# Variational ground states for correlated electron systems: from conducting polymers to high-temperature superconductors

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# Outline

1 Polyacetylene: Dimerization and metal-insulator transition

2 Toy model: Improved variational wave functions

3 Layered cuprates: 2D Hubbard model

Collaborators:

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Main publications on this topic:

D. B. and K. Maki, Phys. Rev. B **31**, 6633 (1985).

D. B., Solid St. Sciences **69**, 183 (1987).

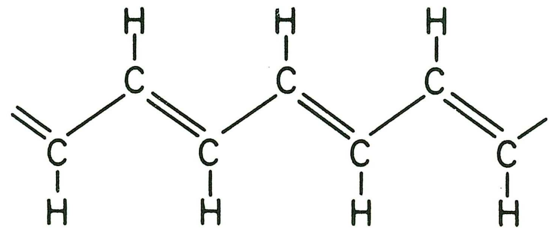
E. Jeckelmann and D. B., Synth. Met. **65**, 211 (1994).

M. Dzierzawa, D. B. and M. Di Stasio, Phys. Rev. B **51**, 1993(R) (1995).

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

# 1 Polyacetylene: Dimerization and metal-insulator transition

## Polyacetylene



## Peierls-Hubbard model

$$\hat{H} = -\sum_{i\sigma} t_{i,i+1}(c^\dagger_{i\sigma} c_{i+1\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$t_{i,i+1} = t_0 + \alpha(u_i - u_{i+1})$$

$$E(\{u_i\}) = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{K}{2}\sum_i u_i^2$$

## Gutzwiller ansatz

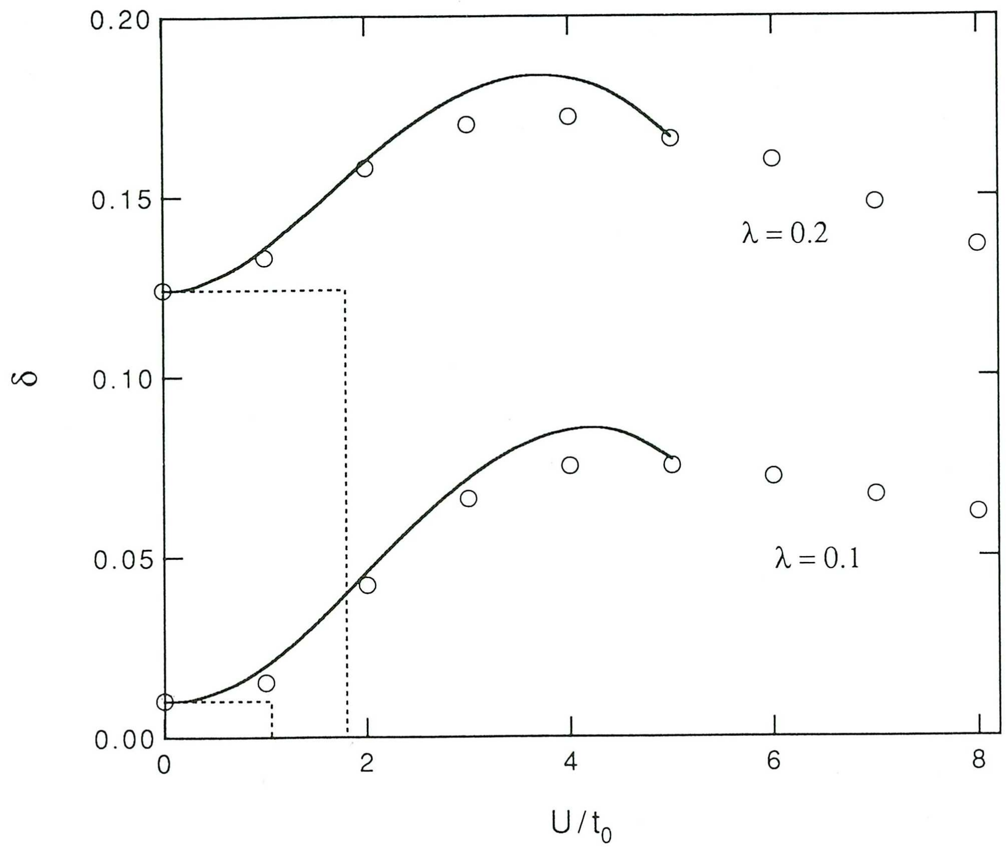
$$|\Psi\rangle = e^{-g\hat{D}}|\mathrm{BOW}\rangle\,,$$

