Variational Monte Carlo for the Hubbard model

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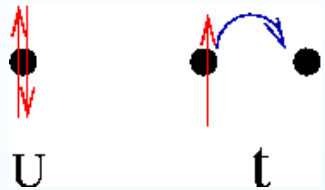
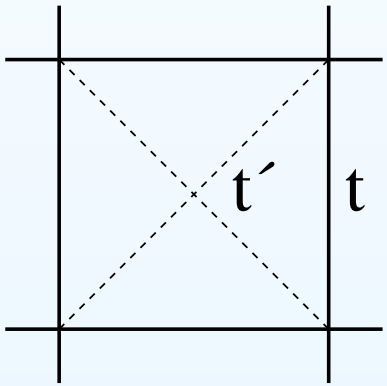
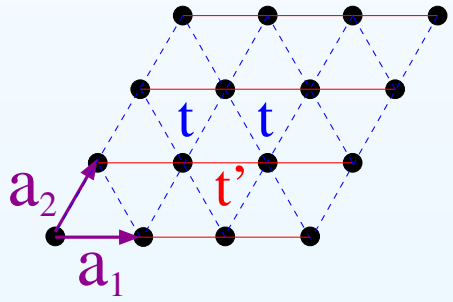
Jülich, 24th September 2026

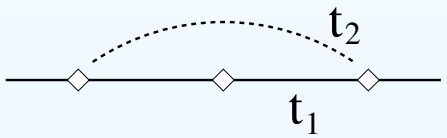
The single-orbital Hubbard model

$$\mathcal{H}_{\text{Hub}} = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.} + \sum_{i} U n_{i,\uparrow} n_{i,\downarrow}$$





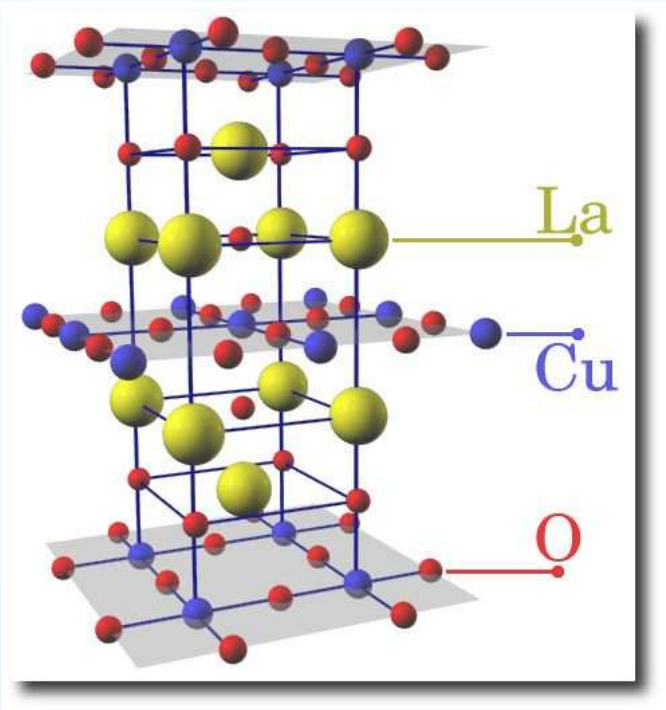


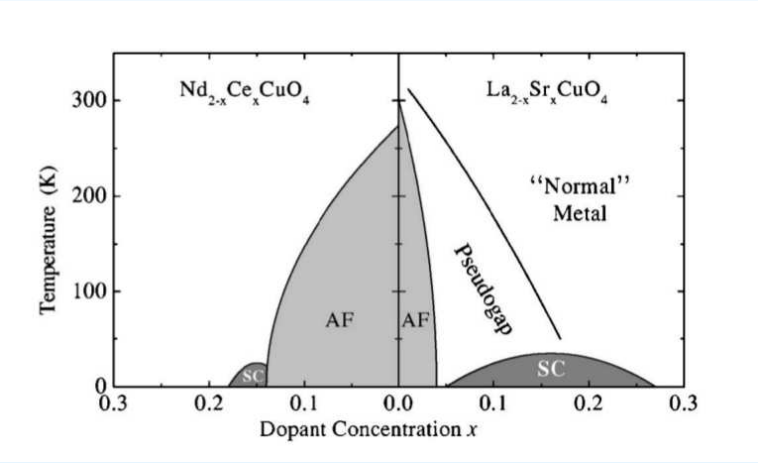


- Correlation: On-site Coulomb repulsion U
- Delocalization: Lattice-dependent competing hoppings
- Doping: Change the average electron density n
  (# electrons divided by the # sites)
- Minimal set of interactions describes complicated phenomena: Mott insulators, magnetism, superconductivity

High-temperature superconductors: cuprates

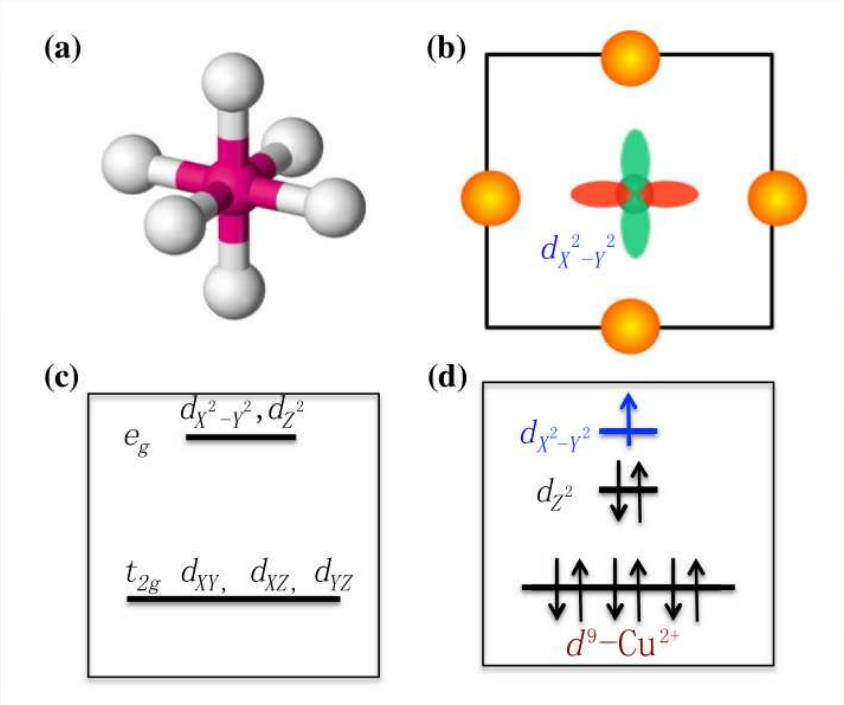
- Cuprates are antiferromagnetic Mott insulators e.g., La_2CuO_4
- Holes are added in the CuO planes, e.g., by replacing trivalent La with divalent Sr ($La_{2-x}Sr_xCuO_4$)
- Superconductivity develops in the CuO planes (that have a square lattice geometry)



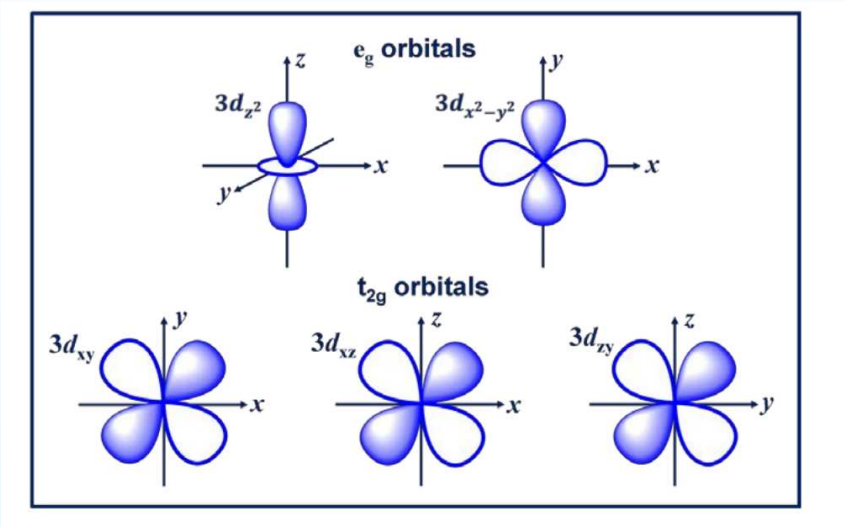


Damascelli *et al.*, RMP 75, 473 (2003)

A single-orbital physics



J. Hu, Sci. Bull. 61, 561 (2016)

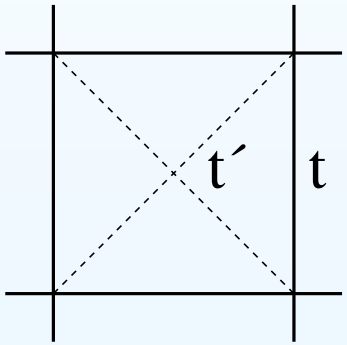


A. Biswas *et al.*, arXiv:1508.04929

- Cu atom surrounded by six oxygens (octahedron)
- Octahedral symmetry favors the t_{2g} orbitals: Lower Coulomb repulsion among electrons in the d orbitals and in the ligands (oxygens)
- Further lattice distortion along z favors the d_{Z^2} over the $d_{X^2-Y^2}$
- 9 electrons per Cu atom leave the $d_{X^2-Y^2}$ orbitals half-filled (one e^- per site)

