Variational Monte Carlo for strongly correlated electron systems

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- Variational Monte Carlo
- The Hubbard model
- Variational wave functions for magnetic and non-magnetic ground states
- Jastrow factors
- Backflow correlations

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Variational Monte Carlo

The variational principle $T = 0$

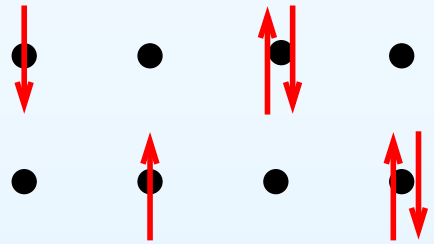
$$E = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{\text{gs}}$$

- $|\Psi\rangle$ is a variational many-body wave function depending on some variational parameters
- Tool to select the best approximation of the ground state: the best approximation gives the lowest expectation value of the energy
- We need a numerical approach to compute expectation values ($\frac{\langle \Psi | \hat{\mathcal{O}} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$) over many-body wave functions:
  Variational Monte Carlo

Variational Monte Carlo

$$E = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \sum_x E_x \bar{P}_x$$

- $E_x = \sum_{x'} \frac{\Psi(x')}{\Psi(x)} H_{x',x}$, the local-energy, depends only on the electronic configuration $|x\rangle$



- Electronic configurations are generated according to the equilibrium probability distribution $\bar{P}_x = \frac{|\Psi(x)|^2}{\sum_{x'} |\Psi(x')|^2}$, using the Metropolis algorithm

Metropolis algorithm

- Start from an initial configuration $|x_0\rangle$
- Choose a new trial configuration $|x_t\rangle$ by moving one particle to a new position
- Accept the new configuration with a probability

$$\mathcal{P}_{x_0 \to x_t} = \min \left[1, \left| \frac{\Psi(x_t)}{\Psi(x_0)} \right|^2 \right]$$

- Repeat this procedure generating a Markov chain (Every configuration $|x_n\rangle$ depends only on the previous $|x_{n-1}\rangle$)
- After a thermalization time M configurations $|x_{n>M}\rangle$ are independent from the initial one x_0 and distributed according to $\bar{P}_x$

Variational Monte Carlo

Monte Carlo samplings of the configurations $\{|x\rangle\}$ has to satisfy two conditions

- Does a stationary $\bar{P}_x$ exist?
- Detailed balance: The number of processes corresponding to the transition $|x\rangle \rightarrow |x'\rangle$ shall be compensated by the number of processes in the reverse sense $|x'\rangle \rightarrow |x\rangle$:

$$\bar{P}_x \mathcal{P}_{x \rightarrow x'} = \mathcal{P}_{x' \rightarrow x} \bar{P}_{x'}$$

$$P^{n+1}_{x_{n+1}} = \sum_{x_n} \mathcal{P}_{x_n \rightarrow x_{n+1}} P^n_{x_n} = \sum_{x_n} \mathcal{P}_{x_n \rightarrow x_{n+1}} \bar{P}_{x_n} = \bar{P}_{x_{n+1}} \sum_{x_n} \mathcal{P}_{x_{n+1} \rightarrow x_n} = \bar{P}_{x_{n+1}}$$

- Metropolis algorithm satisfies the detailed balance condition:

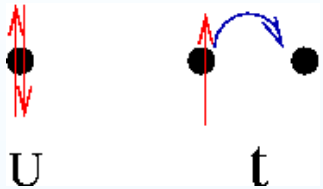
$$|\Psi(x)|^2 > |\Psi(x')|^2 \Rightarrow |\Psi(x)|^2 * |\Psi(x')|^2 / |\Psi(x)|^2 = 1 * |\Psi(x')|^2$$

Variational Monte Carlo

- Under which conditions an arbitrary initial probability distribution $P_x^0 = \delta_{x,x_0}$ will converge to $\bar{P}_x$?
- Ergodicity: Any configuration $|x'\rangle$ can be reached, in a sufficiently large number of steps, starting from any initial configuration $|x\rangle$.
  This implies that $\bar{P}_x$ is the unique equilibrium probability distribution.