where $\hat{D}$ is the number of doubly occupied sites,

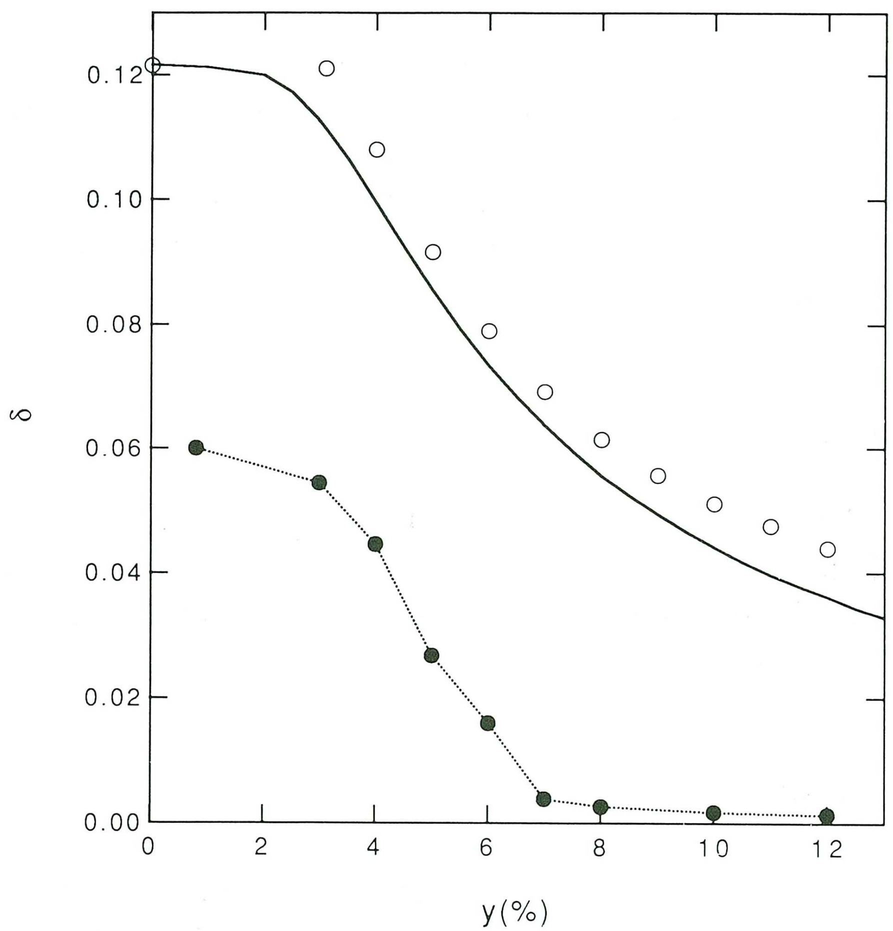
$$\hat{D} = \sum_i n_{i\uparrow}n_{i\downarrow}\,,$$

and $|\mathrm{BOW}\rangle$ stands for a bond-order-wave.

# $U$ increases dimerization, initially



# $U$ induces a metal-insulator transition upon doping



# 2 Toy model: Improved variational wave functions

# Inverting Gutzwiller

$$|\Psi_G\rangle = e^{-g\hat{D}}|\Psi_0\rangle$$

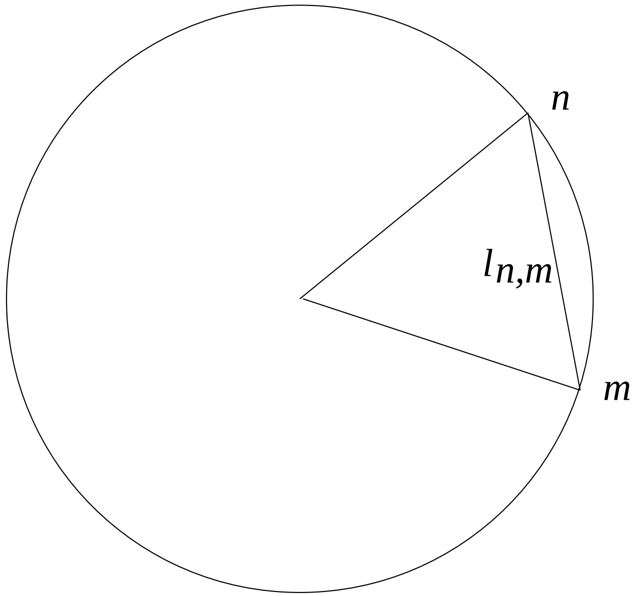
$$|\Psi_B\rangle = e^{-h\hat{T}}|\Psi_\infty\rangle\,,$$

where $\hat{T}$ is the hopping term in $\hat{H} = -t\hat{T} + U\hat{D}$.

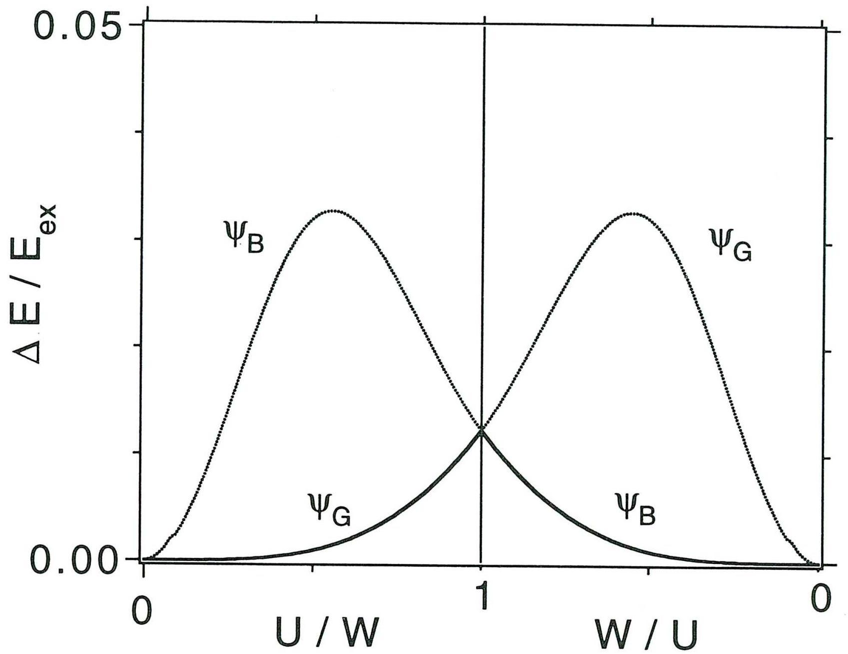
# Toy model: the $1/r$ Hubbard chain

$$\hat{T} = \sum_{\substack{n,m,\sigma \\ m \neq n}} \eta_{n,m} c^{\dagger}_{n\sigma} c_{m\sigma}$$

