Hunting Hamiltonians and Beyond

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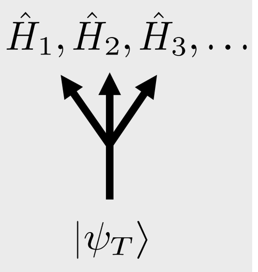
Hunting Hamiltonians

Condensed Matter $\hat{H} \rightarrow |\Psi_0\rangle$

Start with a Hamiltonian, find an interesting ground state.

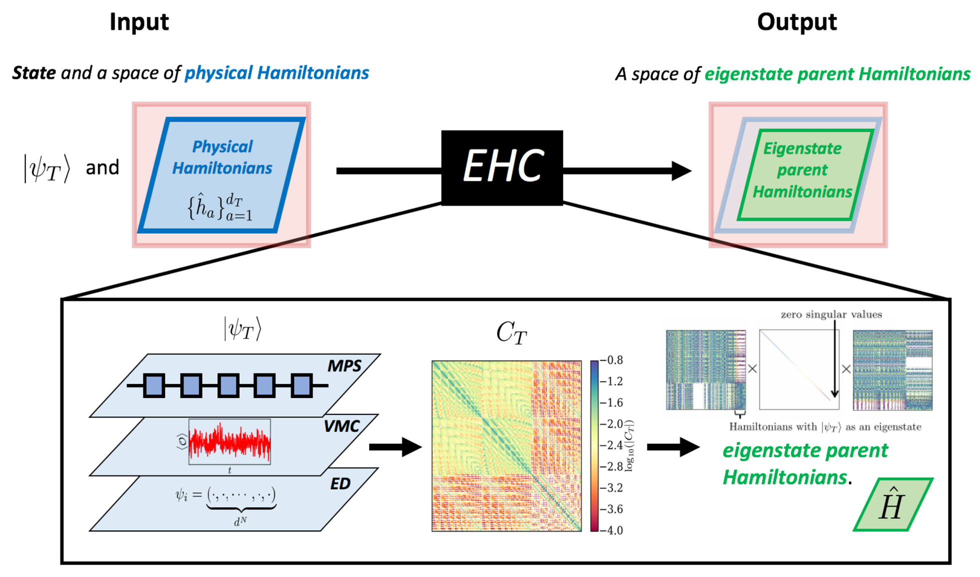
Exponentially costly, limited to a few Hamiltonians, searching for interesting physics in the dark.

Inverse Condensed Matter: *EHC*



Start with an interesting target ground state, find parent Hamiltonians.

Quadratic in cost, finds many Hamiltonians.

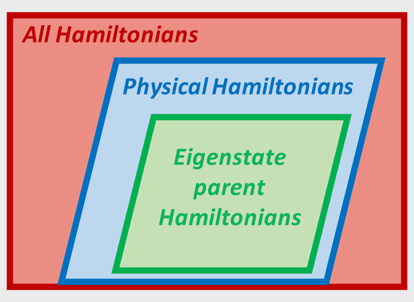


Eigenstate to Hamiltonian Construction (EHC)

The set of ***all Hamiltonians*** forms a vector space.

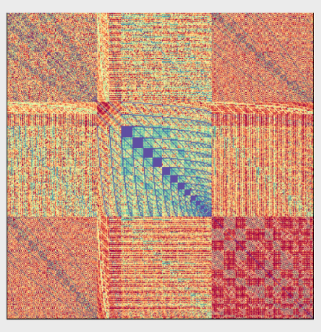
Have: subspace of ***physical Hamiltonians*** $H = \sum_{a=1}^{d_T} J_a \hat{h}_a$ and a ***target eigenstate*** $|\Psi_T\rangle$

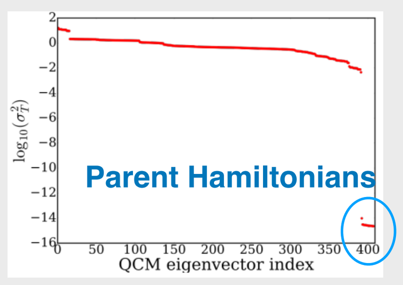
Want: Find the J_a such that $H|\Psi_T\rangle = E|\Psi_T\rangle$



