Title: Dimension reduction of the Functional Renormalization Group

Speakers:

Collection: Machine Learning for Quantum Many-Body Systems

Date: June 12, 2023 - 3:15 PM

URL: https://pirsa.org/23060031

Abstract: ZOOM: https://pitp.zoom.us/j/94595394881?pwd=OUZSSXpzYlhFcGlIRm81Y3VaYVpCQT09

In this work, we use data-driven methods to reduce the dimensionality of the vertex function for the Hubbard model and spin liquid model. By employing a deep learning architecture based on the autoencoder, we show that the functional renormalization group (FRG) dynamics can be efficiently learned. Our approach is compared with other methods, including principal component analysis and dynamic mode decomposition. Our results demonstrate the effectiveness of our proposed approach for understanding the FRG flow in these models.

Dimensional reduction of the Functional Renormalization Group

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6.11, 2023

Acknowledgement

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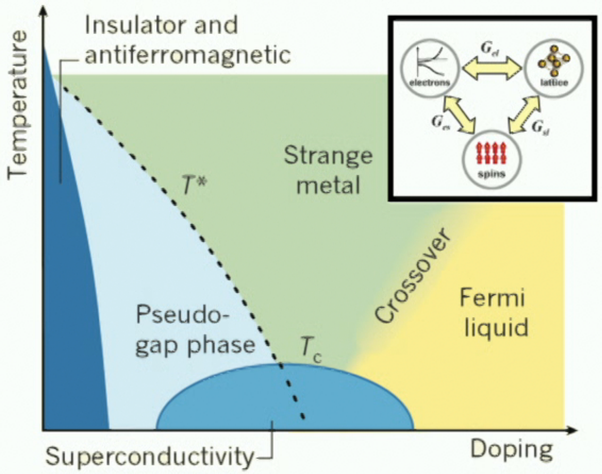
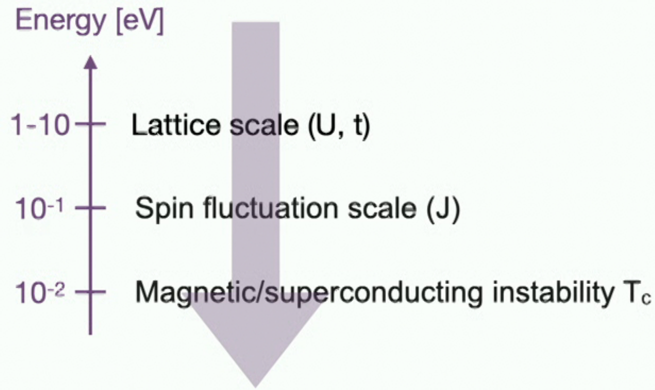
Background - Quantum Systems

- No single-particle picture but collective phenomena
- Require many-body perspective
- Examples:
  - Metal-insulator transition
  - Superconductivity
  - Heavy- fermion behavior
  - Quantum magnetism



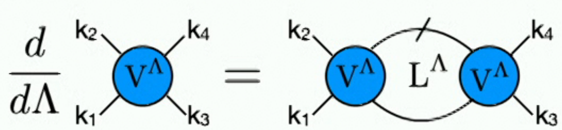
- Archetypal model:
  - Hubbard model $\mathscr{H} = -t\sum_{\langle ij\rangle,\sigma} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$
  - Heisenberg model $\mathscr{H} = J_1\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$

Background - Functional Renormalization Group



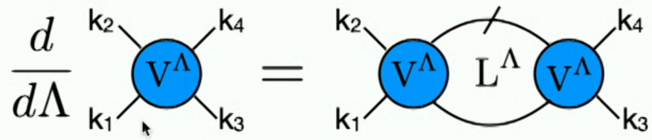
Interacting systems exhibit distinct behaviors on different energy scales.

- fRG (Functional Renormalization Group): A numerical method of systematically coarse-graining a quantum field theory.



