Resonating valence-bond wave functions in the era of neural networks

Federico Becca

Fractionalization and Emergent Gauge Fields in Quantum Matter

Credits to: S. Budaraju, F. Ferrari, R. Rende, and L.L. Viteritti

$$|BCS\rangle = \exp\left\{\sum_k f_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right\} |0\rangle$$

Electron pairing (Cooper pairs)

Bose condensation of pairs

J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **106**, 162 (1957)

$$\Psi(\{z_i\}) = \prod_{i \neq j} (z_i - z_j)^m \exp\{-\frac{1}{4}\sum_i |z_i|^2\}$$

The first topologically ordered state

Fractional excitations

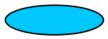
R.B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983)

- **A few variational parameters: easy physical interpretation**
- **Easy construction of low-energy excitations**

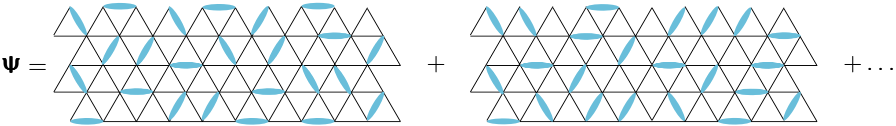
The resonating-valence bond (RVB) picture

Looking for a magnetically disordered ground state

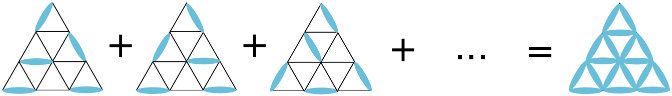
A "quantum liquid" of spins

 $= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

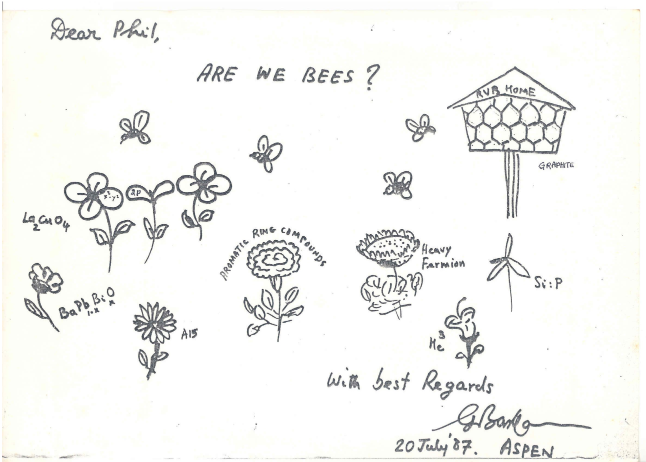
P.W. Anderson, Mater. Res. Bull. **8**, 153 (1973)



Linear superposition of valence-bond (singlet) configurations



G. Baskaran and P.W. Anderson, Phys. Rev. B **37**, 580 (1988)



G. Baskaran, reprinted in *PWA90 A Life Time of Emergence* (World Scientific 2016)

$$\mathcal{H} = \sum_{R,R'} J_{R,R'} \mathbf{S}_R \cdot \mathbf{S}_{R'} \qquad \mathbf{S}_R = \frac{1}{2}\sum_{\alpha,\beta} c^\dagger_{R,\alpha}\sigma_{\alpha,\beta}c_{R,\beta} \qquad \sum_\alpha c^\dagger_{R,\alpha}c_{R,\alpha} = 1$$

- Variational states are constructed from a fermionic auxiliary Hamiltonian

$$\mathcal{H}_0 = \sum_{R,R',\alpha} t_{R,R'} c^\dagger_{R,\alpha} c_{R',\alpha}$$

U(1) gauge fields

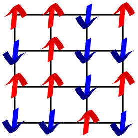
$$c_{R,\alpha} \to e^{i\theta_R} c_{R,\alpha}$$

$$t_{R,R'} \to e^{i(\theta_{R'}-\theta_R)} t_{R,R'}$$

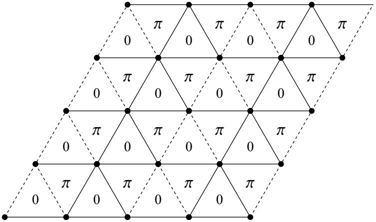
- Fixing the hopping structure = freezing the gauge fluctuations
- The constraint of one-electron per site is inserted by the Gutzwiller projector

