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NEURAL-NETWORK QUANTUM STATES FOR ULTRACOLD FERMI GASES AND DILUTE NUCLEAR MATTER

JANE KIM

Ohio University

Quantum Few- and Many-Body Systems in Universal Regimes, Institute for Nuclear Theory

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In collaboration with:

M. Hjorth-Jensen, A. Lovato, B. Fore, G. Carleo, G. Pescia, J. Nys, and S. Gandolfi

MSU/FRIB/UiO ANL EPFL LANL

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PHY-2310020

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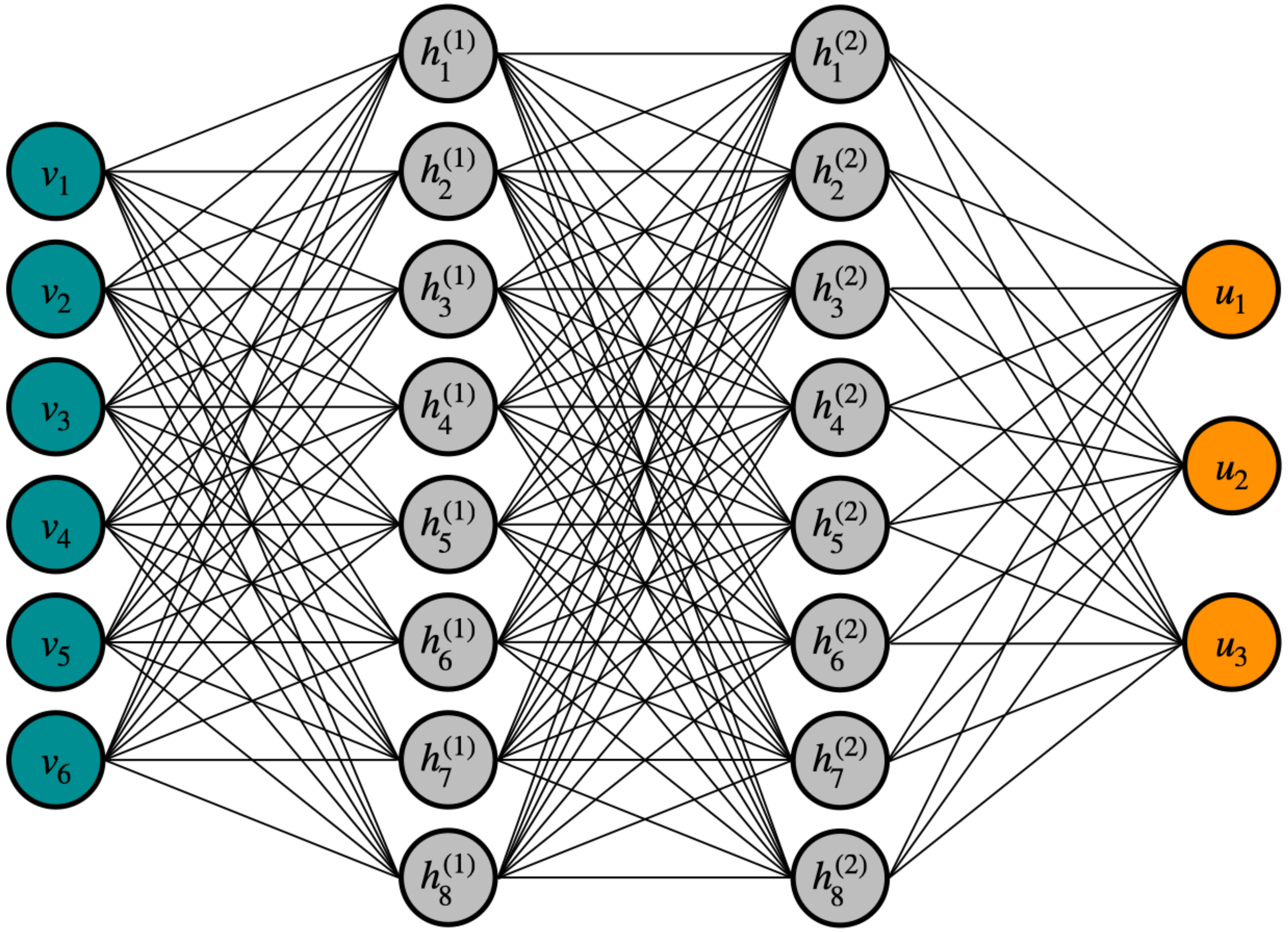
NEURAL-NETWORK QUANTUM STATES (NQS)

- Class of variational wave functions constructed using artificial neural networks
- Introduced by G. Carleo and M. Troyer in 2017
- State-of-the-art NQS usually built using:
    - Densely connect layers (affine)
    - Nonlinear activation functions
    - Pooling operations (destroys ordering)
    - Concatenation operations
    - Determinant



G. Carleo and M. Troyer, Science ***355****, 602-606 (2017).*

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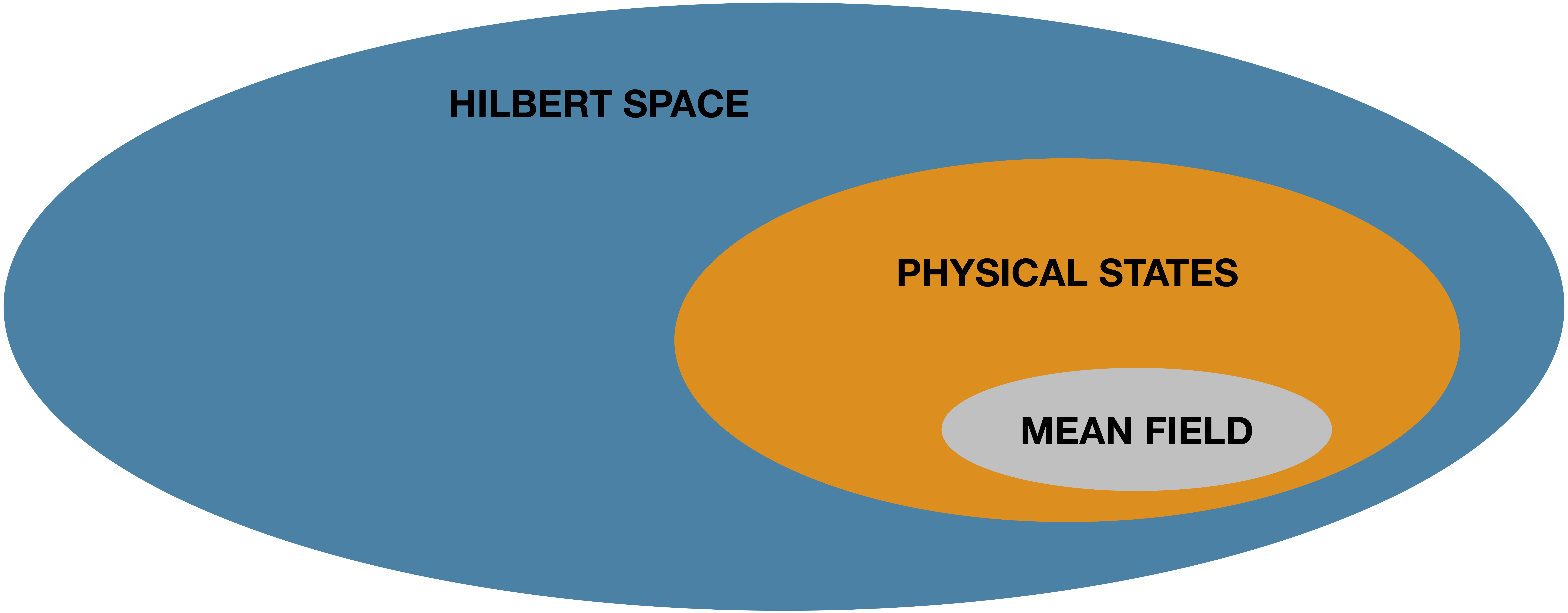

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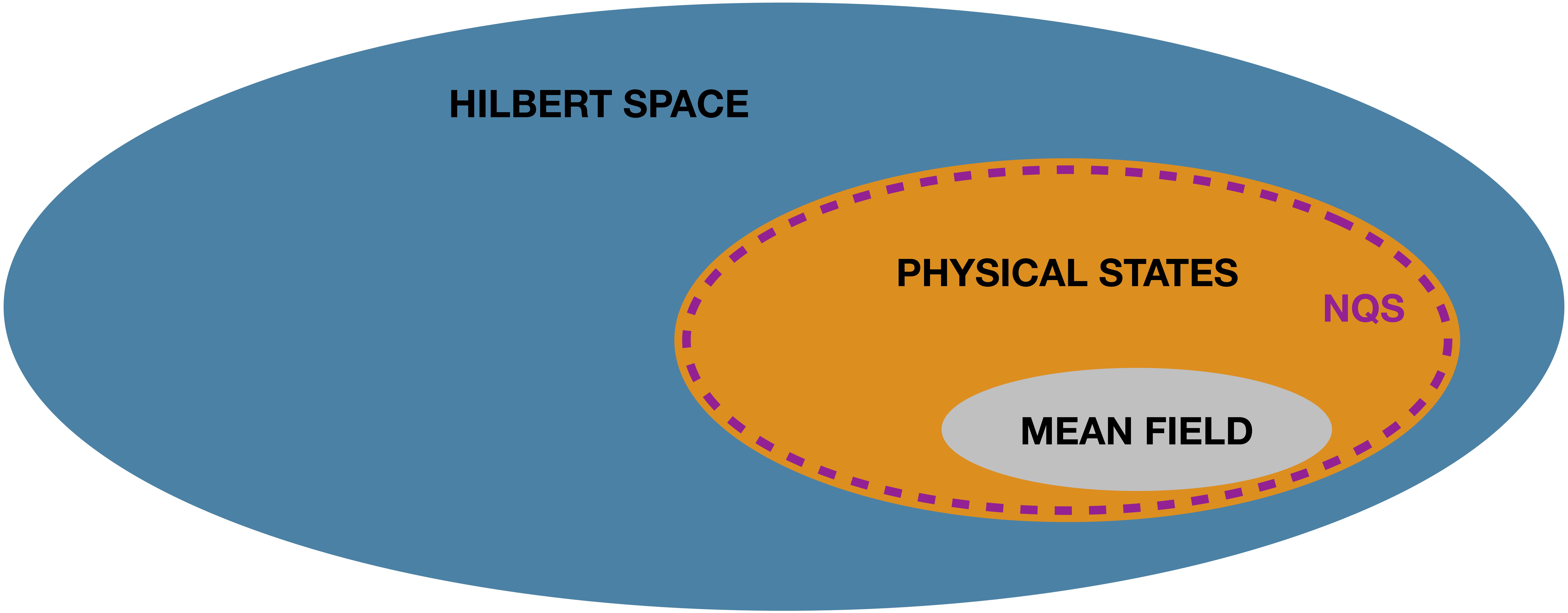

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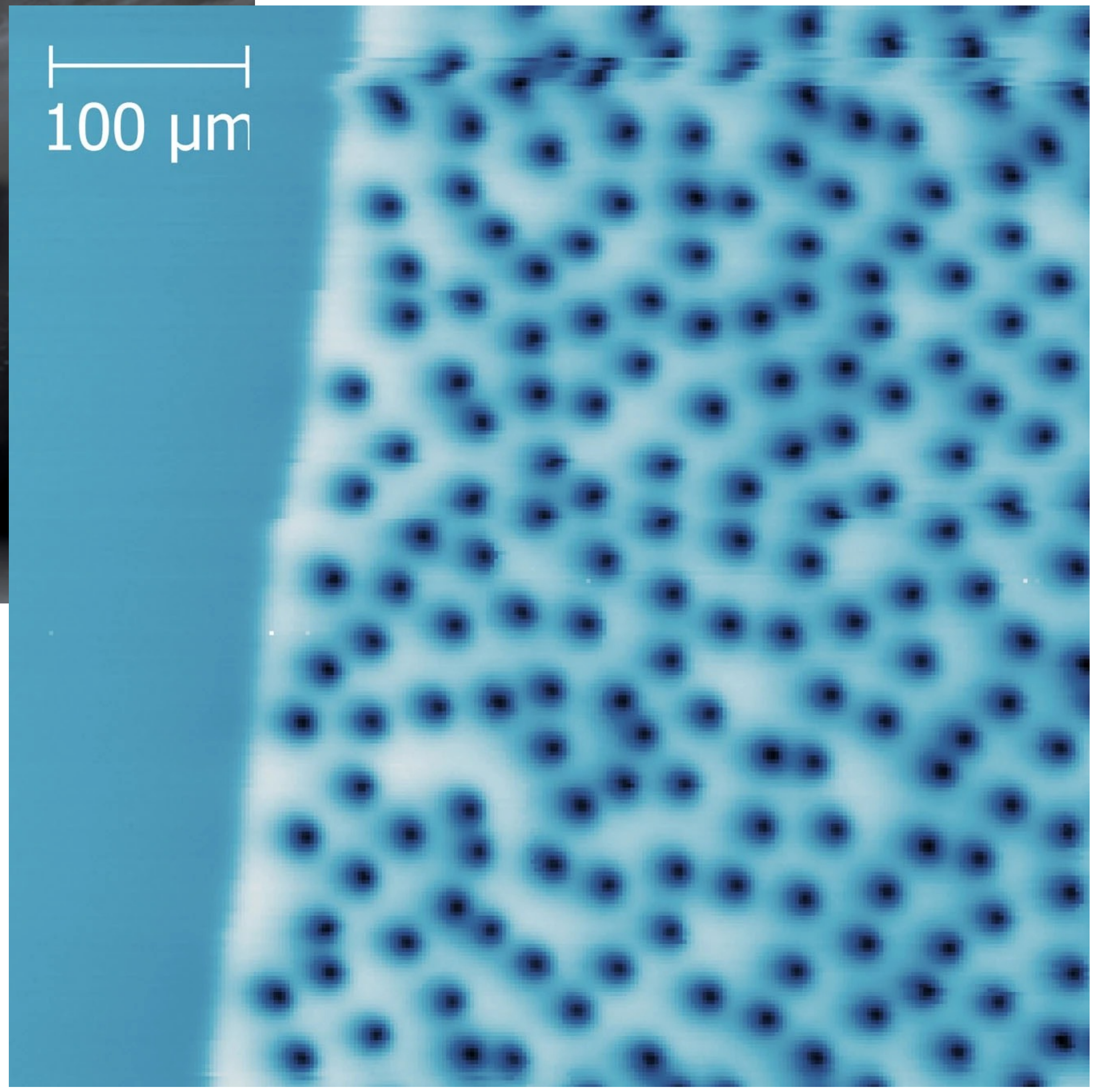
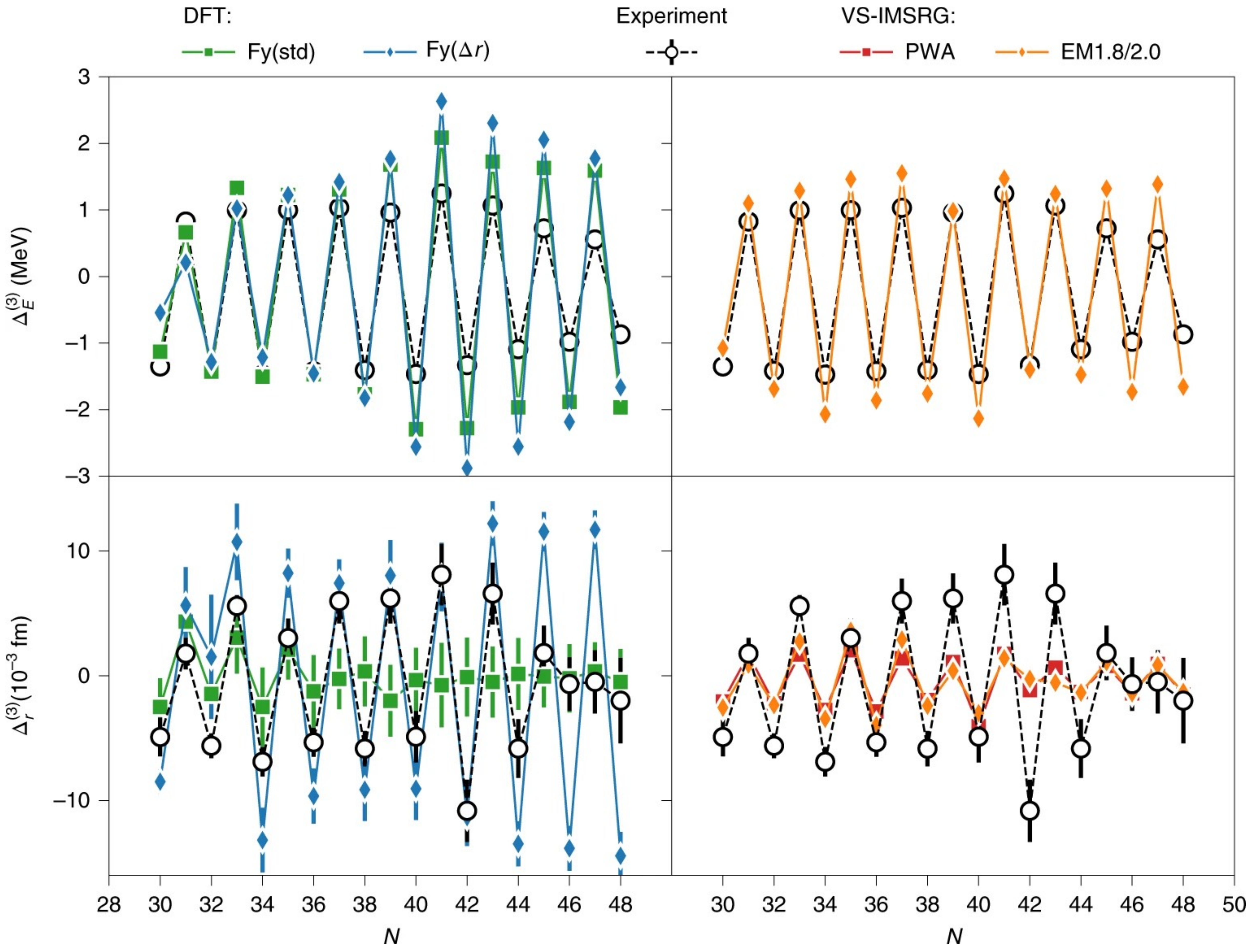
PAIRING PHENOMENA





J. Adam Fenster; Wells et al. Scientific Reports 5, 8677 (2015); de Groote et al., Nature Physics 16, 620-624 (2020)

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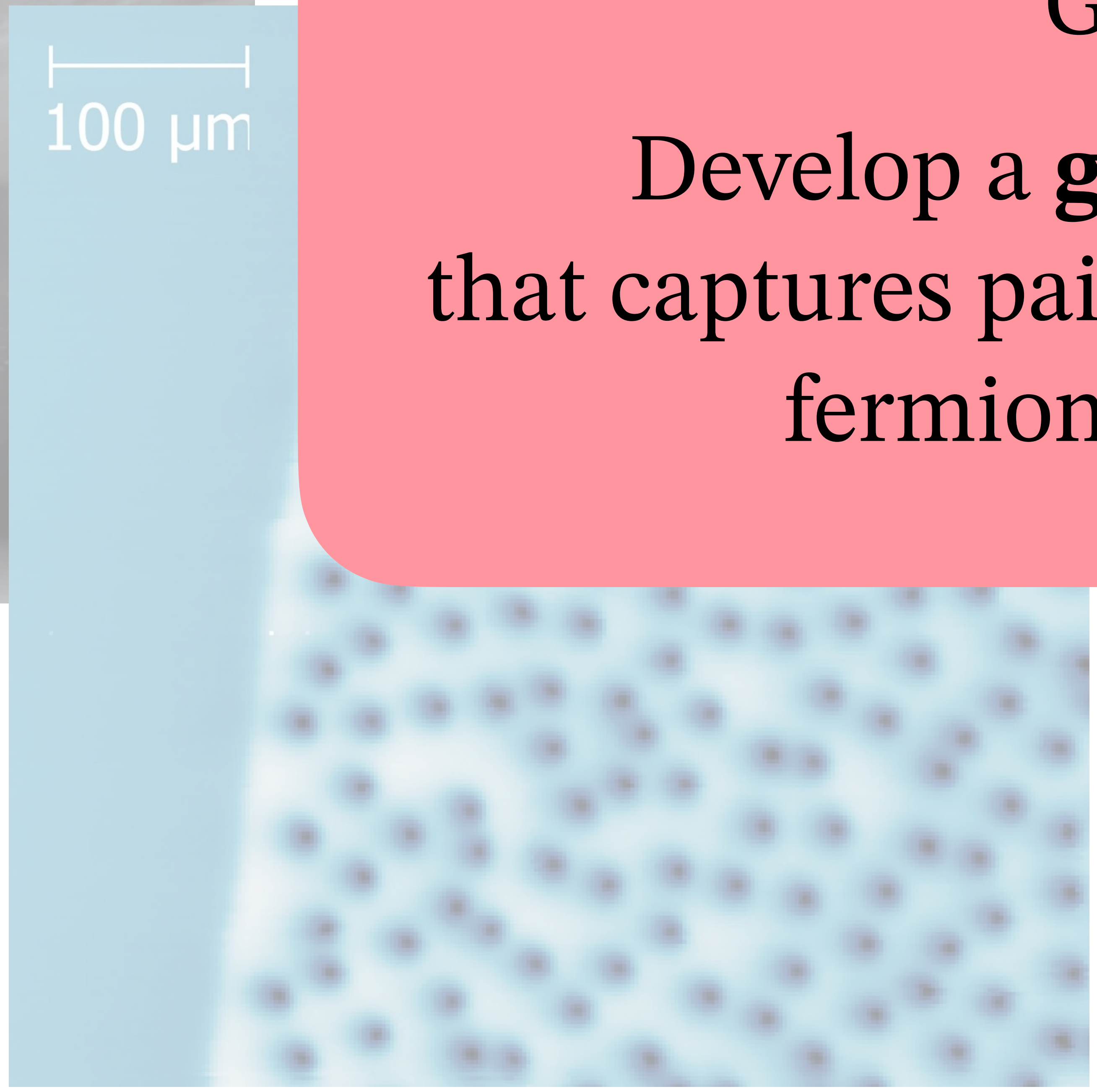

