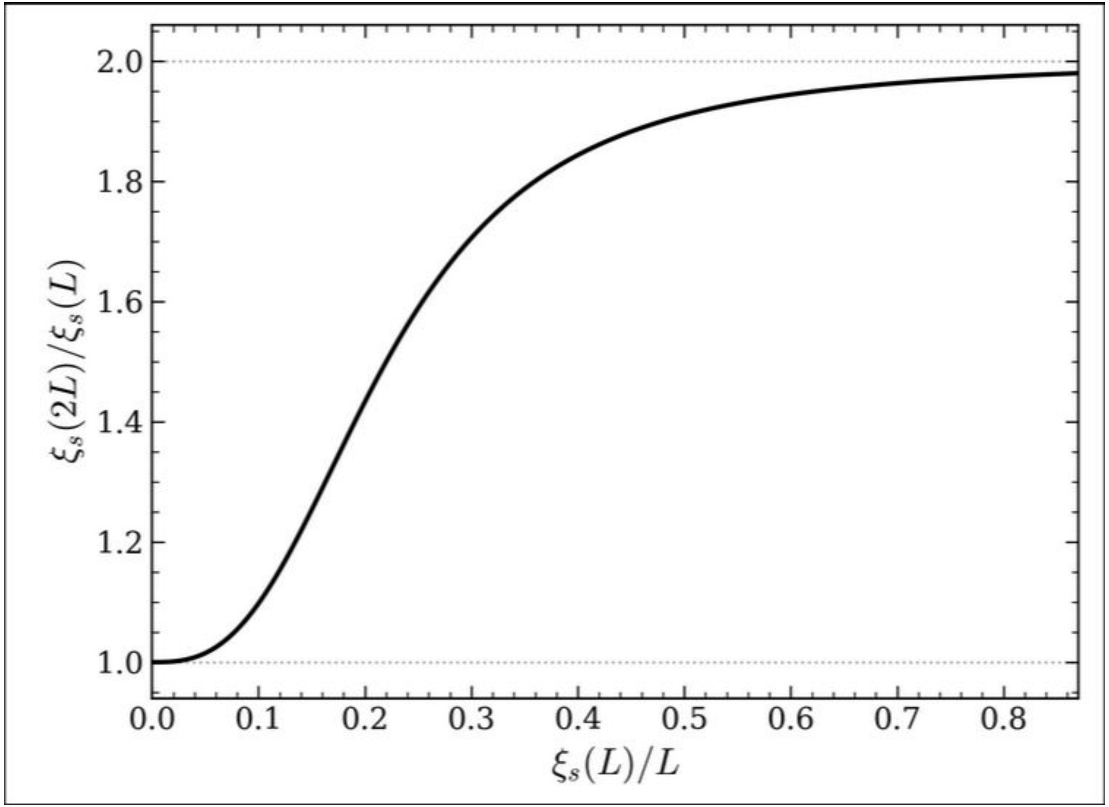
- Comparison with MPS of spatial correlators