Key Tool: Quantum covariance matrix

$$(C_T)_{ab} = \langle\Psi_T|\hat{h}_a\hat{h}_b|\Psi_T\rangle - \langle\Psi_T|\hat{h}_a|\Psi_T\rangle\langle\Psi_T|\hat{h}_b|\Psi_T\rangle$$
$$(a,b) \in \{1, \ldots, d_T\}$$





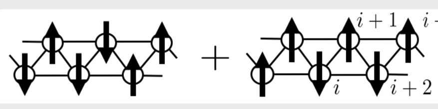
Properties of the QCM

- Hermitian and positive semi-definite (i.e. real, non-negative eigenvalues)
- QCM eigenvalues correspond to variance of Hamiltonians.
- Zero eigenvectors (null vectors) correspond to eigenstate parent Hamiltonians.

Compute: Evaluate the QCM using VMC, DMRG, exact-diagonalization, analytically, etc.

Hamiltonian Discovery

Interesting states can often be built from linear superpositions of ordered states (i.e. dimers).
Here we will consider an equal superposition of frustrated Ising spin configurations on a two leg ladder: $|\Psi_{\rm UFI}\rangle$

$|\Psi_{\rm UFI}\rangle =$  $+ \cdots$

+

Hamiltonians which contain 3-local terms.

EHC

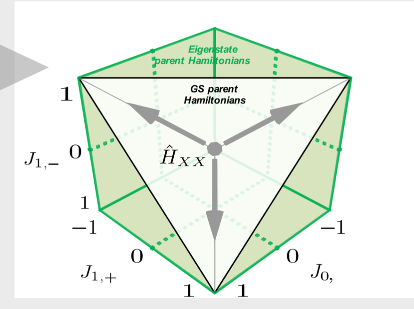
$$H = H_I + J(H^{(1)}_{\rm UFI} + H^{(2)}_{\rm UFI}); 0 < J < 0.175$$
$$\hat{H}_I = \sum_{i=1}^{N}\left(\sigma^z_i\sigma^z_{i+1} + \frac{1}{2}\sigma^z_i\sigma^z_{i+2}\right)$$
$$\hat{H}^{(1)}_{\rm UFI} = \sum_{i=1}^{N}\frac{1}{2}\sigma^z_i\sigma^z_{i+2} + \sigma^x_i\sigma^z_{i+3} + \sigma^x_i\sigma^z_{i+1}\sigma^z_{i+2} - \sigma^z_{i-2}\sigma^x_i\sigma^z_{i+1}$$
$$\hat{H}^{(2)}_{\rm UFI} = \sum_{i=1}^{N}\frac{1}{2}\sigma^z_i\sigma^z_{i+2} + \sigma^x_i\sigma^z_{i+3} + \sigma^z_{i-2}\sigma^z_{i-1}\sigma^x_i - \sigma^z_{i-1}\sigma^x_i\sigma^z_{i+2}$$

More Benchmark Examples

$$\hat{H}_{XX} = \sum_{i=1}^{N}(S^x_i S^x_{i+1} + S^y_i S^y_{i+1})$$ (ground state) $|\Psi_{XX}\rangle$

EHC

$$\hat{h}_a = S^x_i S^x_j, S^y_i S^y_j, S^z_i S^z_j$$



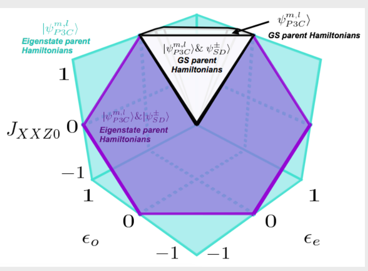
3D ground state manifold of Hamiltonians with $|\Psi_{XX}\rangle$ as the ground state.