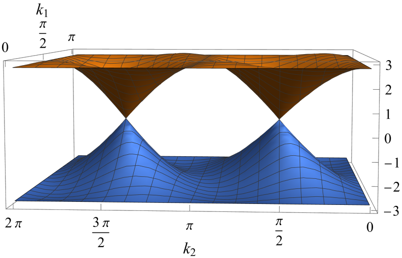
$$\boxed{|\Psi_0\rangle = \mathcal{J}\mathcal{P}_G|\Phi_0\rangle}$$

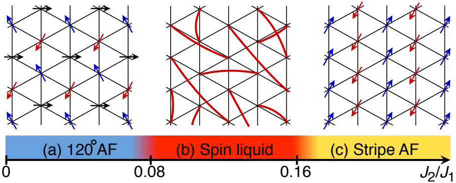
$$\mathcal{P}_G = \prod_R (n_{R,\uparrow} - n_{R,\downarrow})^2$$



This projection partially reintroduces gauge fluctuations



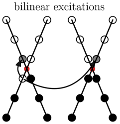


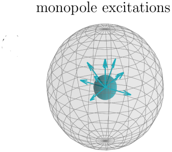


- For $J_2/J_1 = 0.125$, the energy of the π-flux state is $E/J_1 = -0.5019(1)$
  The exact one is estimated to be $E_{\rm ex}/J_1 = -0.5123(2)$

Y. Iqbal, W.J. Hu, R. Thomale, D. Poilblanc, and FB, Phys. Rev. B **93**, 144411 (2016)

- **The low-energy theory is the quantum electrodynamics in $2+1D$**

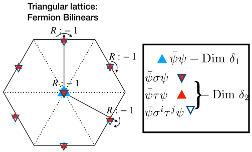


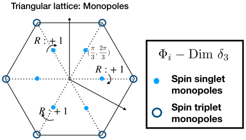


+ Photons

M. Hermele, T. Senthil, M.P.A. Fisher, P.A. Lee, N. Nagaosa, and X.-G. Wen, Phys. Rev. B **70**, 214437 (2004)

- **Symmetry transformation of monopoles**



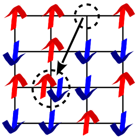


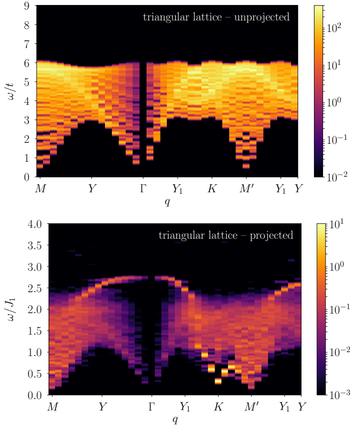
X.-Y. Song, C. Wang, A. Vishwanath, and Y.-C. He, Nat. Comm. **10**, 4254 (2019)

- **Verification by exact diagonalizations**

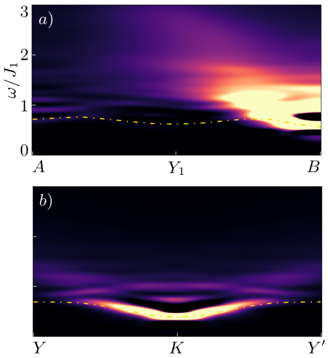
A. Wietek, S. Capponi, and A.M. Läuchli, arXiv:2303.01585

$$|q, R\rangle = \mathcal{P}_G \frac{1}{\sqrt{L}} \sum_{R'} e^{iqR'} \left(c^{\dagger}_{R+R',\uparrow} c_{R',\uparrow} - c^{\dagger}_{R+R',\downarrow} c_{R',\downarrow}\right) |\Phi_0\rangle$$