1) one starts at an ultraviolet (UV) cutoff scale Λ_{UV} and successively takes effects of fermionic fluctuations into account by approaching the infrared (IR) limit $\Lambda_{IR} = 0$.
2) terminate at $T_c > T_{IR}$ if divergence
3) Calculate relative parameters to find the ground state.

Important object: vertex



•the vertex V (k_1 , k_2 , k_3): describes scattering of electrons at (k1,k2) to (k3, k4) plus internal structure. What fRG is doing is keeping track of how this vertex evolves under renormalization.

The vertex is large since it depends on three momenta, making the calculation very computational expensive.

$$\dim\left(V^{\Lambda}\right) = {\rm N_k}^3 = 48^3 \sim 10^5$$

Could we find a compact representation for the complex vertex function?
-> Simplify the fRG calculation
-> Simplify other many body calculation using vertex, such as cluster dynamical mean field calculation and GW approximation.

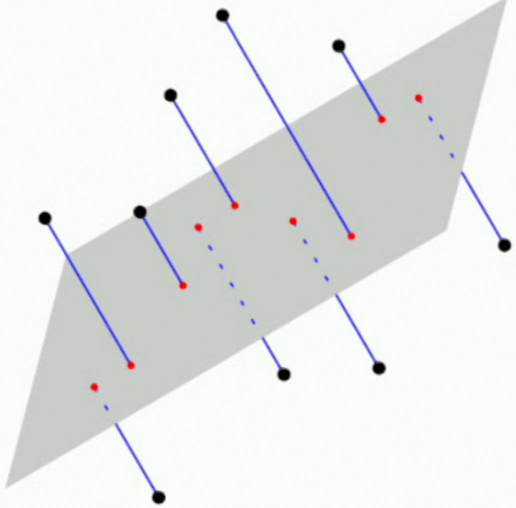
Machine learning- dimensional reduction

- In machine learning, methods:
  - Principal Components Analysis (PCA): linear method
  - AutoEncoder: nonlinear method
  - ..

Principle Component Analysis

- find the best **linear** transformation $\phi : \mathbf{R}^d \to \mathbf{R}^k$ that maintains reconstruction accuracy.

- The k dimensional subspace can be represented by $\vec{q}_1, \ldots, \vec{q}_k \in \mathbf{R}^d$ orthonormal vectors.



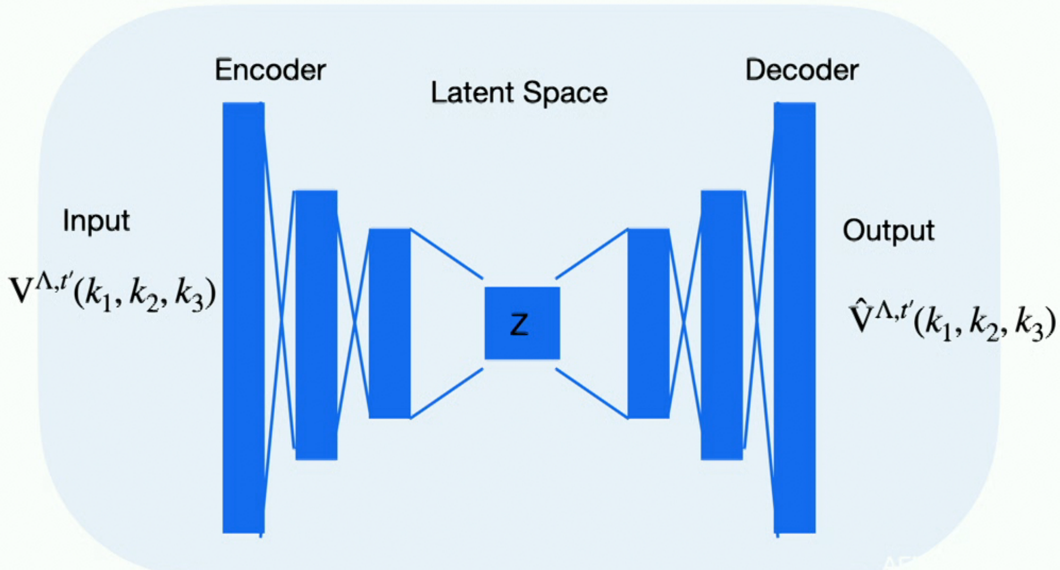
- $$\arg\min_{\substack{Q \in \mathbf{R}^{d\times k} \\ Q^\top Q = I}} \frac{1}{n} \sum_{i=1}^{n} \left\| \vec{v}_i - QQ^\top \vec{v}_i \right\|^2$$

