Metal-insulator transition with Gutzwiller-Jastrow wave functions

Odenwald, July 20, 2010

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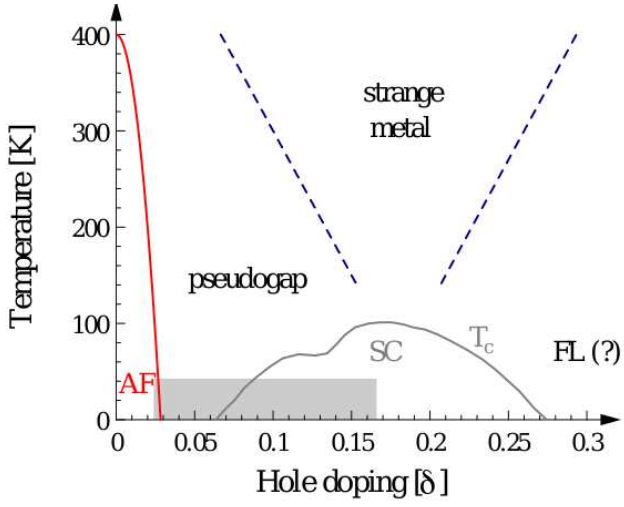
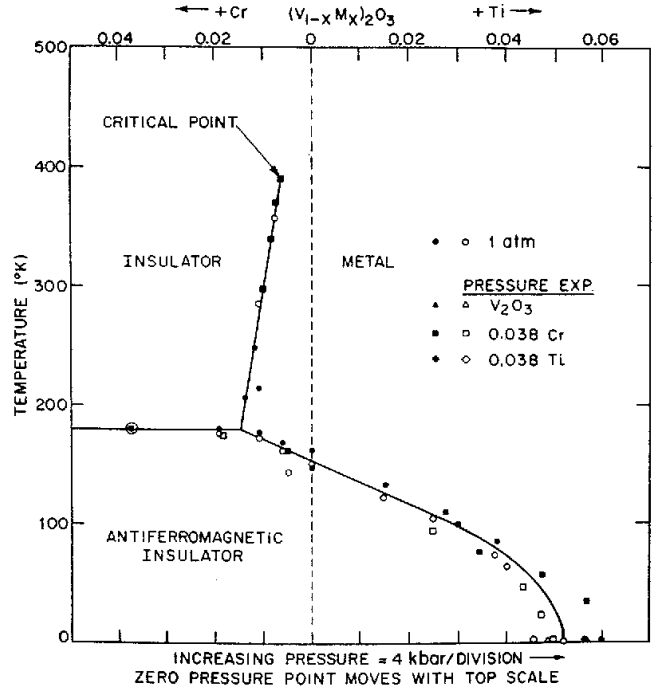
Outline

- Metal-insulator transition for strongly correlated materials
- Variational approach with
  - Gutzwiller-projected wave functions
  - Gutzwiller-projected + Jastrow-correlated wave functions