- Long distance behavior is also captured



Step-scaling curve

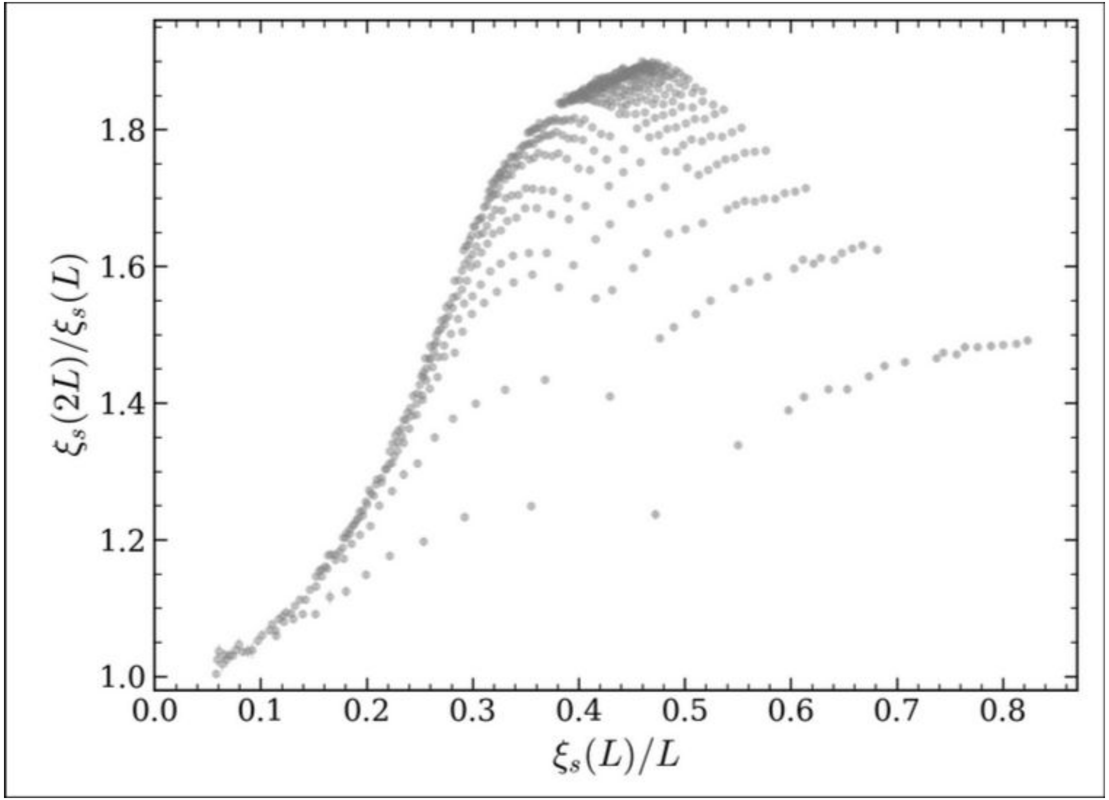
- Plot of ξ□(2L)/ξ□(L) vs ξ□(L)/L



Step-scaling curve

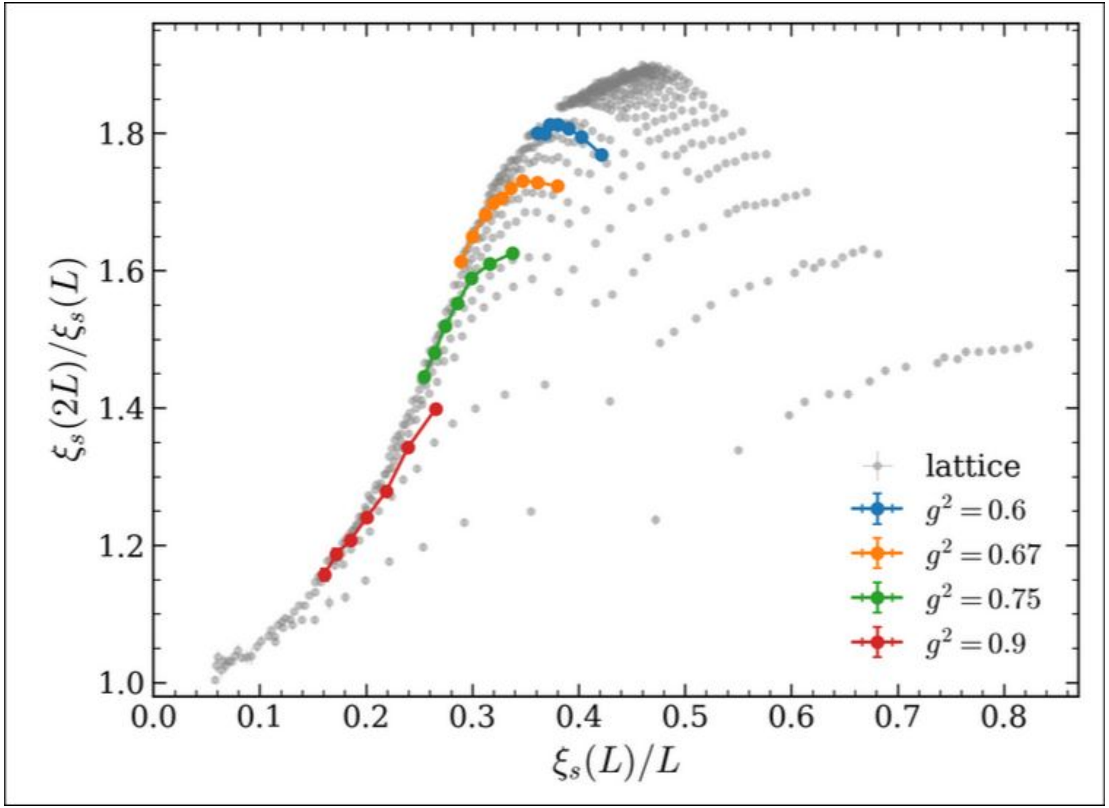