$$Q := \begin{bmatrix} | & & | \\ q_1 & \cdots & q_k \\ | & & | \end{bmatrix}$$

- The solution q_1, q_2.. are called principle components, where the i-th vector is the direction of a line that best fits the data while being orthogonal to the first i-1 vectors

Auto-encoder

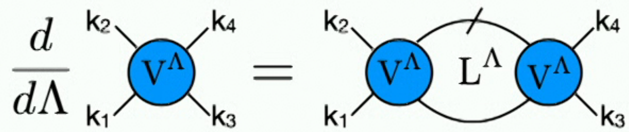
- Auto-encoder learns to reduce the dimension via a **non-linear** way
-



Physics: t-t' Hubbard model

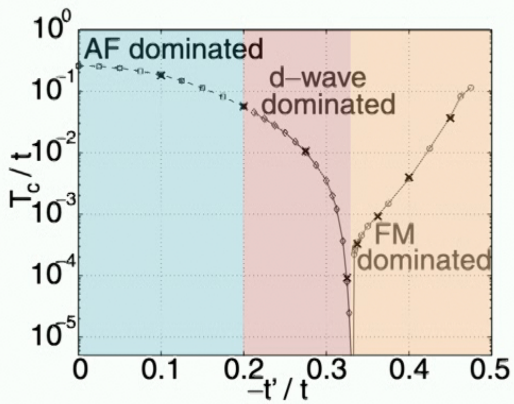
$$H = -t \sum_{\text{nn,s}} c^\dagger_{i,s} c_{j,s} - t' \sum_{\text{nnn,s}} c^\dagger_{i,s} c_{j,s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

at Λ→0, fRG predicts different physical phases:



- Antiferromagnetic (AFM) instability
- d-wave superconducting (d-SC) instability
- Ferromagnetic (FM) instability

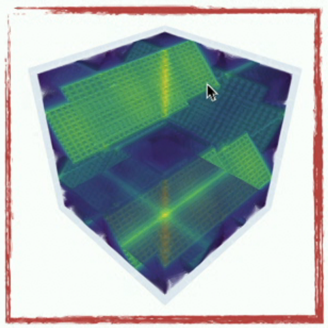
We use the final vertices as the input data, and perform PCA and auto-encoder.



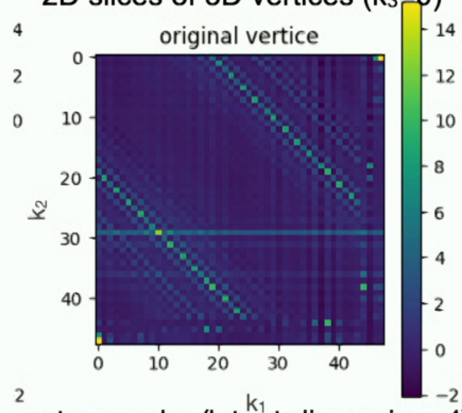
*Honerkamp et al., Phys. Rev. Lett. **87**, 187004 (2001)