Strongly correlated Materials

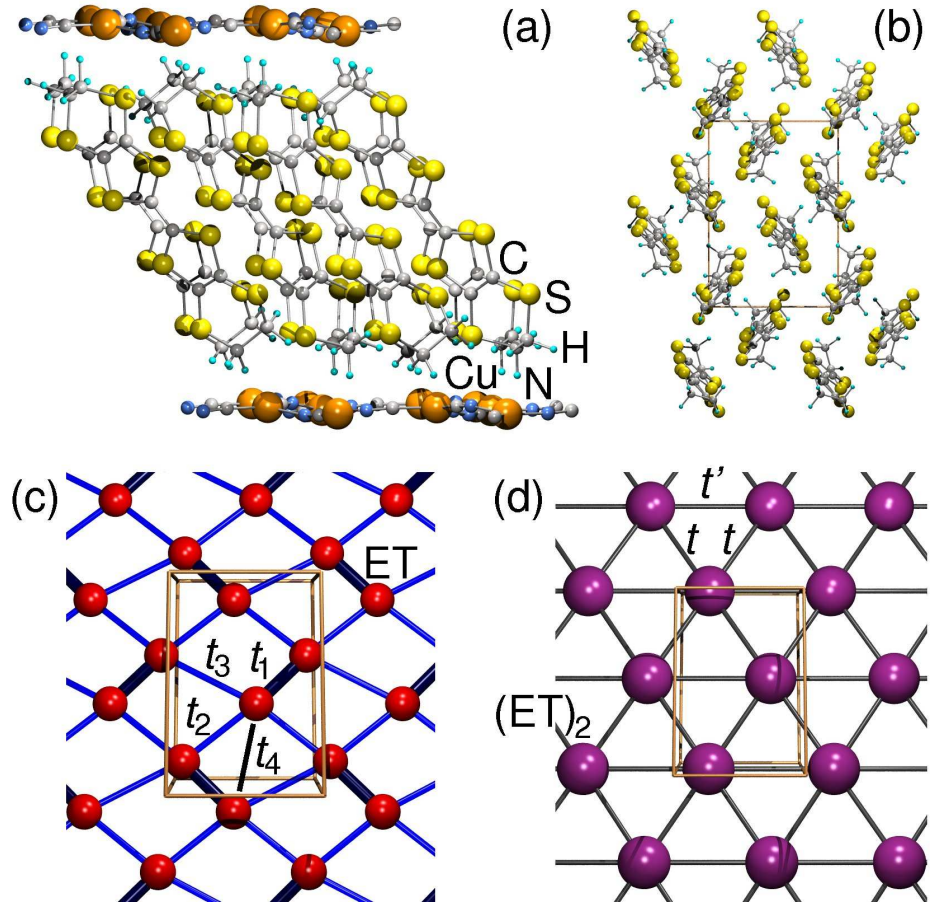


Phase Diagram of the Cuprates



Phase Diagram of $(V_{1-x}M_x)_2O_3$

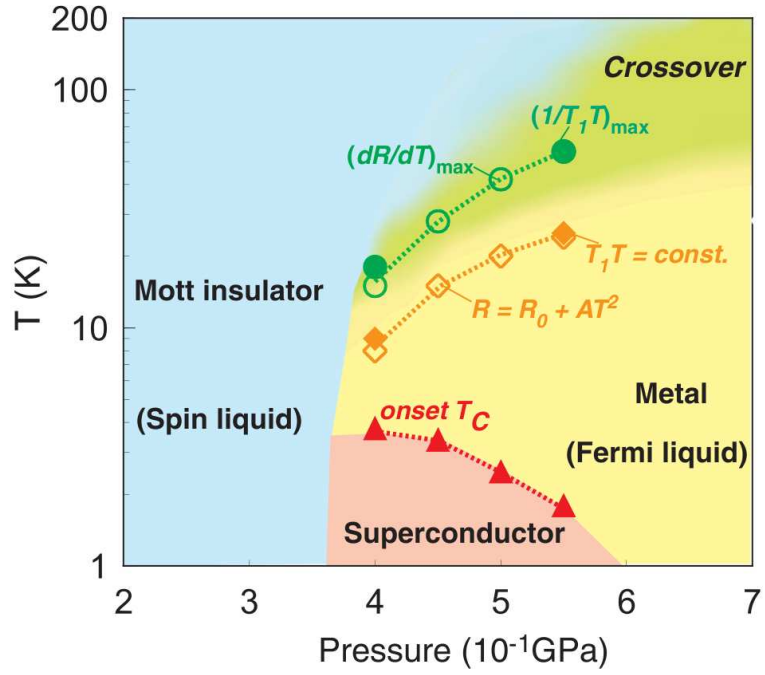
Charge Transfer Salts



$\kappa - (BEDT - TTF)_2 Cu_2 (CN)_3$ [Kandpal 2009]

Geometrical **Frustration** $\Longrightarrow$ Suppression of Long-Range Magnetic Order

Charge Transfer Salts



Experimental Phase Diagram of $\kappa-(ET)_2Cu_2(CN)_3$ [Kanoda 2003, 2005]

Mott Insulator

Fermi Liquid Metal

Why the paramagnetic solution?

The Hubbard model: $H = \sum_{ij\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$

- At $T = 0$ the half-filled solution on unfrustrated square lattices is an AFM-ordered insulator for any $U/t > 0$.

  BUT

- What happens for highly frustrated lattices?
- What happens for room-temperature paramagnetic materials?
- Strong correlations freeze charge degrees of freedom $\Rightarrow$ **MOTT-INSULATOR** for finite U/t.

Strategy: variational approach

The variational principle $T = 0$

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

$|\Psi\rangle$ is a variational wave function with variational parameters.

The best variational wave function gives the lower energy.

Why Projected wave functions?

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$|\Psi\rangle = P|\Psi_0\rangle$

No double occupancies: $P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$:

- ^3He almost localized Fermi Liquid [Vollhardt 1984]

- Applications to the t-J model

  $H_{t-J} = -t \sum_{ij\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \sum_{ij} J \hat{S}_i \cdot \hat{S}_j$

  Applications to the Hubbard model

  $H_{t-J} = -t \sum_{ij\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \sum_i U n_{i\uparrow} n_{i\downarrow}$

  $\Downarrow$

  High T_c superconductors (cuprates, cobaltates...)

Computations with Gutzwiller wave functions

$$|\Psi_G\rangle = P|\Psi_0\rangle = \mathrm{e}^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}|\Psi_0\rangle$$

For $g > 0$, P suppresses the double occupancies $d_i = n_{i\uparrow}n_{i\downarrow}$.

- **Variational Monte Carlo (VMC)**

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_x O_x \bar{P_x}$$

Electronic configurations $|x\rangle$ are generated according to the probability distribution $\bar{P_x} = \frac{|\Psi^2(x)|}{\sum_{x'}|\Psi^2(x')|}$.