The Hubbard model

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



General wave function for a correlated electron system

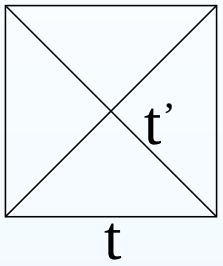
$$|\Psi\rangle = \mathcal{P}(\{v_i\})|D(\{\Delta_i\})\rangle$$

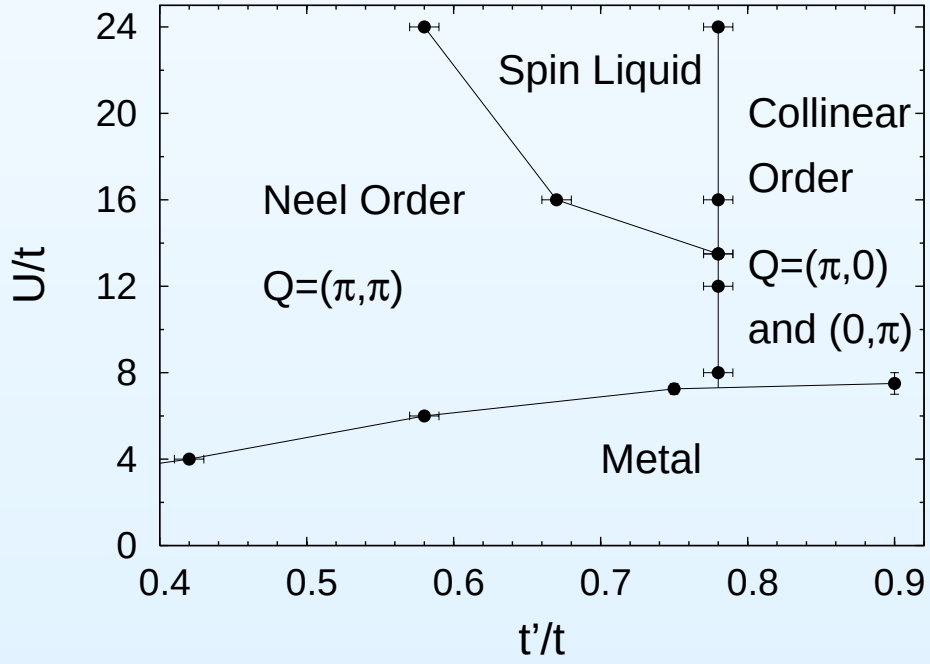
- $\mathcal{P}(\{v_i\})$ correlation factor
- $D(\{\Delta_i\})$ Mean-field Slater determinant
- $\{v_i\}$ and $\{\Delta_i\}$ are variational parameters to be optimized

Phase diagram on the square lattice

Hubbard model on the square lattice with next and nearest-next neighbour hopping

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

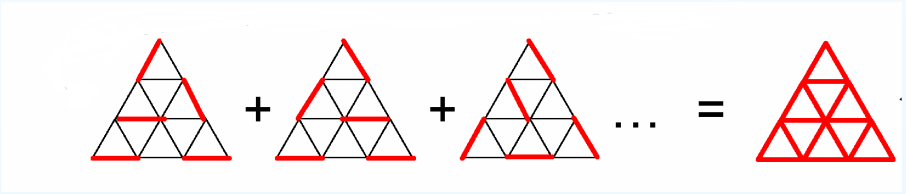




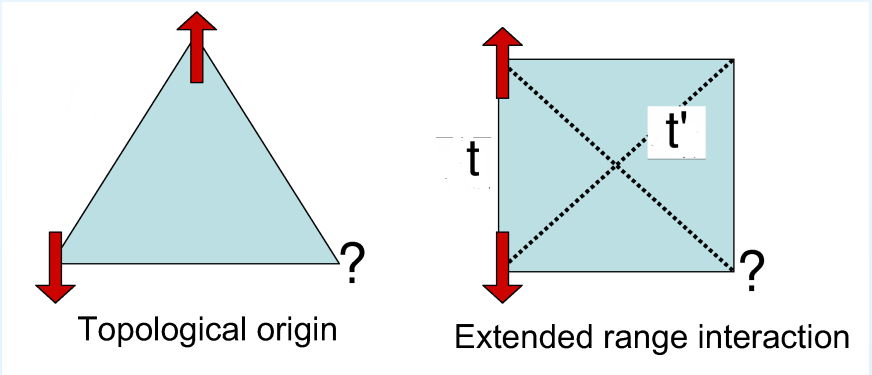
Spin liquid

Spin liquid state= Mott insulating paramagnetic state without any spontaneously broken symmetry at $T = 0$