F. Ferrari and FB, Phys. Rev. X **9**, 031026 (2019)

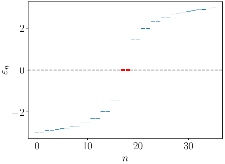


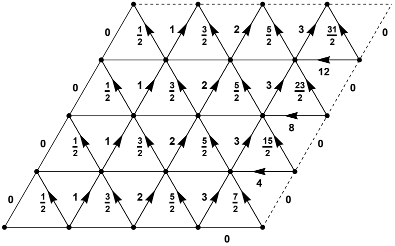
M. Drescher, L. Vanderstraeten, R. Moessner, and F. Pollmann, Phys. Rev. B **108**, L220401 (2023)

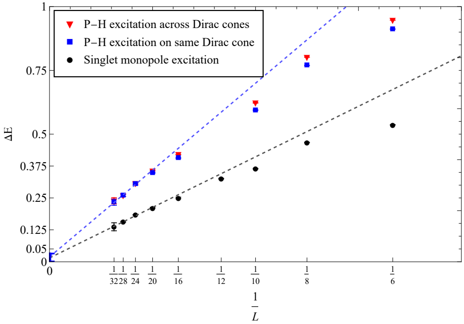
- A 2π flux on top of the Dirac state

X.-Y. Song, C. Wang, A. Vishwanath, and Y.-C. He, Nat. Comm. **10**, 4254 (2019)

A. Wietek, S. Capponi, and A.M. Läuchli, arXiv:2303.01585





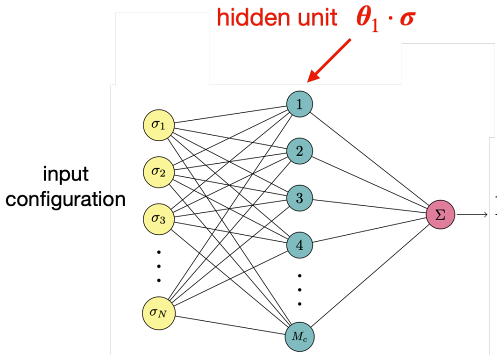


- **The monopole excitations are gapless (as in the large-N limit)**

S. Budaraju, Y. Iqbal, FB, and D. Poilblanc, Phys. Rev. B **108**, L201116 (2023)

S. Budaraju et al., unpublished

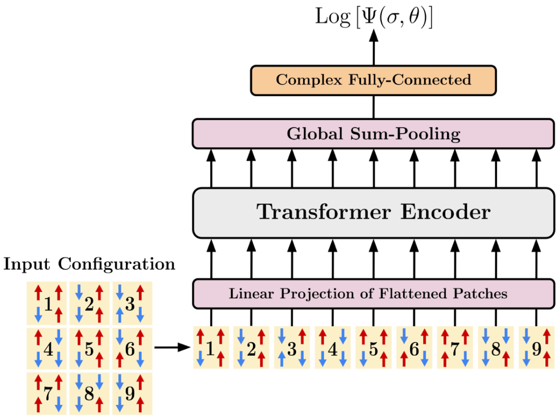
- **Idea: use neural networks to parametrize variational wave functions**
- **The simplest example: a single fully-connected layer**



$$\log \Psi(\boldsymbol{\sigma}) = \sum_{\alpha=1}^{M} g\left(\boldsymbol{\theta}_\alpha \cdot \boldsymbol{\sigma}\right)$$

G. Carleo and M. Troyer, Science **355**, 602 (2017)

- **Not easy interpretation and simple way to compute dynamical correlations**



$$z = \sum_{i=1}^{N} \mathbf{y}_i \qquad z \in \mathbf{R}^d$$

$$\mathbf{y}_1, \cdots, \mathbf{y}_N \qquad \mathbf{y}_i \in \mathbf{R}^d$$

$$\mathbf{x}_1, \cdots, \mathbf{x}_N \qquad \mathbf{x}_i \in \mathbf{R}^d$$

- Map spin configurations into abstract representations using the Transformer
- Apply a complex fully connected layer to predict both amplitude and sign
  [similar to the so-called Visual Transformer (ViT)]

The $J_1 - J_2$ Heisenberg model on the square lattice

- Calculations on the 10×10 cluster with PBC

TABLE I. Ground-state energy on the 10×10 square lattice at $J_2/J_1 = 0.5$.