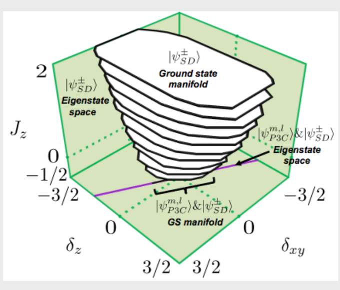
Two leg triangular ladder

$|\Psi^{\pm}_{SD}\rangle$ are singlet dimer states.

$|\Psi^{m,l}_{\rm P3C}\rangle$ are projected 3-coloring states

DEHC





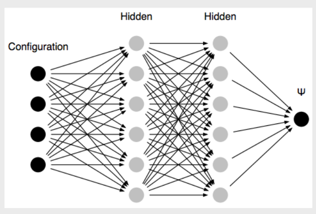
Singlet dimer eigenstate parent Hamiltonians.
3-coloring eigenstate parent Hamiltonians.
Degenerate ES parent Hamiltonians
Ground State parent Hamiltonians

$H_{\rm Heisenberg} = \sum_{\langle ij\rangle} S_i \cdot S_j$ (ground state) $|\Psi_{\rm Heisenberg}\rangle$ EHC $H_{\rm Heisenberg} + \alpha\sum_{n=1}^{N}\cos(2\pi n/N)S_n \cdot S_{n+1}$

Feed-Forward Neural Networks for Wave-functions

Machine learning sans hype.

Wave-function: $\Psi[c] \rightarrow \#$

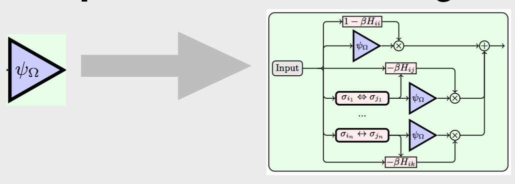


Feed-Forward Neural Nets unlike standard RBM, can change sign.

with Dmitrii Kochkov

Which wave-functions can it represent?

In exponential time: *all ground states*



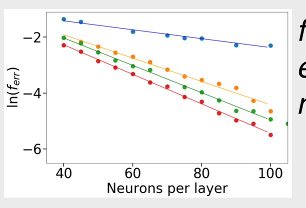
$|\Psi\rangle \rightarrow (1 - \beta H)|\Psi\rangle$

Iterate many times to produce arbitrary ground state.

In polyomial time: *any polynomial ansatz*

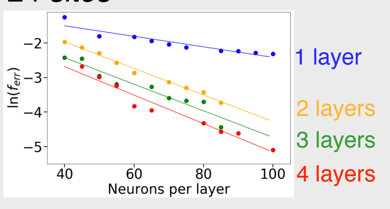
Kagome?

18 sites

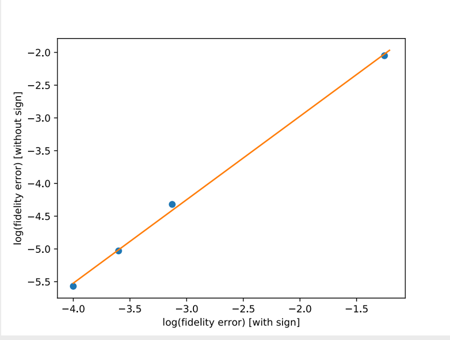


fidelity improves exponentially in neurons

24 sites



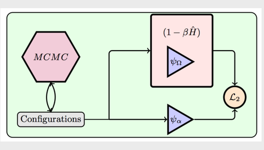
Is the problem the signs?



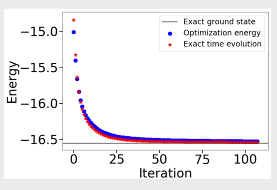
70 neurons

Significantly easier but not trivial.

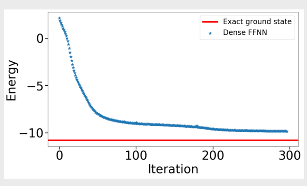
Can we optimize?



Novel wave-function optimization by supervised learning.



Works fine on square lattice (6x4)



But intermediate kagome states aren't representable.