- **Gutzwiller Approximation (GA)**

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = g\frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

The Gutzwiller Approximation (GA)

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projected wave functions

$$|\Psi\rangle = P\,|\Psi_0\rangle = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right) |\Psi_0\rangle$$

projected Hilbert space : $|\Psi\rangle$

pre-projected Hilbert space : $|\Psi_0\rangle$

renormalization scheme

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g\,\frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

renormalization factors

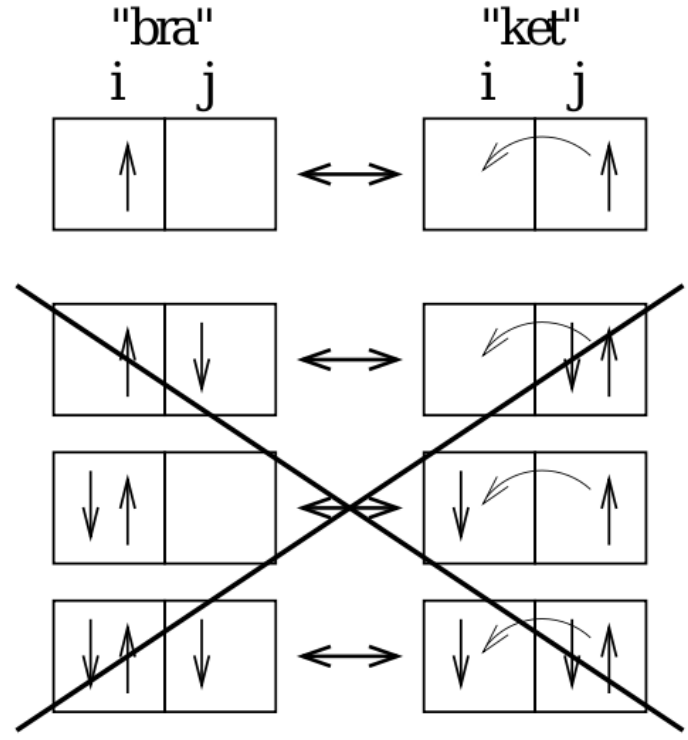
Hilbert-space arguments

Gutzwiller renormalization factors

kinetic energy

$$\frac{\langle\Psi|T_e|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \propto n_\sigma(1-n)$$

$$\frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \propto n_\sigma(1-n_\sigma)$$



$$\frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g_t \frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$g_t = \frac{1-n}{1-n_\sigma} = \frac{1-n}{1-n/2}$$

renormalized Hamiltonian

in pre-projected Hilbert space

The Gutzwiller Approximation

Electronic energy: $E_{e0}/N = g_t e^0 + UD$ with $g_t = 8D(1-2D)$.

- $\dfrac{\partial E_{e0}}{\partial d} = 0 \Longrightarrow$ **Metal-Insulator Transition (MIT)** for $U = U_c = 8|e^0|$.

  Double occupancy d + compressibility $\kappa_{\mathbf{q}=\mathbf{0}}$ vanish for $U \to U_c$.

  METALLIC STATE ($U < U_c$)

  $$d = \frac{1}{4}\left(1 - \frac{U}{U_c}\right) \;\Rightarrow\; g_t = 1 - \left(\frac{U}{U_c}\right)^2 \;\Rightarrow\; \frac{E_{e0}}{N} = e^0\left(1 - \frac{U}{U_c}\right)^2$$

  INSULATING STATE ($U > U_c$)