Extended (single-orbital) Hubbard model

$$\mathcal{H}_{\text{Hub}} = -t \sum_{\langle R,R'\rangle,\sigma} c^{\dagger}_{R,\sigma} c_{R',\sigma} - t' \sum_{\langle\langle R,R'\rangle\rangle,\sigma} c^{\dagger}_{R,\sigma} c_{R',\sigma} + \text{H.c.} + \sum_{R} U n_{R,\uparrow} n_{R,\downarrow}$$



- The Hubbard model on the square lattice is appropriate for the cuprates
- In cuprates there is a realistic next-nearest neighbor hopping t' with $t'/t < 0$, estimated by Density Functional Theory

  Pavarini, Dasgupta, Saha-Dasgupta, Jepsen, and Andersen, PRL 87, 047003 (2001)
- It reproduces an antiferromagnetic Mott insulator at half filling
- Superconductivity emerges by doping the Hubbard model away from half filling (even if competition with charge and spin modulations)

"Solving" the Hubbard model: The variational approach

- The general model is not exactly solvable except in 1D
- Each site has four states: $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow,\downarrow\rangle$
- The Hilbert space grows up exponentially as 4^L: Exact diagonalization only for very small sizes
- Alternative approach: Construct wave functions $|\Psi_{\text{var}}\rangle$ that capture the correct low-energy properties of correlated systems
- Select the best approximation with the variational principle

$$E_{\text{var}} = \frac{\langle\Psi_{\text{var}}|\mathcal{H}|\Psi_{\text{var}}\rangle}{\langle\Psi_{\text{var}}|\Psi_{\text{var}}\rangle} \geq E_0 \text{ (exact energy)}$$

- The best approximation has the lowest energy
- How do we compute these expectation values? Monte Carlo!

Variational Monte Carlo for the ground-state properties of correlated Hamiltonians I

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Main reference: Becca and Sorella: Quantum Monte Carlo Approaches for Corrletaed Systems (Cambridge University Press, 2017)

Variational Monte Carlo (VMC)

Pros:

- Variational principle: the estimated energy is always an upper bound of the exact one
- Non-perturbative in the electonic correlation
- Performances not significantly affected by dimensionality or size of the local Hilbert space
- Spatial correlations and superconductivity can be properly described
- No sign problem

Cons:

- Ground state method: no dynamical correlations. VMC can be extended to work at finite temperatures and time dependent, not discussed here
- Difficult to quantify the systematic errors that come from the choice of the trial state: Results may be biased from the trial state
- Usually not the most accurate estimate for the variational energy. It may improved (e.g. with Green's Function Monte Carlo)

Variational Monte Carlo

- Consider an orthonormalized basis set $\{|x\rangle\}$
- It is convenient to choose a local basis, defined on the lattice sites
- On each lattice site the basis set has four elements (for the Hubbard model): $\{|\xi\rangle_i\} = \{|0\rangle_i, |\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i\}$
- A generic element of the lattice basis set $|x\rangle$ is given by:

$$|x\rangle = |\xi\rangle_1 \cdots |\xi\rangle_L$$

- Convenient choice: There is a small number of non-vanishing matrix elements of the Hamiltonian on this basis since interactions are local in space (Hubbard-U) and hoppings are short range

Variational Monte Carlo

In quantum mechanics, we need to compute expectaction values of operators $\mathcal{O}$, as the energy

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi | \mathcal{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_x \langle \Psi | x \rangle \langle x | \mathcal{O} | \Psi \rangle}{\sum_{x'} \langle \Psi | x' \rangle \langle x' | \Psi \rangle}$$

The number of elements in the sum grows exponentially with the system size (4^L in the Hubbard model): we cannot compute $\langle \mathcal{O} \rangle$ exactly! We can use a Monte Carlo sampling:

- Recast $\langle \mathcal{O} \rangle$ in a more convenient way

$$\langle \mathcal{O} \rangle = \frac{\sum_x |\langle \Psi | x \rangle|^2 \frac{\langle x | \mathcal{O} | \Psi \rangle}{\langle x | \Psi \rangle}}{\sum_{x'} |\langle \Psi | x' \rangle|^2} = \sum_x \mathcal{P}(x) \mathcal{O}_L(x)$$

Variational Monte Carlo

- $\langle \mathcal{O} \rangle$ is the average of the local estimator $\mathcal{O}_L(x)$ of the operator $\mathcal{O}$ over the probability distribution in quantum mechanics (non-negative and normalized, so no sign problem)

$$\langle \mathcal{O} \rangle = \sum_x \mathcal{P}(x) \mathcal{O}_L(x) \quad \mathcal{O}_L(x) = \frac{\langle x|\mathcal{O}|\Psi\rangle}{\langle x|\Psi\rangle} \quad \mathcal{P}(x) = \frac{|\langle \Psi|x\rangle|^2}{\sum_{x'} |\langle \Psi|x\rangle|^2}$$

- We construct a Markov chain (with the Metropolis algorithm) that generates a set of configurations $\{x_n\rangle\}$ distributed according to $\mathcal{P}(x)$
- We compute the quantum expectation value $\langle \mathcal{O} \rangle$ as the average of the random variable $\mathcal{O}_L(x)$:

$$\langle \mathcal{O} \rangle \sim \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}_L(x_n)$$

Zero-variance property

- The most important observable is the energy (variational principle). The local estimator e_L is:

$$e_L(x) = \frac{\langle x|\mathcal{H}|\Psi\rangle}{\langle x|\Psi\rangle}$$

- Assume $|\Psi\rangle$ to be an eigenstate of $\mathcal{H}$ ($\mathcal{H}|\Psi\rangle = E|\Psi\rangle$):

$$e_L(x) = \frac{\langle x|\mathcal{H}|\Psi\rangle}{\langle x|\Psi\rangle} = E\frac{\langle x|\Psi\rangle}{\langle x|\Psi\rangle} = E$$

  E is exact with zero variance

- This is an extreme case, but, in general, the variance decreases when $|\Psi\rangle$ approaches an exact eigenstate.

Metropolis algorithm

A practical way to construct configurations x_n that are distributed according to $\mathcal{P}(x)$, after an initial equilibration time

- Propose a move generating a configuration x' according to a transition probability $T(x'|x)$ (the move can be chosen to be very simple,i.e., flip a spin in the Ising model, move an electron in the Hubbard one)
- Extract a random number $\eta \in (0, 1]$
- Accept the move ($x_{n+1} = x'$) if $\eta < A(x'|x) = \min\left\{1, \frac{\mathcal{P}(x')}{\mathcal{P}(x)}\right\}$. Otherwise $x_{n+1} = x$
- Good news: We only need to know probability ratios $\mathcal{P}(x')/\mathcal{P}(x)$: No need to normalize the probability distribution!

Calculation of observables

- Compute local estimators (e.g., $e_L(x)$ for the energy) every $O(N_e)$ steps (N_e is the number of electrons and one step is the proposal of a single electron move)
- In correlated electron systems, the acceptance probability is usually small $\Rightarrow$ Perform a binning technique to uncorrelate measures
- First write the observables on the hard disk and then perform statistical analysis, since correlation time is unknown

Correlated measures: a bit of statistics

Local estimators are computed every $O(N_e)$ steps. Still, configurations are not independent because the acceptance ratio in the Hubbard model is small!

- Consider the variance estimator s^2 for a single Monte Carlo run

$$s^2 = \frac{1}{N}\sum_i (x_i - \bar{x})^2 = \frac{1}{N}\sum_i x_i^2 - \left(\frac{1}{N}\sum_i x_i\right)^2$$

- Compute its average $\langle s^2 \rangle$:

$$\langle s^2 \rangle = \frac{1}{N}\sum_i \langle x_i^2 \rangle - \frac{1}{N^2}\sum_{i,j} \langle x_i x_j \rangle$$

Correlated measures

- When the $\langle x_i \rangle$ are independent and identically distributed $\langle s^2 \rangle$ is a good estimator of the variance:

  Using $\langle x_i x_j \rangle = \langle x_i \rangle \langle x_j \rangle = \langle x \rangle^2$ for $i \neq j$; $\langle x_i x_j \rangle = \langle x^2 \rangle$ for $i = j$