- Plot of ξ□(2L)/ξ□(L) vs ξ□(L)/L

- Euclidean lattice data in gray



Step-scaling curve

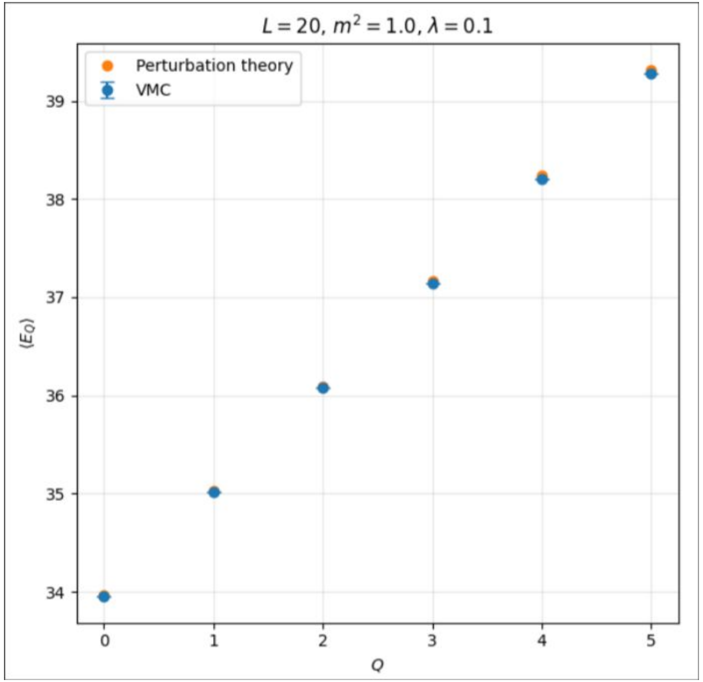
- Plot of ξ□(2L)/ξ□(L) vs ξ□(L)/L
- Euclidean lattice data in gray
- VMC data in color

