Variational Wave Functions for Strongly-Correlated Fermionic Systems

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Autumn School on Correlated Electrons:
Many-Body Methods for Real Materials
Jülich, September 19th

UNIVERSITÀ DEGLI STUDI DI TRIESTE

Band theory + Odd number of el. per unit cell $\Longrightarrow$ Metal

Many materials with an odd number of electrons per unit cell are insulators
for example transition-metal compounds

These are called Mott insulators

We will consider lattice models

GOAL: Describe an insulating state of purely Mott type

In Mott insulators localization is induced by strong correlation
Failure of the single-particle picture

The variational approach gives insight into the ground state properties
Until very recently a consistent Mott insulating state was not available

- Long-range (density) Jastrow factor
- "Backflow" correlations

Main result:

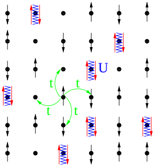
Metal-insulator transition and strong-coupling phase

But also:

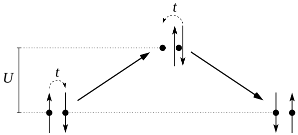
Accurate metallic and/or superconducting phase when doping Mott insulators

Hubbard and Heisenberg models

$$\mathcal{H} = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



The Hubbard model is the prototype for correlated electrons on the lattice
[like the Ising model for classical magnetism]
NO exact solution in D>1



Antiferromagnetic super-exchange

$J = \frac{4t^2}{U}$

NO charge fluctuations, only spin

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

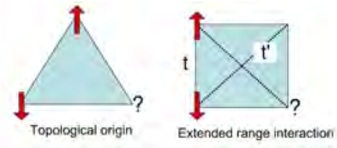
At large U/t there are antiferromagnetic correlations

At $T = 0$ (ground state), magnetic order may be present

- Long-range magnetic order on square and honeycomb lattices (QMC)
  Triangular lattice: convincing evidence from different numerical methods

Magnetic frustration: a way to destabilize magnetic AF order

Non-magnetic ground states may exist



- Evidence for the absence of magnetic order on the kagome lattice
  Frustrated square and triangular lattices: evidence from different numerical methods

THE INFINITE-U LIMIT (HEISENBERG MODEL)

- **Magnetically ordered state: the (spin) Jastrow factor**

$$\mathcal{H}_{\rm cl} = \Delta_{\rm AF} \sum_j \mathbf{S}_j \cdot \mathbf{n}_j \qquad \Longrightarrow |\Phi_{\rm cl}\rangle$$

$\mathbf{n}_j = \{\cos(\mathbf{Q} \cdot \mathbf{R}_j), \sin(\mathbf{Q} \cdot \mathbf{R}_j)\}$

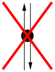
$\mathcal{J}_s = \exp[-\frac{1}{2} \sum_{i,j} u_{i,j} S_i^z S_j^z]$ $\qquad$ $|\Psi_{\rm AF}\rangle = \mathcal{J}_s |\Phi_{\rm cl}\rangle$

Manousakis, Rev. Mod. Phys. **63**, 1 (1991)

- **Non-magnetic state (spin liquid): the Gutzwiller projector**

$$\mathcal{H}_{\rm BCS} = \sum_{i,j,\sigma} t_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} + \sum_{i,j} \Delta_{i,j} [c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + c^\dagger_{j,\uparrow} c^\dagger_{i,\downarrow}] + h.c. \Longrightarrow |\Phi_{\rm BCS}\rangle$$

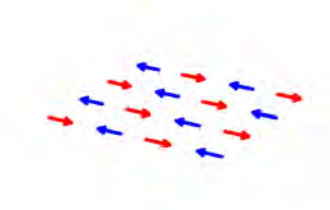
$P_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$



$|\Psi_{\rm SL}\rangle = P_G |\Phi_{\rm BCS}\rangle$

Anderson, Science **235**, 1196 (1987)