24 sites, 3 layers, 80 hidden neurons

Neural Network Backflow

Two approaches to wave-functions:

Brute Force:
DMRG
FFNN
Multi-determinants

Lots of work to even get weakly interacting systems

Originally developed by Feynman for He-4 (sans neural-network)

Mean Field++:

Slater-Determinant $\psi_{SD}(r) = \det[M^{SD,\uparrow}]\det[M^{SD,\downarrow}]$, $M^{SD,\sigma}_{ik} = \phi_{k\sigma}(r_{i\sigma})$

Slater-Jastrow (SJ) $\psi_{SJ}(r) = e^{-U(r)}\psi_{SD}(r)$

SJ Backflow $\phi^b_{k\sigma}(r_{i,\sigma}; r) = \phi_{k\sigma}(r_{i,\sigma}) + a^{NN}_{ki,\sigma}(r)$

Mean field starts by capturing the right physics.

Configuration-dependent correction to single particle orbitals. Generated by neural net.

Q: Can we replace Feynman (and other parameterization) with machine learning?

Input: configuration on input neurons (*N neurons*)

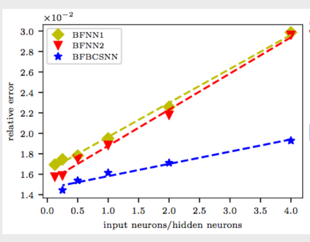
Output: $a^{NN}_{ki,\sigma}(r)$ on output neurons. (*N² neurons*)

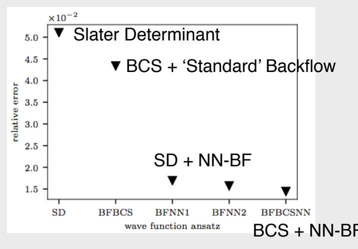
Hidden Layers: Fully Dense + ReLu

One neural net per spin

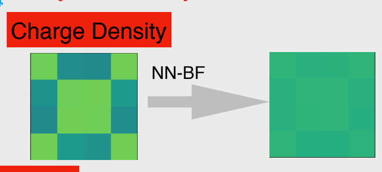
Benchmark: Hubbard Model: U=8, Doping = 0.875

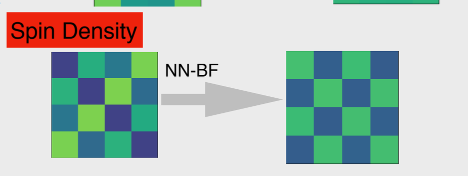
$$H = -t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.) + \sum_i U n_{i\uparrow}n_{i\downarrow}$$

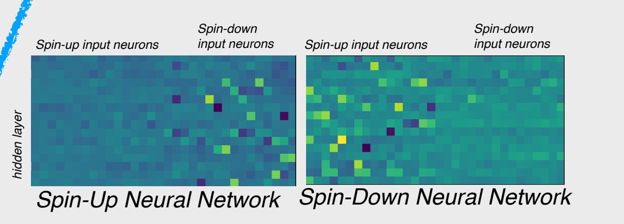




Can we understand (some of) what it learned?



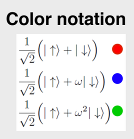




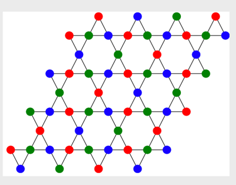
with Di Luo

Frustrated Magnetism

Advertisement *see Hitesh Changlani's poster*

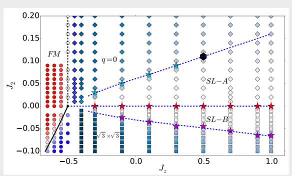


On the kagome lattice, $H = \sum_{\langle ij\rangle} S^x_i S^x_j + S^y_i S^y_j - \frac{1}{2}S^z_i S^z_j$ is exponentially degenerate



All (projected) three-colorings are ground states.

Why? Because the Hamiltonian is frustration free over triangles.