Spin liquid described through a superposition of valence bond states (pattern of singlet pairs) RVB Anderson (1987)



Spin liquid states are favoured by frustrated interaction



Wave function for a magnetic state

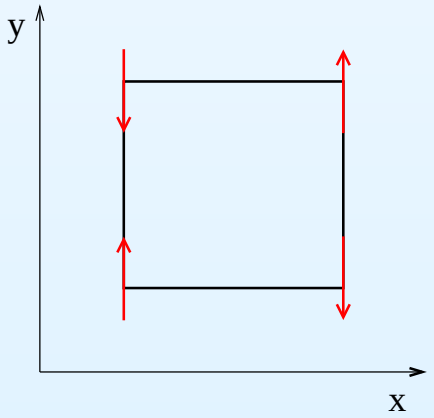
$$|\Psi_{\mathrm{AF}}\rangle = \mathcal{J}_{\int}\mathcal{G}|\mathrm{AF}\rangle$$

$$\mathcal{H}_{\mathrm{AF}} = \sum_{i,j,\sigma} \tilde{t}_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \Delta_{\mathrm{AF}} \sum_{i} \exp[i\boldsymbol{Q}\boldsymbol{R}_i](\boldsymbol{n}_i \boldsymbol{S}_i)$$

$$\mathcal{J}_{\int} = \exp\left[-\frac{1}{2}\sum_{i,j} u_{i,j} S^z_i S^z_j\right]$$

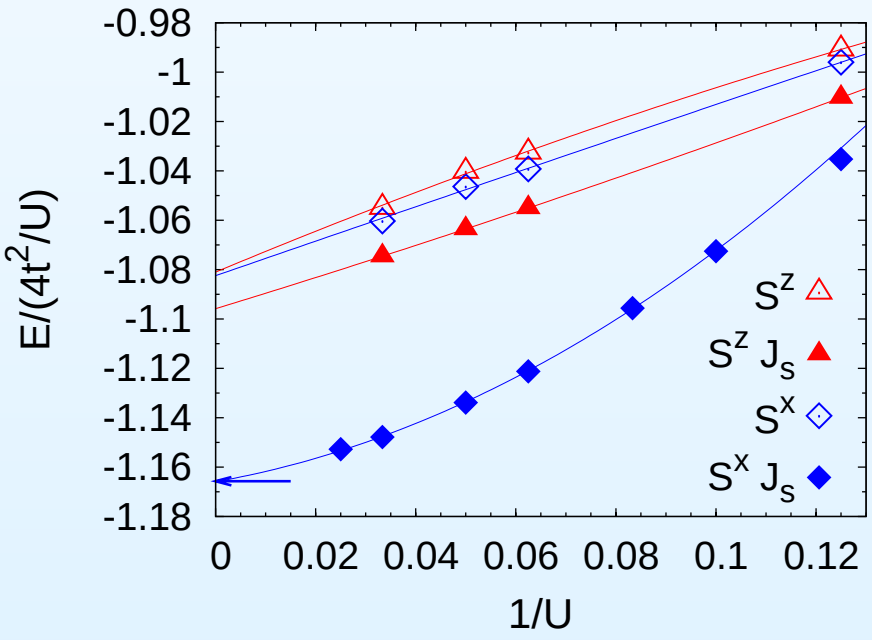
$$\mathcal{G} = \mathrm{e}^{-g\sum_i n_{i,\uparrow} n_{i,\downarrow}}$$

- $\mathcal{G}$ On-site Coulomb repulsion
- $\mathcal{J}_{\int}$ Spin-Jastrow factor Fluctuations orthogonal to the ordering plane (like spin waves)