$$\eta_{n,m} = -i(-1)^{n-m}/\ell_{n,m}$$

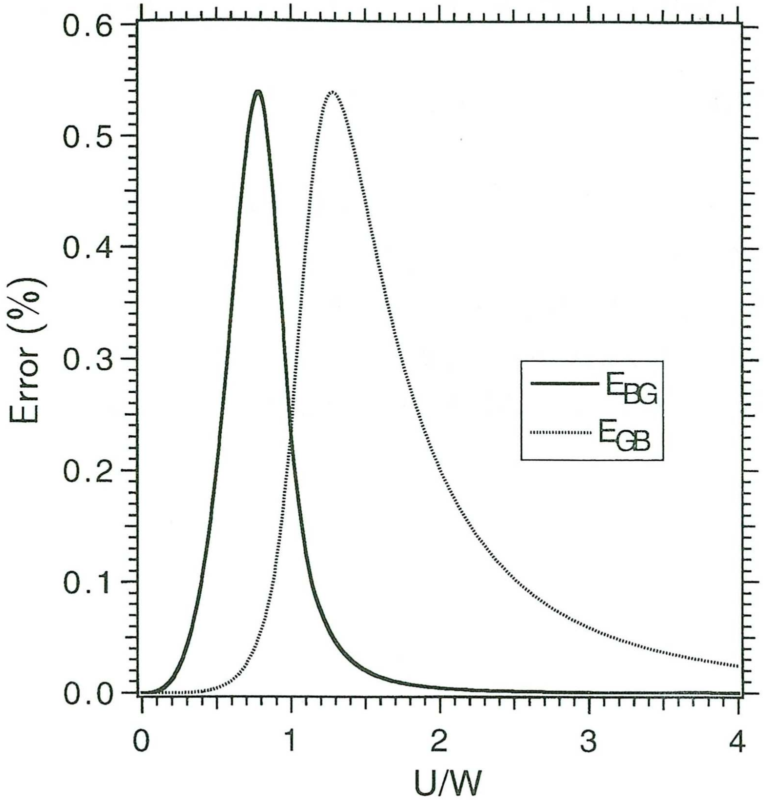


# Mott transition at half filling ($W = 2\pi t$)



# Refined variational wave functions

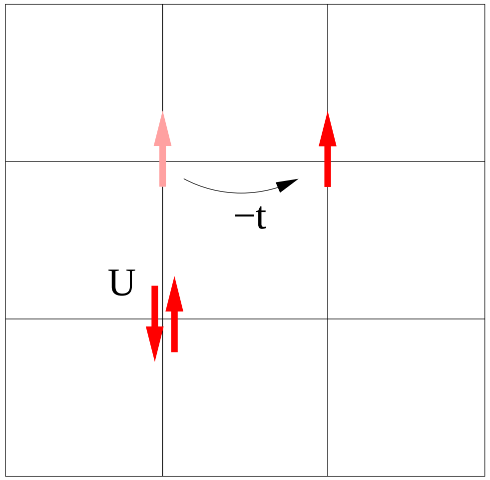
$$|\Psi_{GB}\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |\Psi_0\rangle, \qquad |\Psi_{BG}\rangle = e^{-g\hat{D}} e^{-h\hat{T}} |\Psi_\infty\rangle$$



# 3 Layered cuprates: 2D Hubbard model

## Hubbard Hamiltonian on a square lattice:

$$\hat{H} = -t\hat{T} + U\hat{D}$$




Hopping term: $\hat{T} = \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma})$

Number of doubly occupied sites: $\hat{D} = \sum_i n_{i\uparrow} n_{i\downarrow}, \;\; n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$

- Hubbard-Stratonovich transformation to decouple the exponent:

$$
\begin{aligned}
e^{-g\hat{D}} &= e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}} \\
&= \frac{1}{2}Tr_{\{\tau_i\}}e^{[\sum_i 2a\tau_i(n_{i\uparrow}-n_{i\downarrow})]-\frac{1}{2}g\hat{N}}, \qquad a = \arctan\sqrt{\tanh\frac{g}{4}}
\end{aligned}
$$

$\rightarrow$ Introduction of “Ising spins” $\tau_i \in \{1,-1\}$

- Bogoliubov transformation

$$
|\Psi_0\rangle = \prod_{\vec{k}} \alpha^\dagger_{\vec{k}\uparrow}\alpha^\dagger_{\vec{k'}\downarrow}|0\rangle, \qquad \vec{k'} = \pm\vec{k}
$$