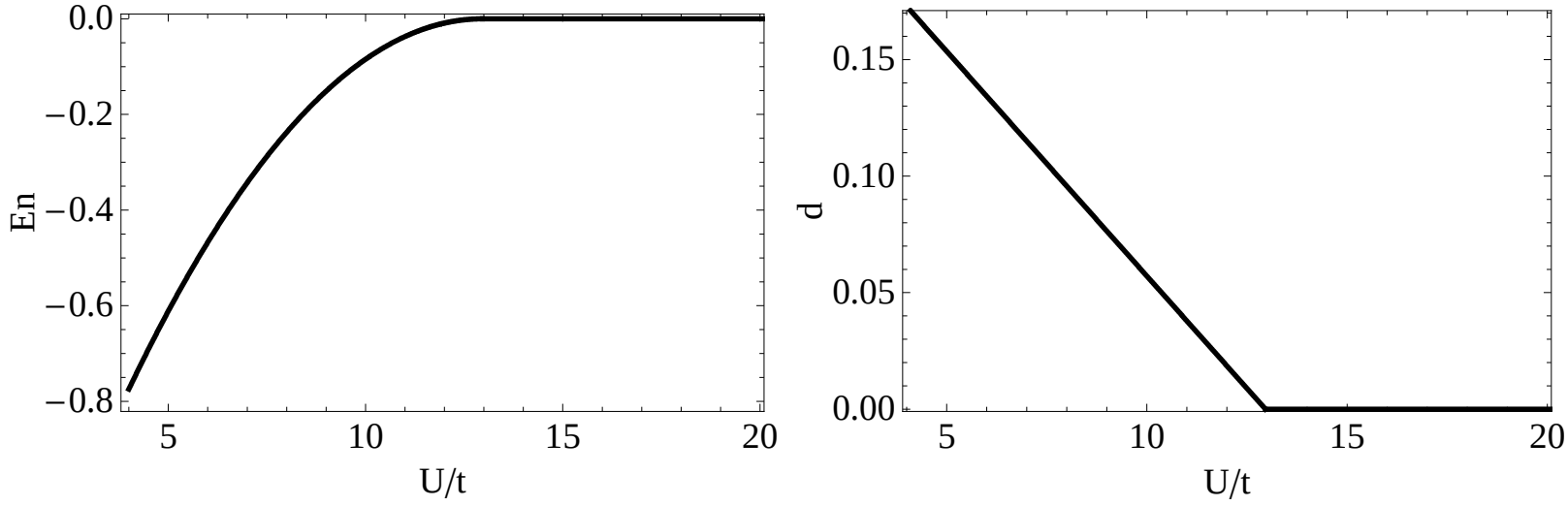
  $$d = 0 \;\Rightarrow\; g_t = 0 \;\Rightarrow\; E_{e0} = 0 \;\Rightarrow\; \kappa_{\mathbf{q}=\mathbf{0}} = 0$$

- The Gutzwiller Approximation finds the MIT but describes the insulating state trivially.

Analytical results in the Gutzwiller Approximation

First studied by [Brinkman-Rice 1970].

$$|\Psi\rangle = P|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}\left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$



Energy and double occupancy as a function of U/t in the GA.

Metal-insulator transition at $U_c = 12.96t$.

In the insulator $E = 0$ and $d = 0$

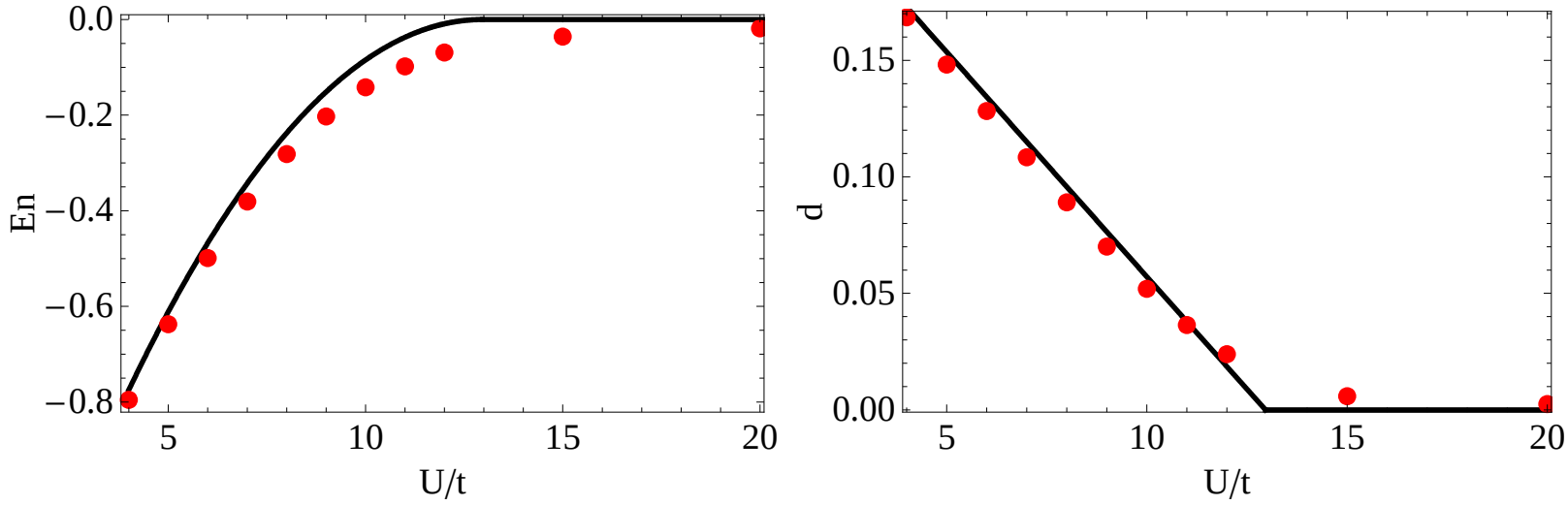
$\Rightarrow$ d order parameter for a 2nd-order phase transition.

VMC results with Gutzwiller wave functions

First studied by [Yokoyama-Shiba 1987].

$$|\Psi\rangle = P|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}\left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$

Results for 242-site lattice in 2D.