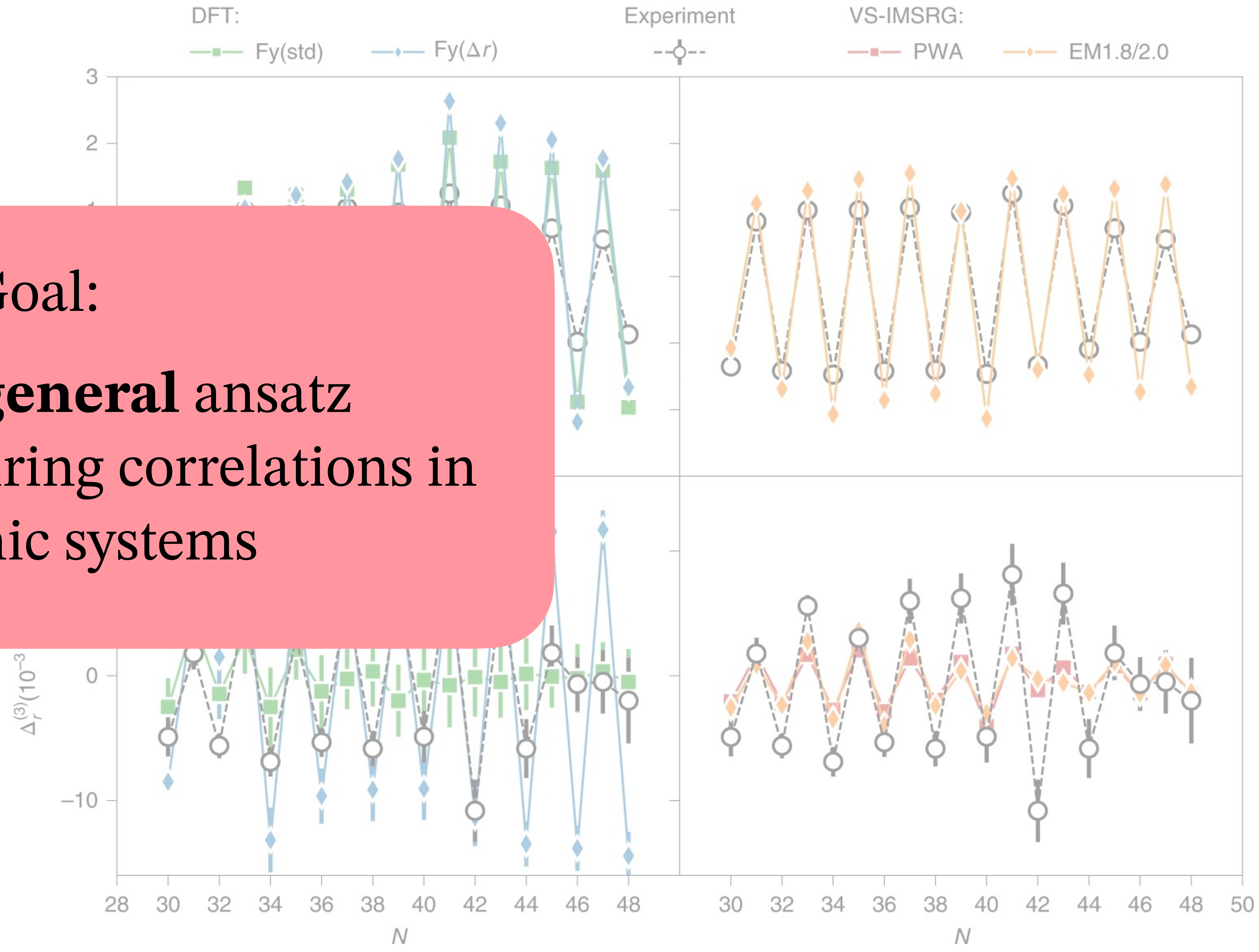

Goal:

Develop a **general** ansatz
that captures pairing correlations in
fermionic systems

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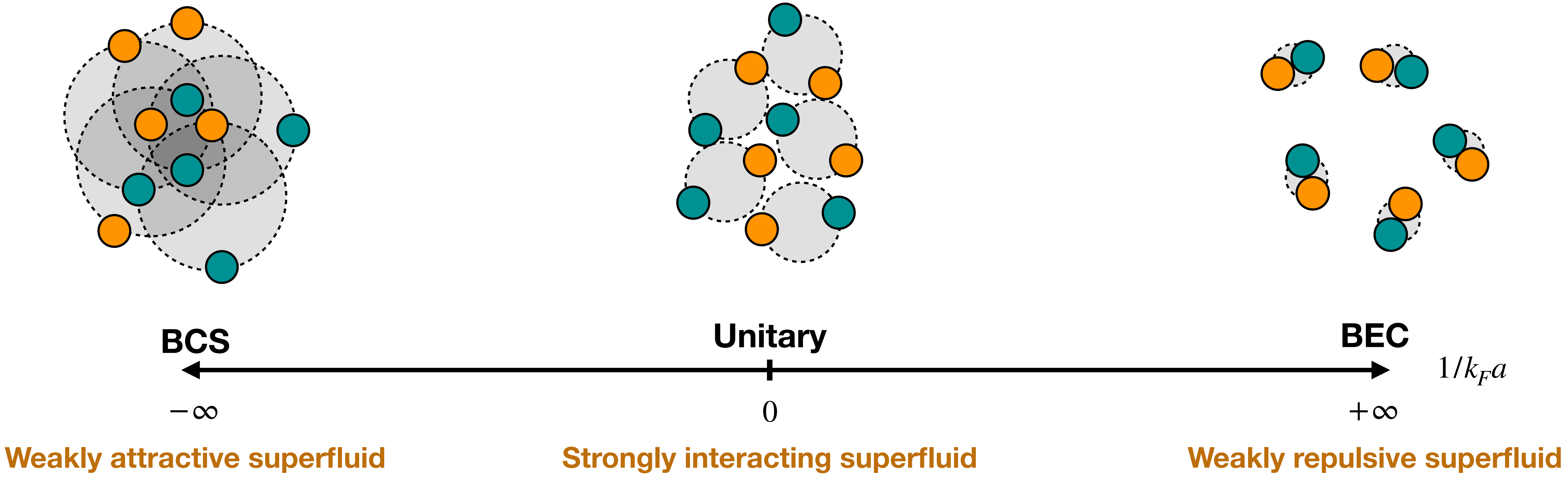
ULTRACOLD FERMI GASES

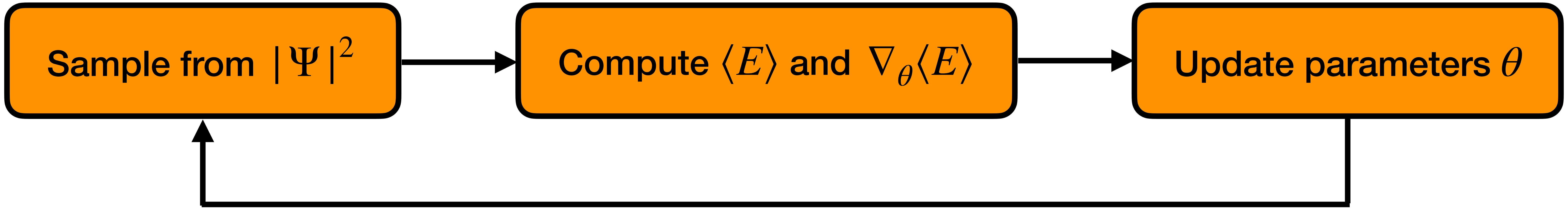
- Characterized by strong, short-range attraction between fermions
- Can be created in the lab by tuning an external magnetic field near a Feshbach resonance



- Unitary Fermi gas: an extreme example of a strongly-paired quantum system

THIS WORK

- Simulate unpolarized gas of N fermions in a periodic box of size L
- Design a neural-network quantum state (NQS) that…
    1. Efficiently encodes pairing and backflow correlations
    2. Naturally enforces fermion antisymmetry and boundary conditions
    3. Has as few variational parameters as possible
- Train NQS using variational Monte Carlo (VMC) with stochastic reconfiguration

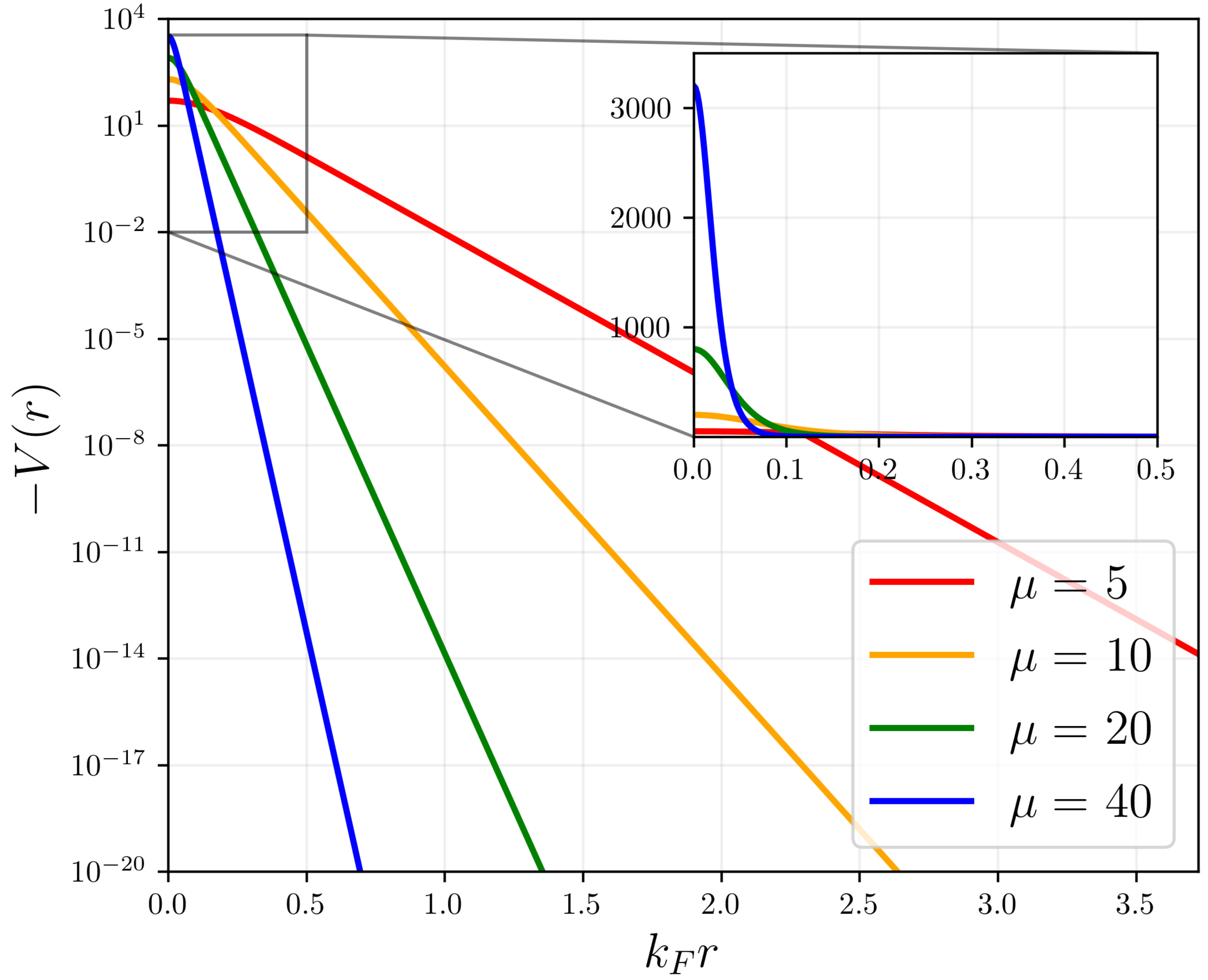


PÖSCHL-TELLER POTENTIAL

- Regularized, short-range attraction

$$V_{ij} = (\delta_{s_i,s_j} - 1)v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij})}$$

- Exact solutions of two-body problem
- At unitarity: $v_0 = 1,\ r_e = 2/\mu$



JK et al., Commun. Phys. **7**, 148 (2024).

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ANTISYMMETRY

- The antisymmetry of the fermionic wave function is constrained by a Pfaffian
- Simplest and most general way to build an antisymmetrized product of pairing orbitals rather than single-particle orbitals

$$\Phi(X) = \mathrm{pf} \begin{bmatrix} 0 & \phi(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \phi(\mathbf{x}_1, \mathbf{x}_N) \\ -\phi(\mathbf{x}_1, \mathbf{x}_2) & 0 & \cdots & \phi(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ -\phi(\mathbf{x}_1, \mathbf{x}_N) & -\phi(\mathbf{x}_2, \mathbf{x}_N) & \cdots & 0 \end{bmatrix}$$

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?

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DETERMINANT VS. PFAFFIAN

Defined for $n \times n$ matrices

$$\det(A) = \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} a_{i,\sigma(i)}$$

$$\det(A^T) = \det(A)$$

$$\det(A)\det(B) = \det(AB)$$

Defined for $2n \times 2n$ skew-symmetric matrices

$$\operatorname{pf}(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} a_{\sigma(2i-1),\sigma(2i)}$$

$$\operatorname{pf}(A^T) = (-1)^n \operatorname{pf}(A)$$

$$\operatorname{pf}(A)\operatorname{pf}(B) = \exp\left(\frac{1}{2}\operatorname{tr}\log(A^T B)\right)$$

$$\det(A) = \operatorname{pf}(A)^2$$

DETERMINANT VS. PFAFFIAN

Example:

$$A = \begin{bmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{bmatrix} \quad \Longrightarrow \quad \operatorname{pf} A = af - be + dc$$

Pfaffian implementation: Wimmer, ACM Trans. Math. Softw. 38, 4 (2012)

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$$\det A = a^2f^2 - 2abef + 2acdf + b^2e^2 - 2bcde + c^2d^2$$

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$$\begin{aligned} \det\ A &= a^2f^2 - 2abef + 2acdf + b^2e^2 - 2bcde + c^2d^2 \\ &= (af - be + dc)^2 \end{aligned}$$

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ANTISYMMETRY

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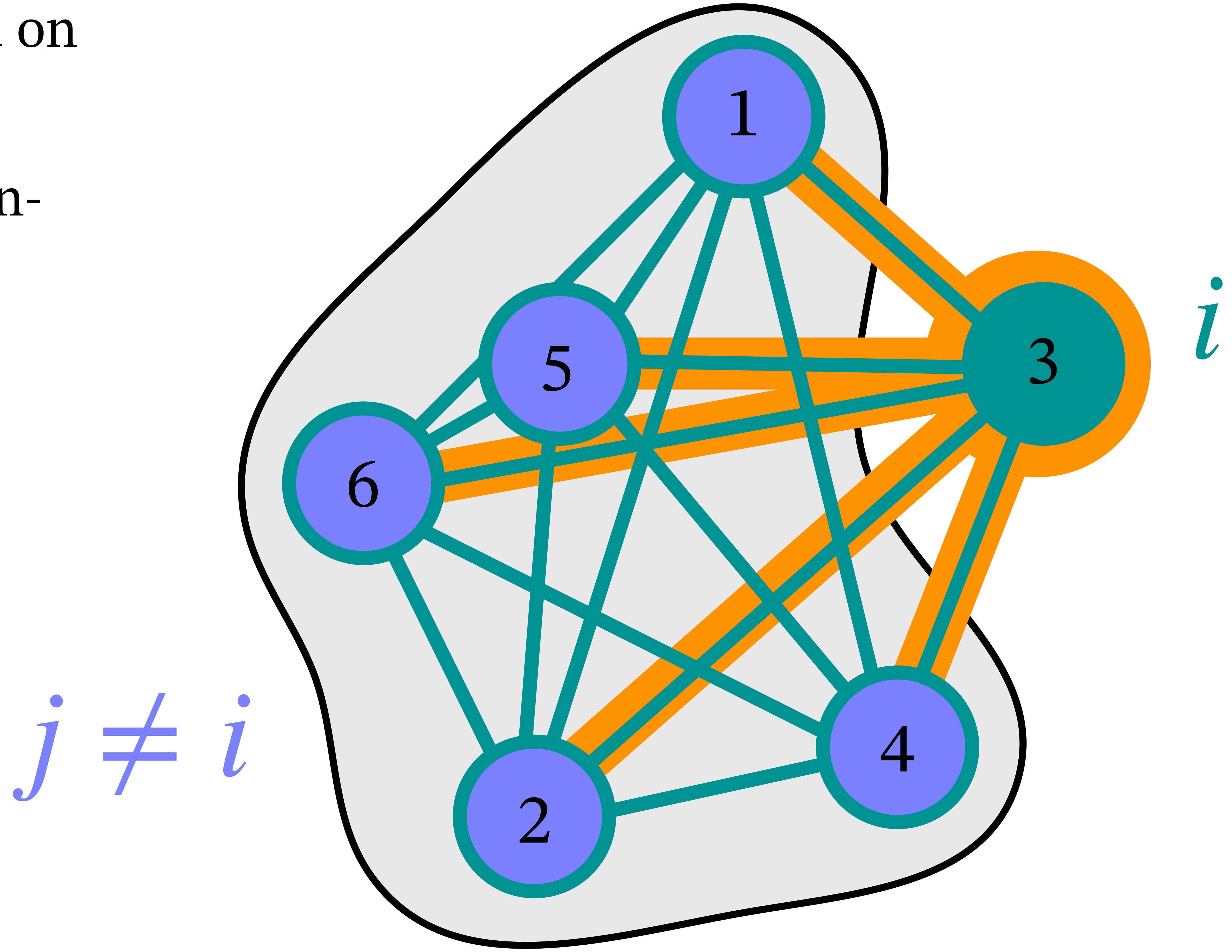
- The pairing orbital into commonly decomposed into explicit singlet and triplet contributions
- We take advantage of universal approximation theorem: $\phi(\mathbf{x}_i, \mathbf{x}_j) \equiv \nu(\mathbf{x}_i, \mathbf{x}_j) - \nu(\mathbf{x}_j, \mathbf{x}_i)$, where ν is a neural network.
- Naturally encodes singlet and triplet pairing because ν takes spins as input

JK et al., *Commun. Phys.* **7**, 148 (2024).