- Start from a (classical) ordered state in the XY plane

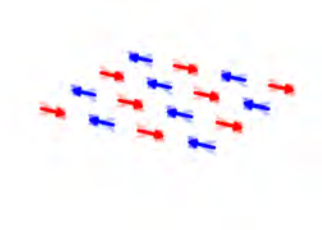


$$|\Phi_{\rm cl}\rangle = \prod_j \left(|\uparrow\rangle_j + e^{iQR_j} |\downarrow\rangle_j \right)$$

No correlation

Q determines the periodicity

- Include a two-body (spin) Jastrow factor to modify the weights



$$|\Psi_{\rm AF}\rangle = \exp\left[-\frac{1}{2} \sum_{i,j} u_{i,j} S_i^z S_j^z \right] |\Phi_{\rm cl}\rangle$$

The Jastrow factor creates correlations

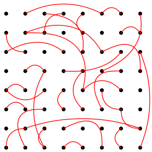
$u_{i,j}$ is a pseudo-potential to be optimized

This wave function corresponds to the one of the spin-wave approximation

- The mean-field wave function has a BCS form

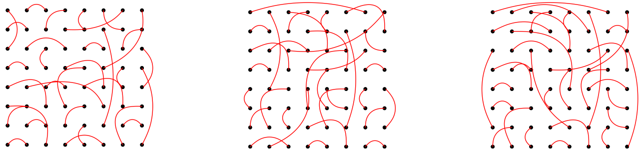
$$|\Phi_{\rm BCS}\rangle = \exp\left\{ \frac{1}{2} \sum_{i,j} f_{i,j} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} \right\} |0\rangle$$

It is a linear superposition of all singlet configurations (that may overlap)



$+ \ldots$

- With $P_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$, only non-overlapping singlets survive



$+ \ldots$

The wave function corresponds to the resonating valence-bond (RVB) state

These wave functions cannot be treated by using analytical approaches

- They can be treated within quantum Monte Carlo

$$E(\Psi) = \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_x P(x) e_L(x) \approx \frac{1}{M}\sum_{i=1}^{M} e_L(x_i)$$

$P(x) = \frac{|\langle x|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$ ("classical" Monte Carlo)

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

Requirements

- $\langle x|\Psi\rangle$ must be efficiently computed
- The Hamiltonian must be local

Becca and Sorella, *Quantum Monte Carlo Approaches for Correlated Systems* (Cambridge University Press, 2017)

Variational Monte Carlo for the Jastrow wave function

- **Magnetically ordered state** $\Longrightarrow |\Phi_{\rm cl}\rangle$ is a product state

$$\mathcal{J}_s = \exp[-\tfrac{1}{2}\sum_{i,j} u_{i,j} S_i^z S_j^z] \qquad |\Psi_{\rm AF}\rangle = \mathcal{J}_s |\Phi_{\rm cl}\rangle$$

$|x\rangle$ is the (Ising) basis with fixed S^z on each site

- $\mathcal{J}_s$ is diagonal and $\langle x|\Phi_{\rm cl}\rangle$ is a number $\Longrightarrow \langle x|\Psi_{\rm AF}\rangle$ computed in $O(N^2)$
- $e_L(x)$ is computed in $O(N^3)$, for a short-range Hamiltonian

Hasting-Metropolis algorithm: Markov chain $|x\rangle \to |x'\rangle$

- $\frac{P(x')}{P(x)}$ is computed in $O(1)$ for local moves!
- $e_L(x)$ is computed in $O(N)$
- Updating is done in $O(N)$

- Size consistent wave function

  $O(N)$ variational parameters (with translational invariance): $u_{i,j} \to u_r$

  $O(N^2)$ scaling for sampling: easy calculations up to $N \approx 500 \div 1000$ (on a desktop)

- The accuracy depends upon the lattice

  Rather good variational energy for unfrustrated lattices: $\Delta E/E_{\rm ex} \approx 1\%$

  Accuracy on observables follows (ϵ on $E \to \sqrt{\epsilon}$ on O): $\Delta M/M_{\rm ex} \approx 10\%$