Reconstruct the vertices

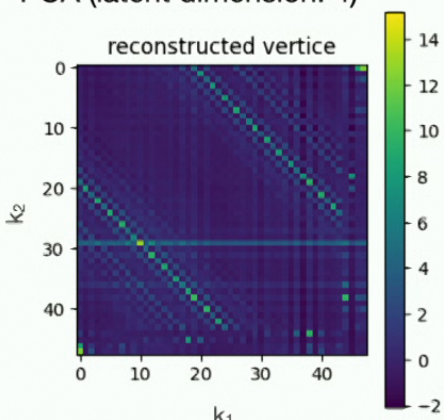
3D plot of vertex function



2D slices of 3D vertices (k_3=0)

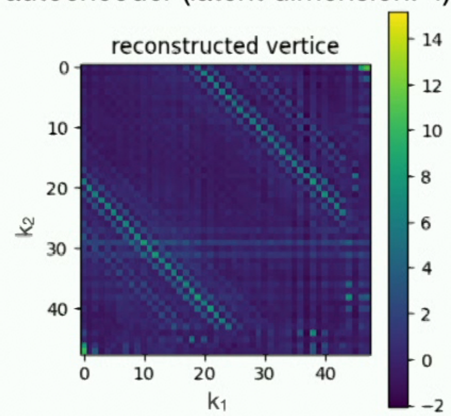


PCA (latent dimension: 4)



Mean square error: ~0.02

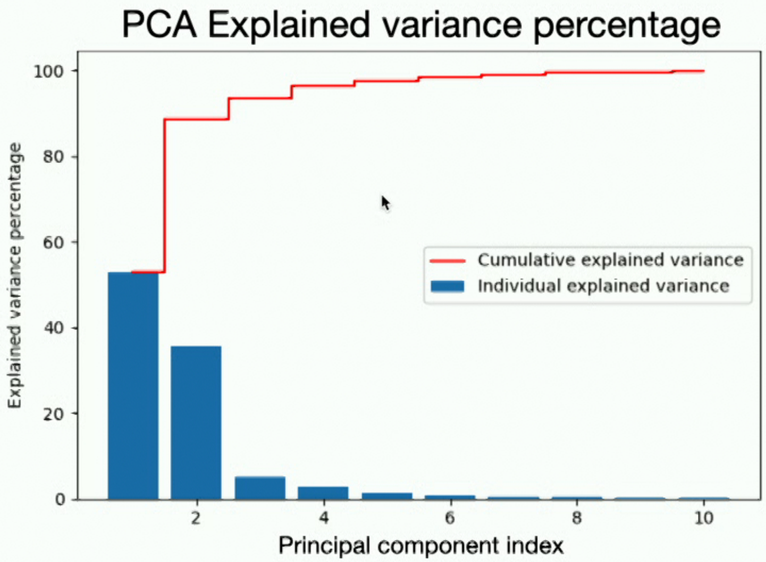
autoencoder (latent dimension: 4)



Mean square error: ~0.07

- PCA and autoencoder both correctly reproduce the vertex.

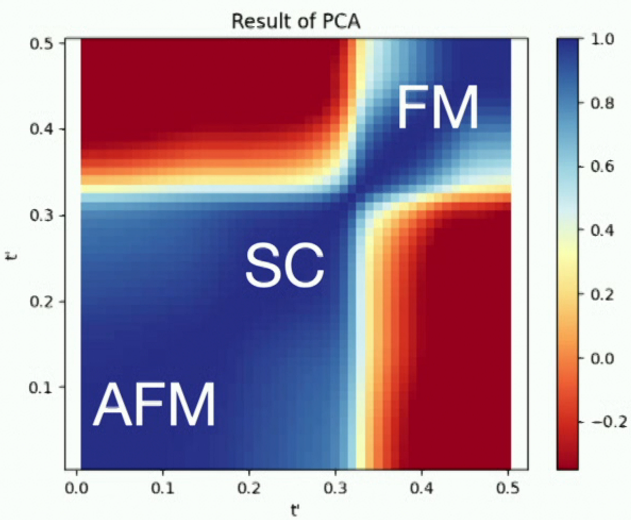
Principle Component Analysis - Result for Hubbard model