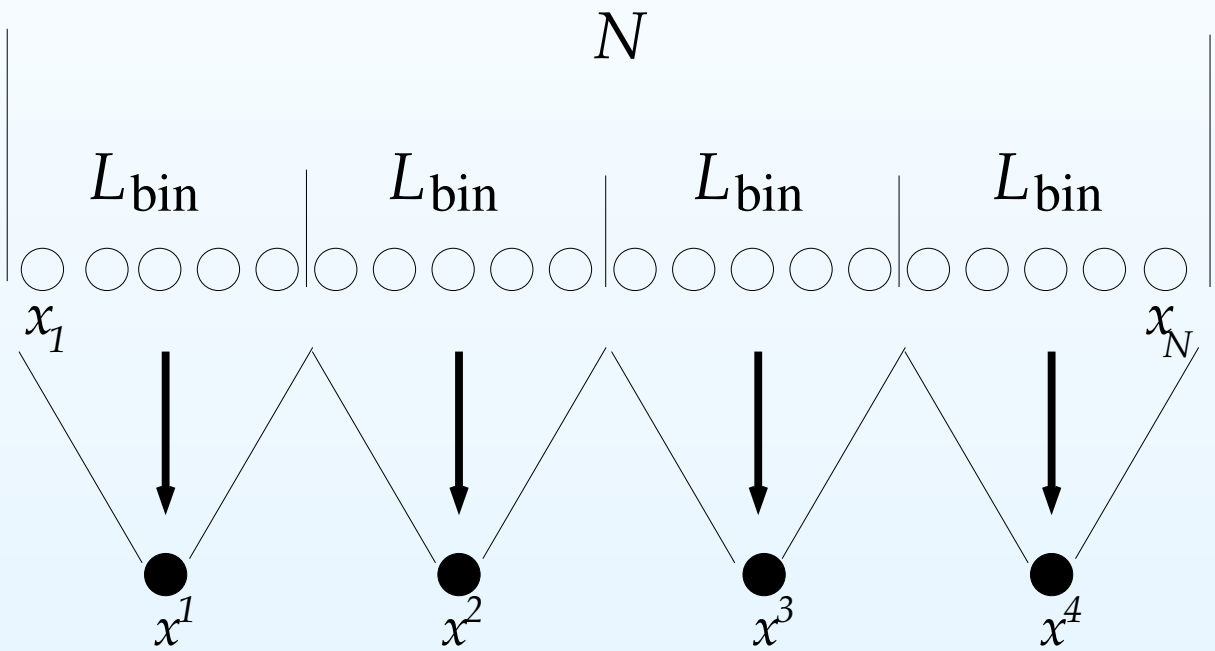
$$\langle s^2 \rangle = \frac{1}{N} \sum_i \langle x_i^2 \rangle - \frac{1}{N^2} \sum_{i,j} \langle x_i x_j \rangle = \left(1 - \frac{1}{N}\right) \left(\langle x^2 \rangle - \langle x \rangle^2\right) =$$

$$= \left(\frac{N-1}{N}\right) \sigma^2$$

- When $\langle x_i x_j \rangle \neq \langle x_i \rangle \langle x_j \rangle$, $\langle s^2 \rangle$ is no longer a proper estimator of the variance
- Solve the problem with the block analysis!

Binning technique (block analysis)

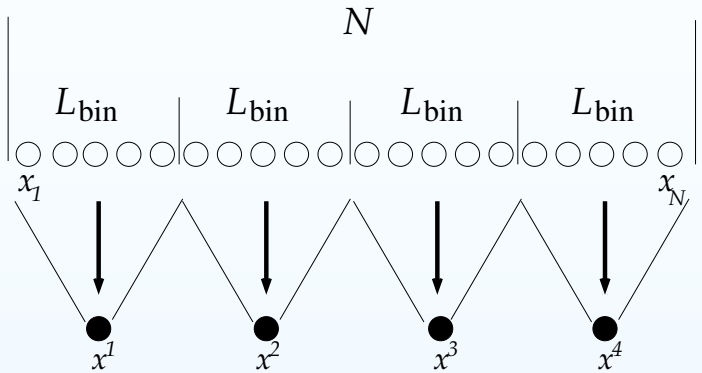
Divide the data set $\{x_i\}$ $i = 1, \ldots, N$ from a Markov chain in N_{bin} bins of length $L_{\text{bin}} = N/N_{\text{bin}}$ to uncorrelate data



- Consider the partial average on each bin j ($j = 1, \ldots, N_{\text{bin}}$)

$$x^j = \frac{1}{L_{\text{bin}}} \sum_{i=(j-1)L_{\text{bin}}+1}^{jL_{\text{bin}}} x_i$$

Binning technique (block analysis)



- The average over the bins is equal to the original average (linearity of the average)

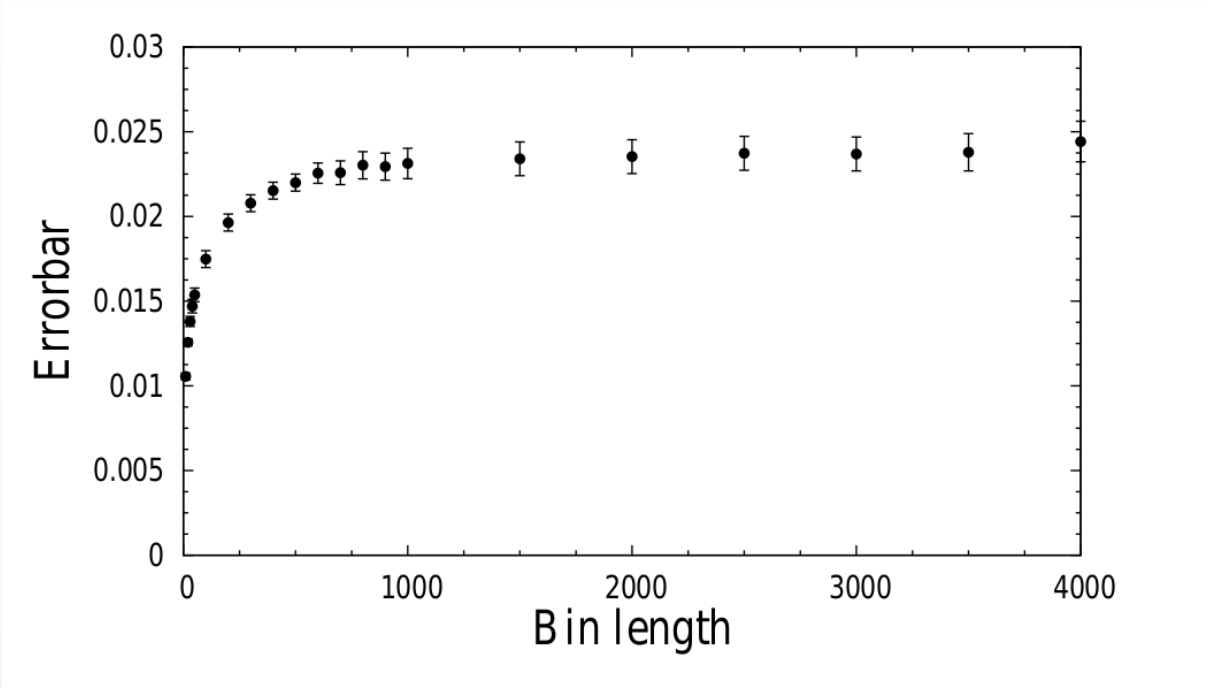
$$\bar{x^j} = \frac{1}{N_{\text{bin}}} \sum_{j=1}^{N_{\text{bin}}} x^j = \bar{x}$$

- If L_{bin} is large enough, the bin averages x^j are independent random variables

$$s^2_{\text{bin}} = \frac{1}{N_{\text{bin}}} \sum_{j=1}^{N_{\text{bin}}} (x^j - \bar{x})^2$$

- The error bar on the average value is given by $s_{\bar{x}} = s_{\text{bin}}/\sqrt{N_{\text{bin}}}$

Binning technique (block analysis)



Error bar on the average $s_{\bar{x}}$ as a function of L_{bin} along a Markov chain

(keeping the length of the Markov chain N fixed)

Variational wave functions for the single-orbital Hubbard model

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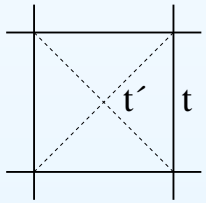
Variational MC: superconductivity and magnetism

Jastrow-Slater wave function: $|\Psi\rangle = \mathcal{J}|\Phi_0\rangle$

$|\Phi_0\rangle$ is the ground state of a non-interacting Hamiltonian $\mathcal{H}_{\text{aux}}$
It contains the relevant physical ingredients!

$\mathcal{J}$ is a Jastrow factor to include correlation effects

$$\mathcal{H}_{\text{aux}} = \mathcal{H}_0 + \mathcal{H}_{\text{BCS}} + \mathcal{H}_{\text{Néel}}$$



$$\mathcal{H}_0 = \sum_{\boldsymbol{k},\sigma} [-2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu] c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}$$

$$\text{H}_{\text{BCS}} = \sum_{\boldsymbol{k}} 2(\Delta_x \cos k_x - \Delta_y \cos k_y) c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow} + \text{H.c.} \quad \text{(superconductivity with } d\text{-wave pairing)}$$

$$\mathcal{H}_{\text{Néel}} = \Delta_{\text{AF}} \sum_R (-1)^{R_x+R_y} \left(c^\dagger_{R,\uparrow} c_{R,\uparrow} - c^\dagger_{R,\downarrow} c_{R,\downarrow} \right) \quad \text{(Néel antiferromagnetism)}$$

Gros, PRB 38, 931 (1988); Yokoyama and Shiba, JPSJ 57, 2482 (1988)

The variational wave functions: Jastrow factor

$$|\Psi\rangle = \mathcal{J}|\Phi_0\rangle$$

$$\mathcal{J} = \exp[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j] \; ; v_{ij} > 0$$

- $\mathcal{J}$ Long-range density-density correlator

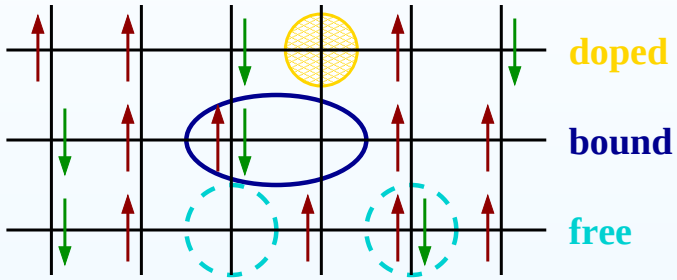
  v_{ij} variational parameters independently optimized for each distance $|i-j|$
- The local term v_{ii} accounts for the local Coulomb repulsion
- The optimal v_{ij} are maximal at short distance and decrease to zero when $|i-j|$ increases
- Long range density-density correlations are crucial to describe strongly correlated physics (see next)