- It breaks spin SU(2) symmetry

  Bad for finite lattices (the ground state is fully symmetric)

  Good for the thermodynamic limit (if the ground state breaks the symmetry)

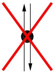
- Goldstone modes from the Feynman construction

  For small momenta: $\langle \Psi_{\rm AF}|S^z_{-q}S^z_q|\Psi_{\rm AF}\rangle/\langle \Psi_{\rm AF}|\Psi_{\rm AF}\rangle \propto q$

  $|\Psi_q\rangle = S^z_q|\Psi_{\rm AF}\rangle$ gives $E_q - E \propto \frac{q^2}{S_q}$

- **Non-magnetic state (spin liquid)** $\Longrightarrow |\Phi_{\rm BCS}\rangle$ is an entangled state

$P_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$



$|\Psi_{\rm SL}\rangle = P_G |\Phi_{\rm BCS}\rangle$

$|x\rangle$ is the basis with one electron per site, fixed S^z on each site

- P_G is the identity and $\langle x|\Phi_{\rm BCS}\rangle$ is a determinant $\Longrightarrow \langle x|\Psi_{\rm SL}\rangle$ computed in $O(N^3)$
- $e_L(x)$ is computed in $O(N^4)$, for a short-range Hamiltonian

Hasting-Metropolis algorithm: Markov chain $|x\rangle \to |x'\rangle$

- $\frac{P(x')}{P(x)}$ is computed in $O(1)$ for local moves!
- $e_L(x)$ is computed in $O(N)$
- Updating is done in $O(N^2)$

- Size consistent wave function

  $O(1)$ variational parameters (few distances): $t_{i,j} \to t_r$ and $\Delta_{i,j} \to \Delta_r$

  $O(N^3)$ scaling for sampling: easy calculations up to $N \approx 100 \div 400$ (on a desktop)

- The accuracy depends upon the lattice

  Rather good variational energy for frustrated lattices: $\Delta E / E_{\rm ex} \approx 1\%$

  Accuracy on observables follows (ϵ on $E \to \sqrt{\epsilon}$ on O)

- It does not break spin SU(2) symmetry

  Good for finite lattices (the ground state is fully symmetric)

  Good for the thermodynamic limit (if the ground state does not break the symmetry)

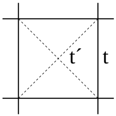
- Fractional $S = 1/2$ spinon excitations and "gauge" excitations

  Free ("deconfined") $S = 1/2$ objects are expected

  In addition, neutral $S = 0$ excitations should exist

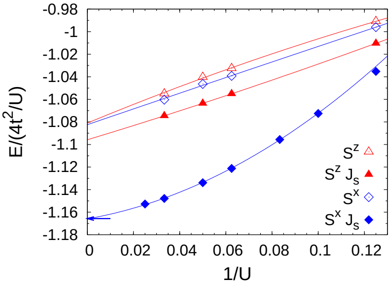
Fradkin, *Field Theories of Condensed Matter Physics*, (Cambridge University Press, 2013)

Magnetic wave function (stable for $t' = 0$ and $U > 0$)



$$\mathcal{H}_{MF} = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. + \Delta_{\rm AF} \sum_j e^{i\mathbf{Q}\cdot\mathbf{R}_j} S^x_j \qquad \Longrightarrow |\Phi_{\rm MF}\rangle$$

$$\mathcal{J}_s = \exp[-\frac{1}{2}\sum_{i,j} u_{i,j} S^z_i S^z_j] \qquad |\Psi_{\rm AF}\rangle = \mathcal{J}_s |\Phi_{\rm MF}\rangle$$



Gutzwiller wave function

$$\mathcal{H}_0 = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. \qquad \Longrightarrow |\mathcal{D}\rangle$$

$$|\Psi_g\rangle = e^{-g \sum_i n_{i,\uparrow} n_{i,\downarrow}} |\mathcal{D}\rangle$$