The exponentially degenerate point is connected to the `Heisenberg' spin liquid.

with Hitesh Changlani, Dmitrii Kochkov, Krishna Kumar and Eduardo Fradkin

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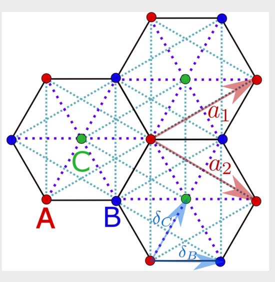
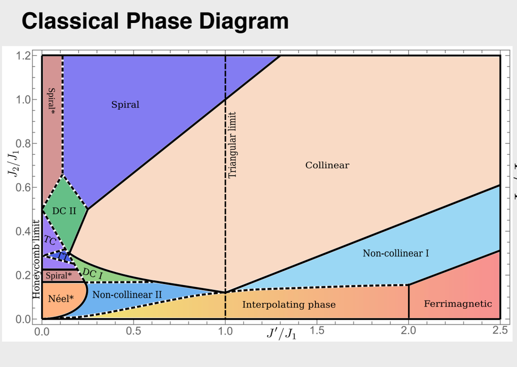
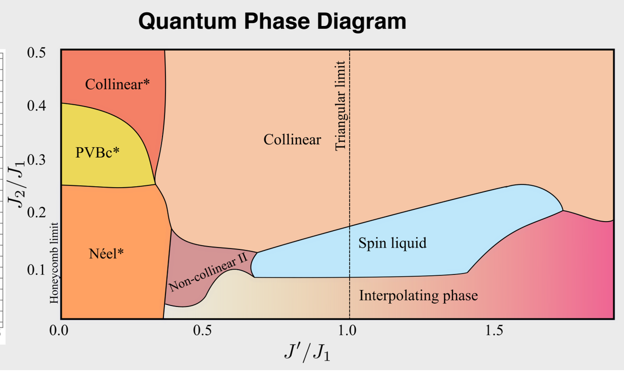


The Stuffed Honeycomb lattice has an exotic classical and quantum phase diagram.

Classical Phase Diagram



Quantum Phase Diagram



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Many-Body Localization

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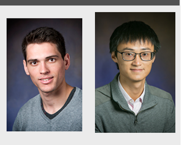
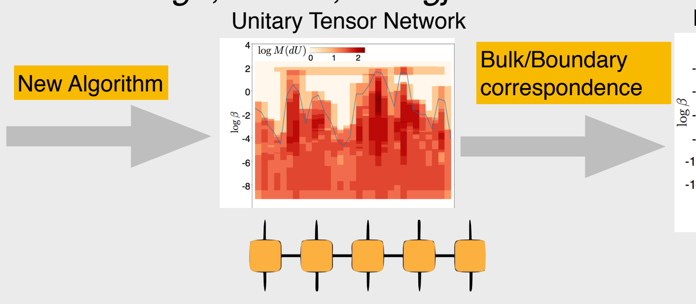


MBL Hamiltonian

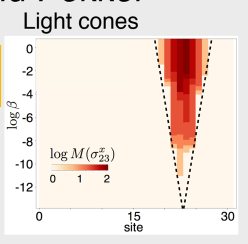
$$H = \sum_i\left(\vec{S}_i \cdot \vec{S}_{i+1} + h_i S^z_i\right),$$
$$h_i \in [-W, W], \quad p(h_i) = 1/(2W)$$

New Algorithm

Unitary Tensor Network

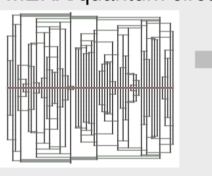


Light cones



New Algorithm

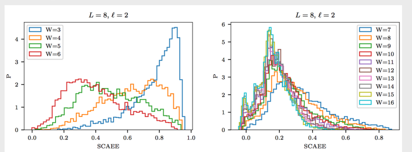
MERA/quantum circuit



Effective Hamiltonians

Beyond MBL: *Simultaneous area law and log-law eigenstates.*

$H = -t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.) + \sum_i U n_{i\uparrow}n_{i\downarrow} + \sum_i h_i S^z_i$



Acknowledgements/References

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