The Jastrow factor $\mathcal{J}$

At half filling, pure Mott insulator, with no antiferromagnetism, above a finite value of U/t

M. Capello *et al.*, PRL 94, 026406 (2005)

Mott-Hubbard insulator: bounded empty and doubly occupied sites



Effective holon-doublon attraction and holon-holon (doublon-doublon) repulsion

$$\mathcal{J} = \exp[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j] \; ; v_{ij} > 0 \text{ and maximal at short distance}$$

$$n_i n_j = D_i D_j + H_i H_j - H_i D_j - D_i H_j + n_i + n_j - 1$$

$$\begin{cases} n_i = n_{i,\uparrow} + n_{i,\downarrow} \\ D_i = n_{i,\uparrow} n_{i,\downarrow} \\ H_i = (1 - n_{i,\uparrow})(1 - n_{i,\downarrow}) \end{cases}$$

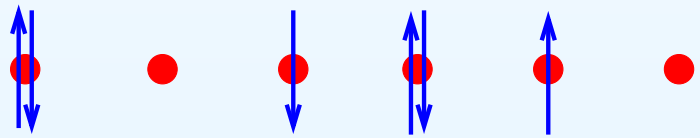
A simpler variational state: Gutzwiller factor

Suppress the weight of configurations with double occupations

Gutzwiller wf $$|\Psi_G\rangle = \mathcal{P}_G|\Phi_0\rangle = \exp[-g\sum_i n_{i,\uparrow}n_{i,\downarrow}]|\Phi_0\rangle; g > 0$$

M.C. Gutzwiller PRL 10, 159 (1963)

Define the basis $\{|x\rangle\}$ of configurations of electrons in the lattice. i.e., $|\bar{x}\rangle$:

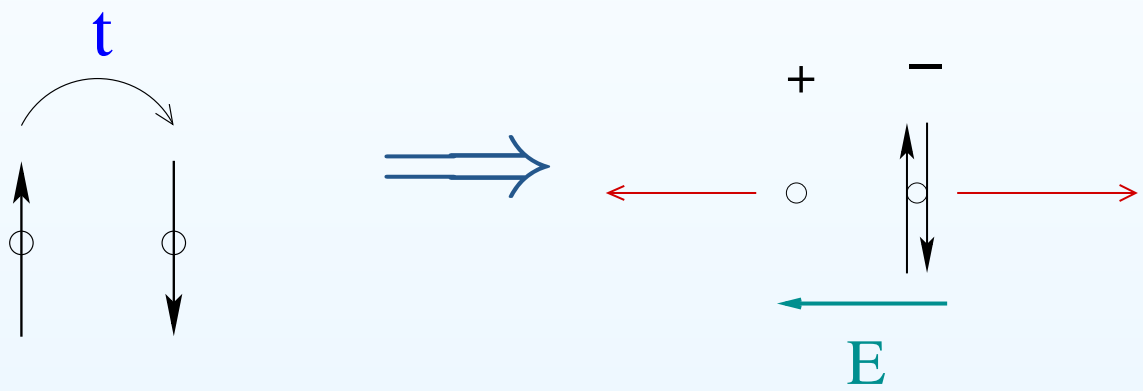


$$\langle x|\Psi_G\rangle = \mathcal{P}_G(x)\langle x|\Phi_0\rangle$$

$\mathcal{P}_G(x) \leq 1$ is a number, smaller when the number of doubly occupied sites in $|x\rangle$ is larger: the amplitude of the non-interacting state $\langle x|\Phi_0\rangle$ is renormalized by $\mathcal{P}_G(x)$

The Gutzwiller factor

At half filling, empty sites (Holons, H) and doubly occupied sites (Doublons, D) play a crucial role for the conduction



H and D must be correlated otherwise E induces a current

The Gutzwiller wf cannot describe a Mott insulator:
The formation of H and D pairs is penalized, but possible once g is finite, and there is no correlation among H and D

We have only a trivial insulator with $g = \infty$

Backflow correlations

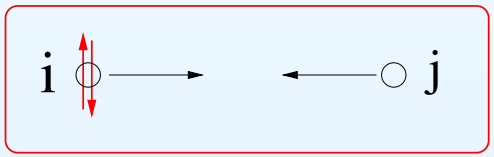
R.P. Feynman and M. Cohen, PR 102, 1189 (1956)

Y. Kwon, D.M. Ceperley, and R.M. Martin, PRB 48, 12037 (1993); M. Holzmann *et al.*, PRE 68, 046707 (2003)

Tocchio, Becca, Parola, Sorella PRB 78, 041101(R) (2008); Tocchio, Becca, Gros PRB 83, 195138 (2011)

$\Longrightarrow$ Many-body effects inside the mean-field variational wave functions $|\Phi_0\rangle$

$$\phi_k^b(r_{i,\sigma}) = \tilde{\epsilon}\phi_k(r_{i,\sigma}) + \eta_1 \sum_{j \text{n.n.} i} D_i H_j \phi_k(r_{j,\sigma}) + \dots$$



ϕ_k single-particle orbital

$D_i = n_{i,\uparrow} n_{i,\downarrow}$ $H_i = h_{i,\uparrow} h_{i,\downarrow}$

$h_{i,\sigma} = (1 - n_{i,\sigma})$

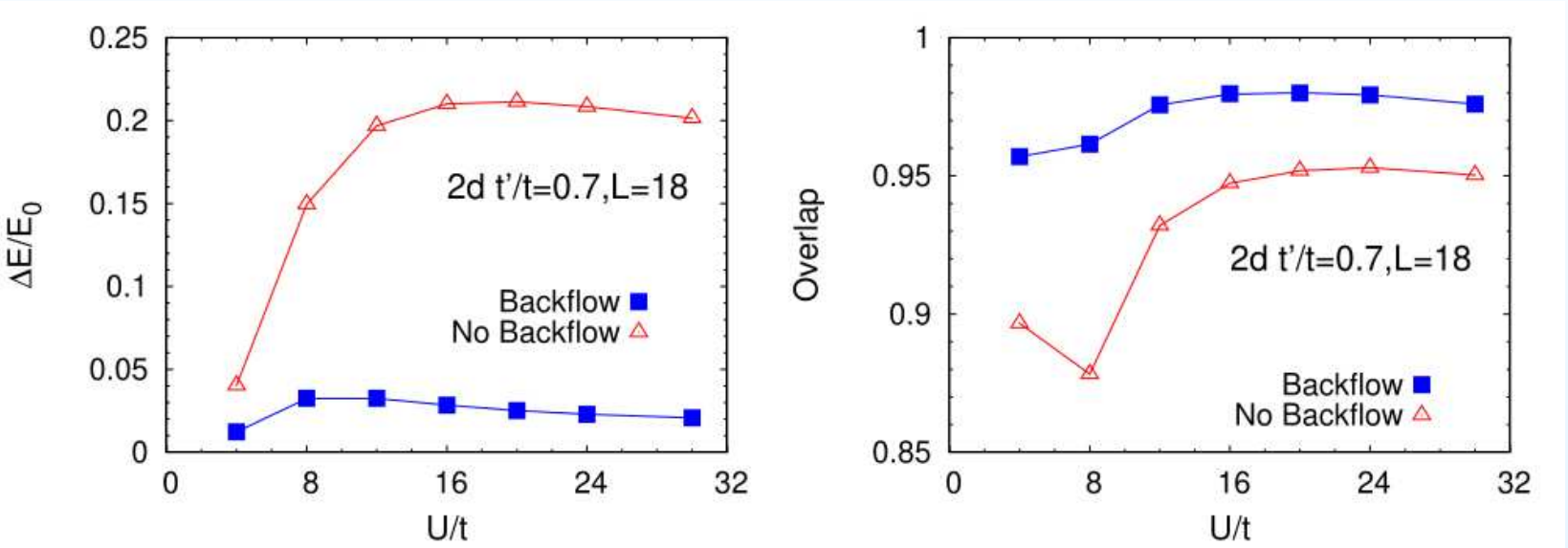
Summing up Slater determinants, according to the many-body configuration in the lattice:

The determinant part of the wave function contains correlation

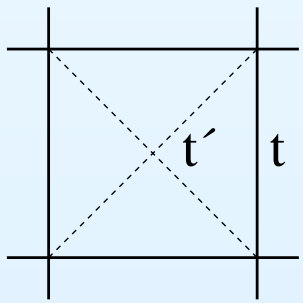
Backflow correlations: accuracy of the variational state

Comparison with exact diagonalization (Lanczos) at half filling

Overlap $\langle \Psi_{\text{var}} | \Psi_0 \rangle$ $\Delta E = E_{var} - E_0$; E_0 exact energy