- $g = 0$, the non-interacting wave function is recovered
- $g = \infty$, the full Gutzwiller projector is obtained

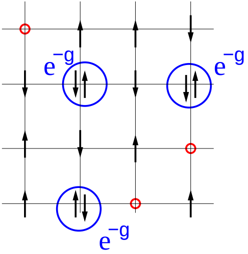
No exact calculations, except 1D

Metzner and Vollhardt, Phys. Rev. B **37**, 7382 (1988)

Gebhard and Vollhardt, Phys. Rev. B **38**, 6911 (1988)

Monte Carlo sampling is possible

Yokoyama and Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987)

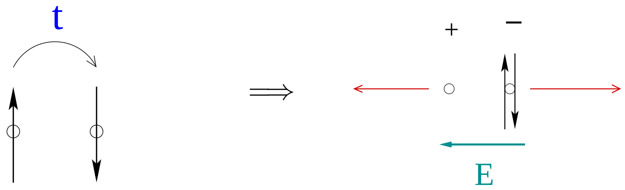


The Gutzwiller wave function is metallic for ANY $g \neq \infty$

It does not correlate charge fluctuations (empty and doubly occupied sites)

In any realistic insulator there are charge fluctuations

Empty sites (Holons, H) and doubly occupied sites (Doublons, D) play a crucial role for the conduction



H and D must be correlated otherwise an electric field would induce a current

Short-range holon-doublon wave function

$$|\Psi_{hd}\rangle = e^{f \sum_{\langle l,m \rangle} h_l d_m} |\Psi_g\rangle = e^{f \sum_{\langle l,m \rangle} h_l d_m} e^{-g \sum_i n_{i,\uparrow} n_{i,\downarrow}} |\mathcal{D}\rangle$$

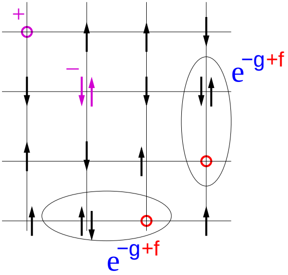
- Put nearest-neighbor correlation among holons and doublons

Exact calculations on small clusters

Kaplan, Horsch, and Fulde, Phys. Rev. B **49**, 889 (1982)

Monte Carlo sampling is possible

Yokoyama and Shiba, J. Phys. Soc. Jpn **59**, 3669 (1990)



H and D farer than nearest neighbors are uncorrelated: metallic for ANY f

The low-energy properties reflect the long-distance behavior
We must change the density-density correlations of the mean-field state at large distance

$$|\Psi\rangle = \mathcal{J}_c|\mathcal{D}\rangle$$

$$\mathcal{J}_c = \exp\left[-\frac{1}{2}\sum_{i,j} v_{i,j} n_i n_j\right] = \exp\left[-\frac{1}{2}\sum_{q} v_q n_{-q} n_q\right]$$

$|\mathcal{D}\rangle$ is an uncorrelated determinant, possibly including BCS pairing

Find the optimal set of parameters $v_{i,j}$ which
minimizes the energy without any a-priori assumption

Capello, Becca, Fabrizio, Sorella, and Tosatti, Phys. Rev. Lett. **94**, 026406 (2005)

Capello, Becca, Yunoki, and Sorella, Phys. Rev. B **73**, 245116 (2006)

Ansatz for the low-energy excitations Feynman, Phys. Rev. **94**, 262 (1954)

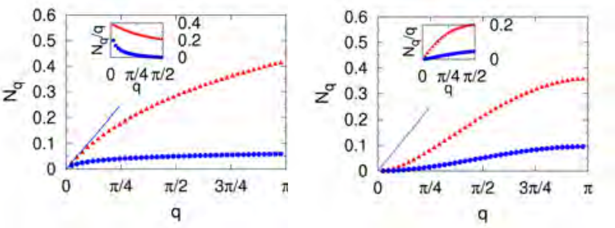
$$|\Psi_q\rangle = n_q|\Psi_0\rangle \qquad N_q = \langle\Psi_0|n_{-q}n_q|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle$$

f-sum rule

$$\Delta_q = \frac{\langle\Psi_q|(H-E_0)|\Psi_q\rangle}{\langle\Psi_q|\Psi_q\rangle} = \frac{\langle\Psi_0|[n_{-q},[H,n_q]]|\Psi_0\rangle}{2N_q} \sim \frac{q^2}{N_q}$$