BACKFLOW CORRELATIONS

- The influence on a particle's coordinates based on coordinates of all other particles
- Backflow transformations must be permutation-equivariant to preserve antisymmetry

$$\mathbf{x}_i \mapsto \mathbf{f}(\mathbf{x}_i; \{\mathbf{x}_j\}_{j \neq i})$$



MESSAGE-PASSING NEURAL NETWORK

- Represent the system as a fully-connected graph
- Iteratively build backflow correlations into new one- and two-body features through trainable permutation-equivariant operations
- Include skip connections to avoid vanishing/exploding gradients
- Visible nodes/one-body features: $\mathbf{v}_i = (s_i)$
- Visible edges/two-body features: $\mathbf{v}_{ij} = (r_{ij}, \mathbf{r}_{ij}, s_i \cdot s_j)$
- Preprocessing step: $\mathbf{h}_i^{(0)} = (\mathbf{v}_i, A\mathbf{v}_i)$

$$\mathbf{h}_{ij}^{(0)} = (\mathbf{v}_{ij}, B\mathbf{v}_{ij})$$

The set-up

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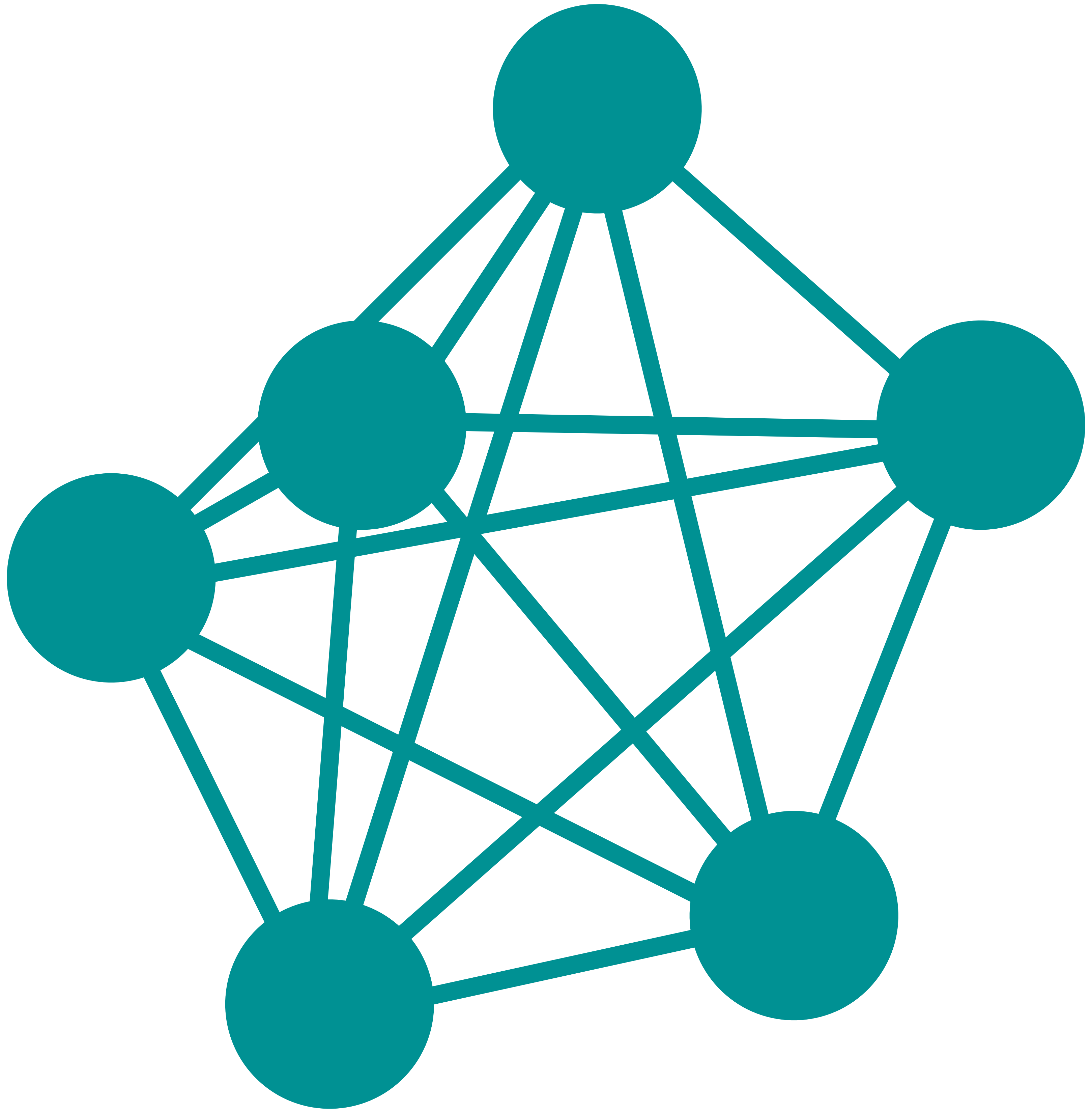

for $t = 1, \ldots, T$:

$$\mathbf{m}_{ij}^{(t)} = \mathbf{M}_t\left(\mathbf{h}_i^{(t-1)}, \mathbf{h}_j^{(t-1)}, \mathbf{h}_{ij}^{(t-1)}\right)$$

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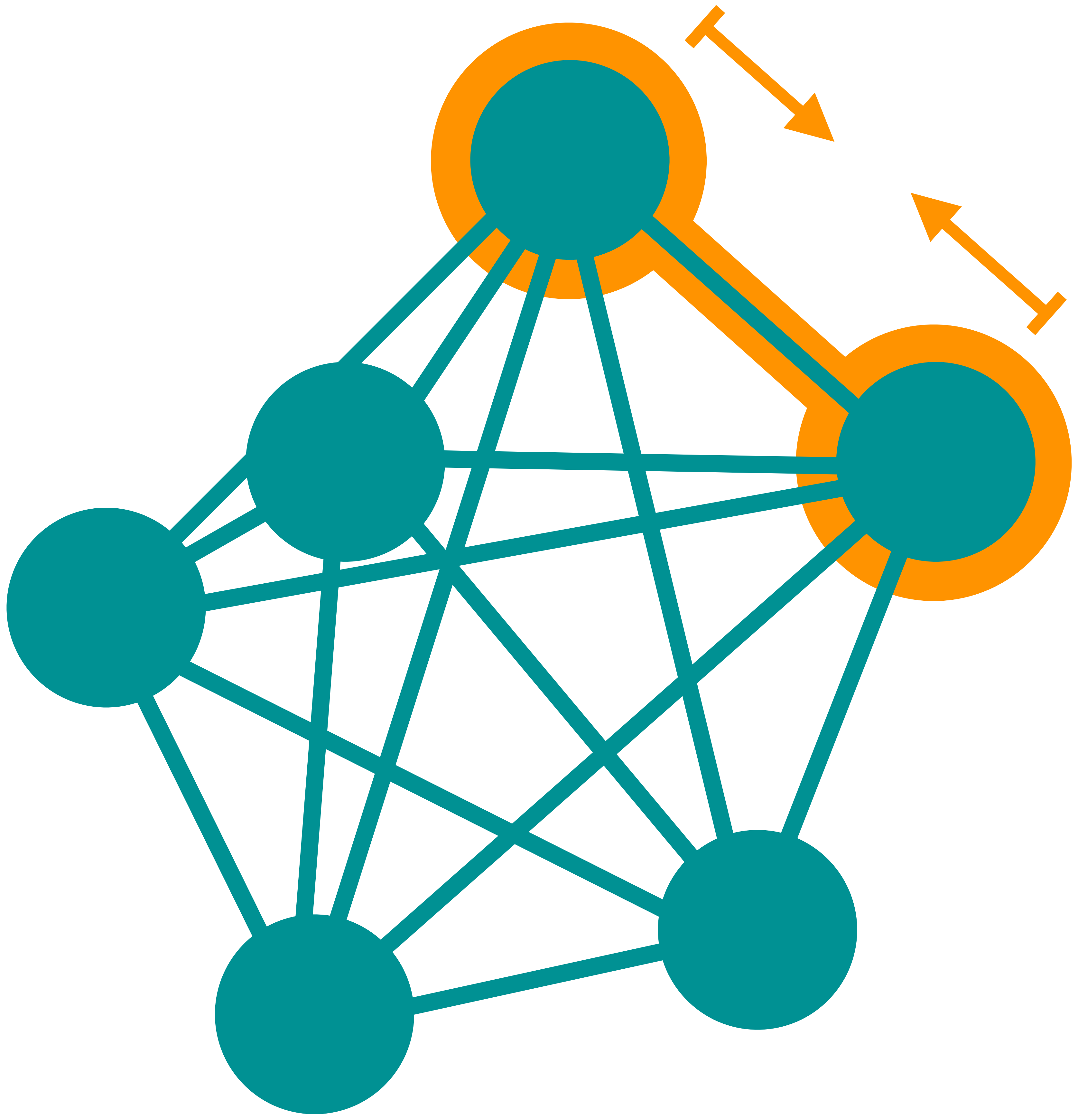

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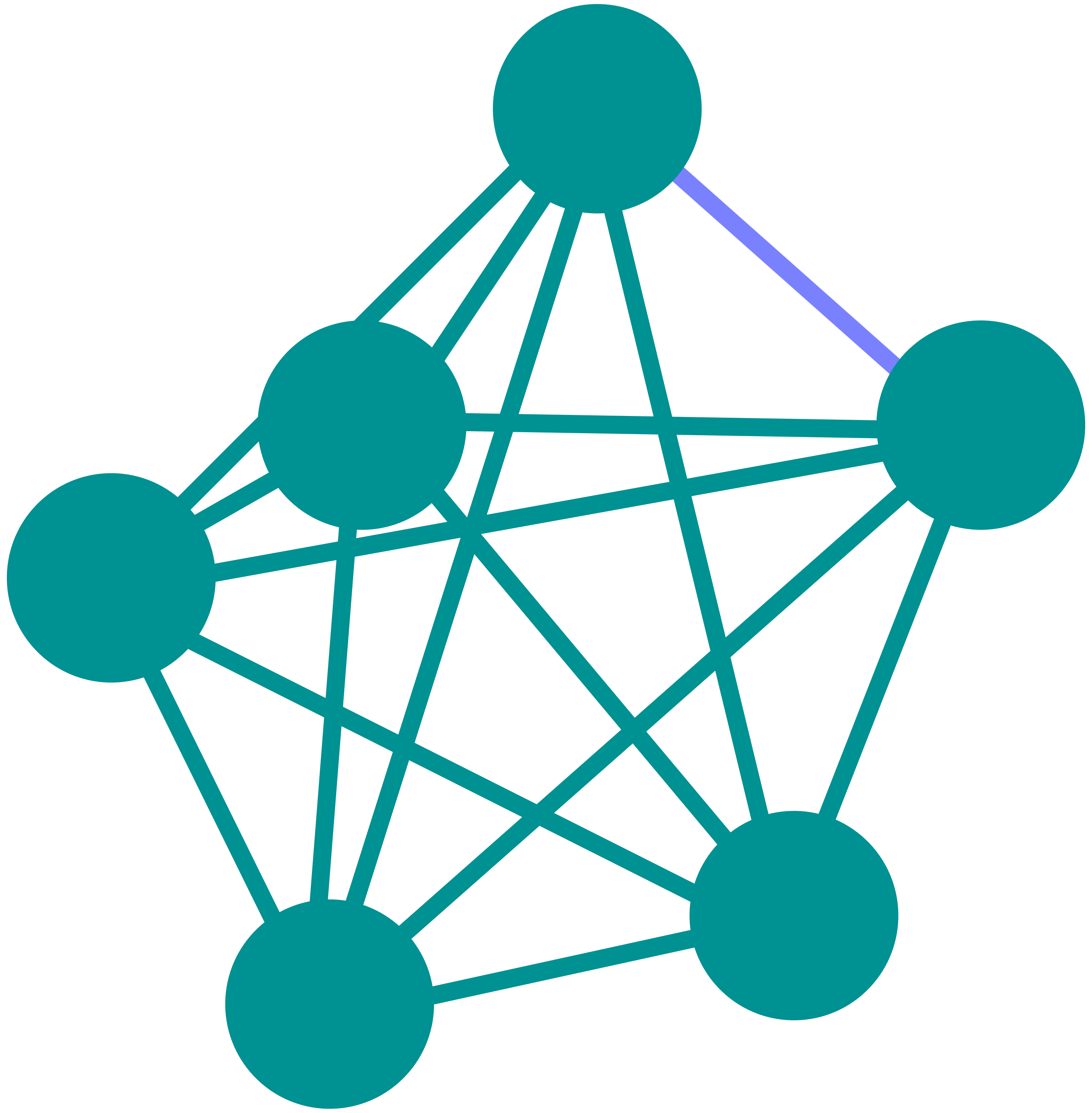

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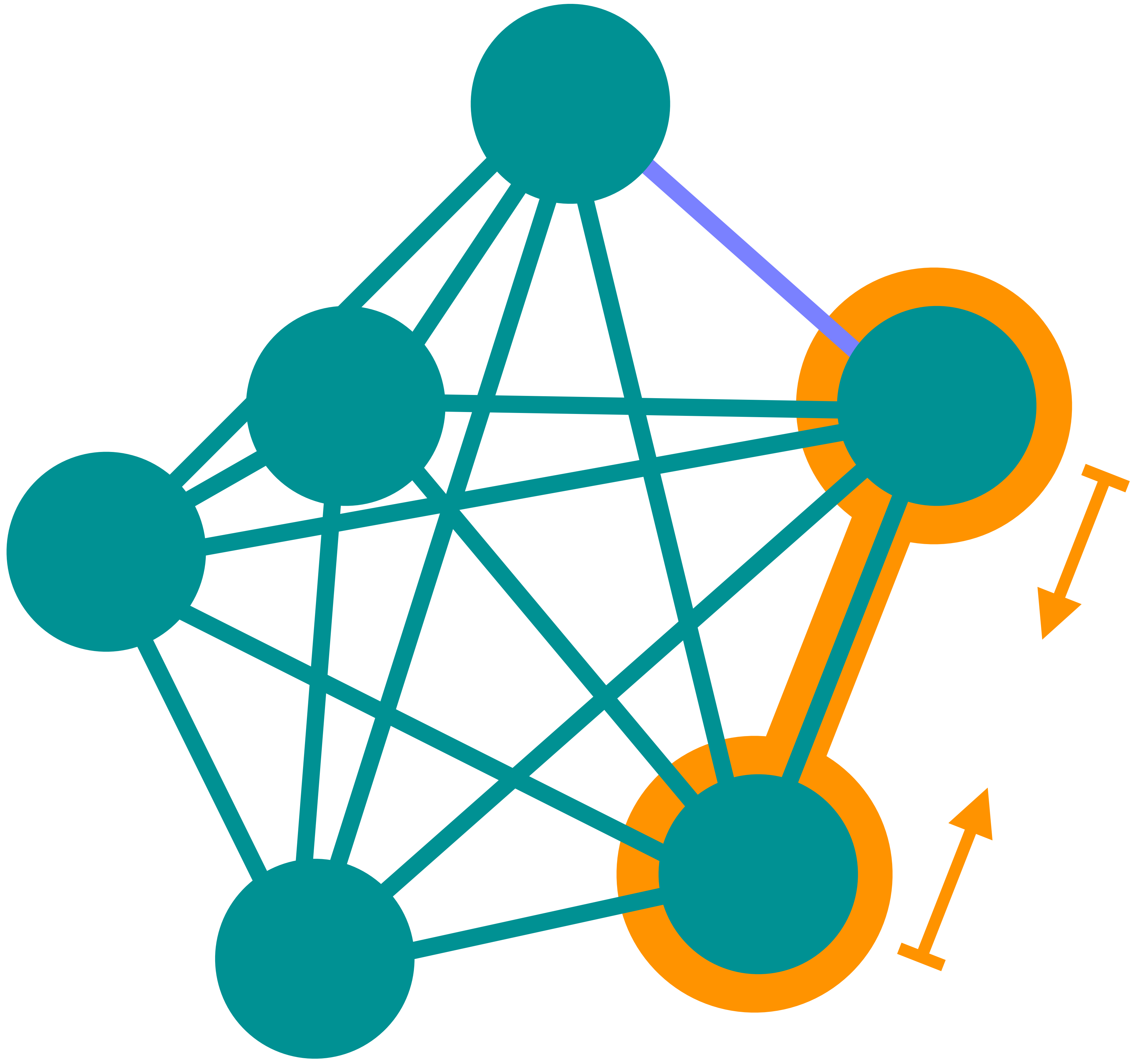

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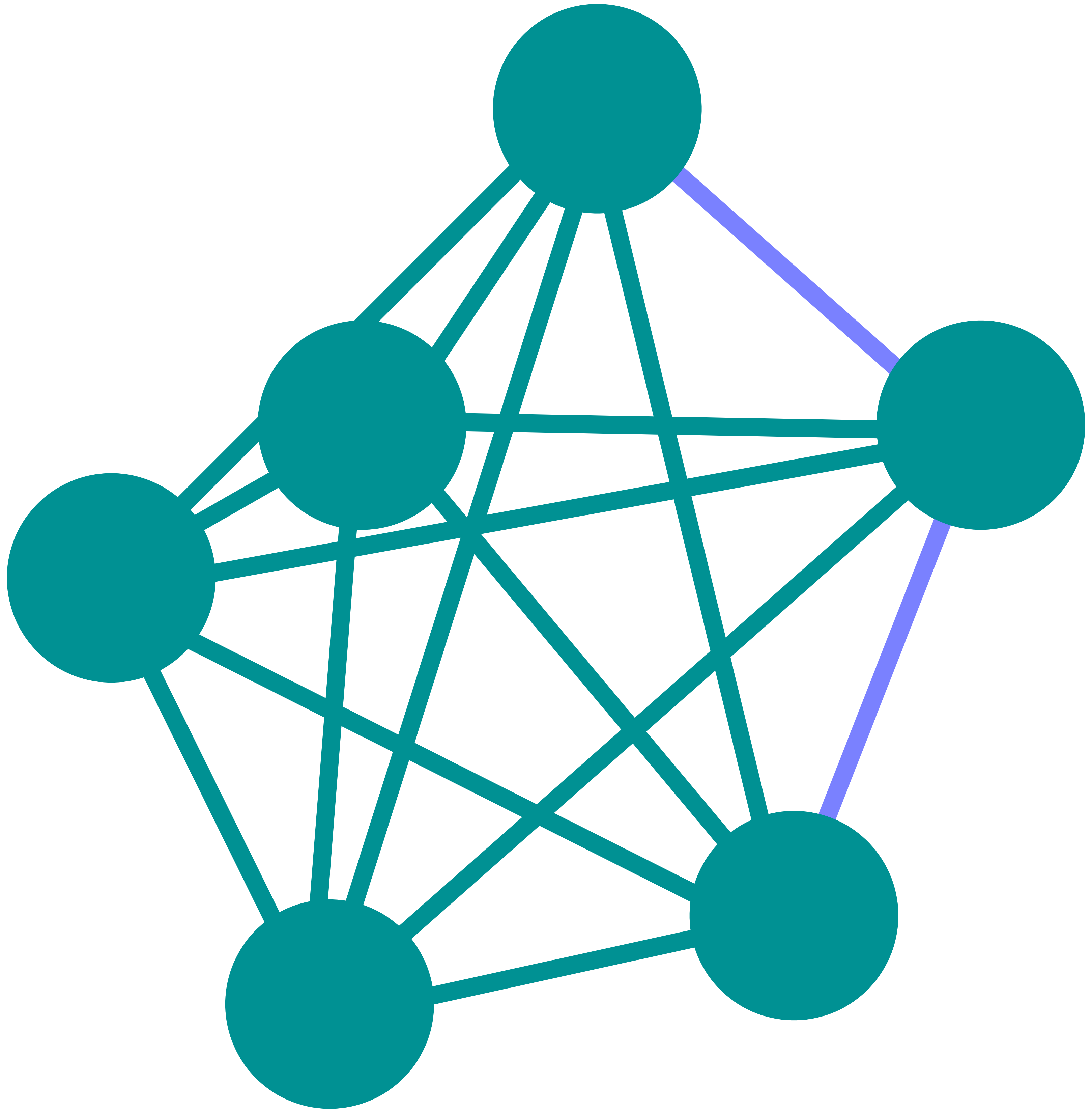

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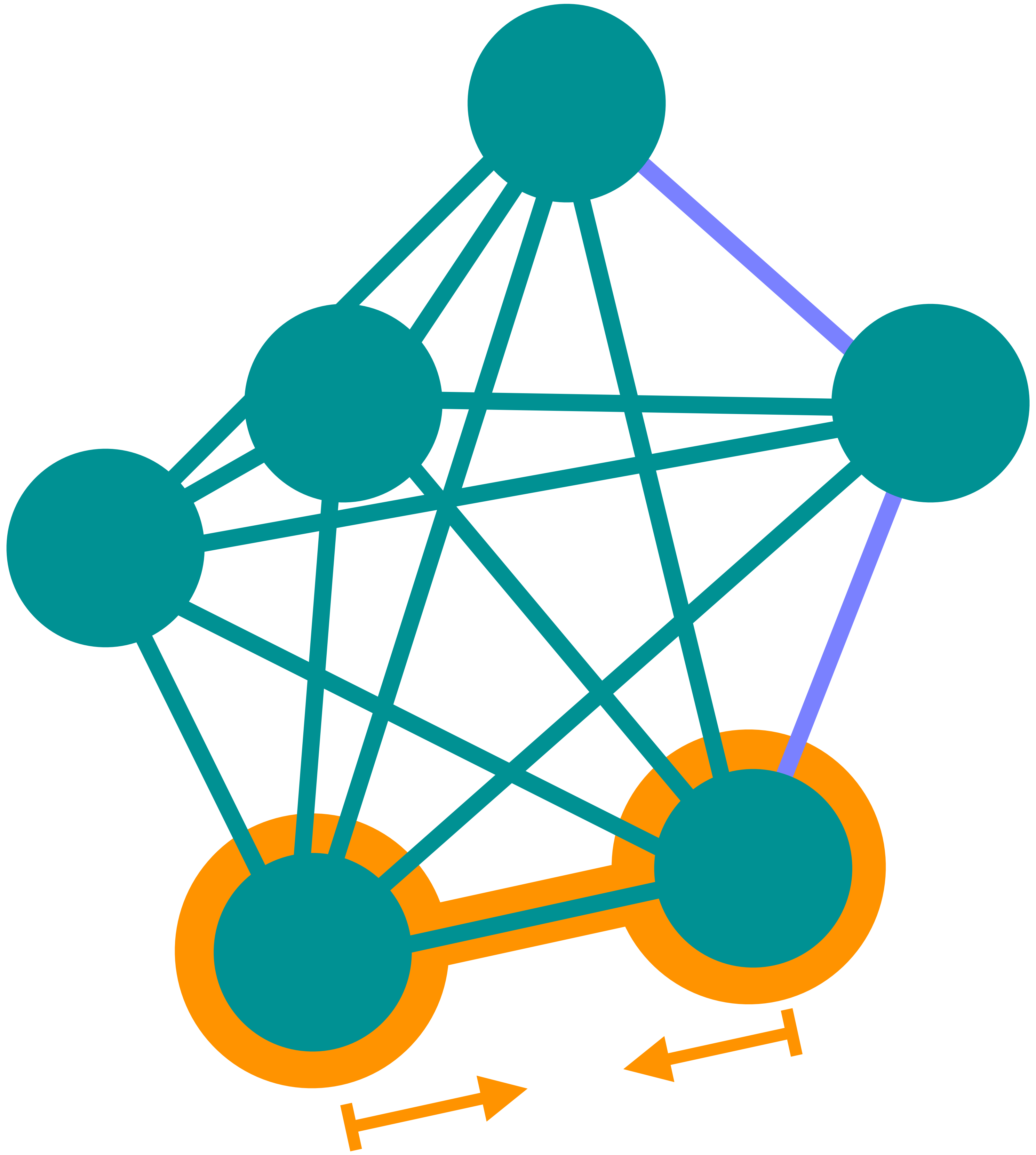