Energy and double occupancy as a function of U/t with VMC (dots) and in the GA (solid line).

VMC results show no evidence of an insulator for finite U/t !

Gutzwiller-Jastrow variational wave functions

Charge fluctuations exist in realistic insulators:

$$|\Psi\rangle = PJ|\Psi_0\rangle$$

- $P = \mathrm{e}^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}$
- $J = e^{-1/2\sum_{ij} v_{ij} n_i n_j}$

  The charge-charge Jastrow term J correlates empty sites (**holons**, h) and doubly occupied sites (**doublons**, d).

Holons and *doublons* play a crucial role for the conduction:
they must be correlated otherwise an applied electric field would induce a current.
The long-range Jastrow factor J correlates h and d and can induce a Metal-Insulator Transition for a finite value of U/t ($v_{ij} > 0$):

$n_i n_j = d_i d_j + h_i h_j - h_i d_j - d_i h_j + n_i + n_j - 1$
$[n_i = 1 + d_i - h_i]$.

metallic vs. insulating states

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Basic property: An insulator has zero d.c. electrical conductivity (at T=0).

Other properties

charge carriers in Mott-Hubbard insulators: bound doublon-holons

Charge density-density correlation function (factor structure):

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

- $N_q \sim q \quad \Rightarrow$ metal
- $N_q \sim q^2 \quad \Rightarrow$ insulator

Jastrow correlator [Fourier Transform]

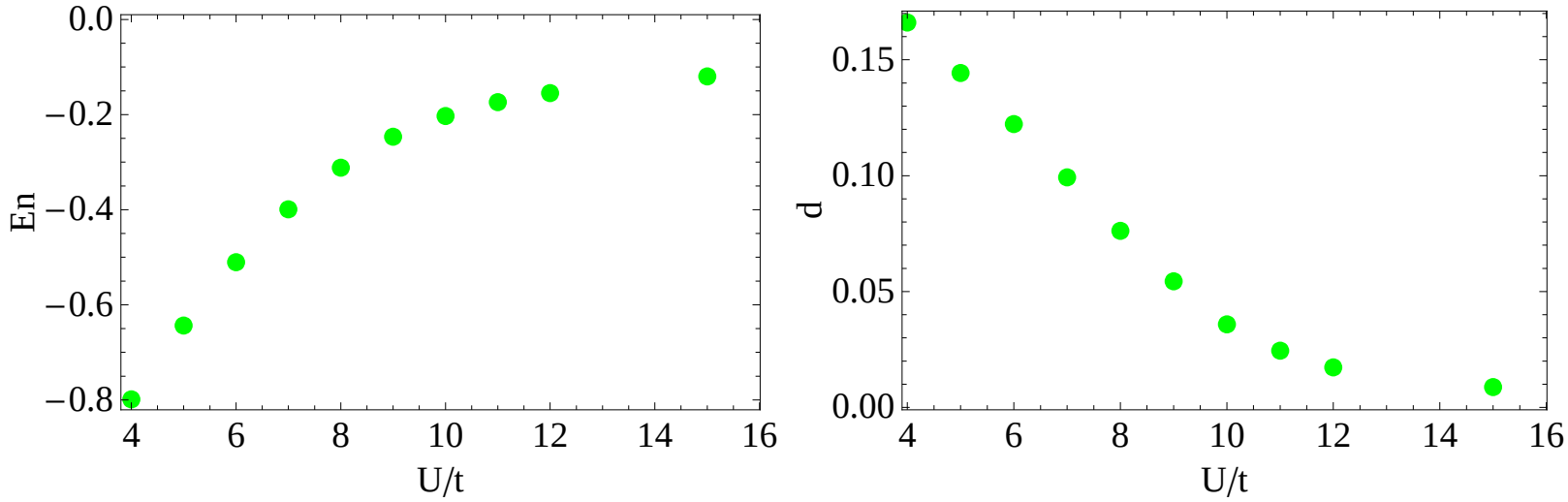
- $V_q \propto 1/q \quad \Rightarrow$ metal
- $V_q \propto 1/q^2 \quad \Rightarrow$ insulator (1D)
- $V_q \propto log(q)/q^2 \quad \Rightarrow$ insulator (2D)

VMC results with Gutzwiller + Jastrow wave functions

First studied by [Capello-Becca 2005].

$$|\Psi\rangle = PJ|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}} \; e^{-\frac{1}{2}\sum_{ij} v_{ij} n_i n_j} \left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$

v_{ij} for $|i-j| = 1$.