$N_q \sim |q| \Rightarrow \Delta_q \to 0 \quad \Rightarrow$ metal

$N_q \sim q^2 \Rightarrow \Delta_q$ is finite $\Rightarrow$ insulator



Gutzwiller (left) and Jastrow (right) wave functions for $U = 4$ and 10

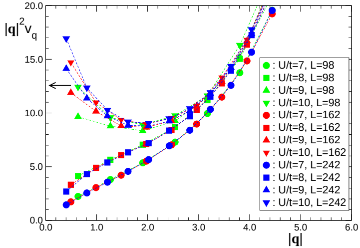
$$N_q = \frac{\langle \Psi | n_{-q} n_q | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

RPA Reatto and Chester, Phys. Rev. **155**, 88 (1967)

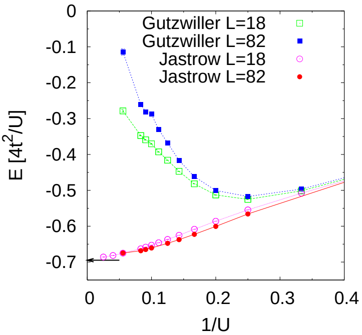
- For continuous systems
- In the weak-coupling regime

$$N_q = \frac{N_q^0}{1 + 2 v_q N_q^0} \approx \frac{1}{v_q}$$

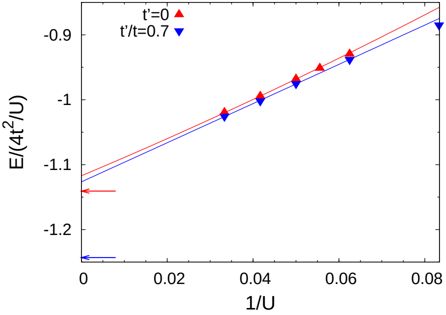
Two-dimensional (paramagnetic) Hubbard model



One dimension



Two dimensions



Poor accuracy in 2D systems: especially in presence of frustration

STANDARD (VERY)-LARGE-U APPROACH

Suppose we have a good ansatz $|\Psi_H\rangle$ for $U = \infty$

$$E = \langle \Psi_H | H_{Heis} | \Psi_H \rangle$$

Then a good ansatz for the Hubbard model in the large-U limit is

$$|\Psi\rangle = e^{iS} |\Psi_H\rangle \quad iS = \frac{1}{U}(T^+ - T^-)$$

MacDonald, Girvin, and Yoshioka, Phys. Rev. B **37**, 9753 (1988)

Difficult to treat

- Expand $e^{iS} \simeq 1 + iS$ (not size consistent)

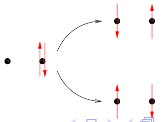
  Paramekanti, Trivedi, and Randeria, Phys. Rev. Lett. **87**, 217002 (2001)

- Perform the Hubbard-Stratonovich decoupling

  D. Eichenberger and D. Baeriswyl, Phys. Rev. B **76**, 180504 (2007)

$$\langle x_0 | \Psi \rangle = \langle x_0 | \Psi_H \rangle$$

$$\langle x_1 | \Psi \rangle = \frac{1}{U} \left\{ \langle x_0^{\uparrow\downarrow} | \Psi_H \rangle + \langle x_0^{\downarrow\uparrow} | \Psi_H \rangle \right\}$$



The backflow wave function in the continuum considers fictitious coordinates of the electrons

$$\mathbf{r}^b_\alpha = \mathbf{r}_\alpha + \sum_\beta \eta_{\alpha,\beta}(\mathbf{r}_\beta - \mathbf{r}_\alpha)$$