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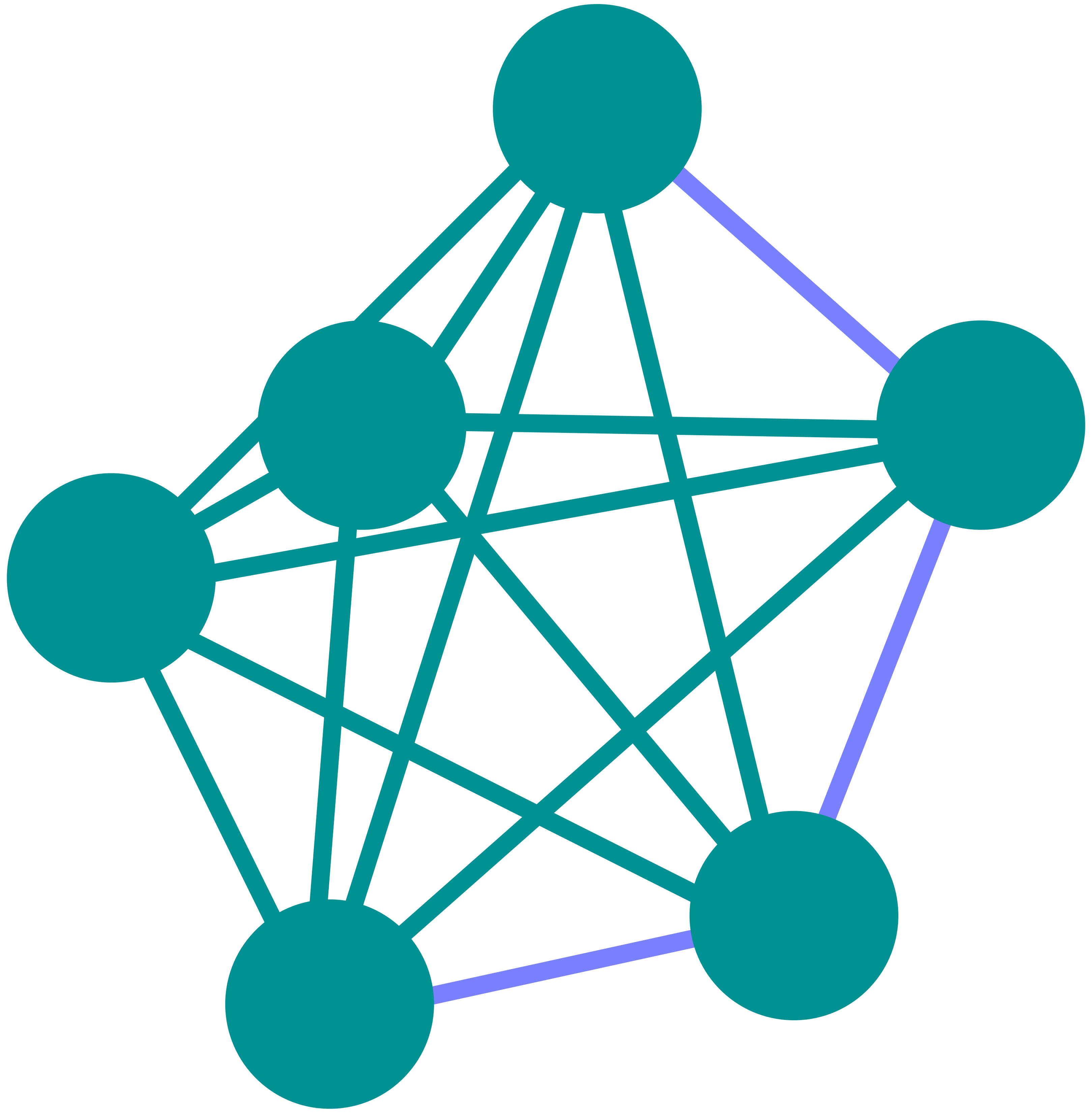

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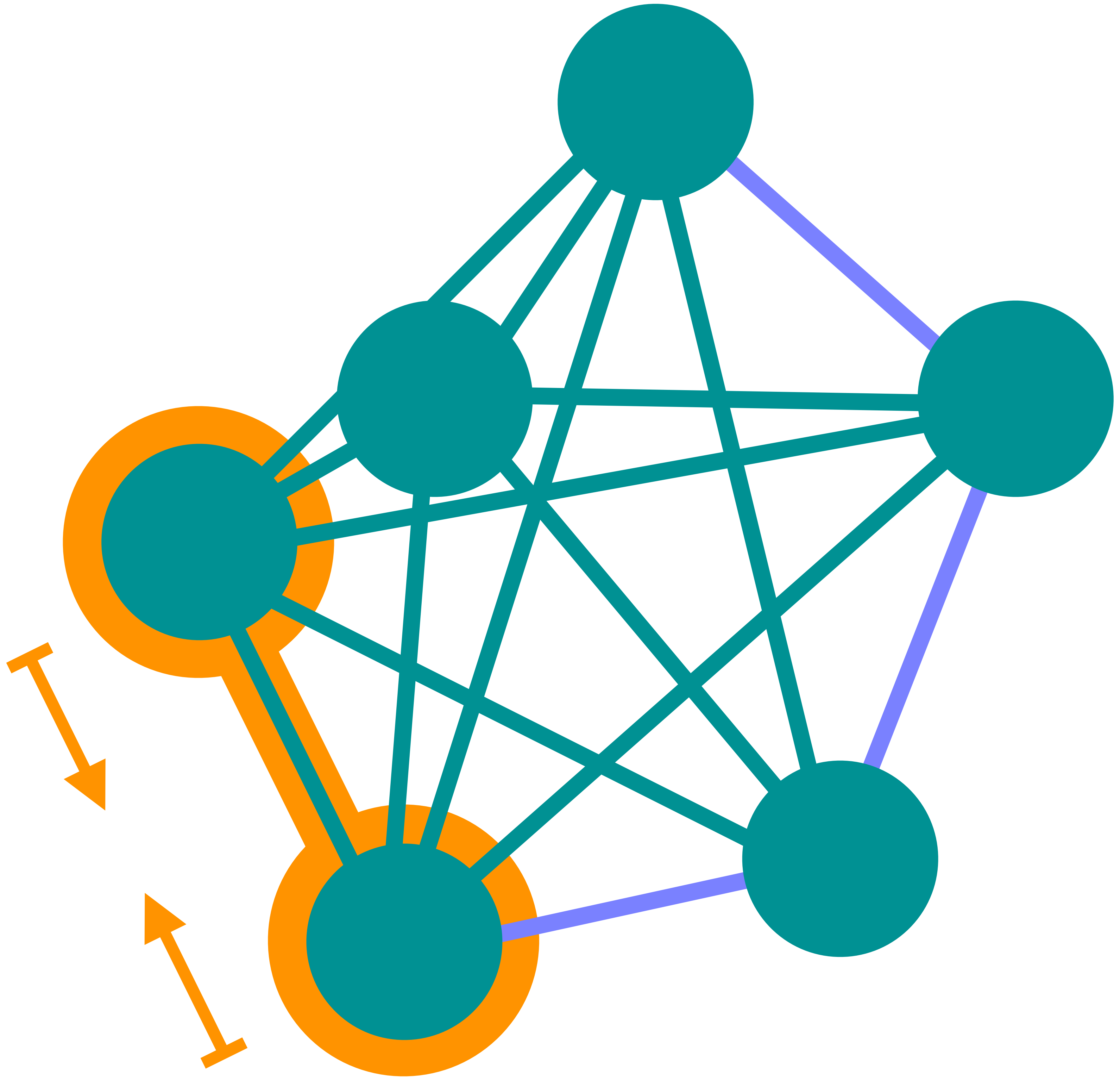

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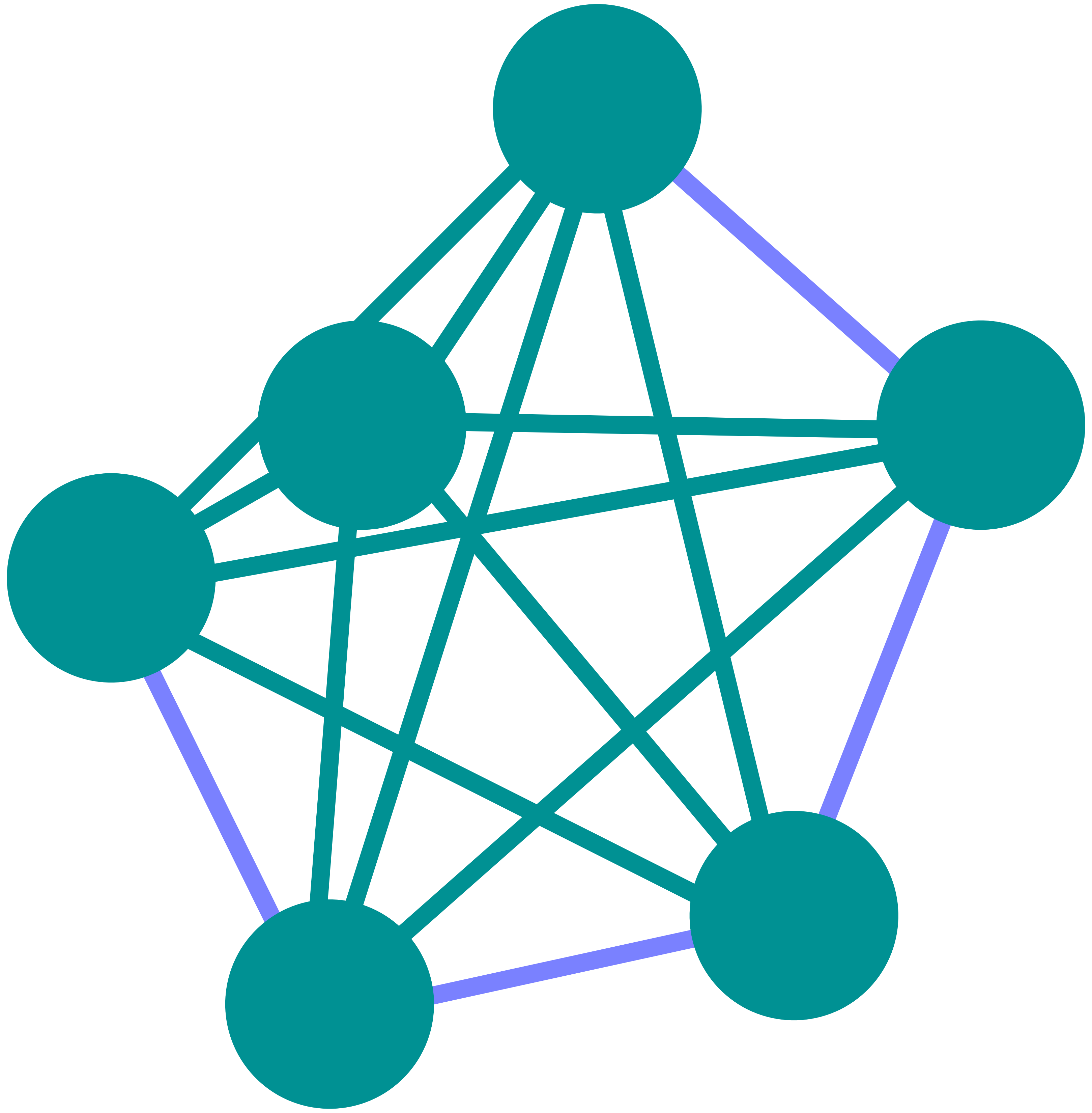

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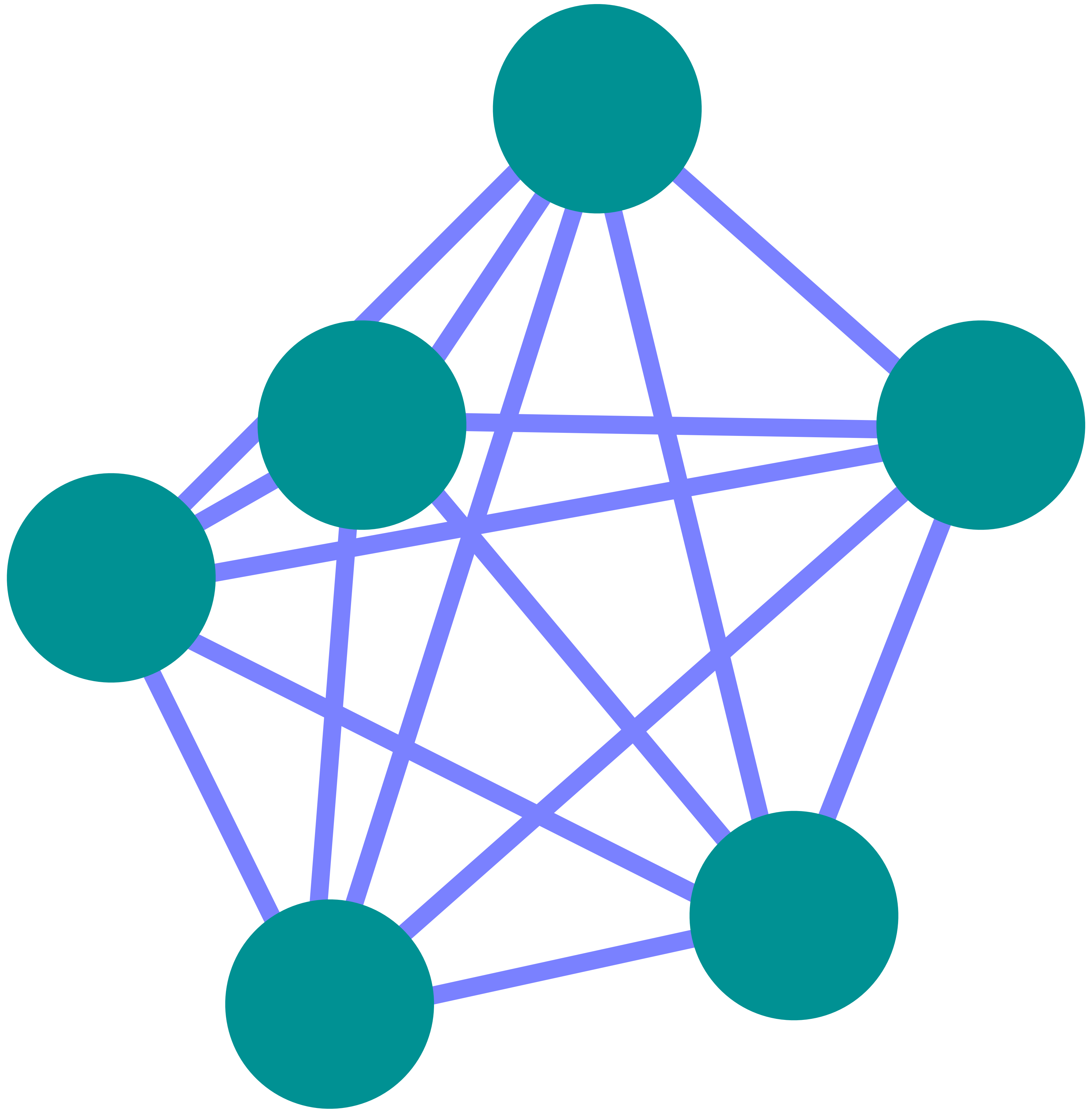

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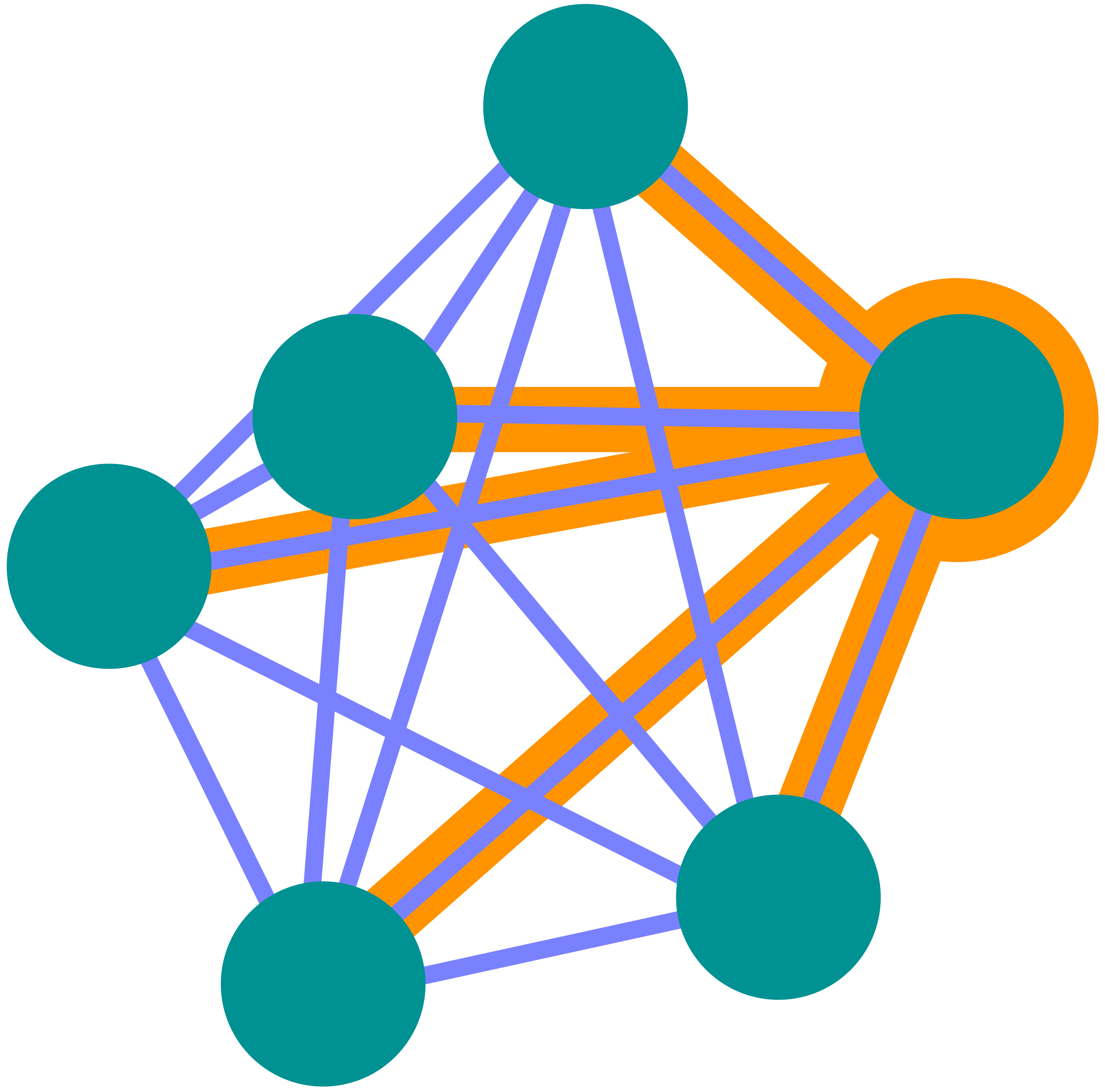

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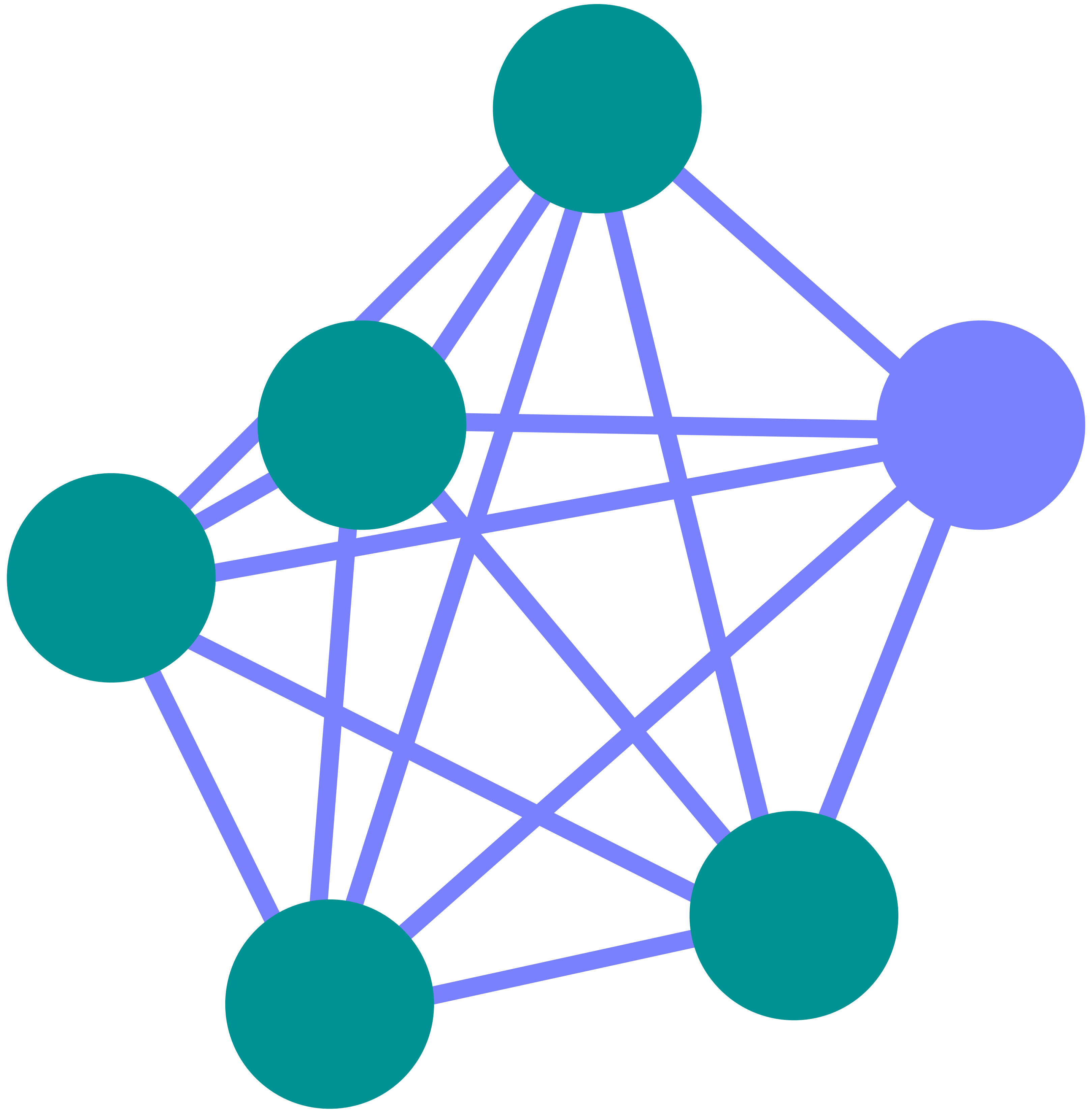