$\longrightarrow$ **Integration over fermionic degrees of freedom**

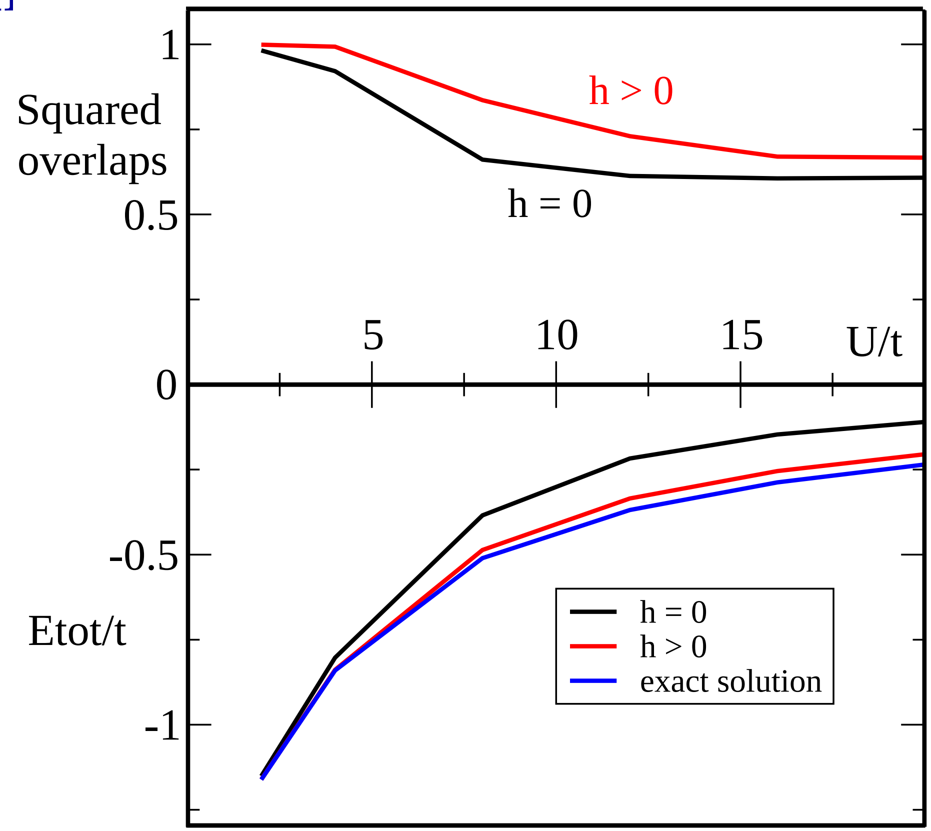
- The trace over 2N Ising spins is performed by a Monte Carlo simulation:

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = Tr_{\{\tau_i\}}\Big[P(\{\tau_i\})E(\{\tau_i\})\Big]$$

where $P(\{\tau_i\})$ is the probability of a particular Ising spin configuration and $E(\{\tau_i\})$ the corresponding energy.

## Comparison with exact diagonalization

$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |FS\rangle$$

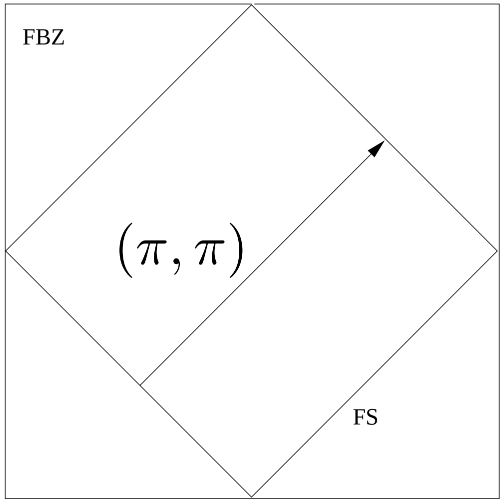



- 10 electrons on 10 sites[a]
- Substantial improvement!

[a] H. Otsuka, J. Phys. Soc. Jpn. **61**, 1645 (1992)

# $n = 1$: antiferromagnetism

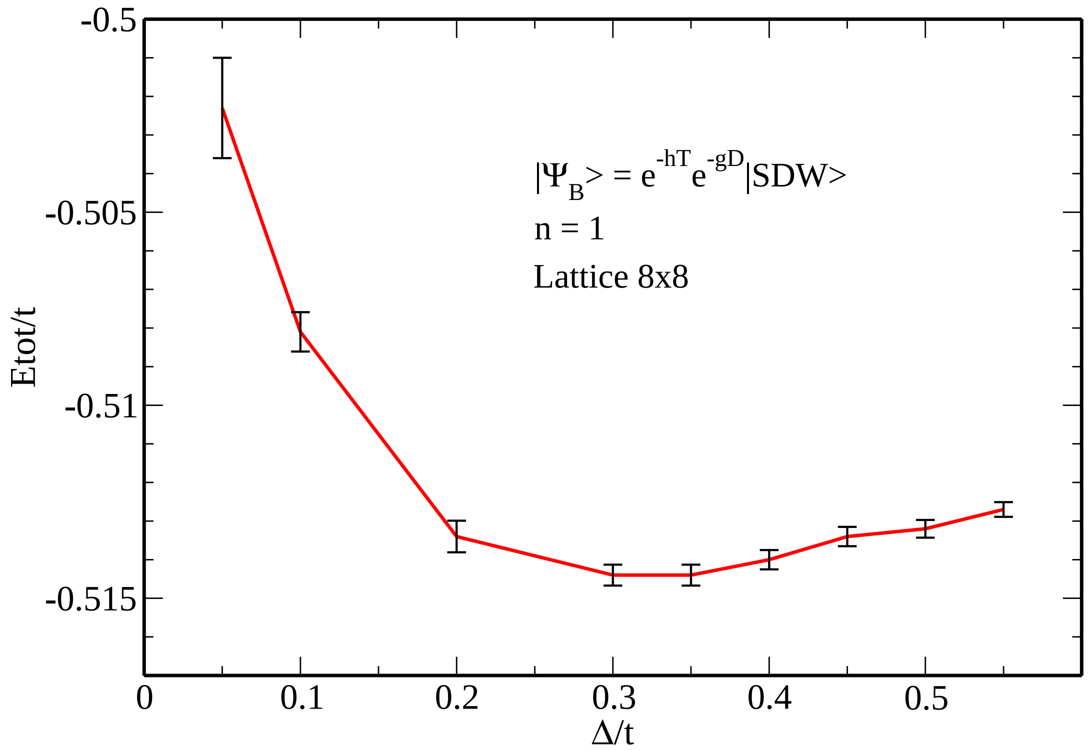
$n = 1$




Variational state:

$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} \underbrace{|SDW\rangle}_{\Delta}$$

where $|SDW\rangle$ is the ground state of the antiferromagnetic mean field Hamiltonian.