- Proposed for roton excitations in liquid Helium

  Feynman and Cohen, Phys. Rev. **102**, 1189 (1956)
- Implemented in Monte Carlo calculations to study bulk ^{3}He

  Schmidt, Lee, Kalos, and Chester, Phys. Rev. Lett. **47**, 807 (1981)
- Used to improve the electron gas

  Kwon, Ceperley, and Martin, Phys. Rev. B **48**, 12037 (1993); Phys. Rev. B **58**, 6800 (1998)

Apply backflow to a lattice model

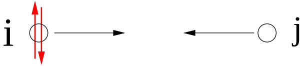
$$\phi_k(\mathbf{r}^b_\alpha) \simeq \phi^b_k(\mathbf{r}_\alpha) \equiv \phi_k(\mathbf{r}_\alpha) + \sum_\beta c_{\alpha,\beta}\phi_k(\mathbf{r}_\beta)$$

ϕ_k = single particle orbitals

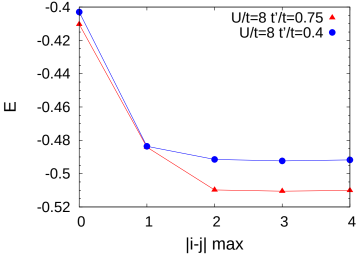
To favor the recombination of neighboring charge fluctuations

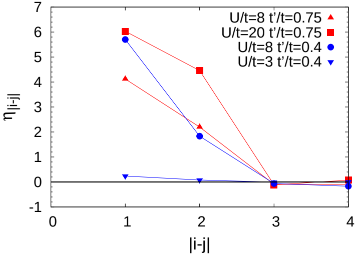
$$\phi_k^b(\mathbf{r}_{i,\sigma}) \equiv \epsilon \phi_k(\mathbf{r}_{i,\sigma}) + \sum_j \eta_{i,j} \, D_i H_j \, \phi_k(\mathbf{r}_{j,\sigma})$$

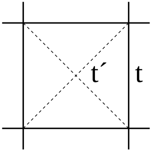
$$D_i = n_{i,\uparrow} n_{i,\downarrow} \quad H_i = (1 - n_{i,\uparrow})(1 - n_{i,\downarrow})$$



- The determinant part of the wave function includes correlations
- Backflow correlations can modify the nodes of the variational wave function
- Jastrow factor can change only amplitudes

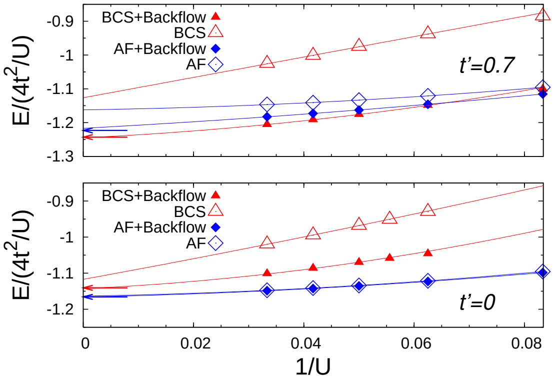






- Important backflow parameters up to the range of the Hamiltonian
- Irrelevant backflow parameters for longer distances
- Backflow parameters are particularly important in the insulating phase

Backflow correlations make it possible to reach the fully-projected state



In the frustrated regime, backflow terms are useful also in the AF wave function

$$H_{\rm kin} = -\sum_{\langle i,j\rangle,\sigma} \sum_{\alpha,\beta} t_{i,j}^{\alpha,\beta} c^\dagger_{i,\alpha,\sigma} c_{j,\beta,\sigma} + h.c.$$

$$H_{\rm int} = U \sum_{i} \sum_{\alpha} n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow} + U' \sum_{i} \sum_{\alpha<\beta} n_{i,\alpha} n_{i,\beta}$$