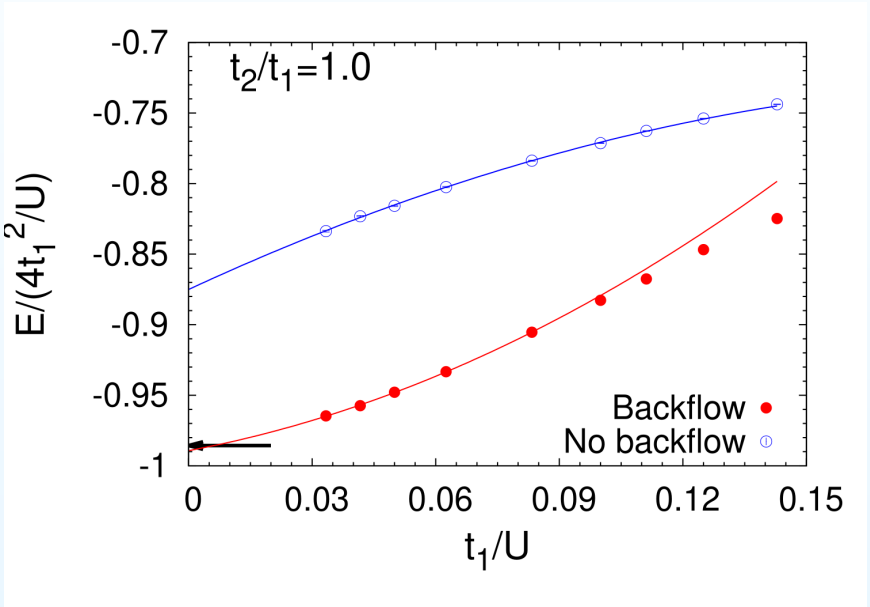
- Energy improvement in the insulating state ($U/t \gtrsim 8$)
- Overlap improvement at the metal-insulator transition



Tocchio, Parola, Becca, Sorella PRB 78, 041101(R) (2008)

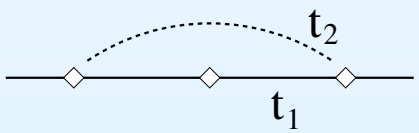
Backflow correlations: accuracy of the variational state

Large U limit in one dimension for the variational energy



- Proper extrapolation to the Heisenberg limit
- Black arrow is Density-matrix renormalization group (DMRG) - Exact in 1D
- Backflow correlations are the starting point for backflow-based neural network states

Luo and Clark, PRL 122,226401 (2019)



Tocchio, Becca, Gros PRB 83, 195138 (2011)

Variational Monte Carlo II

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Variational Monte Carlo

We need to compute:

- Ratio of probabilities for the Metroplis algorithm

$$\frac{\mathcal{P}(x')}{\mathcal{P}(x)} = \left| \frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle} \right|^2$$

- The local estimator, i.e., for the energy:

$$e_L(x) = \frac{\langle x|\mathcal{H}|\Psi\rangle}{\langle x|\Psi\rangle} = \sum_{x'} \langle x|\mathcal{H}|x'\rangle \frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle}$$

a) Is $\langle x|\mathcal{H}|x'\rangle$ hard to compute? No, thanks to the locality of the Hamiltonian: A given $|x\rangle$ is connected only to states that differ for the hopping of one electron from one site to one of its neighbors. Given $|x\rangle$, the non-zero matrix elements of $\langle x|\mathcal{H}|x'\rangle$ are $O(L)$ (# sites L × # bonds ×2 for the spin)

Variational Monte Carlo

b) What about the ratio $\langle x'|\Psi\rangle/\langle x|\Psi\rangle$?

- Let us consider the usual wave function $|\Psi\rangle = \mathcal{J}|\Phi_0\rangle$ ($\langle x|\Psi\rangle = \mathcal{J}(x)\langle x|\Phi_0\rangle$), where $|\Phi_0\rangle$ is the ground state of a quadratic Hamiltonian and $\mathcal{J}$ is the Jastrow factor:

$$\mathcal{J} = \exp(-\frac{1}{2}\sum_{i,j} v_{i,j} n_i n_j)$$

- $\langle x|\Phi_0\rangle$ is a determinant. Using standard linear algebra formulas it scales $O(L!)$. Using the LU decomposition into triangular matrices, it scales $O(L^3)$.
  Important message: Never do linear algebra by yourself, use always the libraries!
- It can be shown that $\langle x'|\Phi_0\rangle/\langle x|\Phi_0\rangle$ scales $O(L^2)$ if $|x'\rangle$ is close to $|x\rangle$

Jastrow ratio computation

- $\mathcal{J}(x) = \exp(-\frac{1}{2}\sum_{i,j} v_{i,j} n_i(x) n_j(x))$ scales $O(L^2)$
- When $|x'\rangle$ is close to $|x\rangle$, it is possible to define a fast computation of $\mathcal{J}(x')/\mathcal{J}(x)$ that is $O(L)$:

$$|x\rangle \equiv |n_1, \ldots, n_k, \ldots, n_l, \ldots, n_L\rangle \qquad |x'\rangle \equiv |n_1, \ldots, n_{k+1}, \ldots, n_{l-1}, \ldots, n_L\rangle$$

$$\frac{\mathcal{J}(x')}{\mathcal{J}(x)} = \frac{\mathcal{J}(n_1, \ldots, n_{k+1}, \ldots, n_{l-1}, \ldots, n_L)}{\mathcal{J}(n_1, \ldots, n_k, \ldots, n_l, \ldots, n_L)} = \frac{\exp(-\sum_i v_{k,i} n_i)}{\exp(-\sum_i v_{l,i} n_i)} e^{v_{k,l} - v_{k,k}}$$

Using $v_{i,j} = v_{j,i}$ and $v_{k,k} = v_{l,l}$ (translational invariance)

- The ratio $\frac{\mathcal{J}(x')}{\mathcal{J}(x)}$ costs $O(1)$ defining $T_{\text{Jastrow}}(j) = \sum_i v_{j,i} n_i$
- Updating $T_{\text{Jastrow}}(j)$ to the new configuration $|x'\rangle$ costs $O(L)$:

$$n'_i = n_i + \delta_{k,i} - \delta_{l,i} \Rightarrow T'_{\text{Jastrow}}(j) = T_{\text{Jastrow}}(j) + v_{k,j} - v_{l,j}$$

- From time to time, recompute $T_{\text{Jastrow}}(j)$ from scratch to avoid rounding errors

VMC summary

- We can compute expectation values of operators with a Monte Carlo sampling

$$\langle \mathcal{O} \rangle = \sum_x \mathcal{P}(x) \mathcal{O}_L(x) \quad \mathcal{O}_L(x) = \frac{\langle x|\mathcal{O}|\Psi\rangle}{\langle x|\Psi\rangle} \quad \mathcal{P}(x) = \frac{|\langle \Psi|x\rangle|^2}{\sum_{x'} |\langle \Psi|x\rangle|^2}$$

- Electronic states $|x_n\rangle$ generated with the Metropolis algorithm $\langle \mathcal{O} \rangle \sim \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}_L(x_n)$
- Binning technique to uncorrelate measures
- Fast computation of ratios of determinants and Jastrow factors

$$\frac{\langle x'|\Psi\rangle}{\langle x|\Psi\rangle} = \frac{\mathcal{J}(x')\langle x'|\Phi_0\rangle}{\mathcal{J}(x)\langle x|\Phi_0\rangle}$$

Optimization of variational parameters

- We have learned how to compute expectation values over a given wave function
- The Jastrow-Slater wave function depends on many variational parameters that can be optimized to minimize the energy

$$|\Psi\rangle = \mathcal{J}|\Phi_0\rangle$$

$$\mathcal{J} = \exp[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j] \; ; v_{ij} > 0$$

- We cannot perform loops over each parameter! We need a method to optimize a large number of parameters at the same time: Stochastic reconfiguration
- More efficient than steepest descent
- Still may have problems with local minima

Stochastic reconfiguration

- Starting state: $|\Psi^0\rangle = |\Psi(\{p_k^0\})\rangle$ with $\{p_k^0\}$ initial set of variational parameters
- Updated state: $|\Psi'\rangle = |\Psi(\{p_k'\})\rangle$ with $\{p_k'\}$ new set of variational parameters

For each variational parameter p_k^0, the update to p_k' is defined as:

$$\delta p_k = \sum_{j=1}^{N_p} S_{jk}^{-1} f_j \qquad p_k' = p_k^0 + \tau \delta p_k.$$

$$S_{jk} = \langle \Psi^0 | \mathcal{O}_j \mathcal{O}_k | \Psi^0 \rangle - \langle \Psi^0 | \mathcal{O}_j | \Psi^0 \rangle \langle \Psi^0 | \mathcal{O}_k | \Psi^0 \rangle$$

$$f_j = \langle \Psi^0 | \mathcal{O}_j | \Psi^0 \rangle \langle \Psi^0 | \mathcal{H} | \Psi^0 \rangle - \langle \Psi^0 | \mathcal{O}_j \mathcal{H} | \Psi^0 \rangle$$

$\mathcal{O}_k$ is the logarithmic derivative of $|\Psi^0\rangle$

$$\mathcal{O}_k(x) = \frac{1}{\Psi^0(x)} \frac{\partial \Psi^0(x)}{\partial p_k} = \frac{\partial \ln \langle x | \Psi^0 \rangle}{\partial p_k}$$