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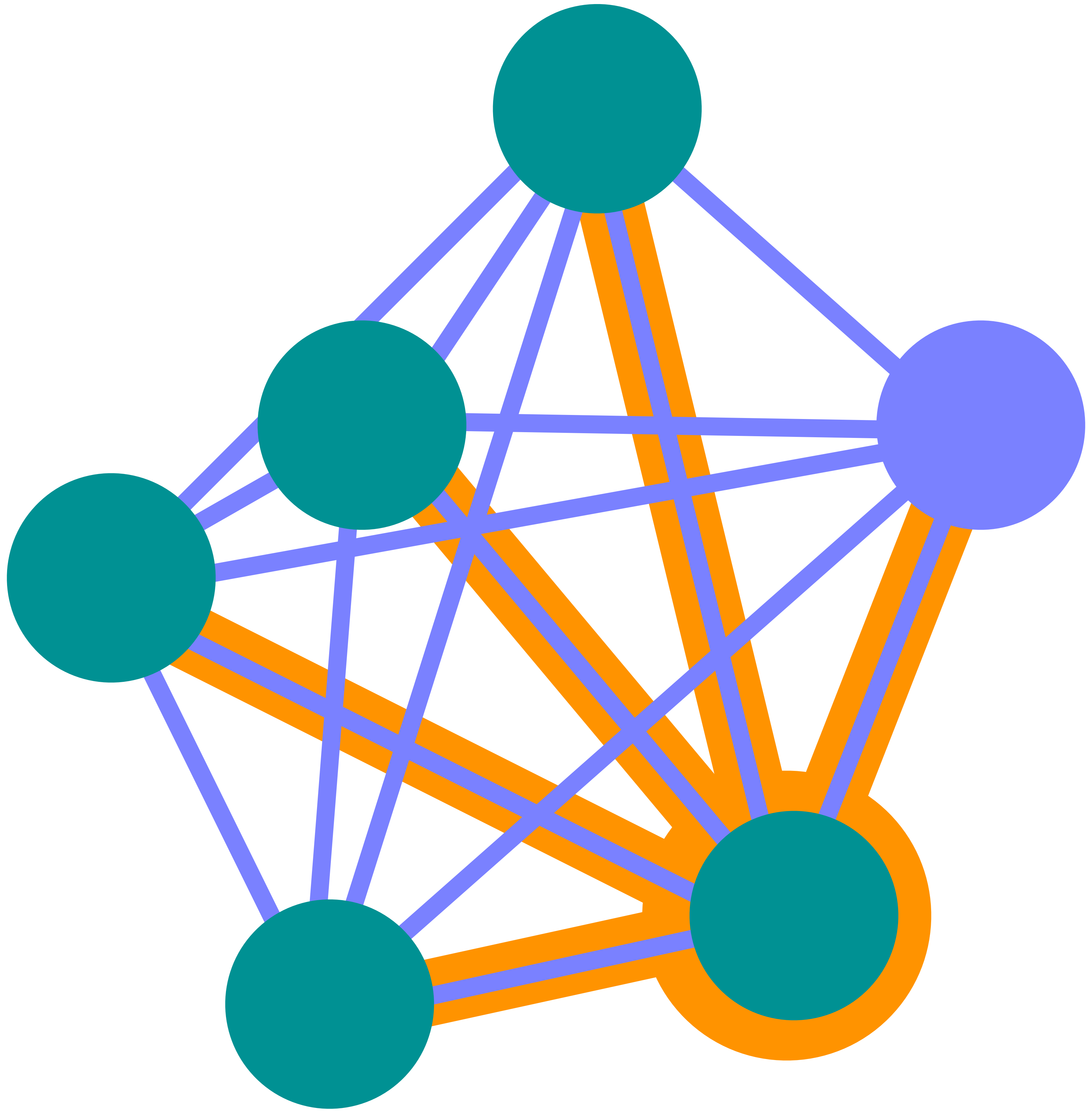

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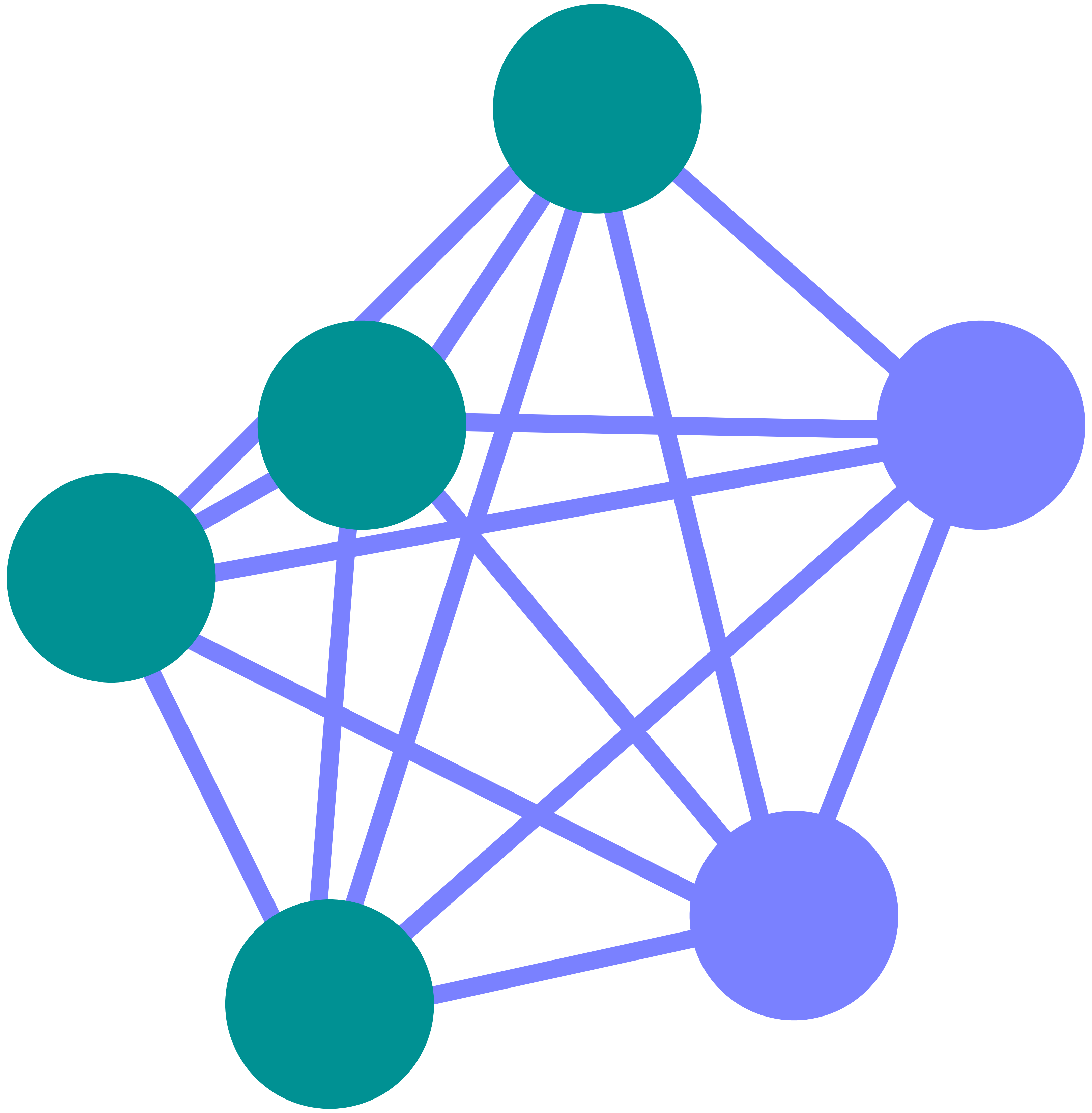
MESSAGE-PASSING NEURAL NETWORK



for $t = 1, \ldots, T$:

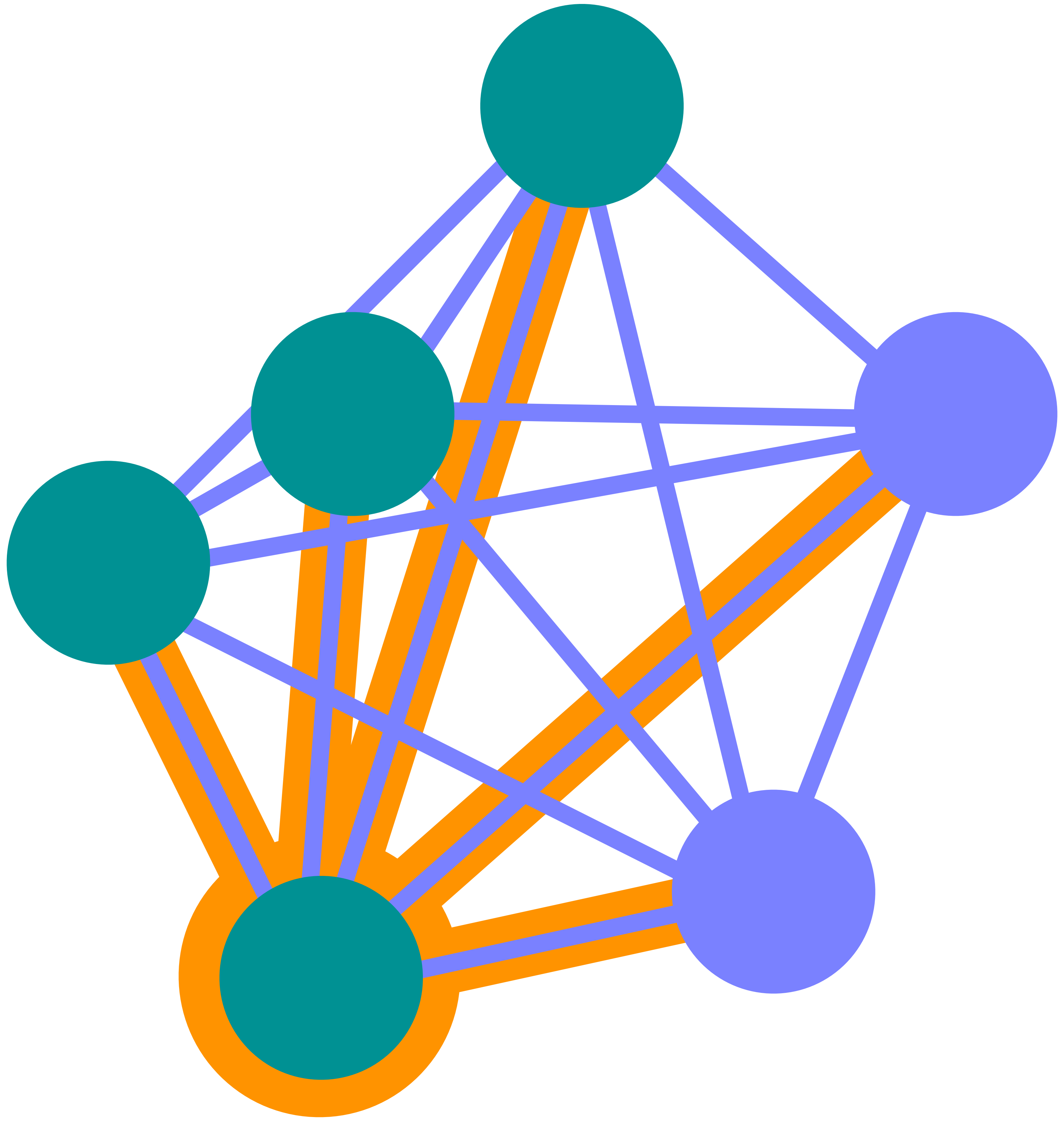
$$\mathbf{m}_{ij}^{(t)} = \mathbf{M}_t\left(\mathbf{h}_i^{(t-1)}, \mathbf{h}_j^{(t-1)}, \mathbf{h}_{ij}^{(t-1)}\right)$$

$$\mathbf{h}_{ij}^{(t)} = \left(\mathbf{v}_{ij}, \mathbf{G}_t\left(\mathbf{h}_{ij}^{(t-1)}, \mathbf{m}_{ij}^{(t)}\right)\right)$$

$$\mathbf{m}_i^{(t)} = \mathrm{Pool}\left(\{\mathbf{m}_{ij}^{(t)} \,|\, j \neq i\}\right)$$

$$\mathbf{h}_i^{(t)} = \left(\mathbf{v}_i, \mathbf{F}_t\left(\mathbf{h}_i^{(t-1)}, \mathbf{m}_i^{(t)}\right)\right)$$

MESSAGE-PASSING NEURAL NETWORK



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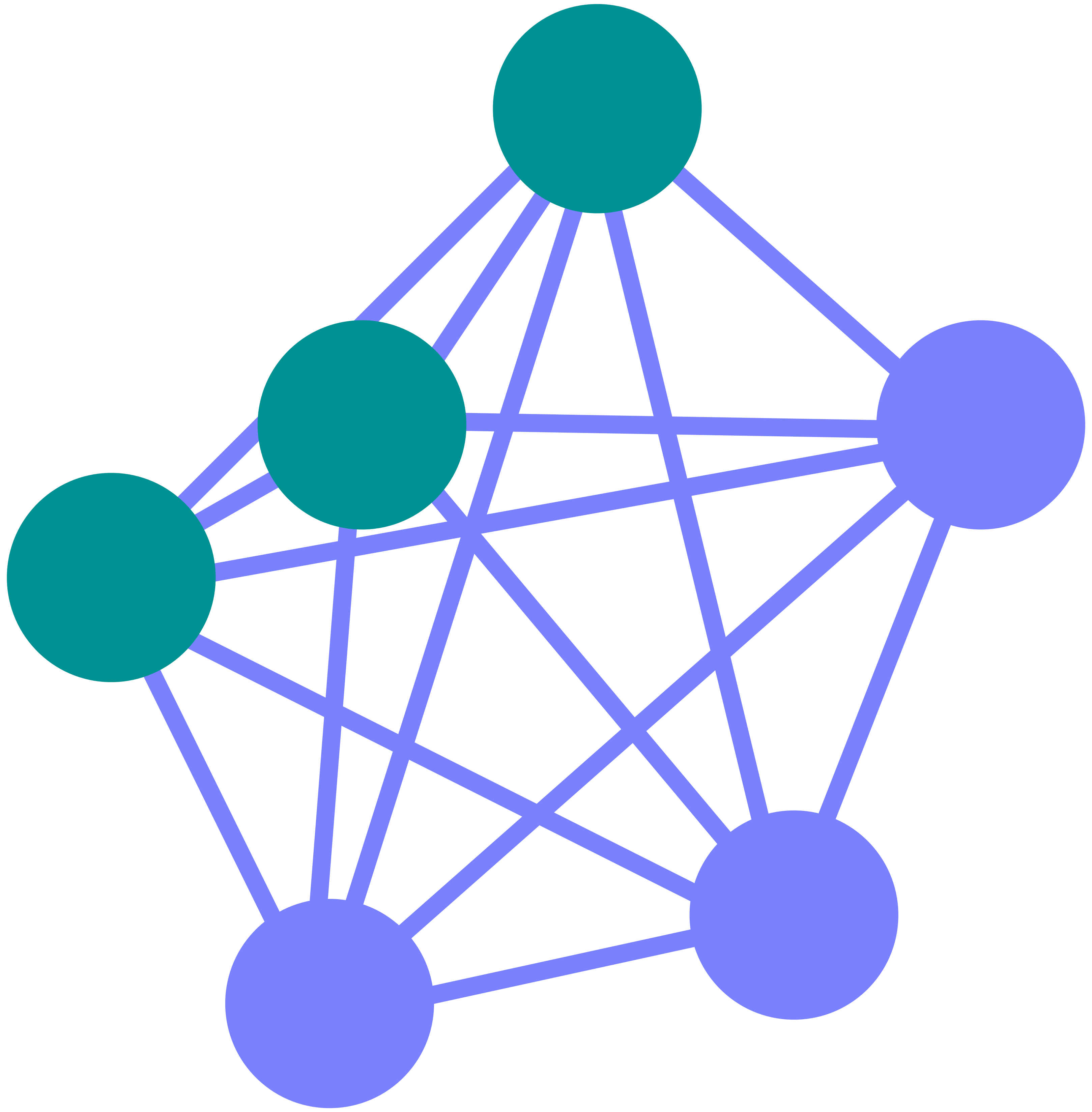
$$\mathbf{m}_i^{(t)} = \mathrm{Pool} \left(\{ \mathbf{m}_{ij}^{(t)} \, | \, j \neq i \} \right)$$

$$\mathbf{h}_i^{(t)} = \left(\mathbf{v}_i, \mathbf{F}_t \left(\mathbf{h}_i^{(t-1)}, \mathbf{m}_i^{(t)} \right) \right)$$

MESSAGE-PASSING NEURAL NETWORK



for $t = 1, \ldots, T:$

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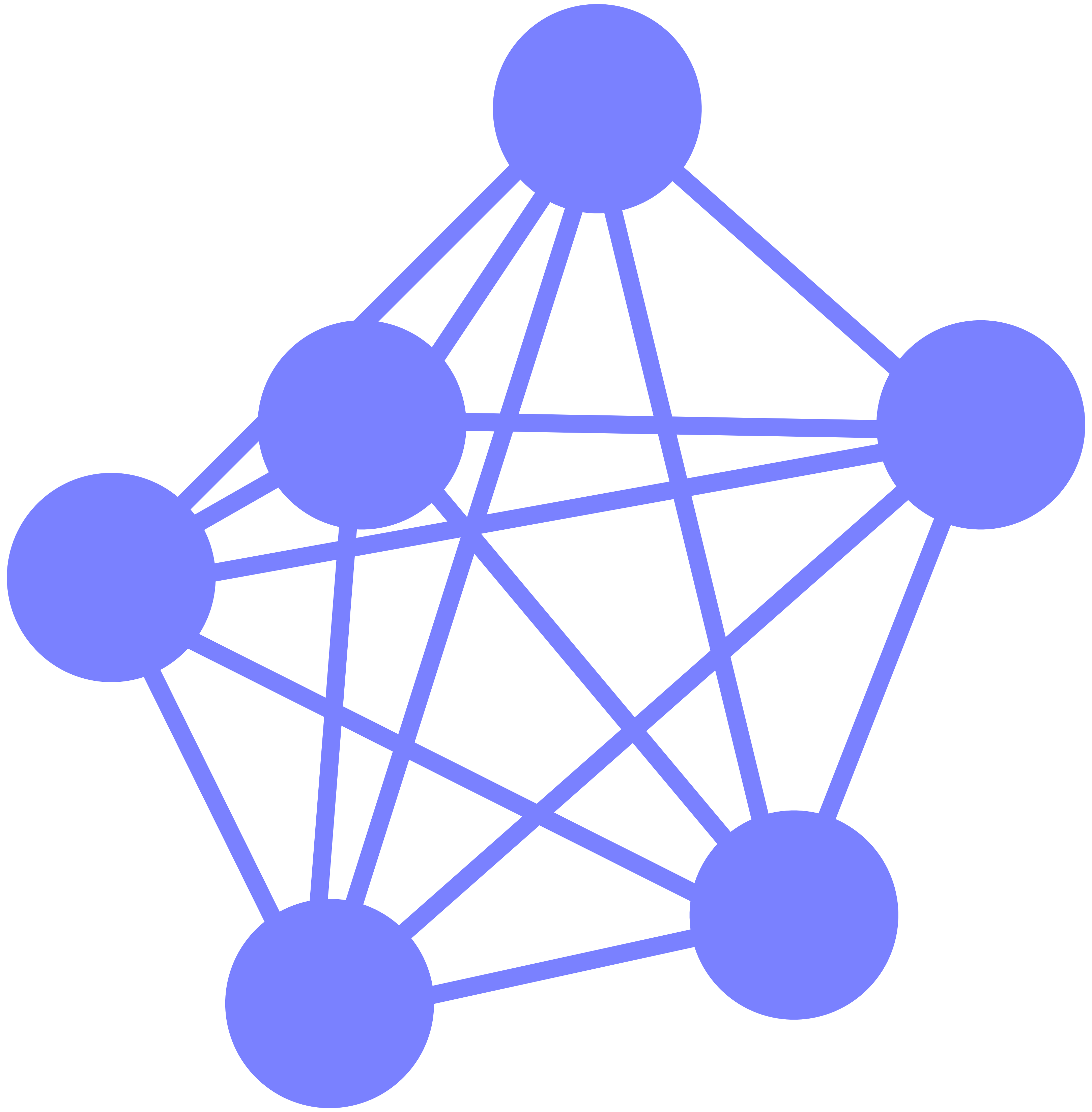
MESSAGE-PASSING NEURAL NETWORK