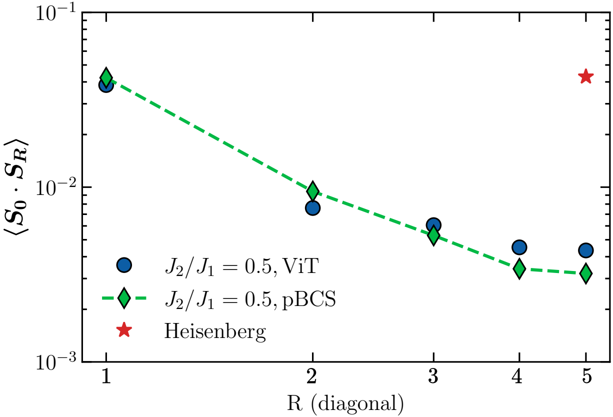
Energy per site	Wave function	# parameters	Marshall prior	Reference	Year
-0.48941(1)	NNQS	893994	Not available	[32]	2023
-0.494757(12)	CNN	Not available	No	[22]	2020
-0.4947359(1)	Shallow CNN	11009	Not available	[21]	2018
-0.49516(1)	Deep CNN	7676	Yes	[20]	2019
-0.495502(1)	PEPS + Deep CNN	3531	No	[33]	2021
-0.495530	DMRG	8192 SU(2) states	No	[31]	2014
-0.495627(6)	aCNN	6538	Yes	[34]	2023
-0.49575(3)	RBM-fermionic	2000	Yes	[15]	2019
-0.49586(4)	CNN	10952	Yes	[35]	2023
-0.4968(4)	RBM ($p = 1$)	Not available	Yes	[36]	2022
-0.49717(1)	Deep CNN	106529	Yes	[28]	2022
-0.497437(7)	GCNN	Not available	No	[27]	2021
-0.497468(1)	Deep CNN	421953	Yes	[30]	2022
-0.4975490(2)	VMC ($p = 2$)	5	Yes	[13]	2013
-0.497627(1)	Deep CNN	146320	Yes	[29]	2023
-0.497629(1)	RBM+PP	5200	Yes	[37]	2021
-0.497634(1)	**Deep ViT**	**267720**	**No**	**Present work**	**2023**

R. Rende, L.L. Viteritti, L. Bardone, FB, and S. Goldt, arXiv:2311.16889

- In one dimension, ViT are sometimes “better” than DMRG (with PBC)

L.L. Viteritti, R. Rende, and FB, Phys. Rev. Lett. **130**, 236401 (2023)

- Calculations on the 10×10 cluster with periodic-boundary conditions



- With 3 parameters (no Lanczos steps): $E/J_1 \approx -0.4946$
- With 267720 parameters: $E/J_1 \approx -0.4976$

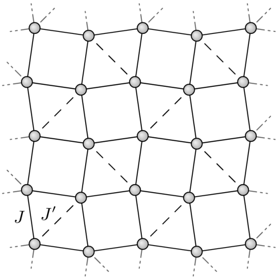
The two-dimensional Shastry-Sutherland model

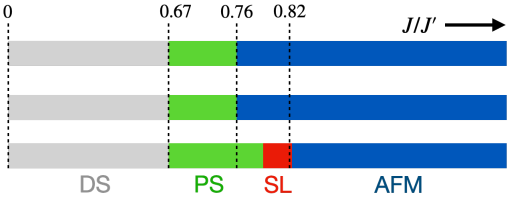
$$\mathcal{H} = J \sum_{\langle R,R' \rangle} \mathbf{S}_R \cdot \mathbf{S}_{R'} + J' \sum_{\langle\langle R,R' \rangle\rangle} \mathbf{S}_R \cdot \mathbf{S}_{R'}$$

The Heisenberg model captures the low-energy properties of $SrCu_2(BO_3)_2$ (dimer phase $J/J' \approx 0.63$)

H. Kageyama *et al.*, Phys. Rev. Lett. **82**, 3168 (1999)

S. Miyahara and K. Ueda, Phys. Rev. Lett. **82**, 3701 (1999)





P. Corboz and F. Mila, PRB **87** 115144 (2013)

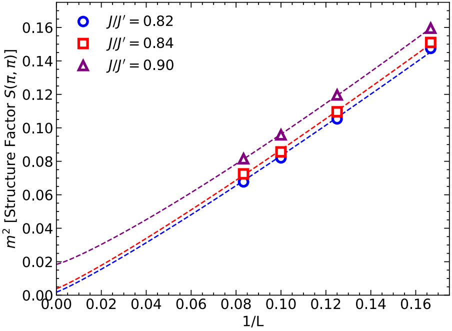
J. Lee, Y. You, S. Sachdev, and A. Vishwanath, PRX **9** 041037 (2019)