$n = 1$

Variational state: $|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |SDW\rangle$

Staggered magnetization: $M = \frac{1}{N} \sum_i (-1)^i \langle n_{i\uparrow} - n_{i\downarrow} \rangle$

| | g | h | $\Delta_{AF}$ | $M$ | E/t |
|---|---|---|---|---|---|
| VMC | 0 | 0 | 3.6(1) | 0.89(1) | -0.466(1) |
| VMC[a] | 0.69 | 0 | 1.3 | 0.86(1) | -0.493(3) |
| VMC | 3.1(1) | 0.101(3) | 0.32(2) | 0.77(1) | -0.514(1) |

2D Hubbard model: $0.42(1) < M < 0.614(1)$ $\longrightarrow$ Spin fluctuations not fully included

[a] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 3582 (1987)

# $n < 1$: $d$-wave superconductivity

## Why $d$-wave?

$$U\langle\hat{D}\rangle = U\sum_i \langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}\rangle \ .$$

$$\text{BCS:} \qquad \langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}\rangle = \langle c^\dagger_{i\uparrow} c_{i\uparrow}\rangle\langle c^\dagger_{i\downarrow} c_{i\downarrow}\rangle + |\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}\rangle|^2.$$

No instability for $U > 0$!

But indifference if $\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}\rangle = 0$, *i.e.* if $\sum_{\mathbf{k}} \Delta(\mathbf{k}) = 0$.
This is the case for $|\Psi\rangle = |d\mathrm{BCS}\rangle$.

If there is superconductivity in the repulsive Hubbard model, this is a true correlation effect (and therefore there is no simple explanation of the "mechanism").

$n < 1$:

## Some previous variational wave functions

*Hubbard model*: Gutzwiller ansatz[a]; Gutzwiller ansatz with additional correlations between empty and doubly occupied sites [b].

*t-J model*: Fully projected Gutzwiller wave function [cd]; Gutzwiller with additional hole-hole correlators[e].

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[a] T. Giamarchi and C. Lhuillier, Phys. Rev. B **43**, 12943 (1991)
[b] H. Yokoyama *et al.*, J. Phys. Soc. Japan **73**, 1119 (2004)
[c] C. Gros, Phys. Rev. B **38**, 931 (1988)
[d] A. Paramekanti, M. Randeria and N. Trivedi, Phys. Rev. B **70**, 054504 (2004)
[e] S. Sorella *et al.*, Phys. Rev. Lett. **88**, 117002 (2002)

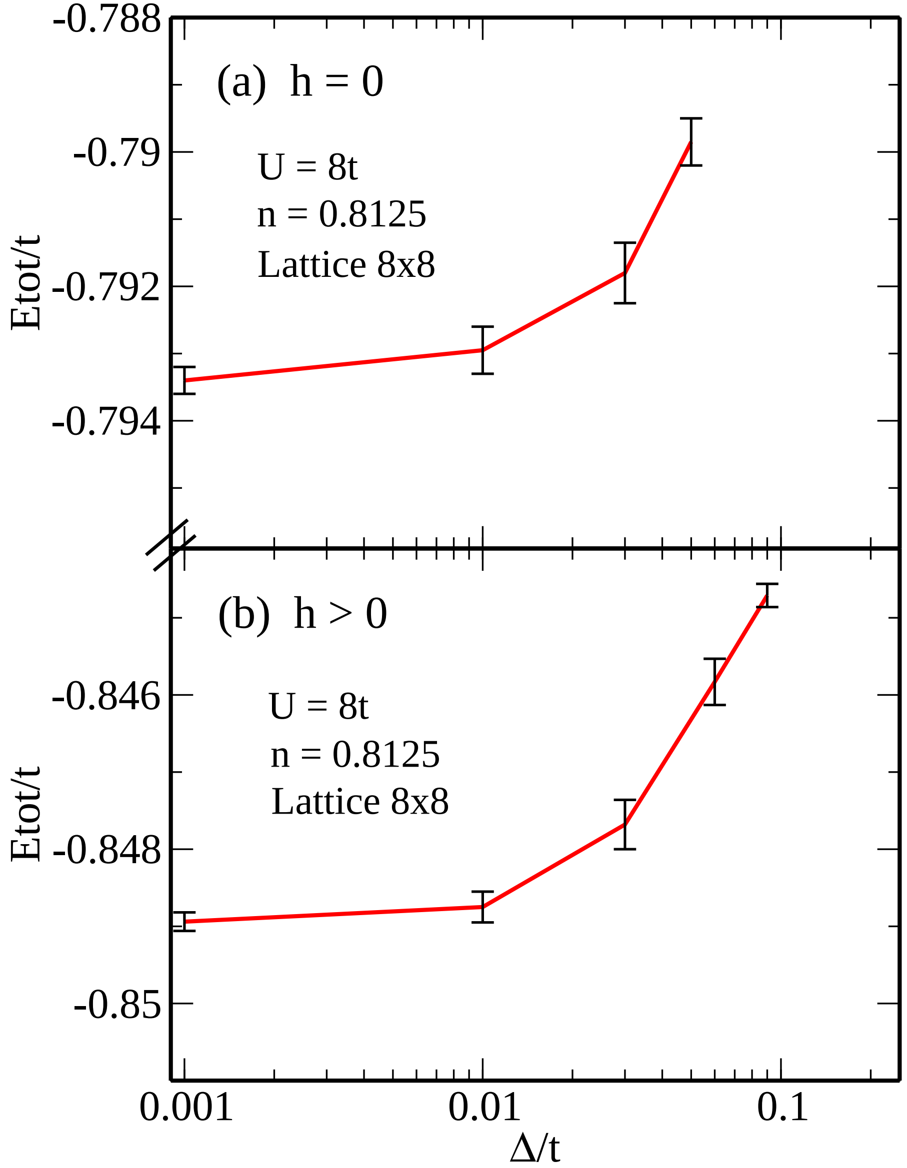
$n < 1$:

Refined variational wave function:

$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} \underbrace{|dBCS\rangle}_{\Delta,\mu}$$

- Additional variational parameter $\Delta$
- The "chemical potential" allows to fix the average density

$\rightarrow$ No pairing instability for a 8x8 system at $n = 0.8125$!



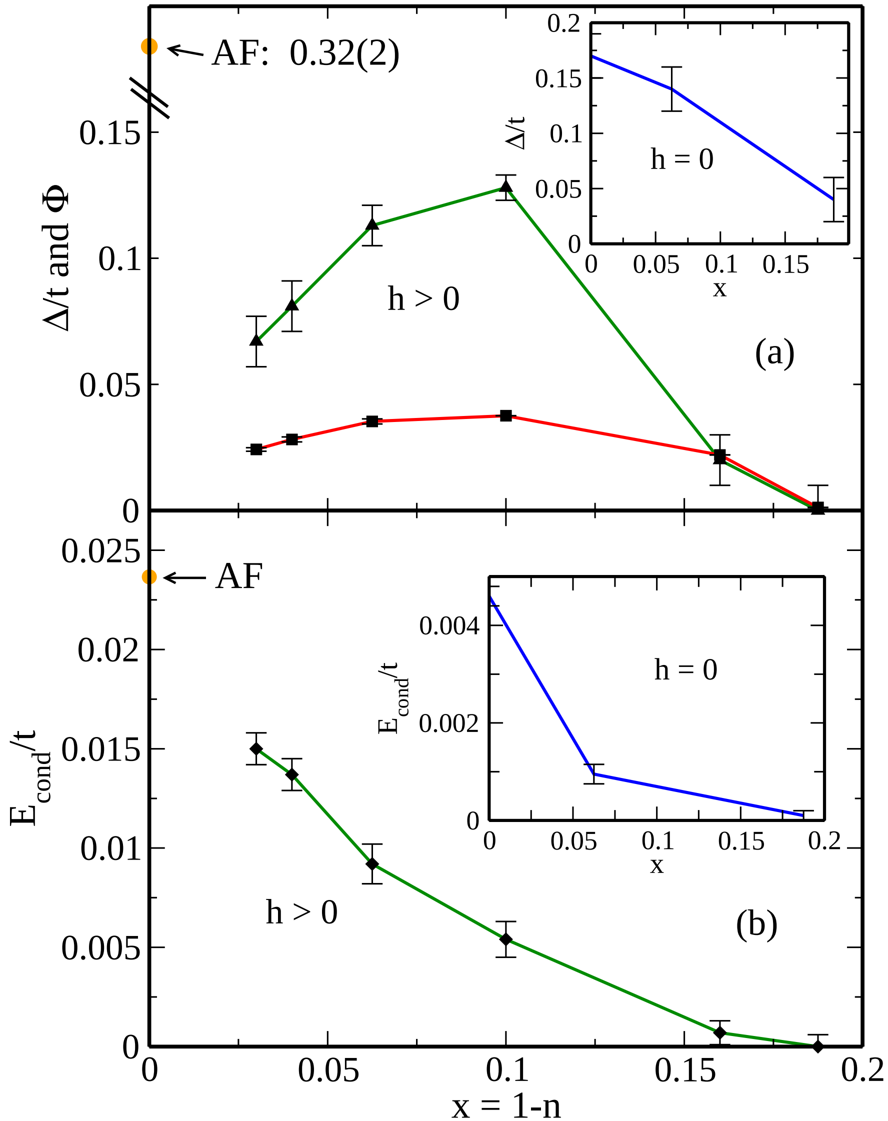
$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |dBCS\rangle$$