$$H_{\rm Hund} = -J \sum_{i,\sigma,\sigma'} \sum_{\alpha<\beta} c^\dagger_{i,\alpha,\sigma} c_{i,\alpha,\sigma'} c^\dagger_{i,\beta,\sigma'} c_{i,\beta,\sigma} - J' \sum_{i} \sum_{\alpha<\beta} c^\dagger_{i,\alpha,\uparrow} c^\dagger_{i,\alpha,\downarrow} c_{i,\beta,\uparrow} c_{i,\beta,\downarrow} + h.c.$$

$$|\Psi\rangle = \mathcal{J}_c |\mathcal{D}\rangle$$

- Orbital-dependednt Jastrow factor:

$$\mathcal{J}_c = \exp\left(-\frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} v_{i,j}^{\alpha,\beta} n_{i,\alpha} n_{j,\beta} \right)$$

(Similar for the spin Jastrow factor)

Towards the exact ground state

How can we improve the variational state?
By the application of a few Lanczos steps!

$$|\Psi_{p-LS}\rangle = \left(1 + \sum_{m=1,\ldots,p} \alpha_m \mathcal{H}^m\right) |\Psi\rangle$$

- For $p \to \infty$, $|\Psi_{p-LS}\rangle$ converges to the exact ground state, provided $\langle \Psi_0 | \Psi \rangle \neq 0$
- On large systems, only a FEW Lanczos steps are affordable:

  $\langle x | \mathcal{H}^m | \Psi \rangle$ (with $m = 1, \ldots, p$) must be computed for a given $|x\rangle$

  We can do up to $p = 2$

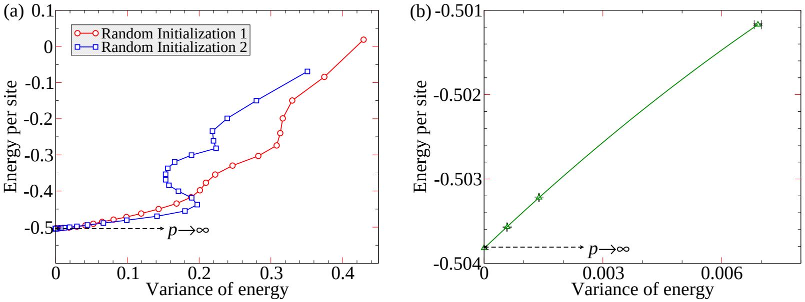
- A zero-variance extrapolation can be done

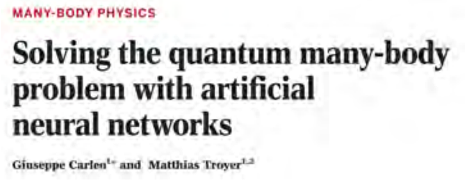
Whenever $|\Psi\rangle$ is sufficiently close to the ground state:

$$E \simeq E_0 + \text{const} \times \sigma^2$$

$$E = \langle \mathcal{H} \rangle / N$$
$$\sigma^2 = (\langle \mathcal{H}^2 \rangle - E^2)/N$$

How does it work?





MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

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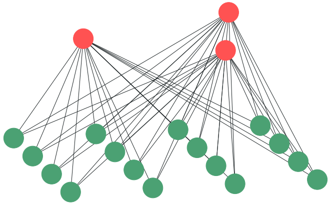

$$|\Psi_{\rm RBM}\rangle = \sum_{h_a=\pm 1} \exp\left[\sum_{i,a} W_{i,a} S_i^z h_a + \sum_a b_a h_a\right] |\Phi_{\rm cl}\rangle$$

$$|\Psi_{\rm RBM}\rangle \propto \prod_a \exp\left\{\log\cosh\left[b_a + \sum_R W_{i,a} S_i^z\right]\right\} |\Phi_{\rm cl}\rangle$$

- Hidden spin variables $(h_1, \dots, h_\alpha)$
- Network parameters (b, W)
- Generalization of the Jastrow factor that includes many-body interactions