Main message: minimization through computing expectation values

Multiorbital Hubbard model

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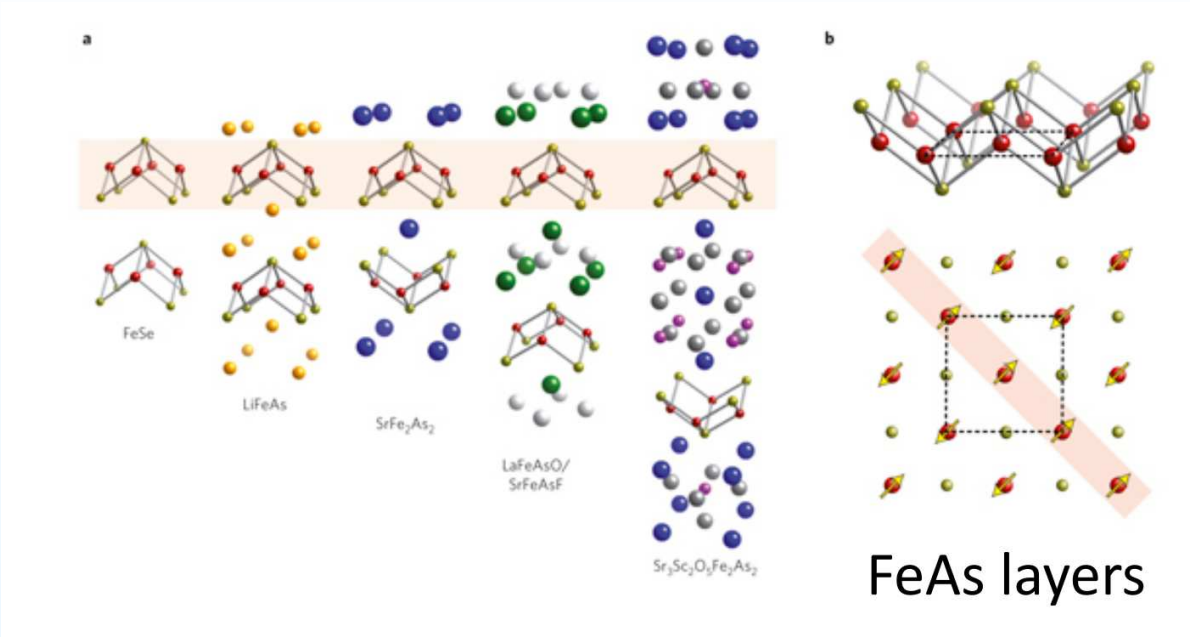
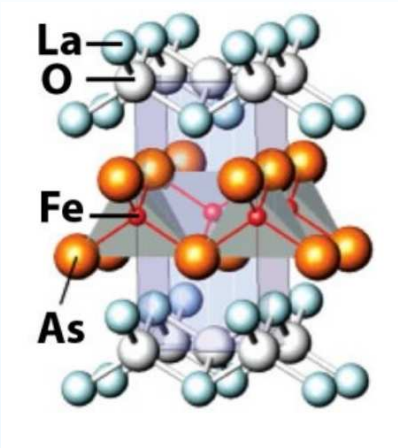
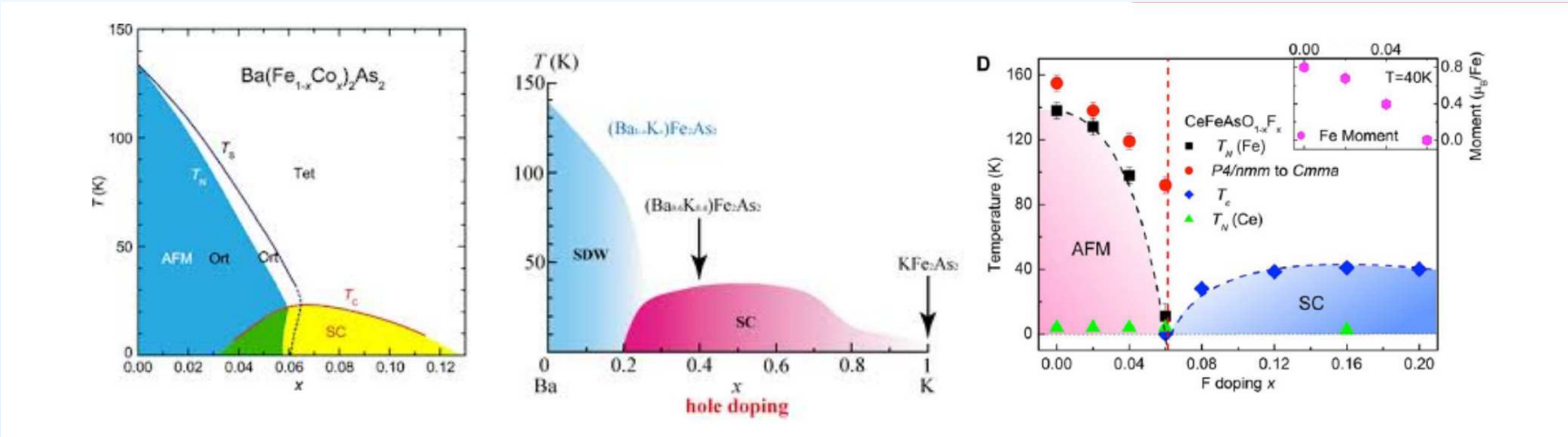
The iron pnictide superconductors

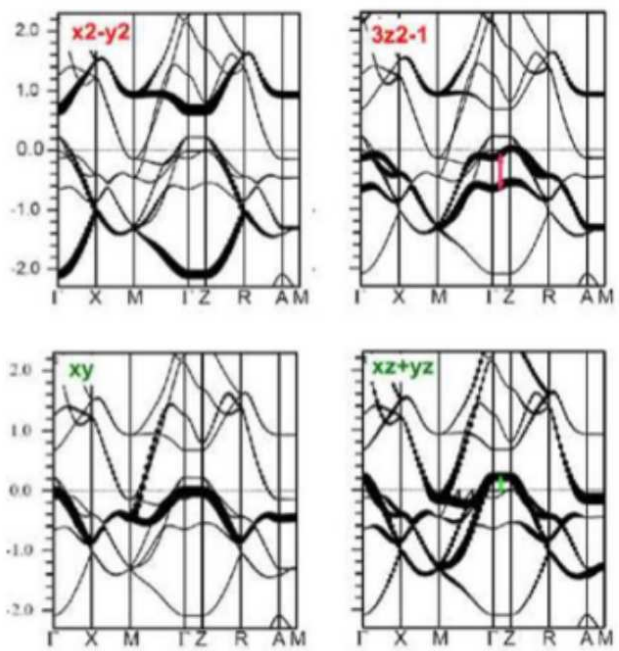






Paglione and Green, Nat. Phys. 6, 645 (2010); Stewart, Rev. Mod. Phys. 83, 1589 (2011)

The multiorbital physics



All the 5 d orbitals are close to the Fermi level. Multiorbital description is necessary

- Effective model with only the d_{xy}, d_{xz} and d_{yz} orbitals
  (light enough for numerics, but keeps main features of Iron-based superc.)
- Role of Hund's physics (correlation) and band structure

The 3-orbital Hubbard model $\mathcal{H}_k + \mathcal{H}_{\text{int}}$

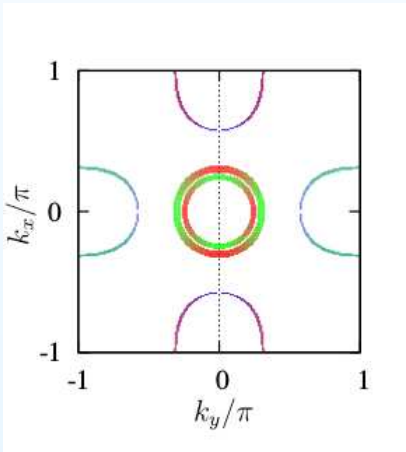
$$\mathcal{H}_k = \sum_k \sum_\sigma \sum_{\alpha,\beta} c^\dagger_{k\alpha\sigma} T_{\alpha\beta}(k) c_{k\beta\sigma}$$

α, β are orbital indices for the $1 = xz, 2 = yz, 3 = xy$ orbitals of Fe

$$T_{11}(k) = 2t_2 \cos k_x + 2t_1 \cos k_y + 4t_3 \cos k_x \cos k_y$$
$$T_{22}(k) = 2t_1 \cos k_x + 2t_2 \cos k_y + 4t_3 \cos k_x \cos k_y$$
$$T_{33}(k) = 2t_5(\cos k_x + \cos k_y) + 4t_6 \cos k_x \cos k_y + \Delta_{xy}$$
$$T_{12} = (T_{21})^* = 4t_4 \sin k_x \sin k_y$$
$$T_{13} = (T_{31})^* = 2it_7 \sin k_x + 4it_8 \sin k_x \cos k_y$$
$$T_{23} = (T_{32})^* = 2it_7 \sin k_y + 4it_8 \sin k_y \cos k_x$$

Orbital d_{xy} has a crystal field

Orbtials d_{xz} and d_{yz} exchange x and y directions



Fermi surface at $n = 4$ (parent compound in the three-orbital model)

Minimal model to reproduce qualitative features of Fermi surface

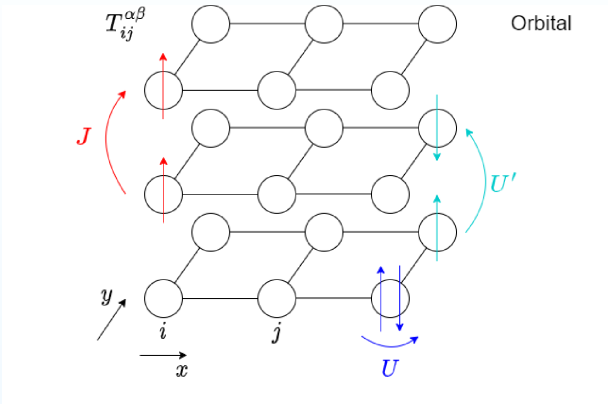
Daghofer *et al.*, PRB 81, 014511 (2010); Fanfarillo *et al.*, PRL 125, 177001 (2020).