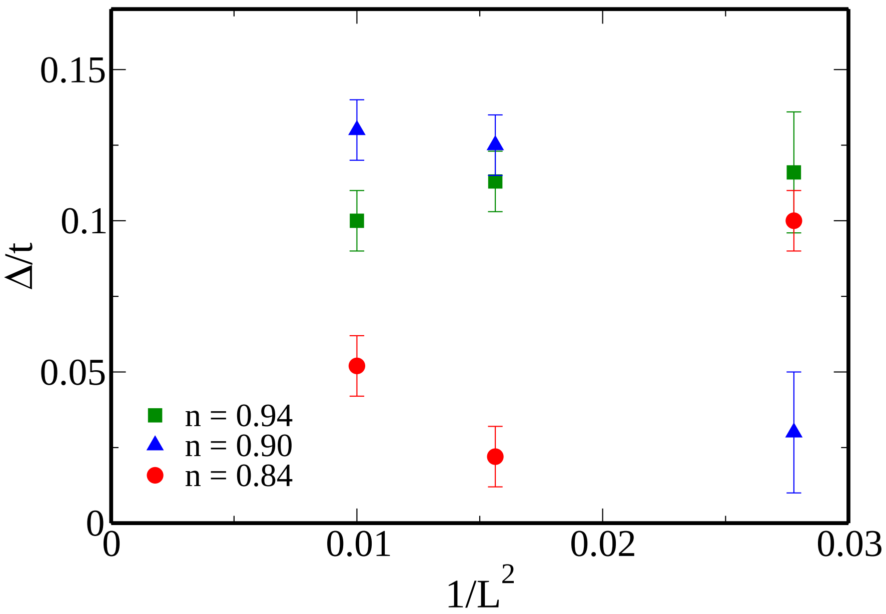
- Order parameter:

$$\Phi = \langle c^\dagger_{0\uparrow} c^\dagger_{1n\downarrow} \rangle$$

- Condensation energy:

$$E_{cond} = E_{tot}(0) - E_{tot}(\Delta)$$






Size dependence

- fixed set of configurations to reduce the computation time[a]

[a] C. J. Umrigar *et al.*, Phys. Rev. Lett. **60**, 1719 (1988)