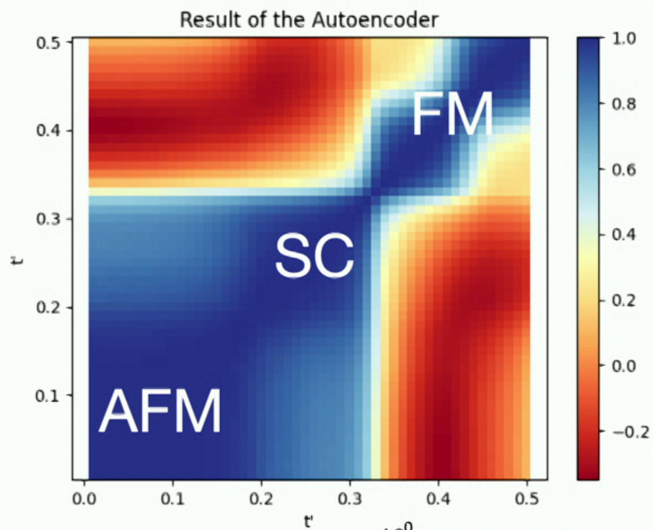


- the explained variance plot: it visually represents the proportion of total variance captured by each successive principal component.
  - First component: ~ 52%
  - Second component ~ 35%
- 4 components already capture above 95% variance of the original data

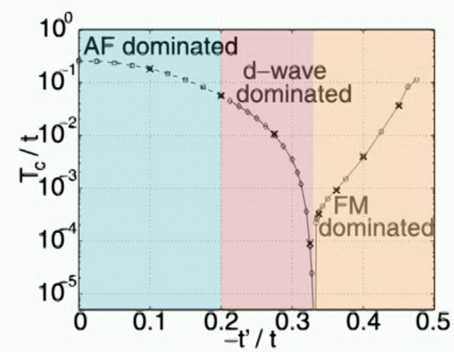
Ground state

$$\mathcal{C}(t'_1, t'_2) = \frac{\mathbf{z}(t'_1) \cdot \mathbf{z}(t'_2)}{\|\mathbf{z}(t'_1)\| \|\mathbf{z}(t'_2)\|}$$





- Three correlated blocks appear in the latent correlation matrix
- Precisely matches fRG predictions of transition points and order
- Correctly predicts similarity between AFM and d-SC phases
- PCA and autoencoder give similar results



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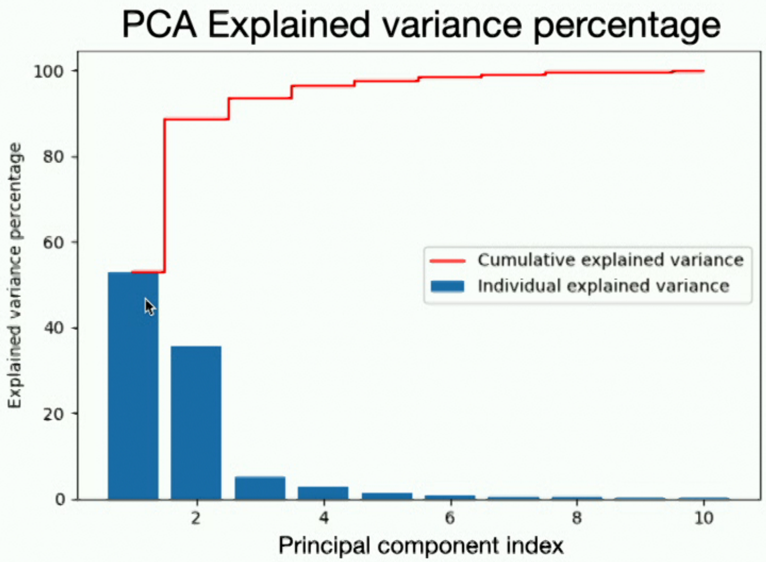