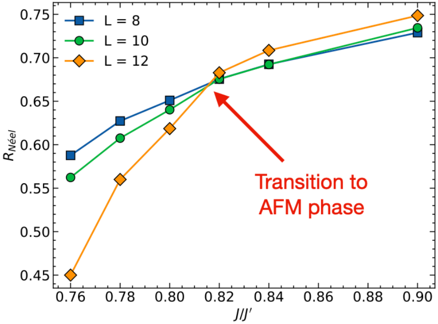
J. Yang, A. Sandvik, and L. Wang, PRB **105** L060409 (2022)

$$S_L(\mathbf{k}) = \frac{1}{L^2} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \mathbf{S}_0 \cdot \mathbf{S}_R \rangle$$

$$m^2(L) \equiv S_L(\pi, \pi)$$

$$R_{\mathrm{Neel}} = 1 - \frac{S_L(\pi, \pi + 2\pi/L)}{S_L(\pi, \pi)}$$

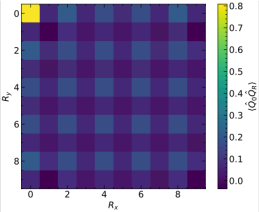




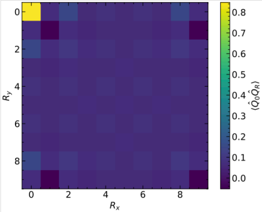
$$C(\mathbf{R}) = \langle Q_0 Q_R \rangle \qquad Q_R \equiv \frac{1}{2}[P_R + P_R^{-1}]$$

P_R is a cyclic permutation operator on the four spins of a plaquette at $\mathbf{R}$

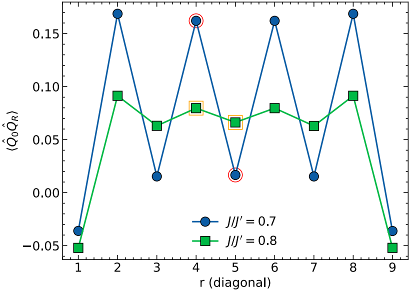
$J/J' = 0.7$



$J/J' = 0.8$



$$m_p(L) \equiv |C(L/2, L/2) - C(L/2-1, L/2-1)|$$



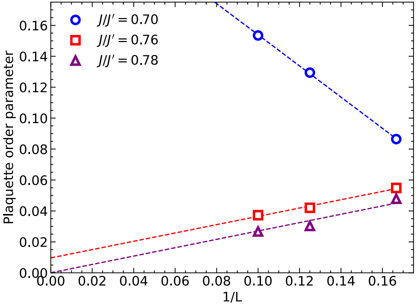
Our phase diagram

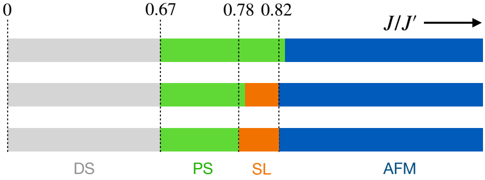
The size scaling of the plaquette order parameter predicts a transition at

$$J/J' \approx 0.77$$

The size scaling of the AFM order parameter predicts a transition at

$$J/J' \approx 0.82$$





W.-Y. Liu *et al.*, arXiv:2309.10955

J. Yang, A. Sandvik, and L. Wang, PRB **105** L060409 (2022)

L.L. Viteritti, R. Rende, A. Parola, S. Goldt, FB, arxiv:2311.16889

At present, no simple RVB states have been found for the intermediate region

Conclusions

- **RVB states (and bees) are extremely useful**

Transparent interpretation in terms of “elementary objects”

Not always very accurate to reach a definite conclusion

- **Neural-network states are extremely accurate and powerful**

No transparent understanding (at the moment)

They are becoming the paradigm to study two-dimensional systems