The 3-orbital Hubbard model $\mathcal{H}_k + \mathcal{H}_{\text{int}}$

$$\mathcal{H}_{\text{int}} = U \sum_R \sum_\alpha n_{R\alpha\uparrow} n_{R\alpha\downarrow} + U' \sum_R \sum_{\alpha \neq \beta} n_{R\alpha\uparrow} n_{R\beta\downarrow} +$$

$$+ (U' - J) \sum_R \sum_{\alpha > \beta} \sum_\sigma n_{R\alpha\sigma} n_{R\beta\sigma} +$$

$$- J \sum_R \sum_{\alpha \neq \beta} c^\dagger_{R\alpha\uparrow} c_{R\alpha\downarrow} c^\dagger_{R\beta\downarrow} c_{R\beta\uparrow} + J \sum_R \sum_{\alpha \neq \beta} c^\dagger_{R\alpha\uparrow} c^\dagger_{R\alpha\downarrow} c_{R\beta\downarrow} c_{R\beta\uparrow}$$



- Intra-orbital Coulomb repulsion U
- Inter-orbital Coulomb repulsion U'
- Hund's coupling J (including spin-flip and pair-hopping terms)

Rotational invariance $U' = U - 2J$

Georges, de' Medici, Mravlje, Annu. Rev. Condens. Matter Phys. 4, 137 (2013)

The variational wave function (Jastrow factors)

$$|\Psi\rangle = \mathcal{J}_U \mathcal{J}_{U'} \mathcal{J}_J |\phi_0\rangle.$$

$|\phi_0\rangle$ is the ground state of a non-interacting Hamiltonian $\mathcal{H}_{\text{BCS}}$
$\mathcal{J}$ is a Jastrow factor to include correlation effects:

Capello, Becca, Fabrizio, Sorella, and Tosatti, PRL 94, 026406 (2005)

Generalization to a multiorbital model

$$\mathcal{J}_U = \exp\Big(-\frac{1}{2}\sum_{\alpha}\sum_{R,R'} v^{\alpha,\alpha}_{R,R'} n_{R\alpha} n_{R'\alpha}\Big)$$ Long-range intra-orbital density-density correlator

$$\mathcal{J}_{U'} = \exp\Big(-\frac{1}{2}\sum_{\alpha\neq\beta}\sum_{R,R'} v^{\alpha,\beta}_{R,R'} n_{R\alpha} n_{R'\beta}\Big)$$ Long-range inter-orbital density-density correlator

$$\mathcal{J}_J = \exp\Big(-\frac{1}{2}\sum_{\alpha\neq\beta} u^{\alpha,\beta}\sum_{R} S^z_{R\alpha} S^z_{R\beta}\Big)$$ On-site inter-orbital spin-spin correlator: Hund's coupling

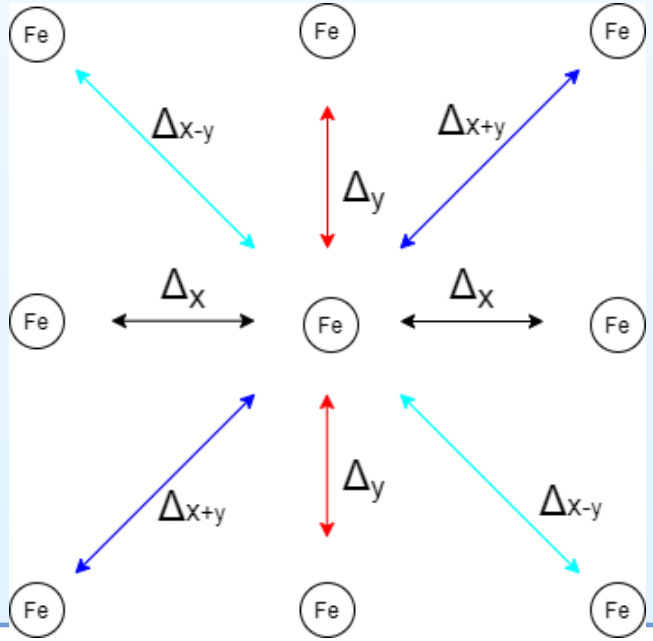
Marino, Scazzola, Becca, Capone, Tocchio, PRL 134, 196502 (2025)

The variational wf ($|\phi_0\rangle$ as ground state of $\mathcal{H}_{\text{BCS}}$)

$$\mathcal{H}_{\text{BCS}} = \mathcal{H}_k - \sum_{R,\alpha,\sigma} \mu_\alpha c^\dagger_{R\alpha\sigma} c_{R\alpha\sigma} + \sum_{R,\alpha,\delta} \left[\Delta_{\alpha,\delta} \left(c_{R,\alpha,\downarrow} c_{R+\delta,\alpha,\uparrow} - c_{R,\alpha,\uparrow} c_{R+\delta,\alpha,\downarrow} \right) + \text{h.c.} \right]$$

$$(\delta = \pm x, \pm y, \pm(x+y), \pm(x-y))$$

- The hopping term $\mathcal{H}_k$ is the same as in the Hubbard Hamiltonian
- Intraorbital pairing amplitudes with no a priori symmetry (optimized along the simulation): (no interorbital pairing Misawa and Imada, Nat Comm 5, 5738 (2014))



Correlation functions

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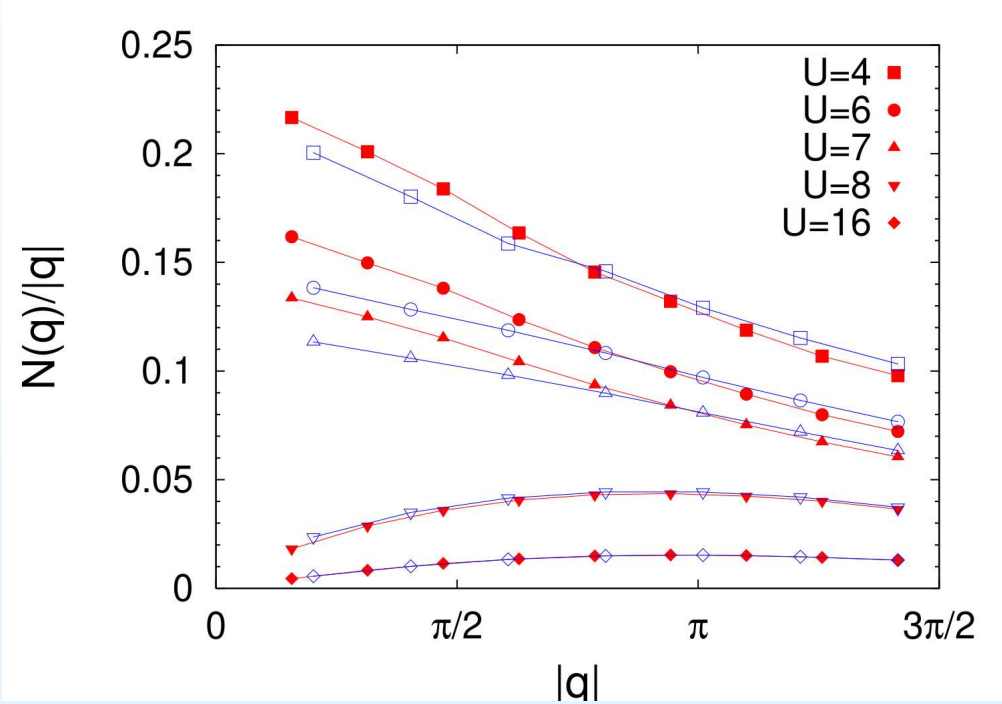
Metal or insulator?

Density-density correlations $N(\boldsymbol{q}) = \frac{1}{L}\sum_{R,R'}\langle n_R n_{R'}\rangle e^{i\boldsymbol{q}\cdot(\boldsymbol{R}-\boldsymbol{R}')}$

Excited state $|\Psi_{\boldsymbol{q}}\rangle = n_{\boldsymbol{q}}|\Psi\rangle \Rightarrow$ Charge gap $\propto \lim_{|\boldsymbol{q}|\to 0} \frac{\boldsymbol{q}^2}{N(\boldsymbol{q})}$

Metal: $N(\boldsymbol{q}) \propto |\boldsymbol{q}|$ for $|\boldsymbol{q}| \to 0$ Insulator: $N(\boldsymbol{q}) \propto |\boldsymbol{q}|^2$ for $|\boldsymbol{q}| \to 0$