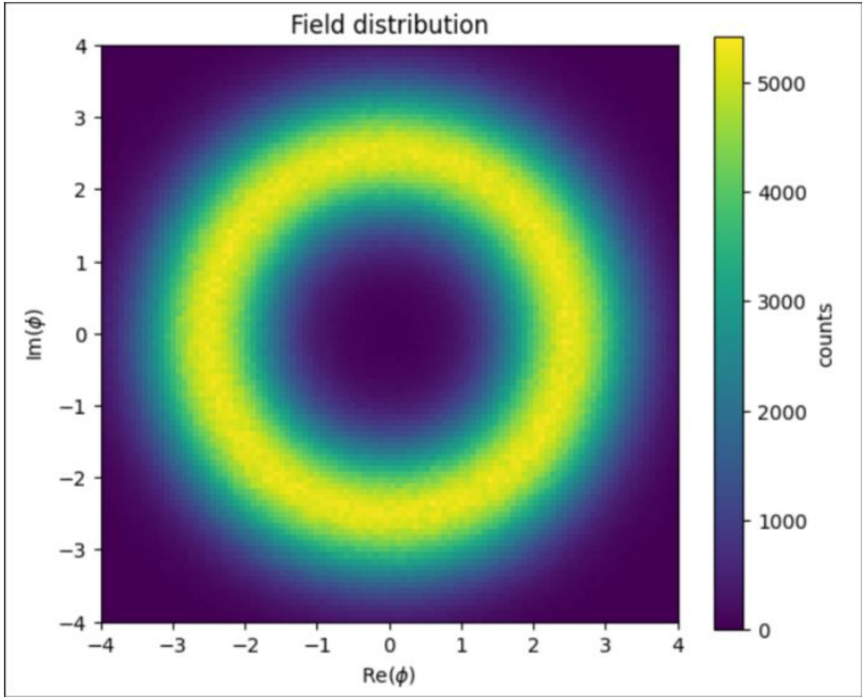


Conclusion

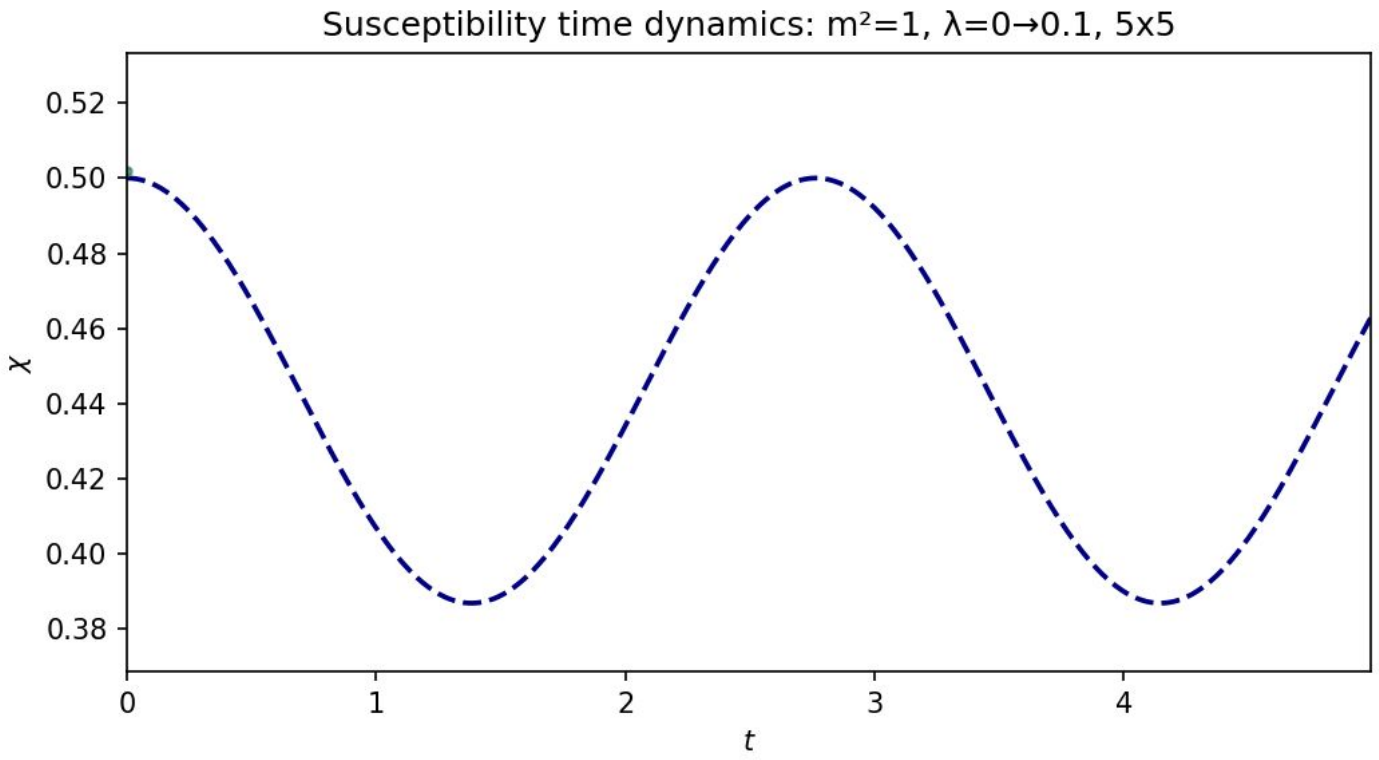
- Variational calculations are feasible in field theory
- Generalizable to finite density by fixing charge sectors in the ansatz
- Real-time evolution possible through time dependent variational Monte Carlo