Wave function for a magnetic state

- A spin-Jastrow factor orthogonal to the ordering plane allows to reproduce the correct spin-spin correlations at large distance Franjic and Sorella Prog.Theor.Phys. 97, 399 (1997)
- A spin-Jastrow factor orthogonal to the ordering plane correctly describes the strong-interacting limit of the Hubbard model (comparison with a spin-Jastrow factor parallel to the ordering plane)



Wave function without magnetism

Charge-Jastrow factor over the ground state of a BCS Hamiltonian

Appropriate for both a metallic state with superconducting fluctuations and an insulator without magnetic order (spin liquid)

$$|\Psi_{\text{BCS}}\rangle = \mathcal{J}|\text{BCS}\rangle$$

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

$$\mathcal{H}_{\text{BCS}} = \sum_{i,j,\sigma} \tilde{t}_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma} + \sum_{i,j} \Delta_{ij} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + \text{H.c.}$$

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

$n_i = 0, 1, 2$

Jastrow factor in real space

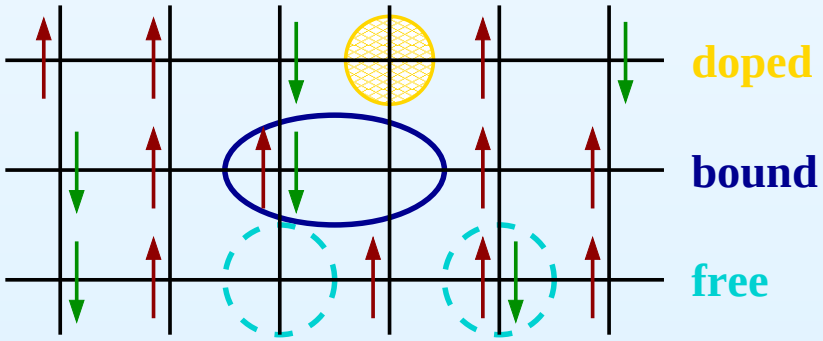
$$\mathcal{J} = \exp[-\tfrac{1}{2}\sum_{i,j} v_{ij} n_i n_j] \; ; v_{ij} > 0$$

The long-range Jastrow J correlates empty and doubly occupied sites, inducing a Metal-Insulator Transition at a finite U/t

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

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

- $D_i D_j + H_i H_j$ repulsion between doublons and between holons
- $-H_i D_j - D_i H_j$ attraction between holons and doublons

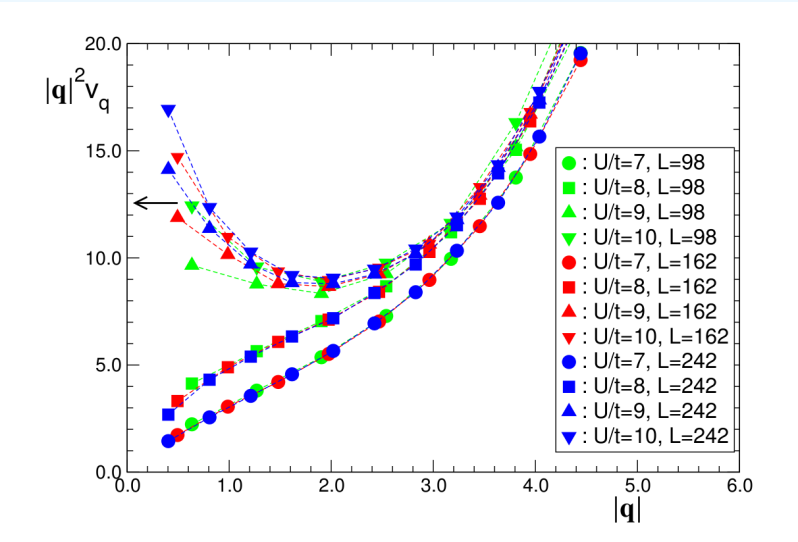


Jastrow factor in $q-$space

$$\mathcal{J} = \exp[-\tfrac{1}{2}\textstyle\sum_{q\neq 0} v_q n_q n_{-q}]$$

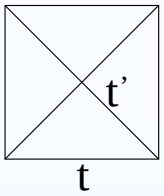
$$V_q \propto \begin{cases} 1/q & : \text{ metal} \\ 1/q^2 & : \text{ insulator (1D)} \\ \log(q)/q^2 & : \text{ insulator (2D)} \end{cases}$$