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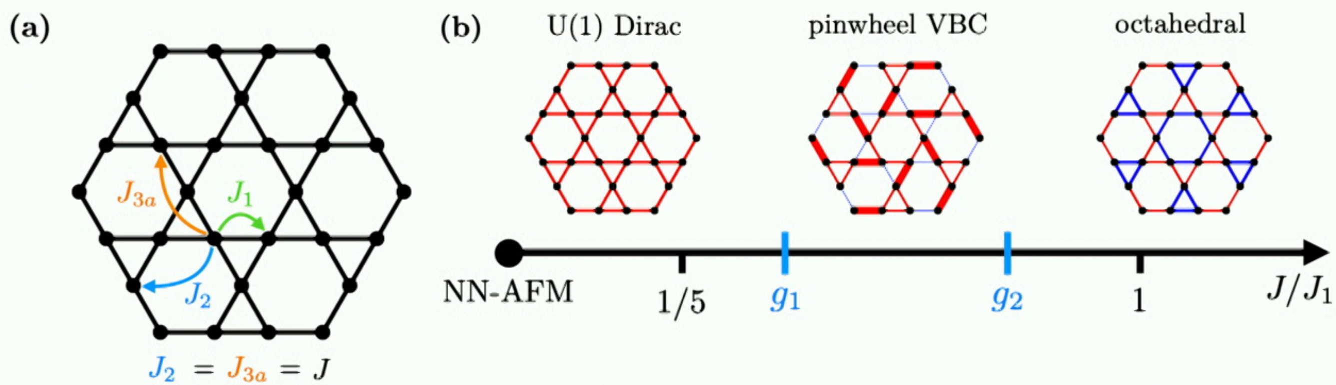
Model2: Heisenberg antiferromagnet on the kagome lattice

$$\mathscr{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J_1}{2} \sum_{\triangle,\nabla} \left(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3\right)^2 - J_1 N \qquad S_i^\mu = \frac{1}{2} \sum_{\alpha,\beta} f_{i,\alpha}^\dagger \sigma_{\alpha,\beta}^\mu f_{i,\beta}$$

at $\Lambda \to 0$, fRG predicts different physical phases:

- U(1) Dirac, pinwheel valence bond crystal (VBC) and octahedral order.



Kiese, Dominik, et al. Physical Review Research 5.1 (2023): L012025.

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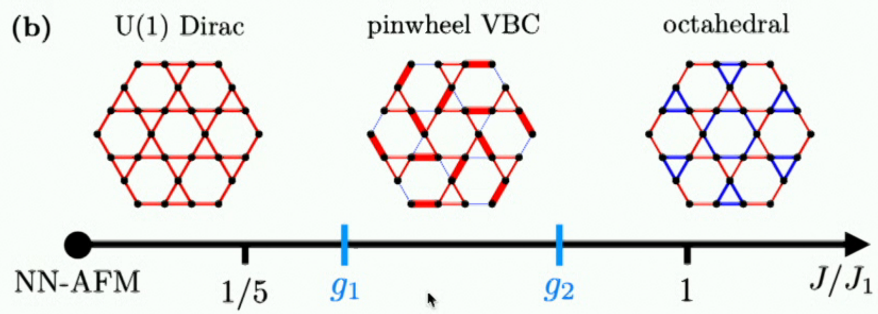
- In fRG, the boundary between VBC and octahedral order (g2) shows a deviation with other methods.