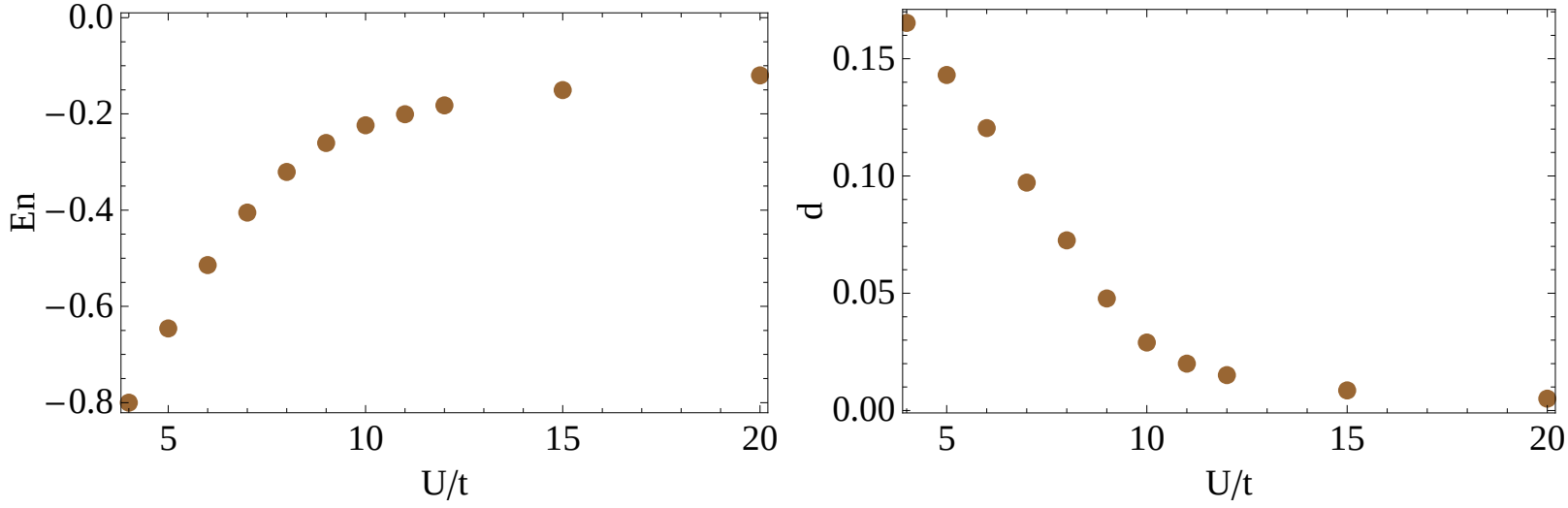


No evidence of an insulator for finite U/t also in this case.

VMC results with Gutzwiller + Jastrow wave functions

$$|\Psi\rangle = PJ|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}} \; e^{-\frac{1}{2}\sum_{ij} v_{ij} n_i n_j} \left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$

v_{ij} for $|i-j| = 2$.



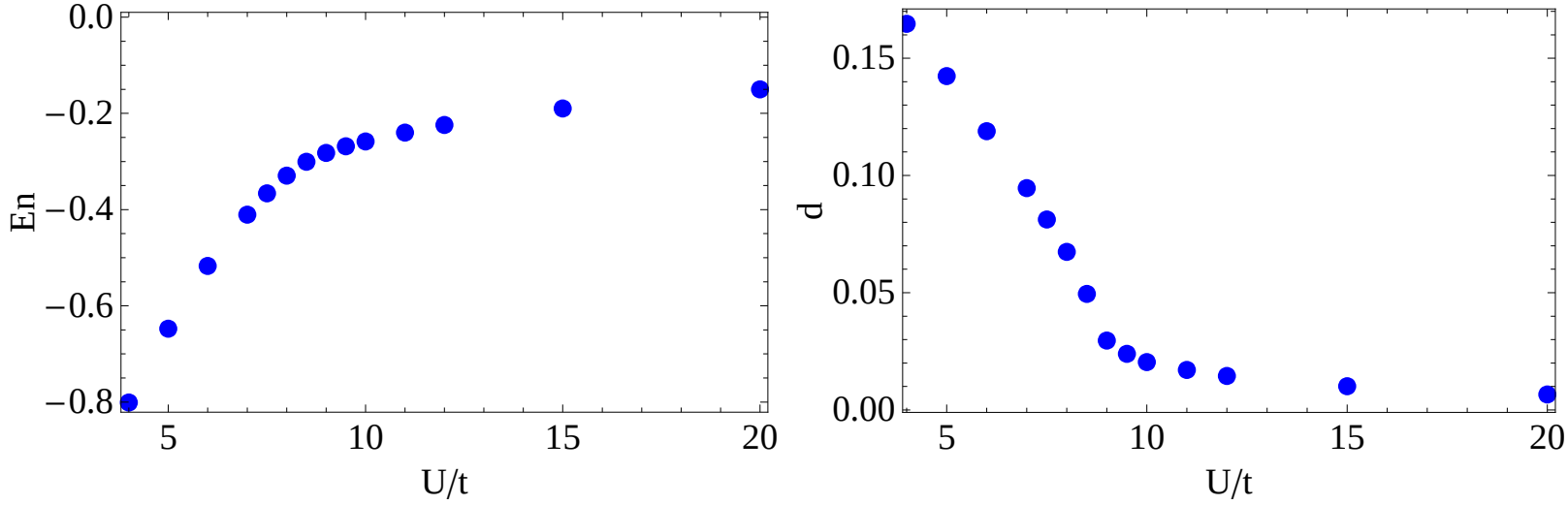
No evidence of an insulator for finite U/t also in this case.

but something is changing...