Metal-insulator transition with a $J|\text{BCS}\rangle$ wave function on a 2D square lattice Capello *et al.* PRB 73, 245116 (2006)

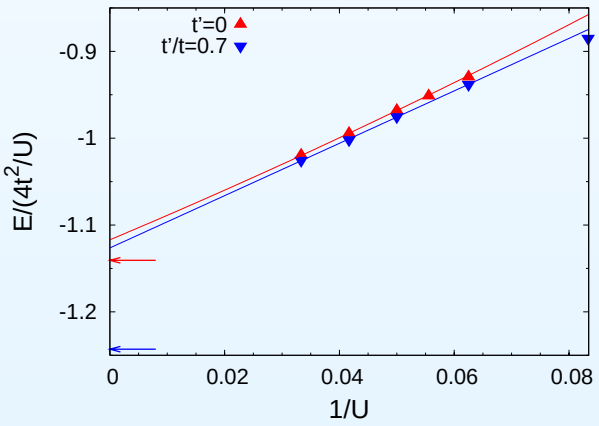


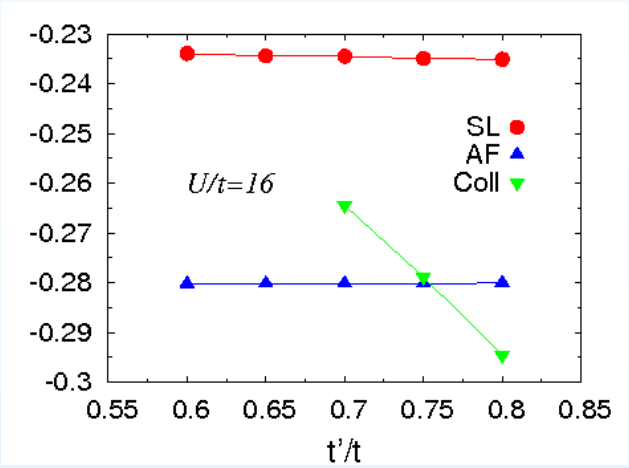
Jastrow factor

The $\mathcal{J}|\mathrm{BCS}\rangle$ wave function can be poorly accurate in the insulating phase



- Bad description of the strongly interacting limit of the Hubbard model
- Poor accuracy with respect to the magnetic wave functions





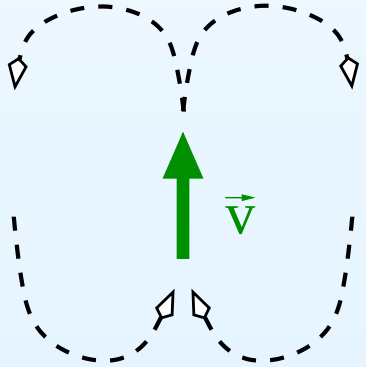
- We need to include correlation in the determinant $|\mathrm{BCS}\rangle$
- A large Δ_{AF} satisfies the single-occupancy constraint

Backflow correlations

- Proposed by Feynman and Cohen to describe a roton excitation in liquid ^{4}He
  PR 102, 1189 (1956)
- Fictitious coordinates of the particles, $\boldsymbol{r}_\alpha^b$

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

- Creates a return flow of current, opposite to the motion of the excitation



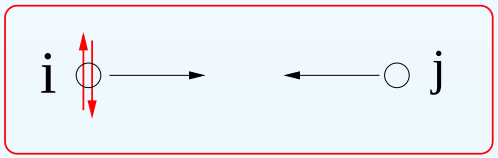
- Applied to electron jellium and metallic hydrogen by Ceperley and coworkers
  PRB 48, 12037 (1993), PRB 58, 6800 (1998), PRE 68, 046707 (2003)