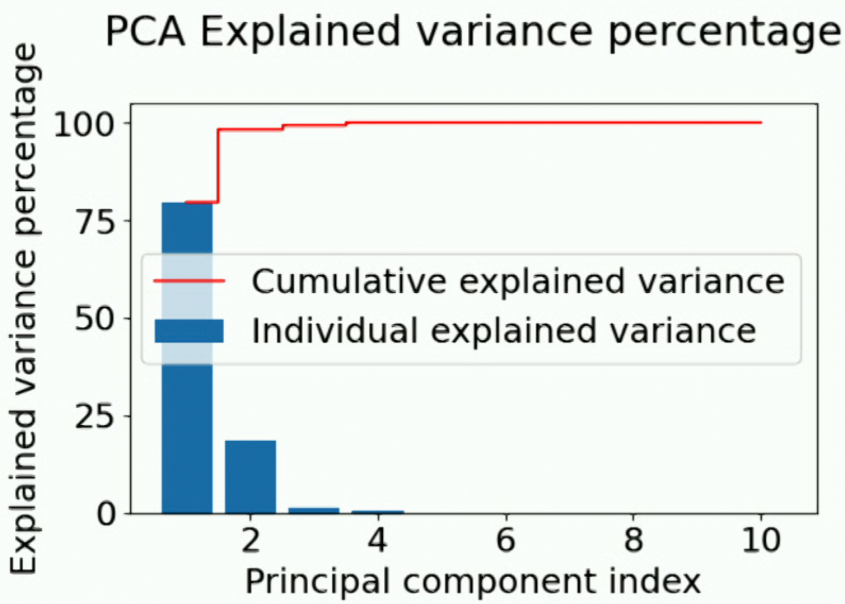
	g_1	g_2
VMC	0.26(1)	0.51(1)
mVMC	0.32(3)	0.51(1)
DMRG	0.27(1)	0.51(1)
pf-FRG	0.30(2)	0.80(5)*



Kiese, Dominik, et al. Physical Review Research 5.1 (2023): L012025.

PCA result

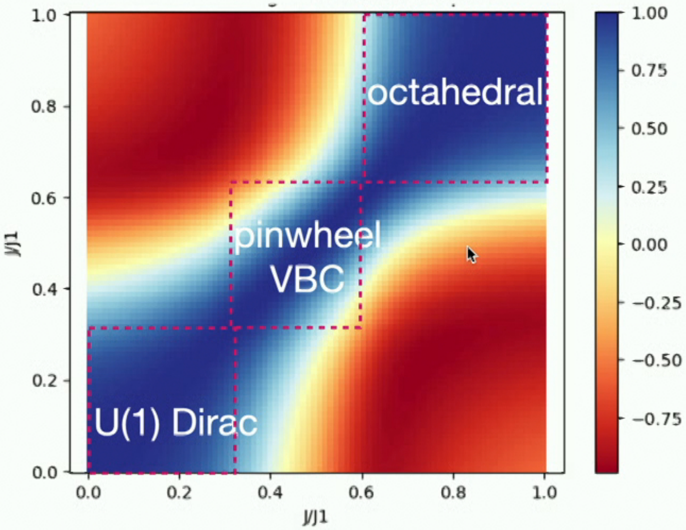
- PCA again shows that we only need a few components to capture the major information in vertex.