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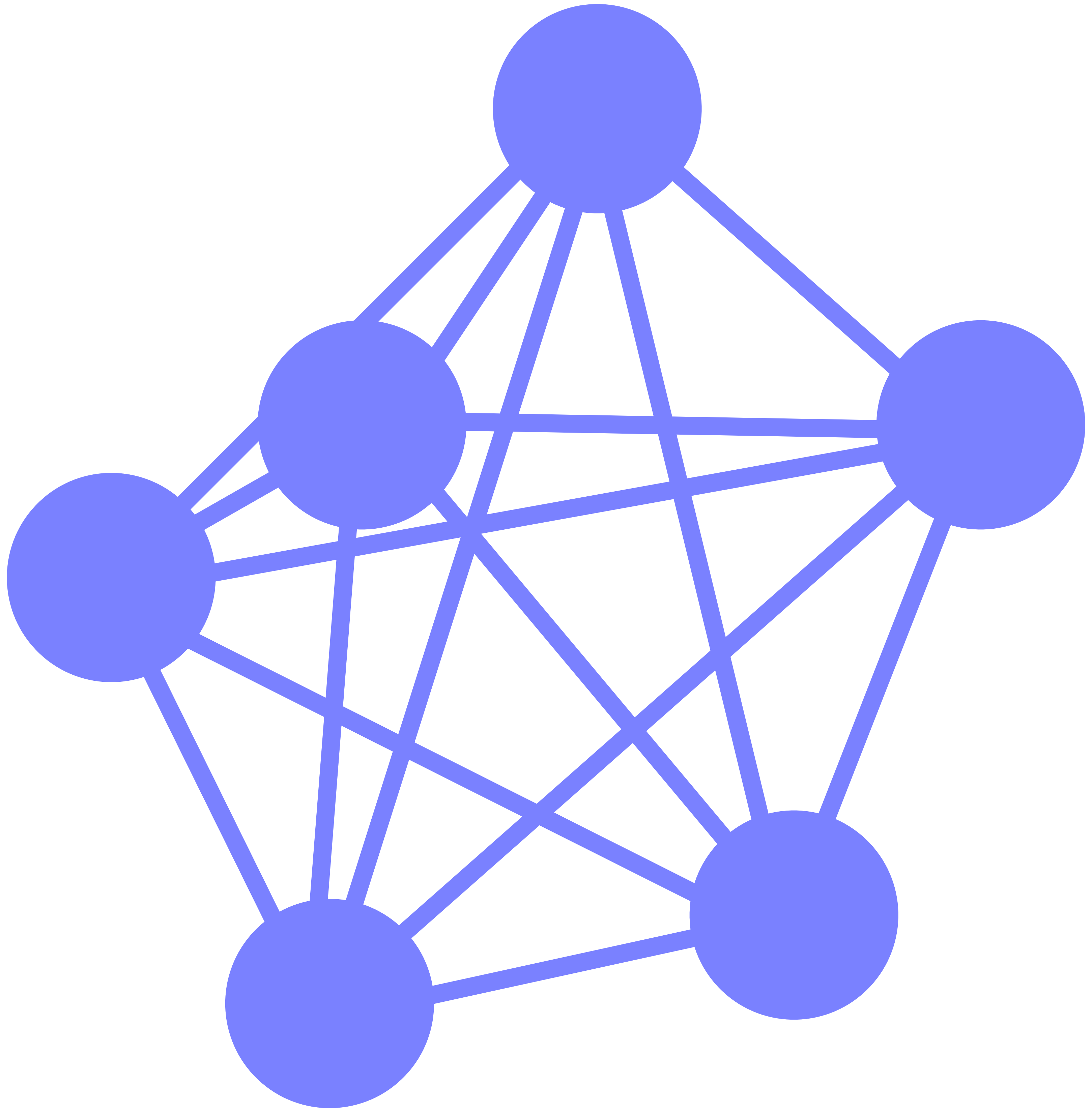
MESSAGE-PASSING NEURAL NETWORK



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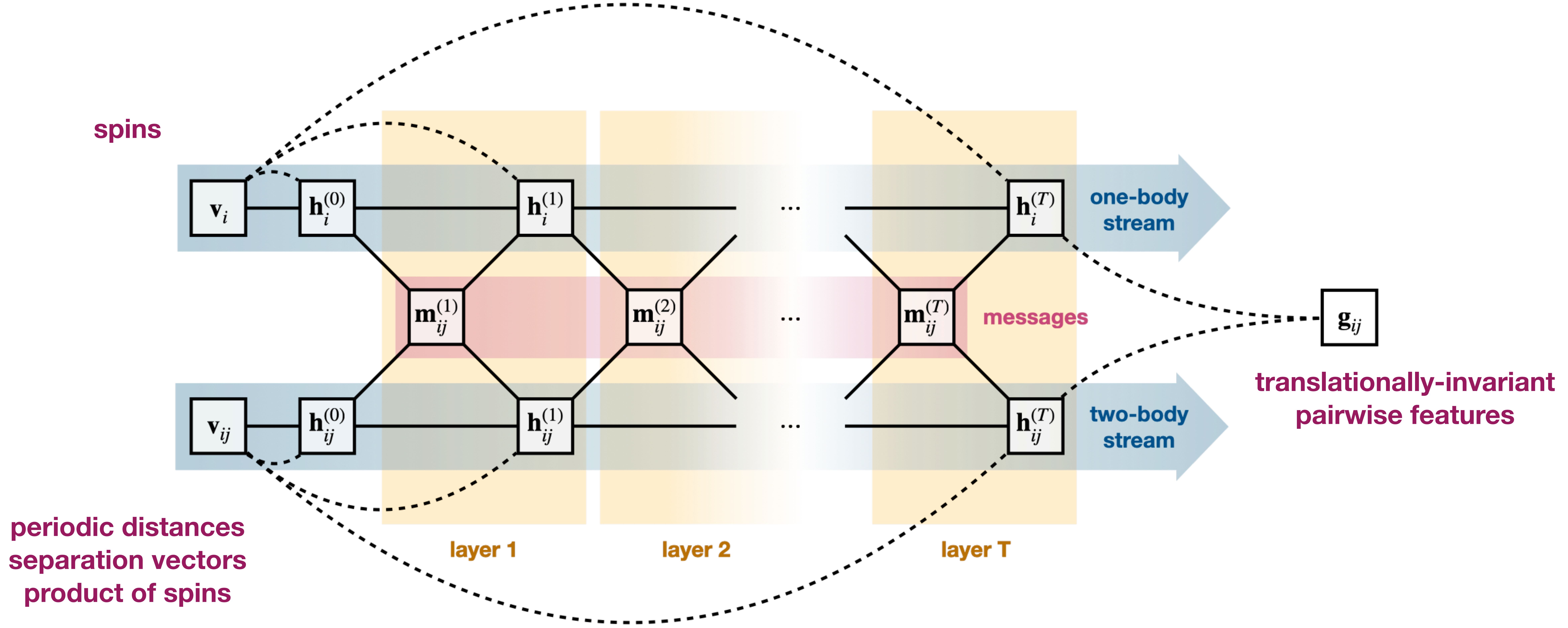
Feedforward neural networks

JK et al., Commun. Phys. ***7****, 148 (2024); G. Pescia, JK, et al., Phys. Rev. B* ***110****, 035108 (2024).*

MESSAGE-PASSING NEURAL NETWORK



FULL ANSATZ

- Use the output of the MPNN as input to the pairing orbital:

$$\Phi(X) = \mathrm{pf}\left[\phi(\mathbf{x}_i, \mathbf{x}_j)\right] \;\mapsto\; \Phi(X) = \mathrm{pf}\left[\phi(\mathbf{g}_{ij})\right]$$

- Jastrow correlator is a Deep Set:

$$J(X) = \rho\left(\mathrm{Pool}\left\{\zeta(\mathbf{g}_{ij})\right\}\right)$$

- Full ansatz: $$\Psi(X) = e^{J(X)}\Phi(X)$$

- We also enforce periodicity, translational invariance, parity and time-reversal symmetries

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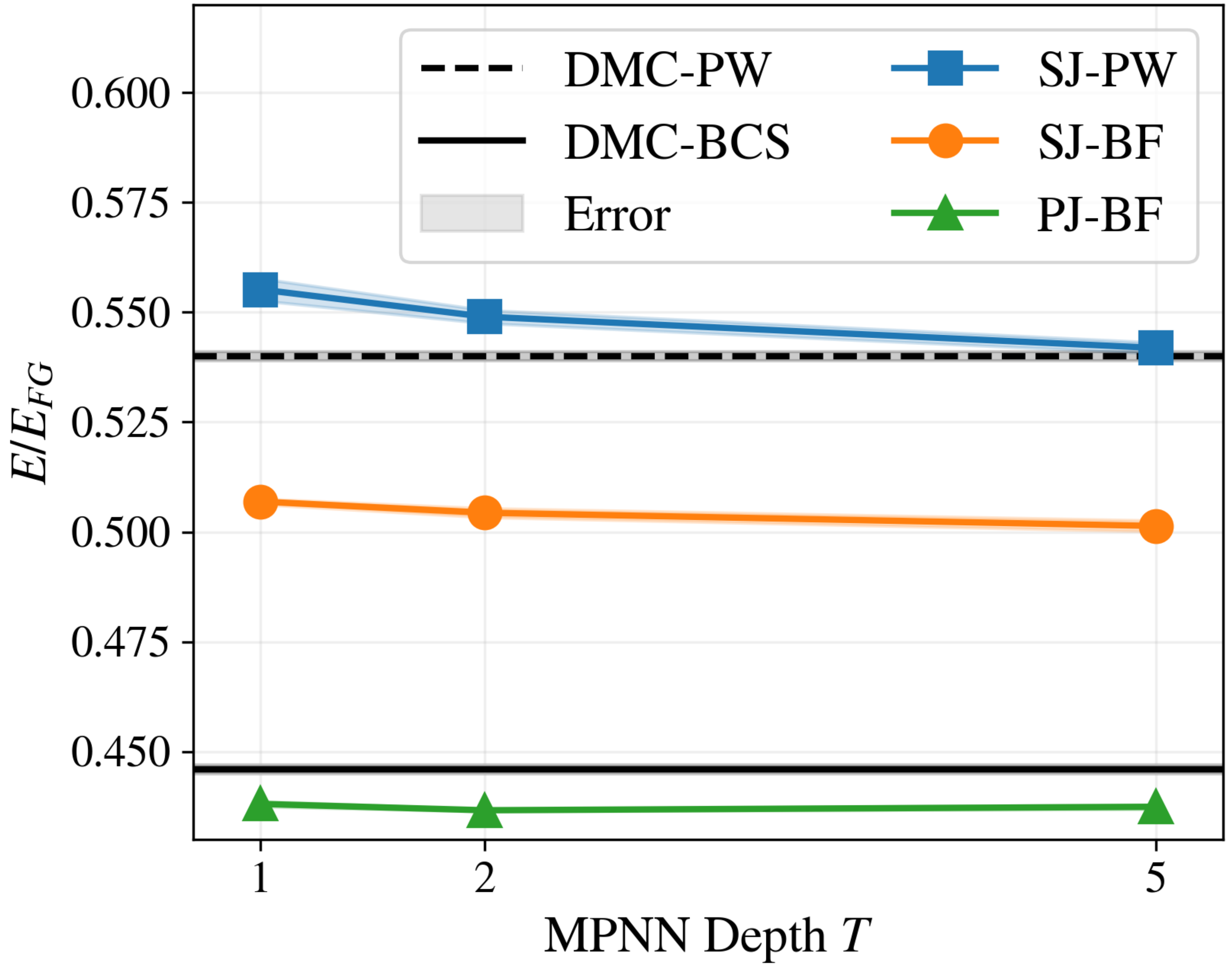
INITIAL COMPARISON WITH DMC



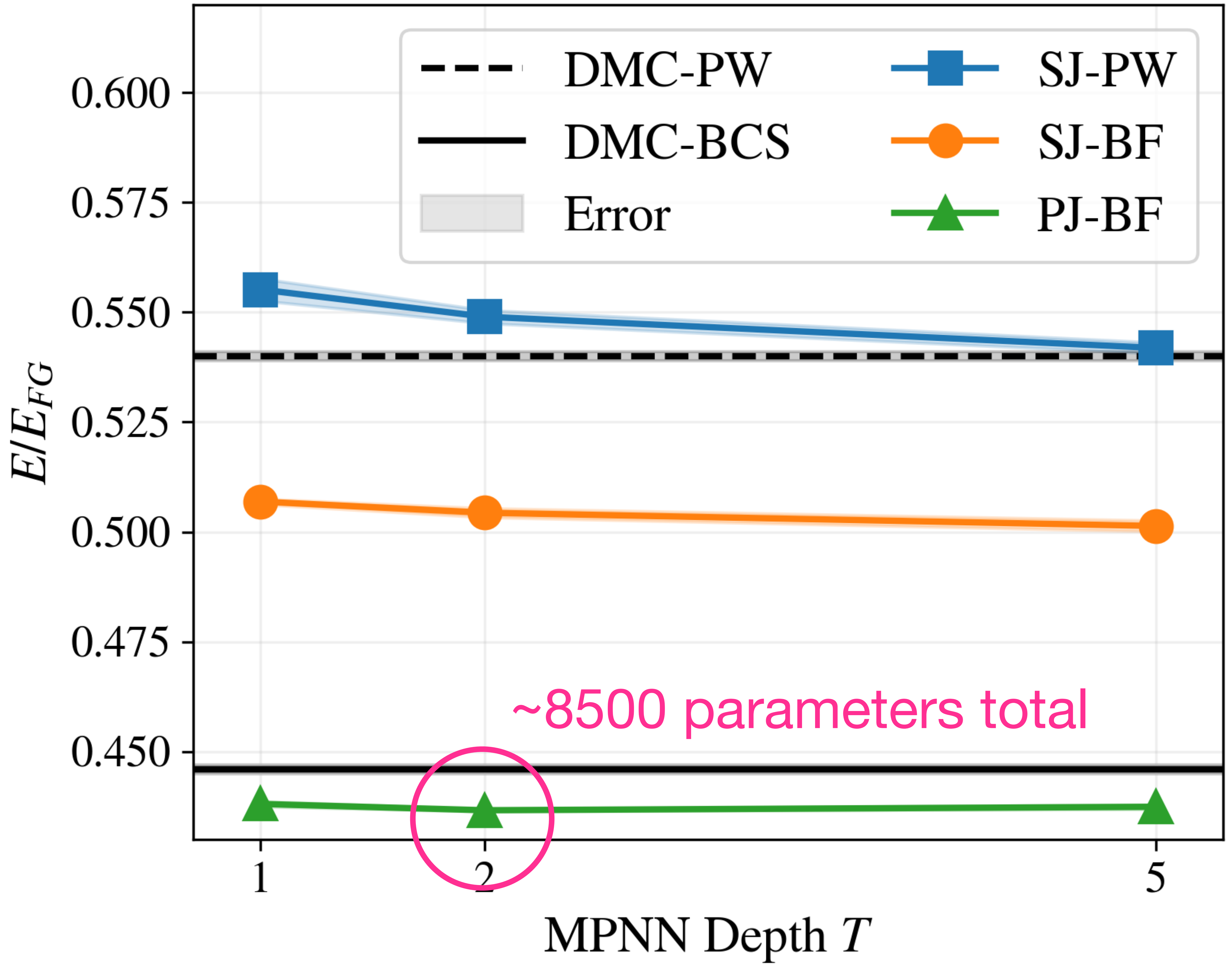
First stage of transfer learning

$$k_F r_e = 0.4$$

$$1/ak_F = 0$$

$$N = 14$$

INITIAL COMPARISON WITH DMC



First stage of transfer learning

$$k_F r_e = 0.4$$

$$1/ak_F = 0$$

$$N = 14$$

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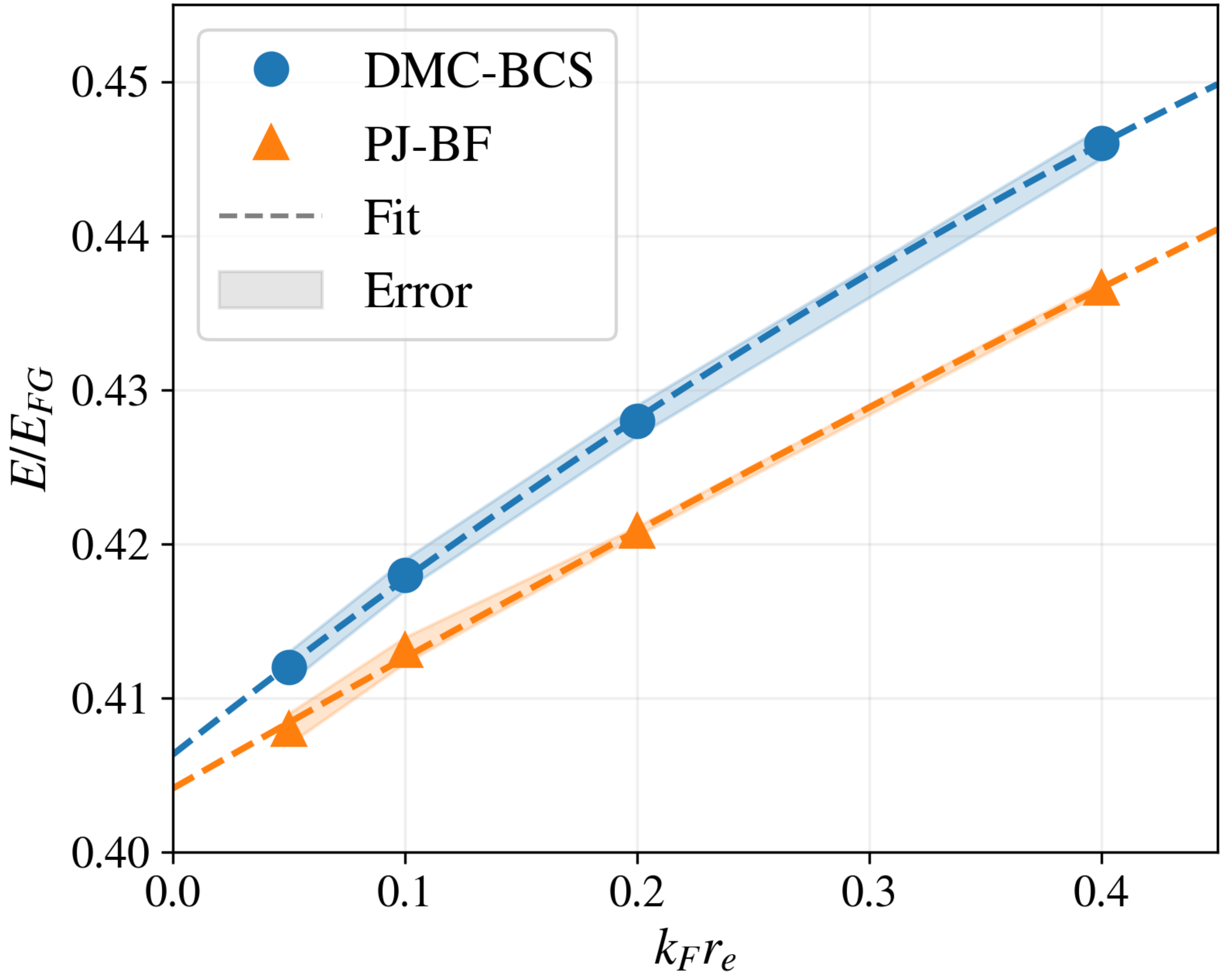
EXTRAPOLATION TO ZERO EFFECTIVE RANGE