VMC results with Gutzwiller + Jastrow wave functions

$$|\Psi\rangle = PJ|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}} \; e^{-\frac{1}{2}\sum_{ij} v_{ij} n_i n_j} \left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$

v_{ij} for $|i-j| = 10$.



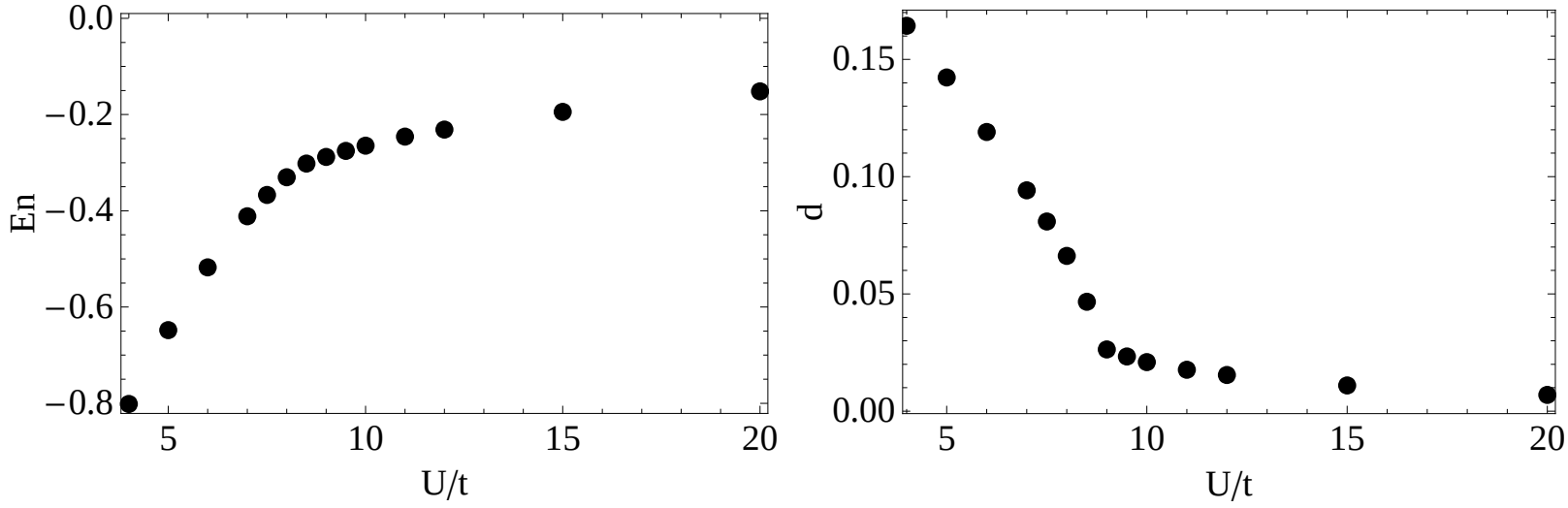
Transition at $U_c \approx 8.5t$ **!**

- **KINK** in the Energy
- **KINK** in the Double Occupancy
- insulator (zero d.c. conductivity)

VMC results with Gutzwiller + Jastrow wave functions

$$|\Psi\rangle = PJ|\Psi_0\rangle = e^{-g\sum_i n_{i\uparrow}n_{i\downarrow}} \; e^{-\frac{1}{2}\sum_{ij} v_{ij} n_i n_j} \left[\prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k},-\sigma}|0\rangle\right].$$