Backflow correlations in the Hubbard model

Correlation between empty sites and doubly occupied sites *inside* the mean-field variational wave function $|\mathrm{BCS}\rangle$ and $|\mathrm{AF}\rangle$

$$\boldsymbol{r}^b_{i,\sigma} = \epsilon \boldsymbol{r}_{i,\sigma} + \eta \sum_j t_{ij} D_i H_j (\boldsymbol{r}_{j,\sigma} - \boldsymbol{r}_{i,\sigma})$$

$$D_i = n_{i,\uparrow} n_{i,\downarrow} \qquad H_j = (1-n_{j,\uparrow})(1-n_{j,\downarrow})$$



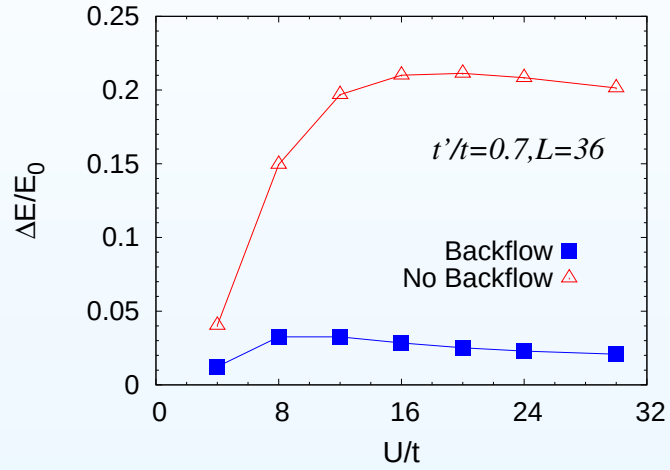
On a lattice electronic positions are limited to lattice sites: an alternative definition, based on single-particle orbitals, is implemented

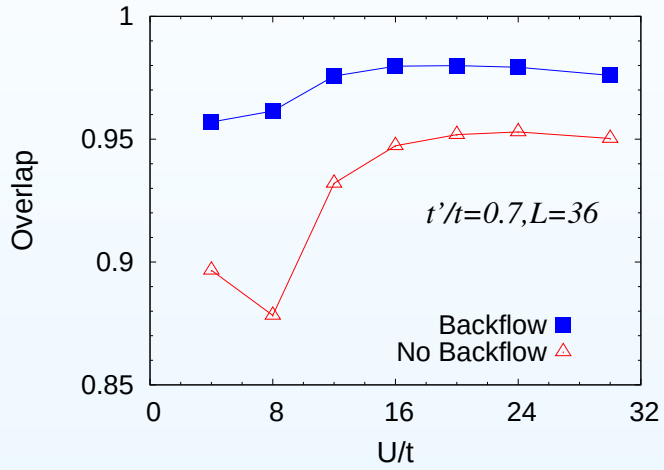
Tocchio *et al.* PRB 78, 041101(R) (2008)

$$\phi^b_k(\boldsymbol{r}_{i,\sigma}) = \epsilon \phi_k(\boldsymbol{r}_{i,\sigma}) + \eta \sum_j t_{ij} D_i H_j \phi_k(\boldsymbol{r}_{j,\sigma})$$

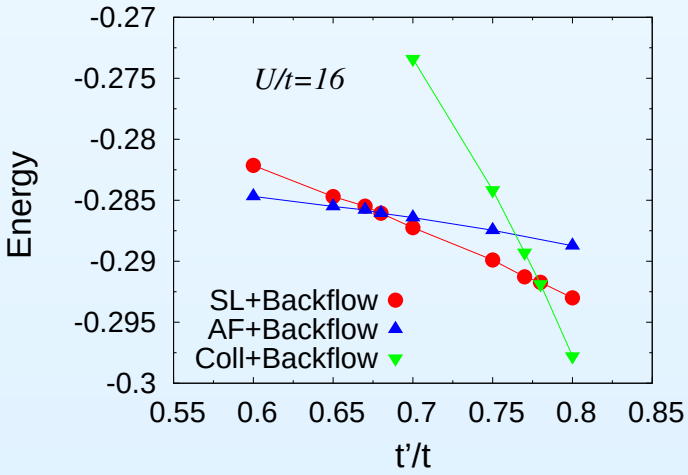
Are backflow correlations important?