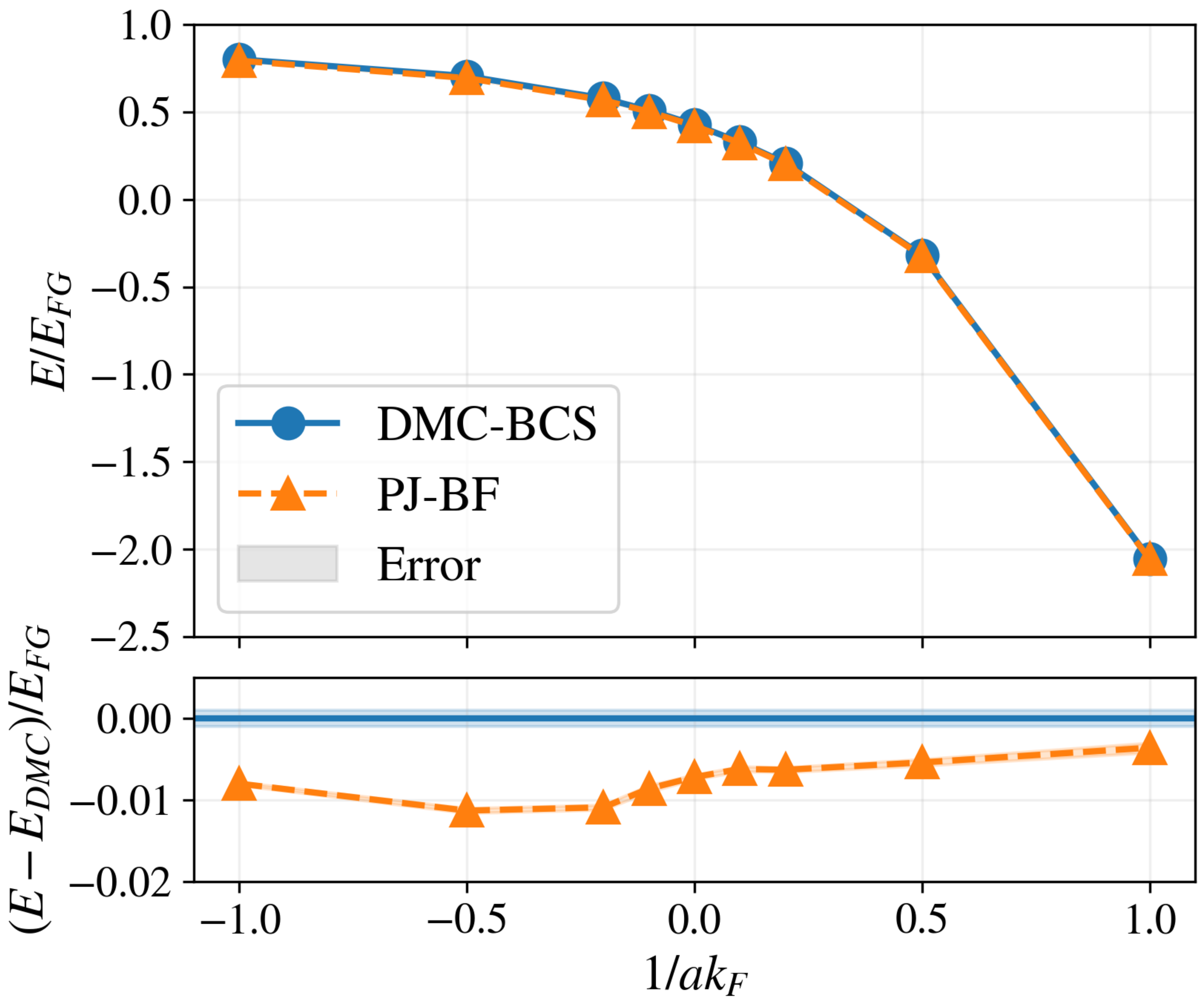


Transfer learning: gradually reduce r_e

$$1/ak_F = 0$$

$$N = 14$$

EXPLORING THE BCS-BEC CROSSOVER



Transfer learning: move away from unitarity

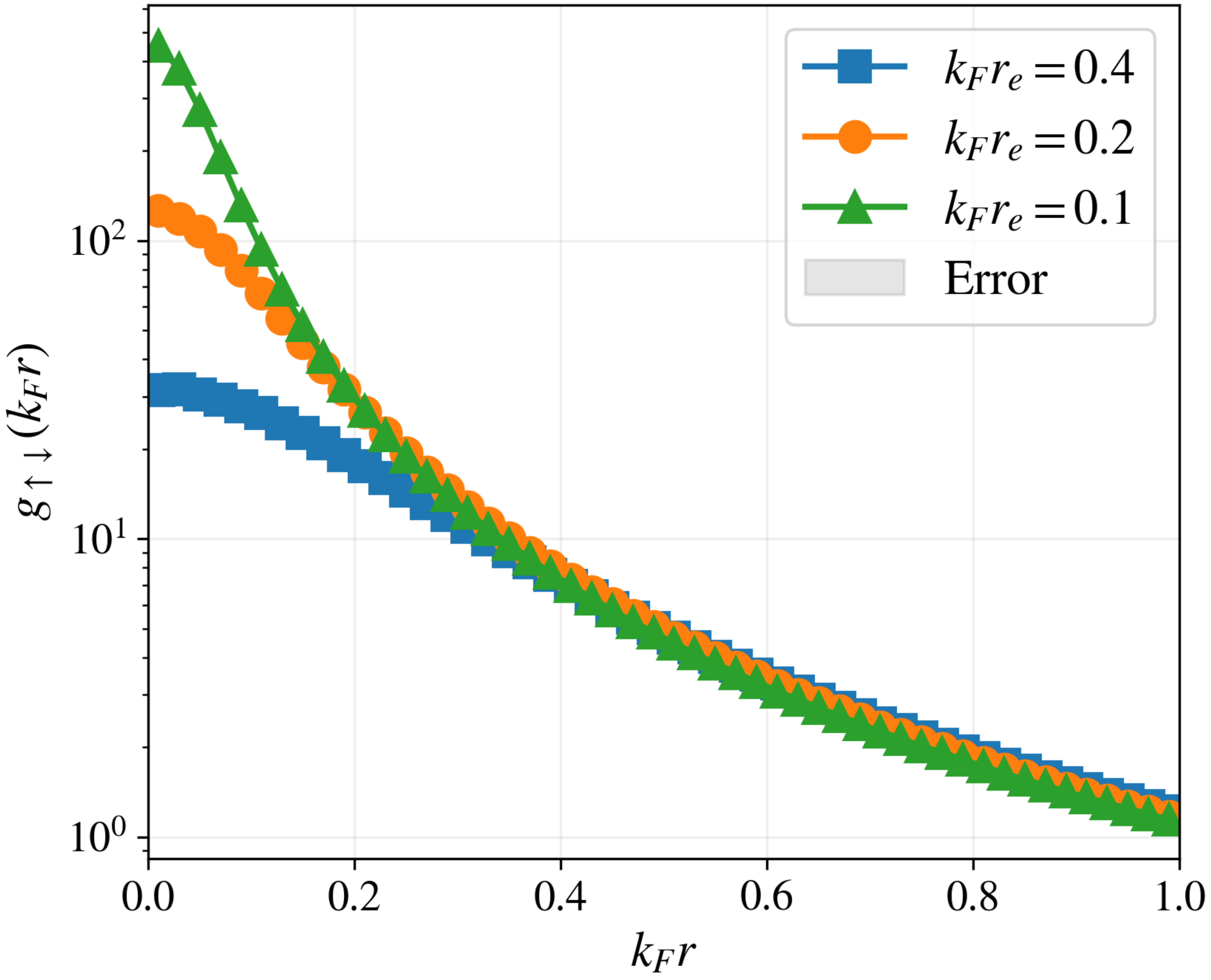
$$k_F r_e = 0.2$$

$$N = 14$$

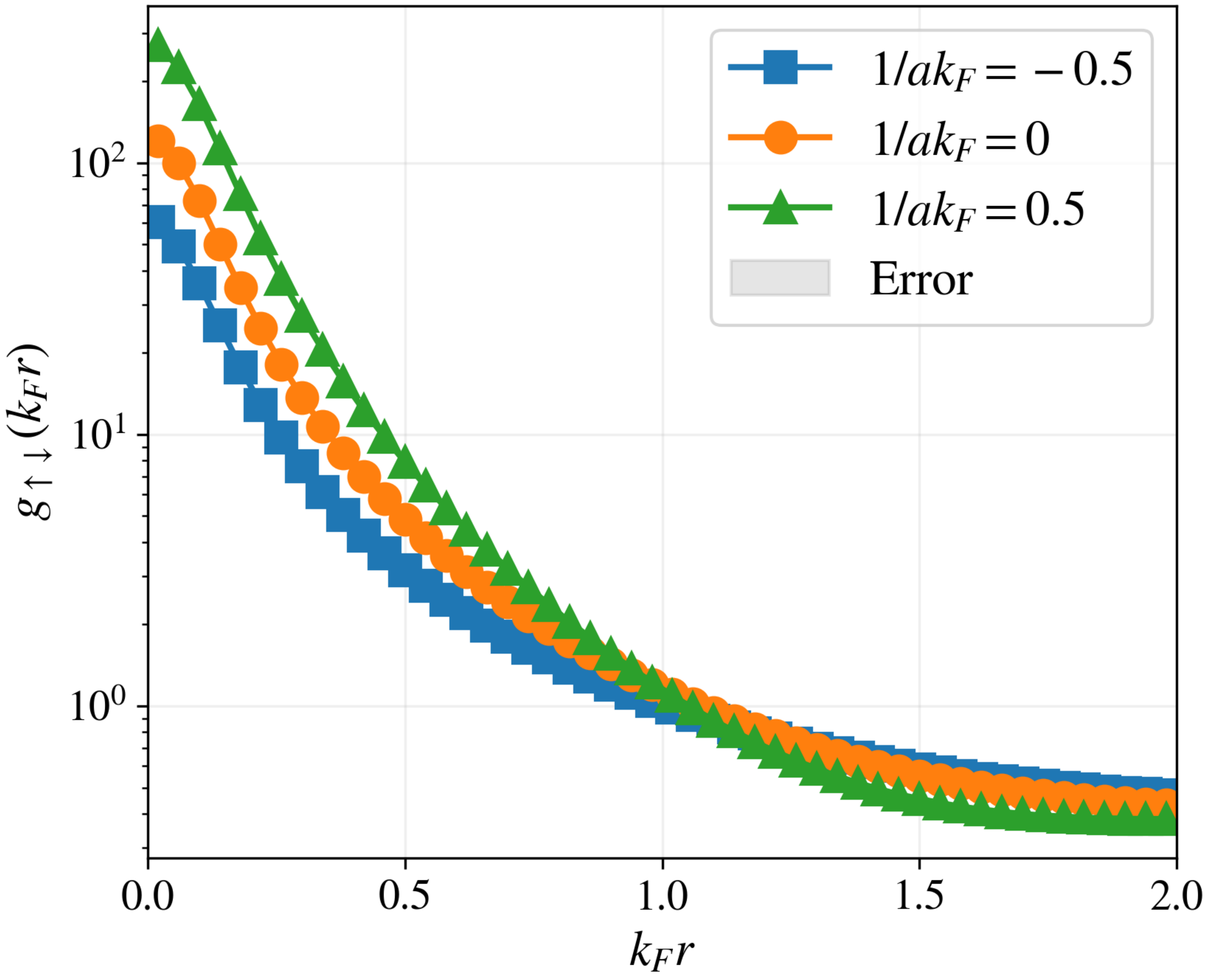
JK et al., *Commun. Phys.* **7**, 148 (2024).

OPPOSITE-SPIN PAIR DISTRIBUTIONS

Different effective ranges at unitarity



Different scattering lengths with fixed effective range



JK et al., Commun. Phys. ***7****, 148 (2024).*

N-INDEPENDENCE

- The total number of parameters for even N:

$$\big(T(3D+7)+3D+5\big)H^2+\big(T(4d+3D+10)+6d+3D+14\big)H+2$$

Spatial dimension

- Hyperparameters:

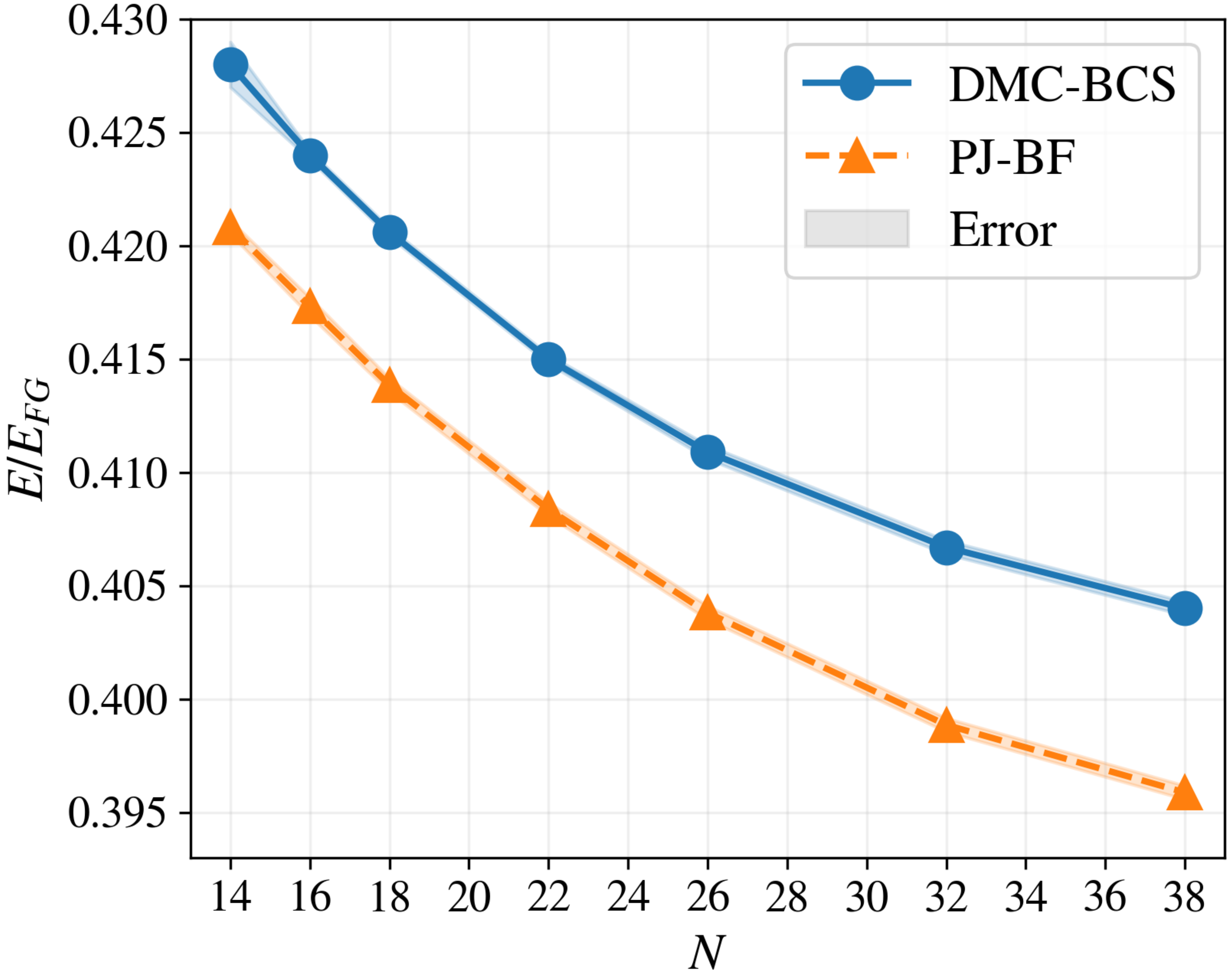
$T =$ Number of message-passing iterations

$D =$ Number of dense hidden layers in a single feedforward neural network

$H =$ Number of hidden nodes in a single dense layer

JK et al., Commun. Phys. ***7****, 148 (2024).*

TOWARDS THE THERMODYNAMIC LIMIT



Transfer learning: increase N

$$k_F r_e = 0.2$$

$$1/ak_F = 0$$

JK et al., Commun. Phys. **7**, 148 (2024).

ODD N

- Require one additional neural network for the unpaired single-particle orbital

$$\Phi(X) = \mathrm{pf}\begin{bmatrix} 0 & \phi(\mathbf{g}_{12}) & \cdots & \phi(\mathbf{g}_{1N}) & \psi(\mathbf{x}_1) \\ -\phi(\mathbf{g}_{12}) & 0 & \cdots & \phi(\mathbf{g}_{2N}) & \psi(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ -\phi(\mathbf{g}_{1N}) & -\phi(\mathbf{g}_{2N}) & \cdots & 0 & \psi(\mathbf{x}_N) \\ -\psi(\mathbf{x}_1) & -\psi(\mathbf{x}_2) & \cdots & -\psi(\mathbf{x}_N) & 0 \end{bmatrix}$$

- Even- and odd-N cases share the same pairing orbital structure (transferrable learning)
- In practice… $\psi(\mathbf{x}_i) \mapsto \psi(\mathbf{r}_i, \mathbf{h}_i^{(T)})$

One-body output of MPNN

PAIRING GAP

- Odd-even staggering: $$\Delta(N) = E(N) - \frac{1}{2}\left(E(N+1) + E(N-1)\right)$$
- Reference values: $$\Delta_{exp} = 0.45(5)\ \varepsilon_F$$ $$\Delta_{DMC-BCS}(66) = 0.50(2)\ \varepsilon_F$$

$\Delta(15)$ →

$1/ak_F$	DMC-BCS	PJ-BF	Diff.
-0.5	0.434(6)*	0.426(7)*	-0.008(9)
0	0.577(8)*	0.519(8)*	-0.06(1)
0	0.988(8)	0.918(8)	-0.07(1)
0.5	1.058(6)*	0.962(8)*	-0.10(1)

* = broken translational symmetry

JK et al., Commun. Phys. ***7****, 148 (2024).*

SUMMARY AND OUTLOOK

- This Pfaffian NQS is very flexible, compact, and scalable
- Current work: comparison with auxiliary-field QMC for a larger system $N = 66$
    - Repeat extrapolation to zero-effective range
    - Estimate Bertsch parameter
    - Compute condensation fraction
- **Very few changes required to reuse ansatz for different Hamiltonians—even those that exchange spin!**

JK et al., Commun. Phys. ***7****, 148 (2024).*

NEUTRON STAR CRUSTS

- Neutron-neutron scattering length: $a_{nn} = -18.63(84)$ fm
- Dilute neutron matter is similar to unitary Fermi gas: $r_e \ll n^{1/3}$
- Even simple pionless effective field theory Hamiltonians exchange spin and isospin at leading order:

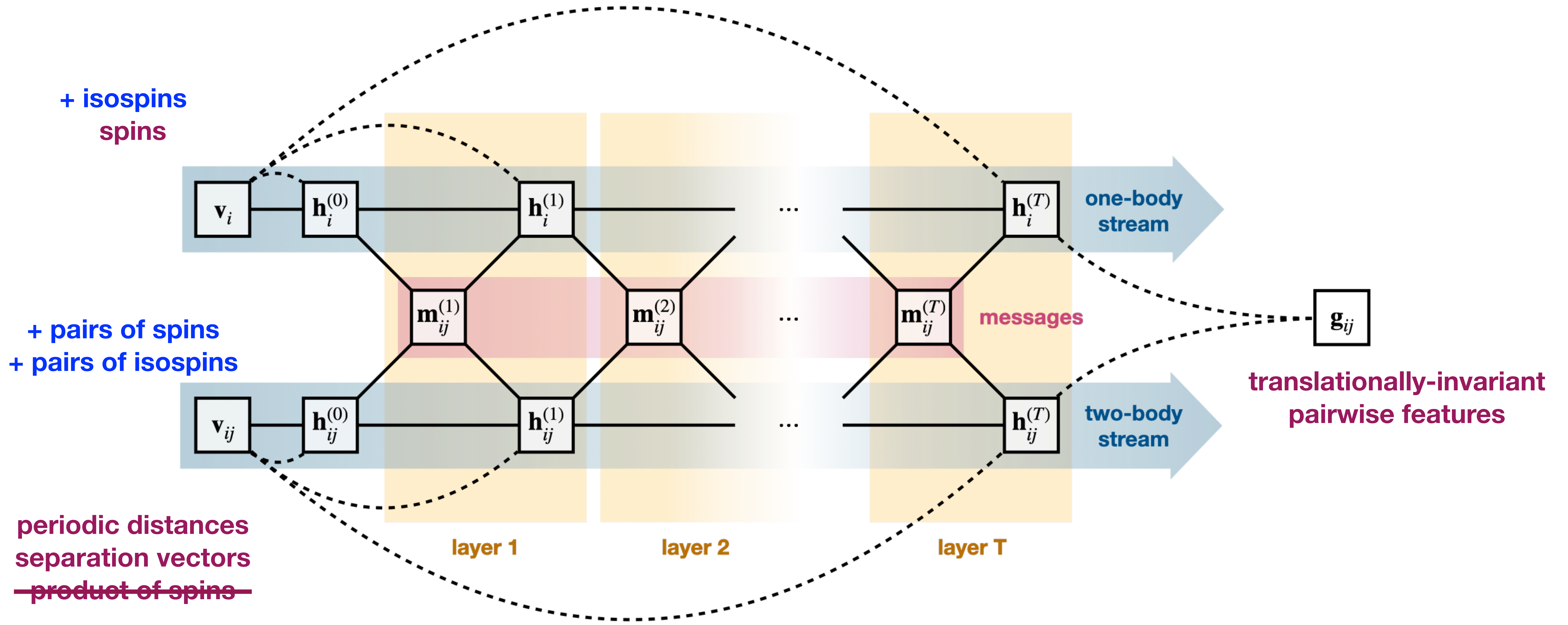
$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{cyclic\ i<j<k} V_{ijk}$$

Masses different for protons and neutrons

Contains operators 1, $(\sigma_i \cdot \sigma_j), (\tau_i \cdot \tau_j), (\sigma_i \cdot \sigma_j)(\tau_i \cdot \tau_j)$