$h = 0$: Gutzwiller wave function

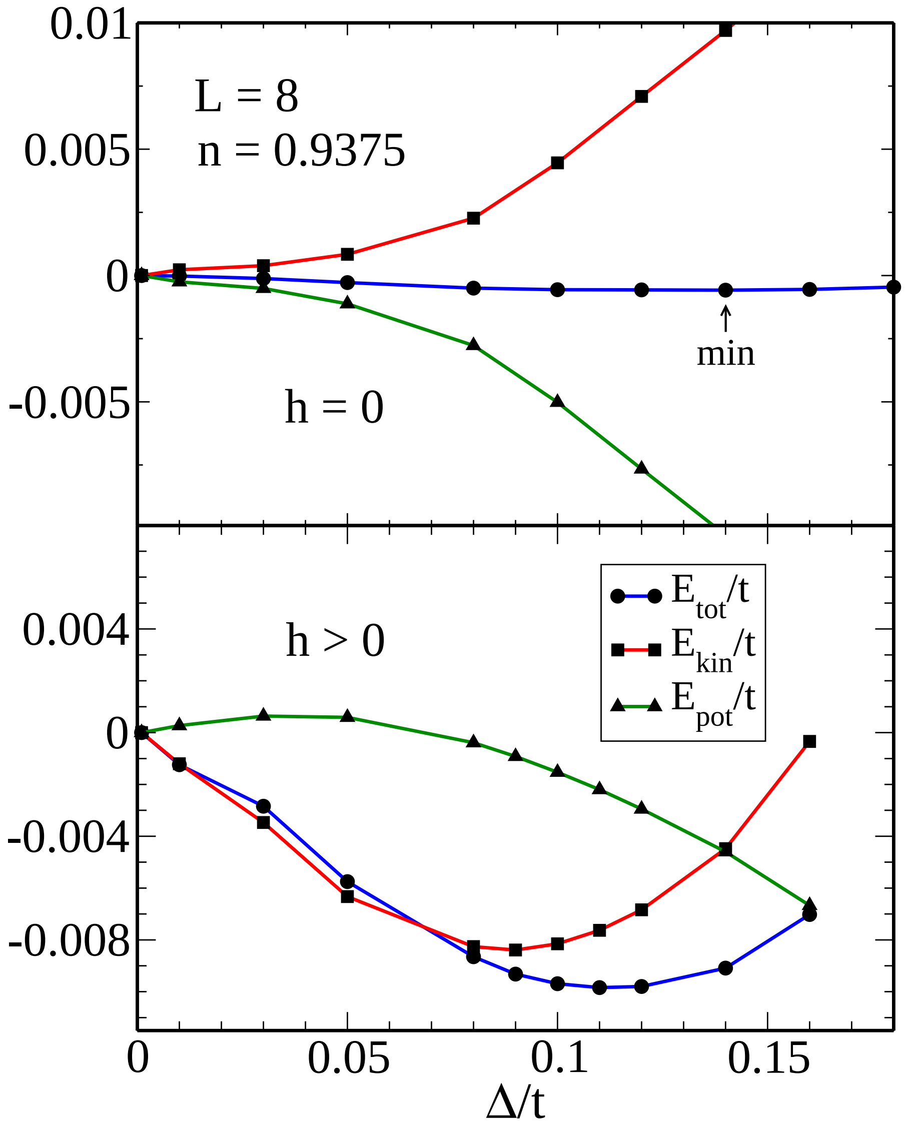
- Gain in the potential energy

$\longrightarrow$ BCS-like behaviour

$h \neq 0$

- strong gain in kinetic energy
- small gain in potential energy

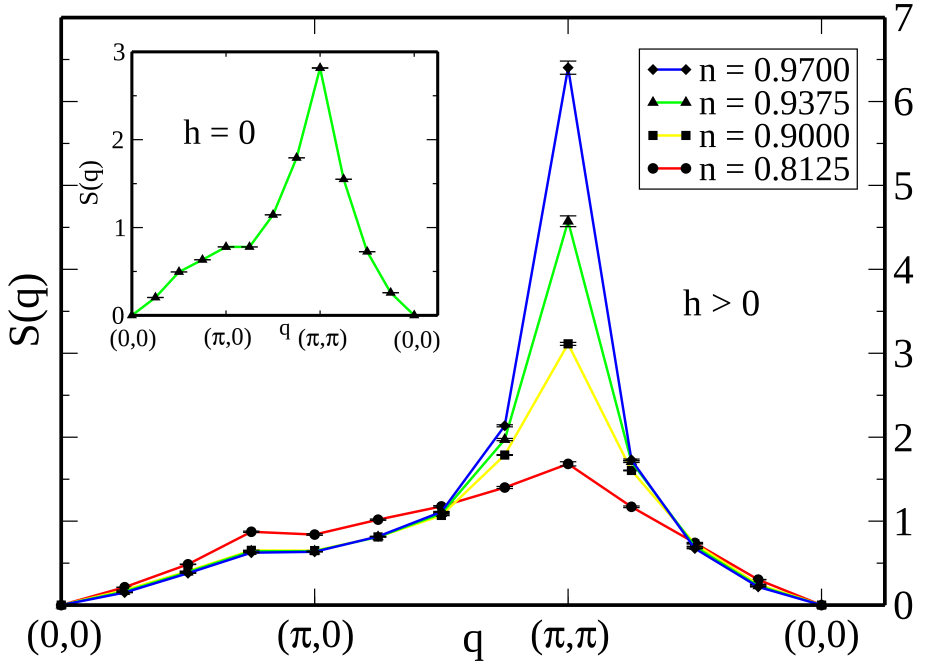
$\longrightarrow$ non-BCS behaviour!



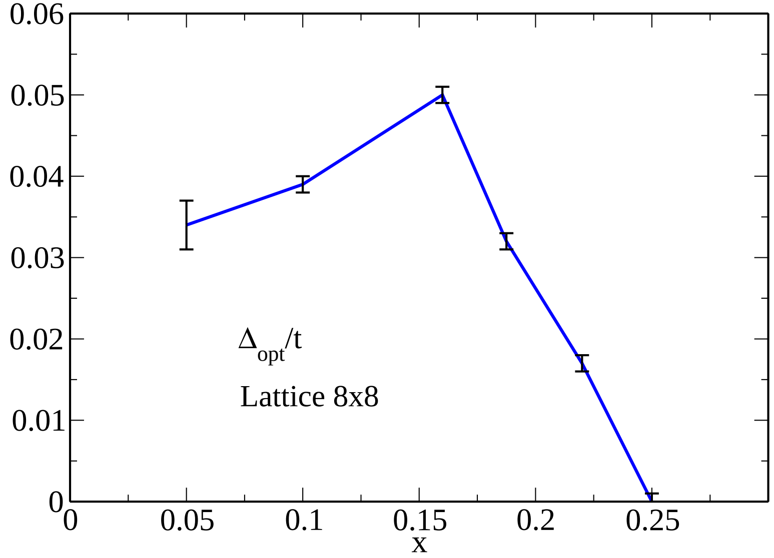
$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |dBCS\rangle$$

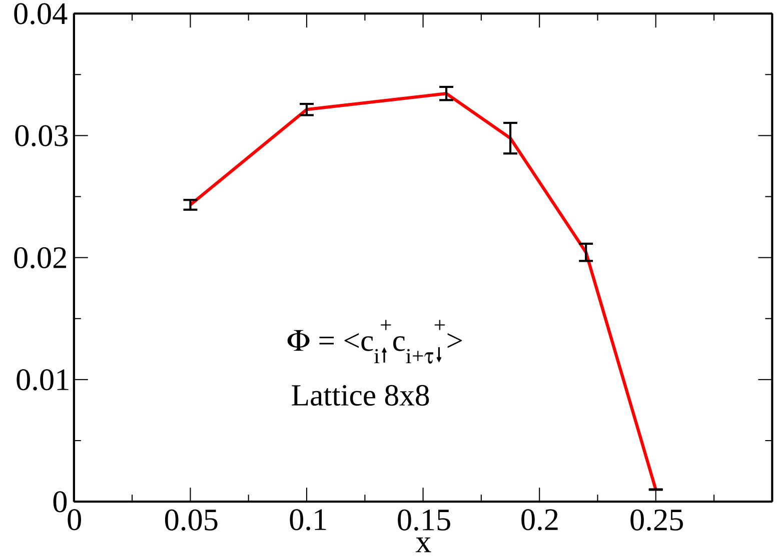
- Magnetic structure factor:

$$\begin{aligned} S(\mathbf{q}) &= \frac{1}{N} \sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R_i}-\mathbf{R_j})} \\ &\cdot \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle \end{aligned}$$



# Including next-nearest-neighbor hopping



# Comparison to layered cuprates

- Antiferromagnetism at half filling
- Superconducting dome
- $d$-wave pairing symmetry
- Right order of magnitude of the gap
- Condensation energy larger than determined from specific heat
- Kinetic energy driven (in agreement with some experiments)
- Persistent antiferromagnetic correlations in the superconducting phase

## Polyacetylene

- Peierls semiconductor
- Bond alternation
- Charged and neutral solitons
- Soliton lattice
- Metallic phase at large $x$
- $U$ quite important

## Layered cuprates

- Mott insulator
- Resonant valence bonds
- Holons and spinons
- Charge stripes
- Fermi liquid at large $x$
- $U$ essential