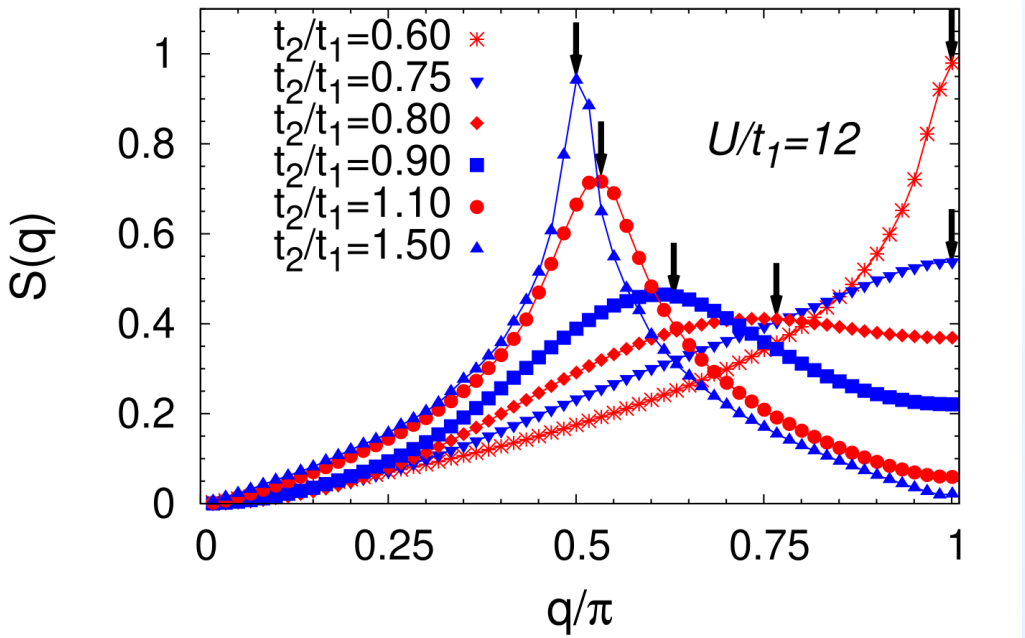
Feynman PR 94, 262 (1954); Tocchio, Becca, Gros, PRB 83, 195138 (2011)

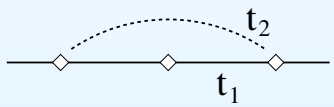


- Single-orbital Hubbard model on the square lattice with $t'/t = 0.75$
- Insulator for $U/t \geq 8$; Metal for $U/t \leq 7$ Tocchio, Parola, Becca, Sorella PRB 78, 041101(R) (2008)

Charge or magnetic order

- Spin-spin correlations $S(\boldsymbol{q}) = \frac{1}{L} \sum_{R,R'} \langle S^z_R S^z_{R'} \rangle e^{i\boldsymbol{q}\cdot(\boldsymbol{R}-\boldsymbol{R}')}$
- Density-density correlations $N(\boldsymbol{q}) = \frac{1}{L} \sum_{R,R'} \langle n_R n_{R'} \rangle e^{i\boldsymbol{q}\cdot(\boldsymbol{R}-\boldsymbol{R}')}$
- Long-range Order: Peak at $\boldsymbol{Q}$, diverging with the system size
- Short-range correlations: Peak at $\boldsymbol{Q}$, *non* diverging with the system size





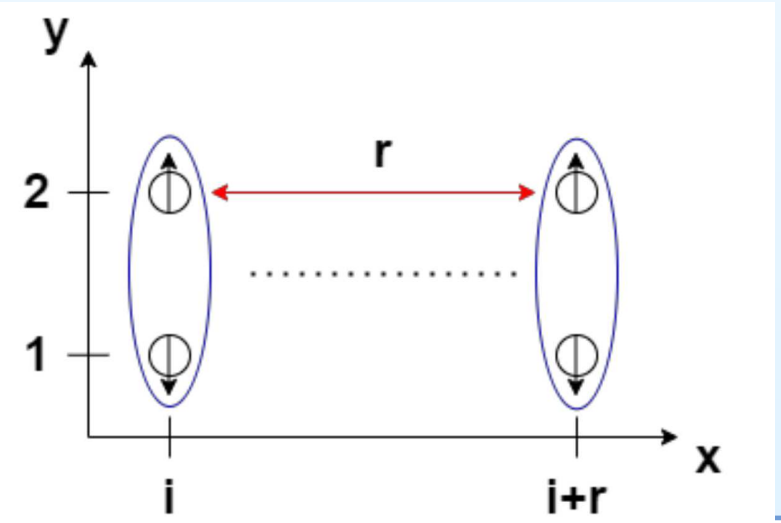
- Example for the 1D Hubbard model: No long-range order in 1D, only short-range spin-spin correlations Tocchio, Becca, Gros PRB 81, 205109 (2011)

Superconductive singlet-singlet correlations

- Finite pairing amplitudes $\Delta_{\alpha,\delta}$ in the variational wave function are necessary condition for superconductivity
- Superconductivity is present when singlet-singlet correlations are finite at large distances

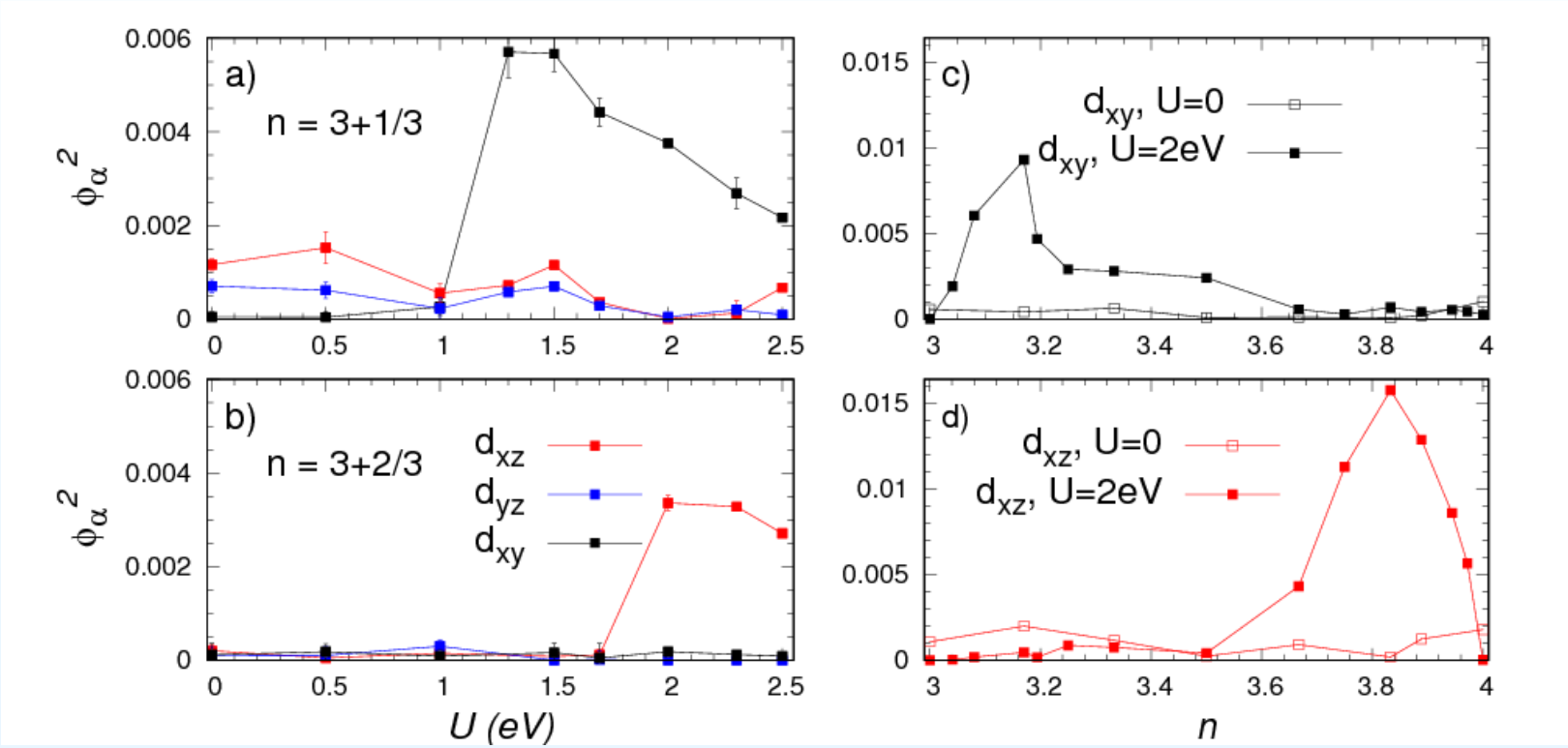
$$D_\alpha(r) = \frac{1}{L}\sum_R \langle P_{R,\alpha} P^\dagger_{R+rx,\alpha}\rangle \quad P_{R,\alpha} = c_{R+y,\alpha,\downarrow} c_{R,\alpha,\uparrow} - c_{R+y,\alpha,\uparrow} c_{R,\alpha,\downarrow}$$

Finite order parameter ϕ_α: $\lim_{r\to\infty} D_\alpha(r) = \phi_\alpha^2$ for superconductivity



Superconductivity in the multiorbital model

Marino, Scazzola, Becca, Capone, Tocchio, PRL 134, 196502 (2025)



- Superconductivity in one of the three orbitals, for U larger than a critical value d_{xy} for $3 < n \lesssim 3.5$; d_{xz} for $3.5 \lesssim n < 4$
- Compare with the finite-size effects at $U = 0$ (Role of U and J (not shown) in driving superconductivity)

Quo vadis VMC?

- Computation of physical observables over a variational approximation of the true ground state
- One path: Apply simple Jastrow-Slater states to multi-orbital Hubbard models where nonperturbative approaches are lacking

  Di Sante *et al.*, Kagome metals, RMP 98, 015002 (2026)
- Another path: Improve the variational states with neural-network quantum states based on the transformer architecture (at the moment limited to single-orbital Hubbard models on simple lattice geometries)

  Viteritti *et al.*, arXiv:2604.21978