Repulsive three-body term prevents collapse

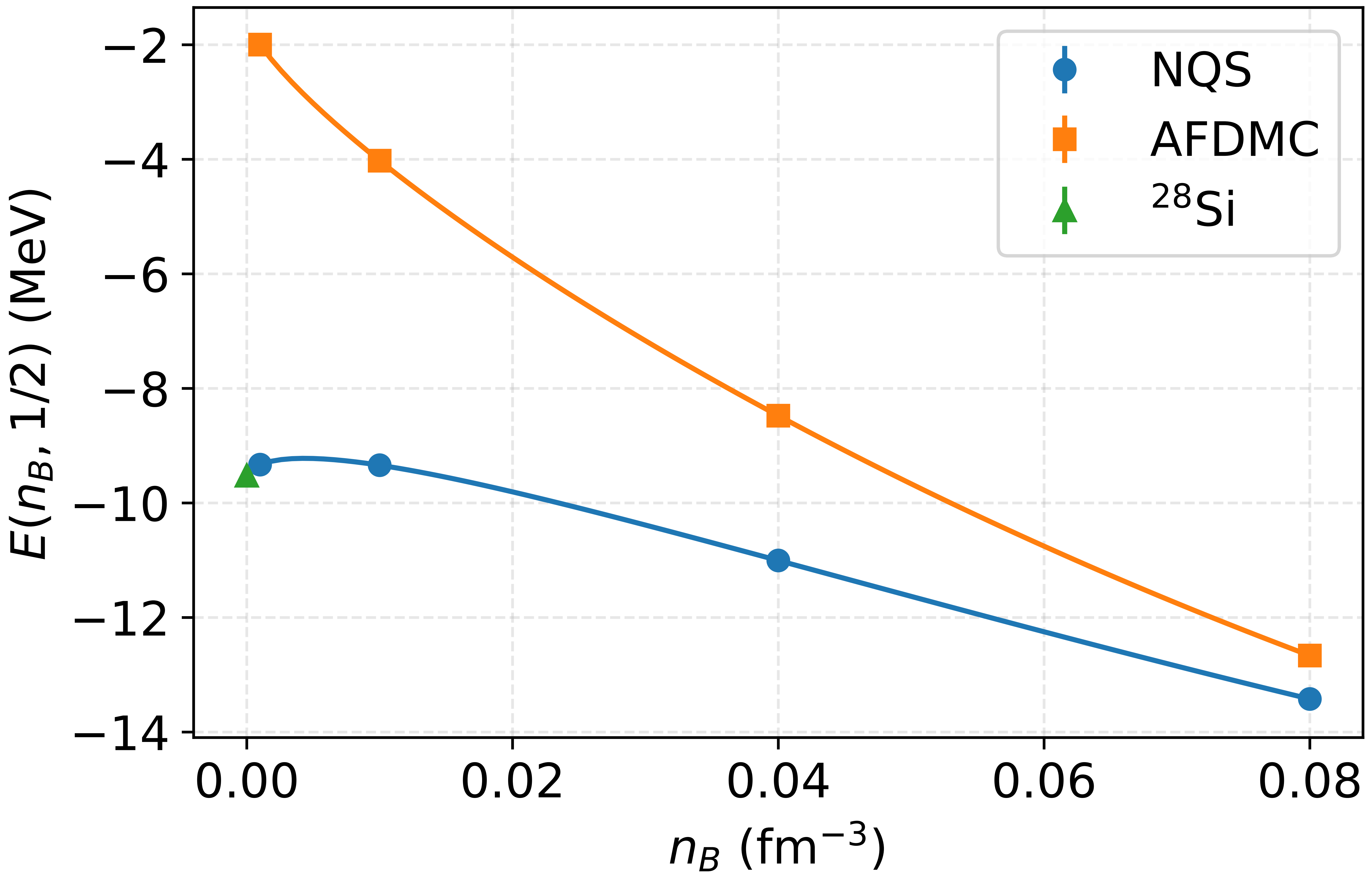
MESSAGE-PASSING NEURAL NETWORK



B. Fore, JK, et al., arXiv:2407.21207 (2024).

SYMMETRIC NUCLEAR MATTER

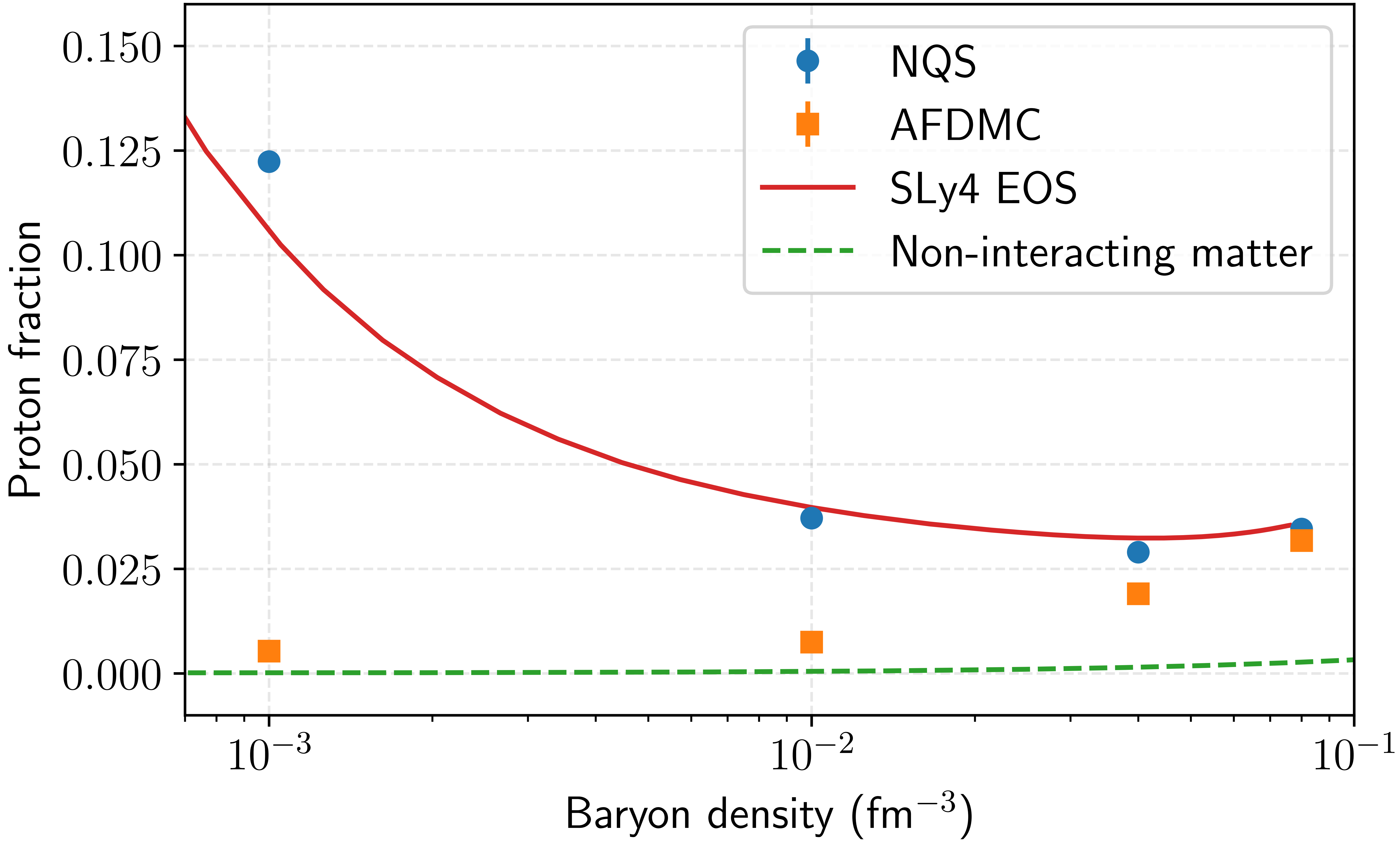
- Comparison with AFDMC for densities between 0.001 fm^{-3} and 0.08 fm^{-3}
- $N = 28,\ N_p = 14$
- Assume lectromagnetic contribution is screened by electrons
- Pfaffian NQS shows formation of ^{28}Si at low densities
- Evidence of clustering, but significant finite-size effects



B. Fore, JK, et al., arXiv:2407.21207 (2024).

BETA-EQUILIBRATED MATTER

- Impose charge neutrality and beta equilibrium conditions
- Proton fraction predicted by Pfaffian NQS agrees better with phenomenological Skryme models than AFDMC



B. Fore, JK, et al., arXiv:2407.21207 (2024).

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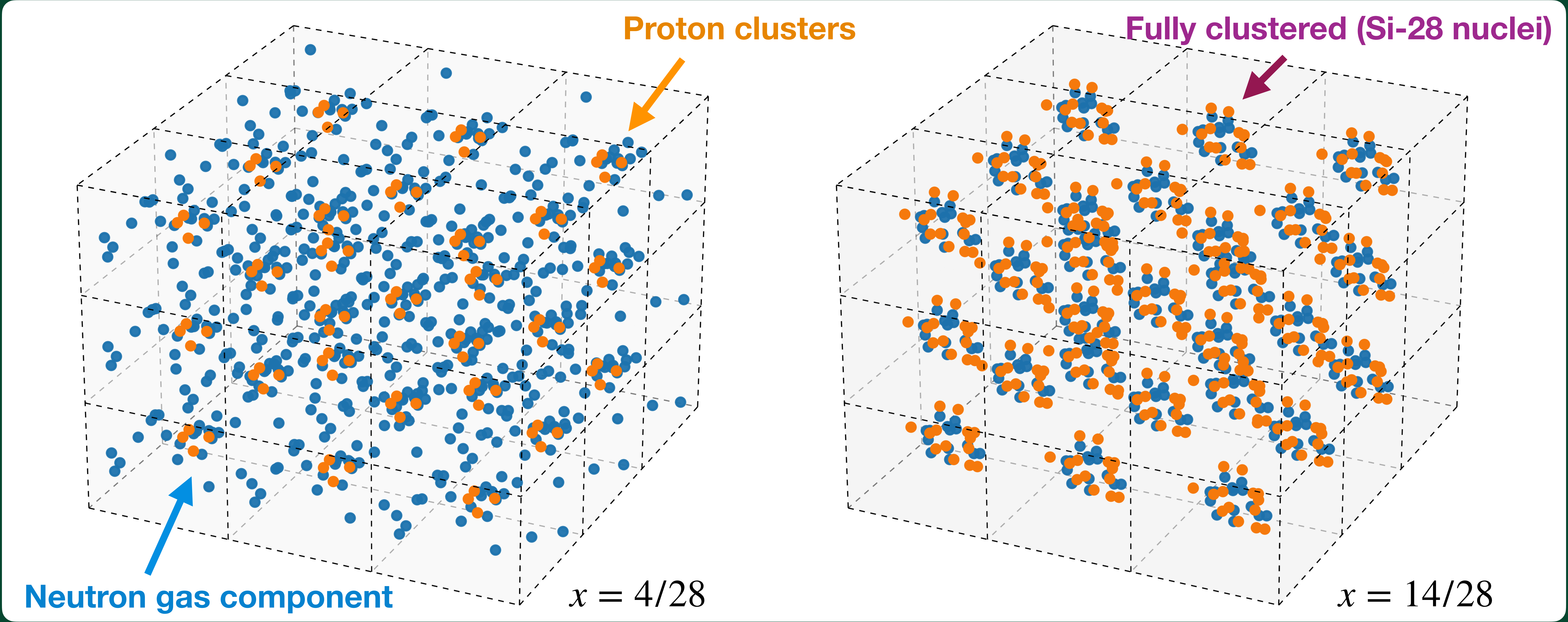
CLUSTERING



B. Fore, JK, et al., arXiv:2407.21207 (2024).

FOREVER OHIO

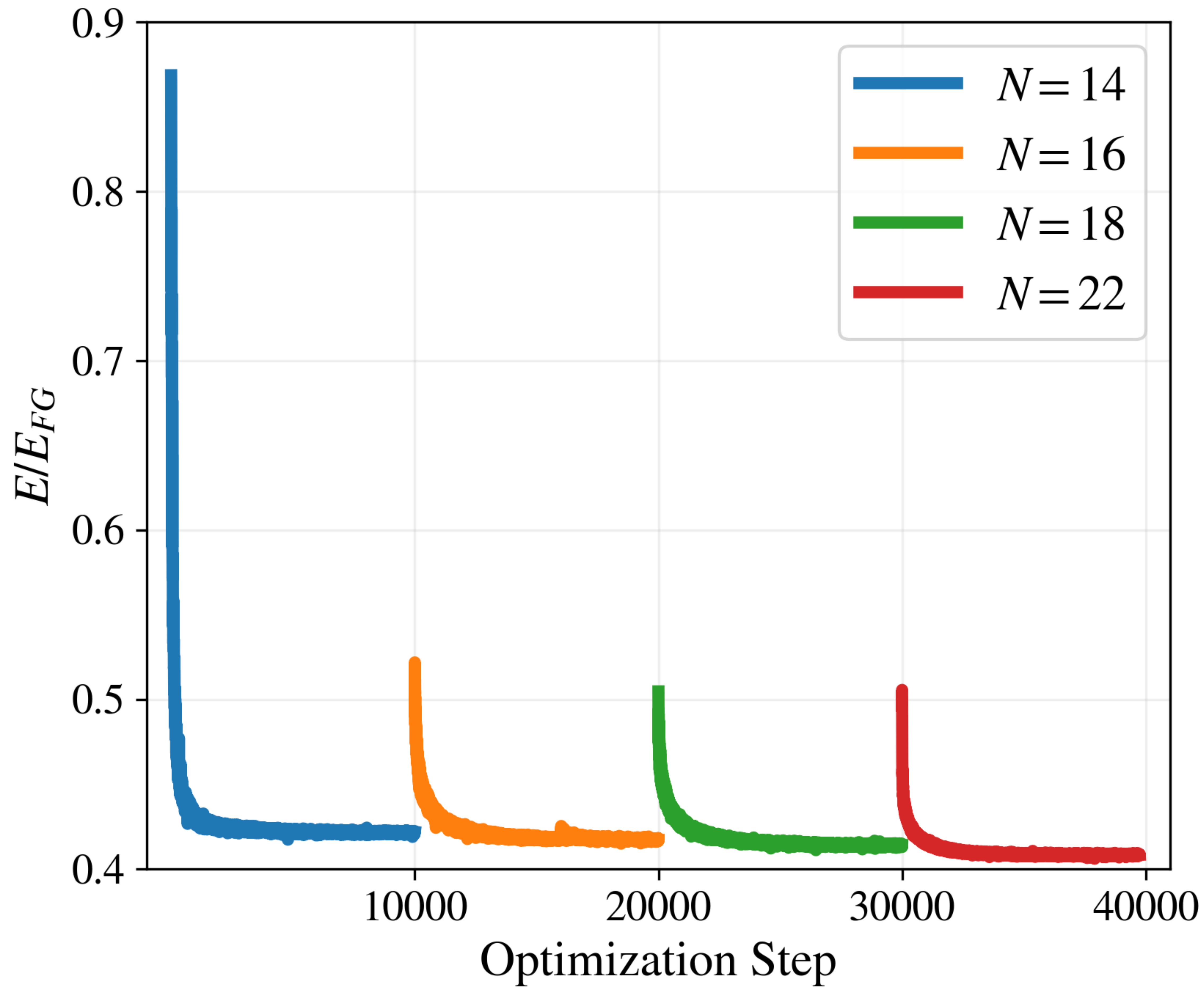
CONCLUSIONS

- This Pfaffian NQS is very flexible, compact, and scalable
- Does not explicitly depend on the number of particles $\rightarrow$ Facilitates transfer learning
- Odd-N and even-N cases handled in a unified manner
- Designed to handle strong pairing, shown to handle clustering and coexistence of clusters and free gas
- Very general, easy to adapt to different Hamiltonians

THANK YOU!

JK et al., *Commun. Phys.* **7**, 148 (2024).

TRANSFER LEARNING



Transfer learning: increase N

$$k_F r_e = 0.2$$

$$1/ak_F = 0$$

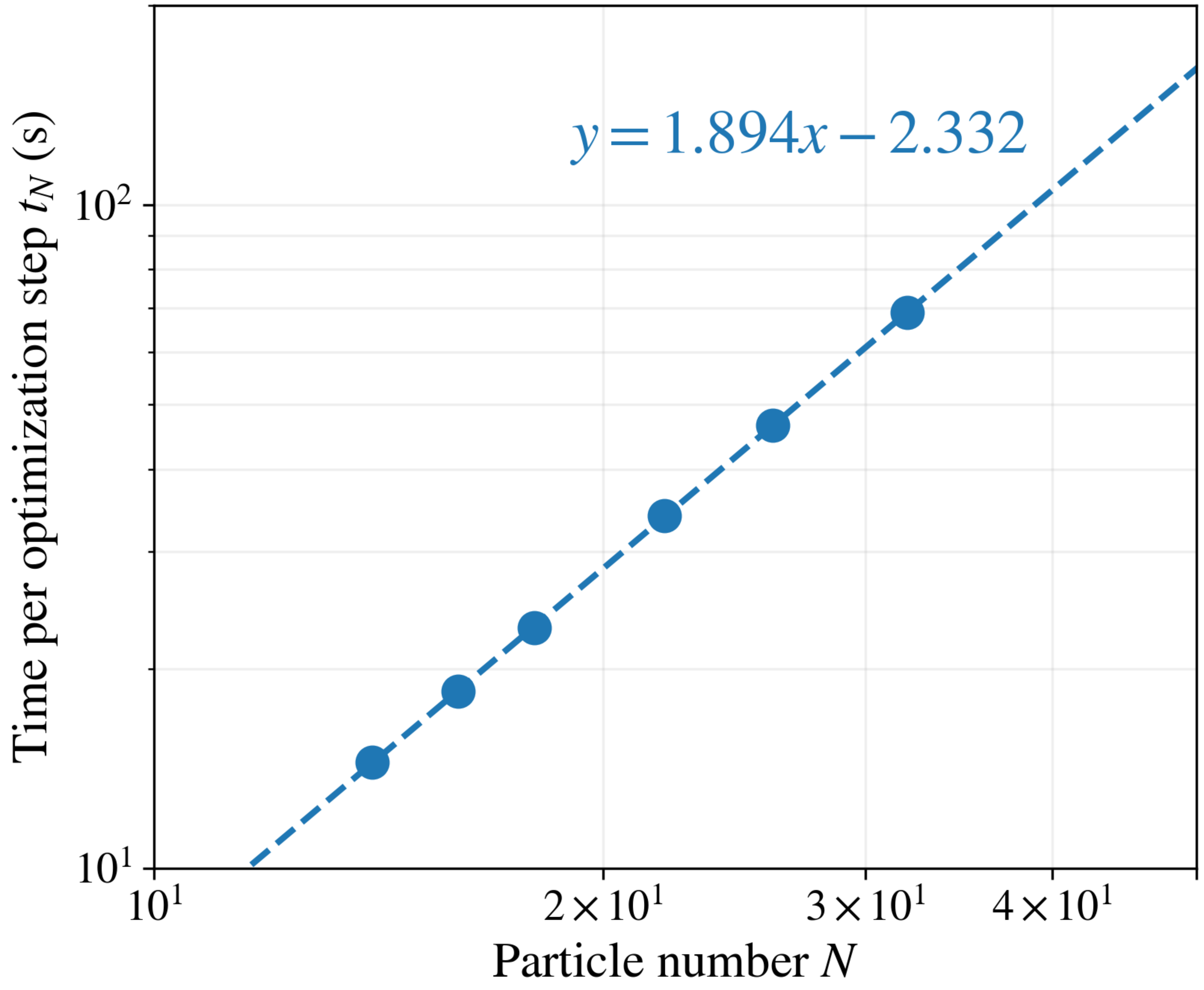
JK et al., *Commun. Phys.* ***7**, 148 (2024).*

COMPUTATIONAL SCALING

Using 4 NVIDIA-A100s for $N \leq 32$

Empirical scaling $\mathcal{O}(N^{1.894})$

(Our updated code seems to scale even better, analysis TBD)



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PERIODIC BOUNDARY CONDITIONS

- Minimum-image convention
- For nuclear matter, we also sum the interaction over nearby boxes
- Periodic separation vectors: $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \quad \mapsto \quad \tilde{\mathbf{r}}_{ij} = \left(\cos\left(\frac{2\pi}{L}\mathbf{r}_{ij}\right),\ \sin\left(\frac{2\pi}{L}\mathbf{r}_{ij}\right) \right)$
- Periodic distance: $r_{ij} = \|\mathbf{r}_{ij}\| \quad \mapsto \quad \tilde{r}_{ij} = \left\| \sin\left(\frac{\pi}{L}\mathbf{r}_{ij}\right) \right\|$

PARITY AND TIME-REVERSAL

- For the unpolarized systems:

$$\Psi^P(R,S) = \Psi(R,S) + \Psi(-R,S)$$

$$\Psi^{PT}(R,S) = \Psi^P(R,S) + (-1)^{N/2}\Psi^P(R,-S)$$

where

$$R = \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}$$

$$S = \{s_1, s_2, \ldots, s_N\}$$

JK et al., Commun. Phys. ***7****, 148 (2024).*

BCS WAVE FUNCTION

- Used for unpolarized systems with strong singlet pairing correlations
- Relies on separating spin-up and spin-down particles (cannot be used for nuclear systems)

$$\Phi(X) = \det \begin{bmatrix} \phi(\mathbf{x}_{1\uparrow}, \mathbf{x}_{1\downarrow}) & \phi(\mathbf{x}_{1\uparrow}, \mathbf{x}_{2\downarrow}) & \cdots & \phi(\mathbf{x}_{1\uparrow}, \mathbf{x}_{N/2\downarrow}) \\ \phi(\mathbf{x}_{2\uparrow}, \mathbf{x}_{1\downarrow}) & \phi(\mathbf{x}_{2\uparrow}, \mathbf{x}_{2\downarrow}) & \cdots & \phi(\mathbf{x}_{2\uparrow}, \mathbf{x}_{N/2\downarrow}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\mathbf{x}_{N/2\uparrow}, \mathbf{x}_{1\downarrow}) & \phi(\mathbf{x}_{N/2\uparrow}, \mathbf{x}_{2\downarrow}) & \cdots & \phi(\mathbf{x}_{N/2\uparrow}, \mathbf{x}_{N/2\downarrow}) \end{bmatrix}$$

- Can expand matrix to include unpaired orbitals for spin-polarized systems

JK et al., Commun. Phys. ***7****, 148 (2024).*

LO $\not{\pi}$EFT Hamiltonian

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{cyclic\ i<j<k} V_{ijk}$$

$$v_{ij} = v_{ij}^{EM} + v_{ij}^{CI}$$

$$v_{ij}^{CI} = C_0(r)P_0^\tau + C_1(r)P_1^\tau$$

$$C_\alpha(r) = \frac{1}{\pi^{3/2}R_\alpha^3} e^{-(r/R_\alpha)^2}$$

$$V_{ijk} = c_E \frac{f_\pi^4}{\Lambda_\chi} \frac{(\hbar c)^6}{\pi^3 R_3^6} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$

Pion decay constant $f_\pi = 92.4$ MeV

Breaking scale $\Lambda_\chi = 1$ GeV

LECs c_E fit for different choices of $R_3 \sim 1$ - 2.5 fm

R. Schiavilla, et al., Phys. Rev. C **103**, 054003 (2021).