Preliminary – Finite Density

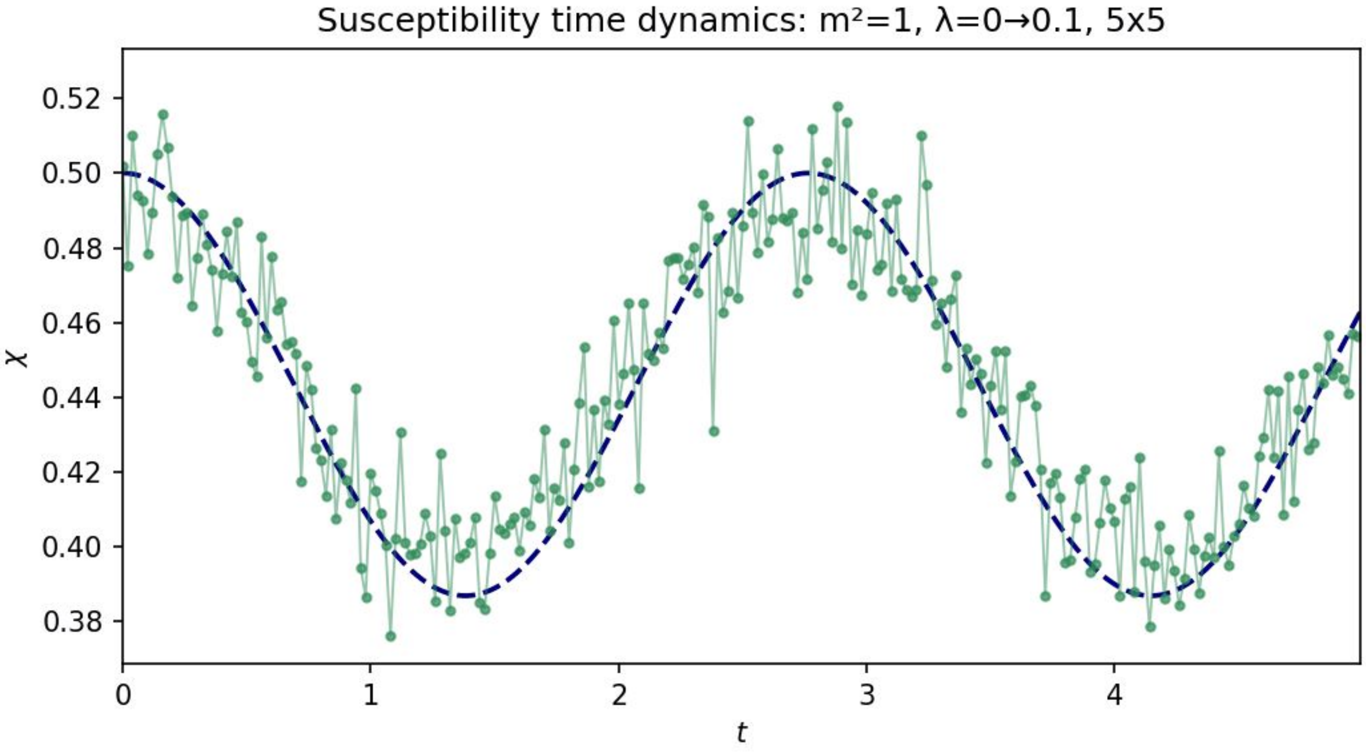




Preliminary – Realtime



Preliminary – Realtime (in case gif doesn't work)



Thank you

Questions?