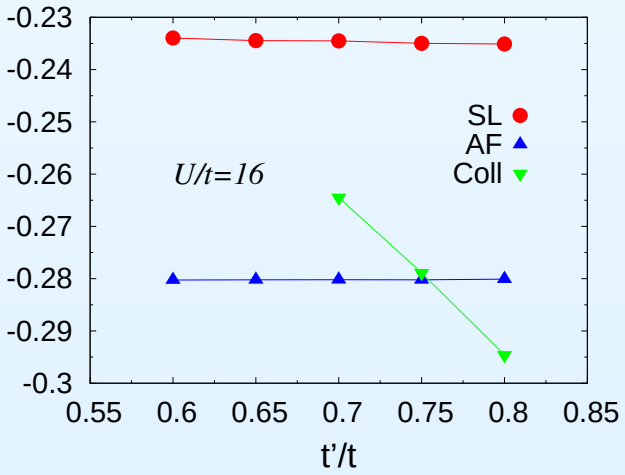
Comparison with exact diagonalization





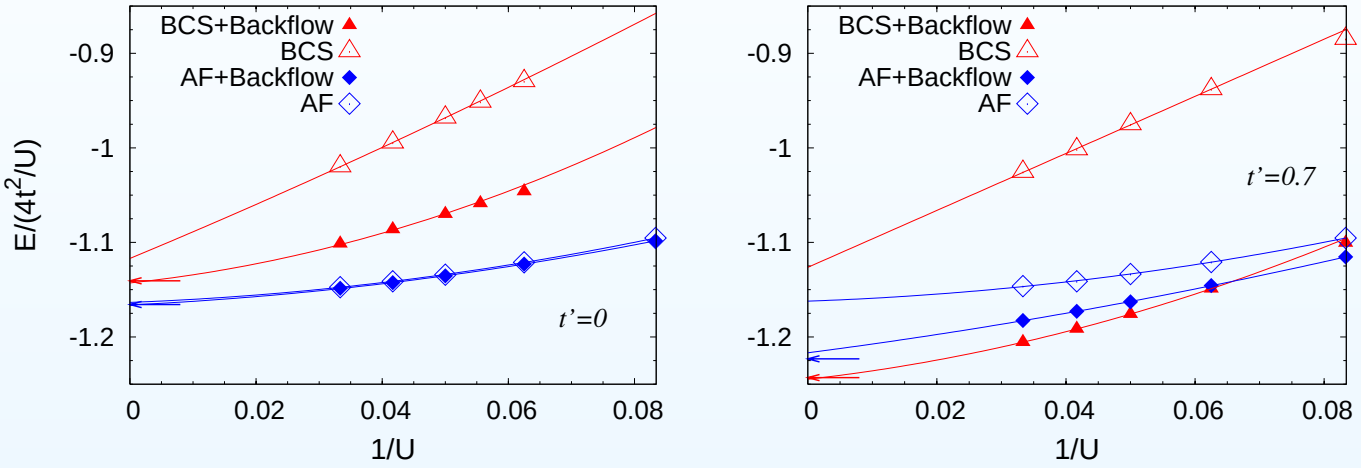
Spin-liquid wave function competitive with the magnetic ones





Are backflow correlations important?

Proper description of the strongly-interacting limit



Tocchio *et al.* PRB 78, 041101(R) (2008)

Becca *et al.* J.Phys.Conf.Ser. 145, 012016 (2009)

Conclusions

- Variational Monte Carlo to study ground-state properties of correlated Hamiltonians
- $\exp[-\frac{1}{2}\sum_{i,j} u_{i,j} S_i^z S_j^z]|\mathrm{AF}\rangle$ to describe a magnetic ground state
- $\exp[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j]|\mathrm{BCS}\rangle$ to describe a non-magnetic ground state
- Charge-Jastrow factor: Metal-Insulator Transition at a finite U/t
- Backflow correlations: How to correlate a non-magnetic wave function; a spin-liquid state can be stabilized in presence of frustration