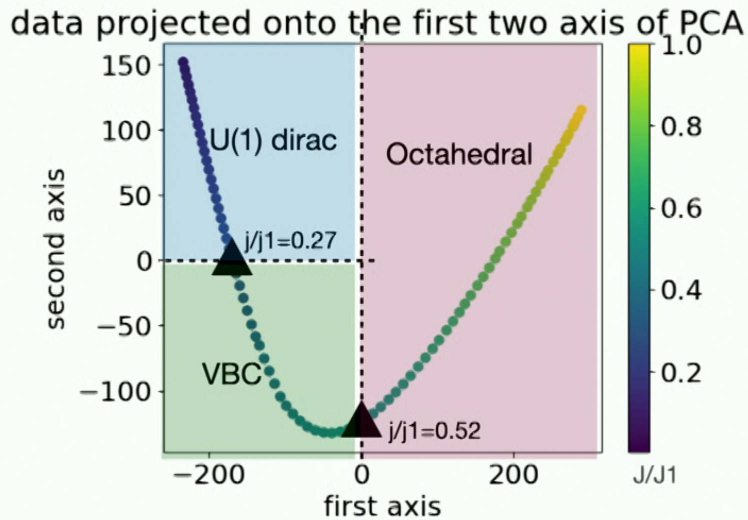


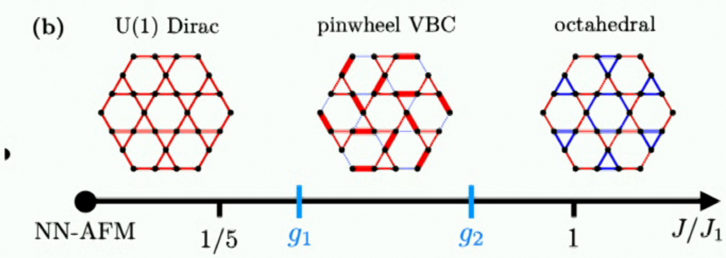
PCA result - ground state

- It shows indication of the phase boundary

$$\mathcal{C}(t_1', t_2') = \frac{\mathbf{z}(t_1') \cdot \mathbf{z}(t_2')}{\|\mathbf{z}(t_1')\| \|\mathbf{z}(t_2')\|}$$







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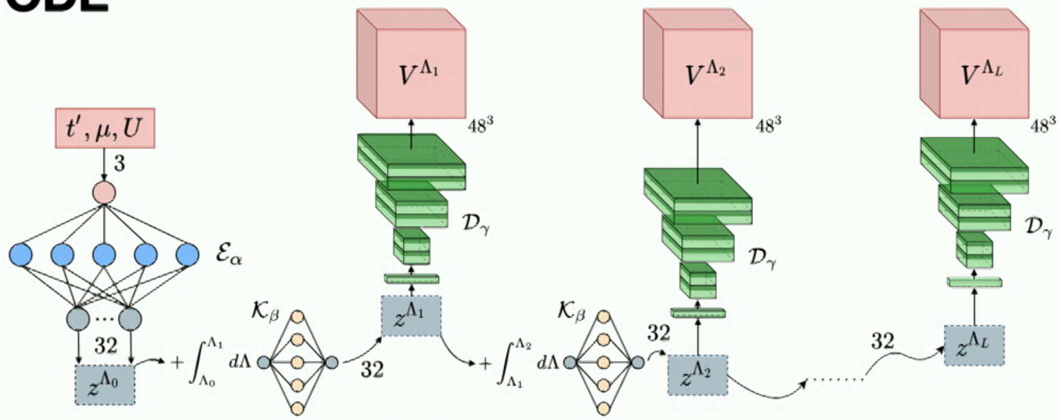
Neural ODE



- Neural Ordinary Differential Equations architecture:
  - Encoder ϵ_α: map initial condition to a low-dimensional latent space
  - NODE K: defines a differential equation propagation rule for latent variables in Λ.
  - Decoder D: at each step of the flow, the decoder maps the latent representation to a reconstructed vertex.

$$\mathbf{z}^{\Lambda_0} = \epsilon_\alpha\left(t', U, \mu\right); \quad \frac{\mathrm{d}\mathbf{z}^\Lambda}{\mathrm{d}\Lambda} = K_\beta\left(\mathbf{z}^\Lambda\right); \quad \hat{\mathrm{V}}^\Lambda = D_\gamma\left(\mathbf{z}^\Lambda\right)$$

Di Sante, D., Medvidović, et al, PRL 129, 136402 (2022)

Summary

- The data-driven method shows that we only need a few parameters to capture the important aspects of the vertex function.

  - PCA gives a more accurate result than the auto-encoder.

- In both the Hubbard model and the Heisenberg antiferromagnet model, the low dimension latent space shows the indication of the boundaries of different ground states.

- Future question:

  - In a Fermi liquid model that doesn't have divergence, could we still use a few parameters to describe the whole space?

  - Could we incorporate PCA into the neural ODE framework?