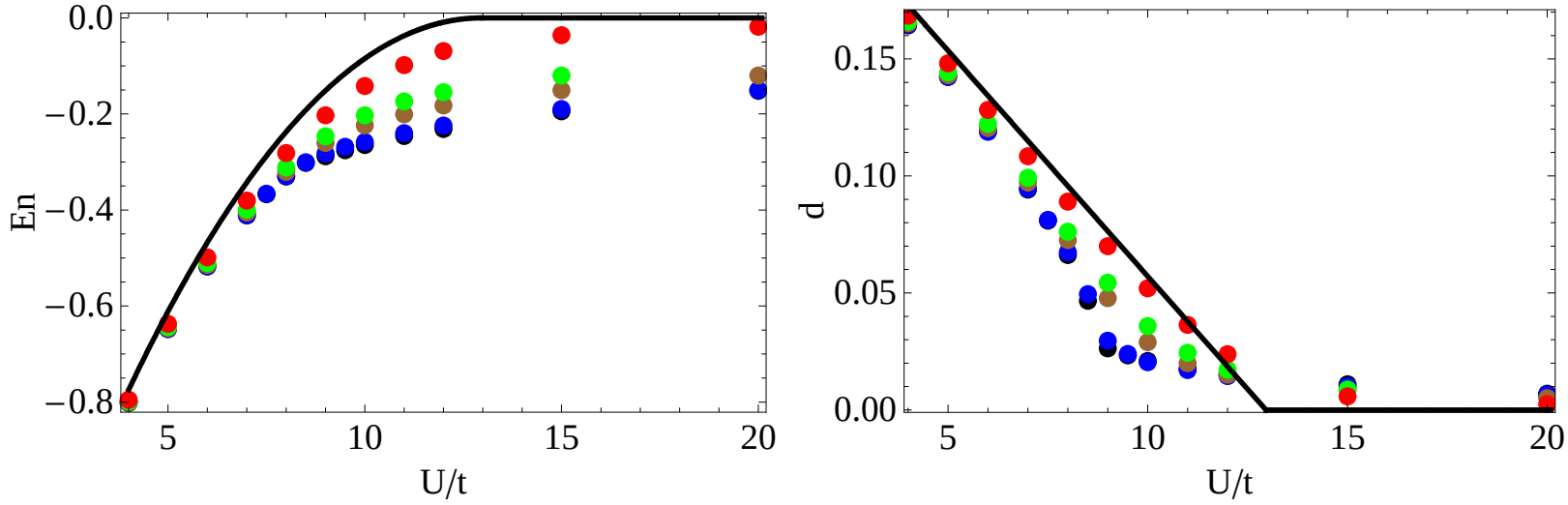
v_{ij} up to the longest possible distance.



Transition at $U_c \approx 8.5t$**.**

- **KINK** in the Energy
- **KINK** in the Double Occupancy
- insulator (zero d.c. conductivity)

SUMMARY!



Energy and double occupancy as a function of U/t.

Gutzwiller wave functions in GA (solid black line)

Gutzwiller wave functions in VMC (red dots)

Gutzwiller + very short-range Jastrow wave functions (green dots)

Gutzwiller + short-range Jastrow wave functions (brown dots)

Gutzwiller + medium-range Jastrow wave functions (blue dots)

Gutzwiller + long-range Jastrow wave functions (black dots)

Outlook

- Metal-Insulator transition with Gutzwiller wave functions is an artifact of the Gutzwiller Approximation!

- The transition is obtained correctly using variational wave functions which include a long-range charge-charge correlation [**Jastrow correlators**].

Basic References

- M. C. Gutzwiller, *Phys. Rev.* **137**, A1726 (1965).
- W. F. Brinkman and T. M. Rice, *Phys. Rev. B* **2**, 4302 (1970).
- H. Yokoyama and H. Shiba, *J. Phys. Soc. Jpn.* **56**, 1490 (1987).
- M. Capello, F. Becca, M. Fabrizio, S. Sorella and E. Tosatti, **94**, 026406-1 (2005).

Gutzwiller Method

The Hubbard model: $H = \sum_{ij\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$

- GZW TRIAL STATE: $|\psi_G\rangle = P|\Psi_0\rangle$

  $|\Psi_0\rangle \rightarrow$ uncorrelated state

  $P = \mathrm{e}^{-g\sum_i n_{i\uparrow}n_{i\downarrow}}$

  For $g > 0$, P suppresses the double occupancies $d_i = n_{i\uparrow}n_{i\downarrow}$.

- GUTZWILLER APPROXIMATION (GA) $\Longrightarrow$

  $E_e = \langle\psi_G|H_e|\psi_G\rangle \approx \sum_{ij\sigma} t_{ij} g_{tij\sigma} \langle\Psi_0|c^{\dagger}_{i\sigma}c_{j\sigma}|\Psi_0\rangle + \sum_i U d_i$

  $g_{tij\sigma}[n_{i\sigma}, n_{i,-\sigma}, d_i] \rightarrow$ GA renormalized hopping factors

Gutzwiller Projected wave functions

- **Totally projected wave function:**

  $|\Psi\rangle = P|\Psi_0\rangle$

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

  $|\Psi_0\rangle \rightarrow$ uncorrelated state

  For single particle (hole) excitations with respect to $|\Psi\rangle \Longrightarrow$ generalized GA.

- **Partially projected wave function:**

  $|\Psi'_\gamma\rangle \;=\; P'_\gamma|\Psi_0\rangle$

  $P'_\gamma = \prod_{i\neq\gamma}(1 - n_{i\uparrow} n_{i\downarrow})$

  Double occupancy is projected out on all sites, but for the **reservoir site γ.**

  In computations with projected excited states $\Rightarrow$ partially projected states arise:

  for example, $\quad P c_{\gamma\sigma}|\Psi_0\rangle = c_{\gamma\sigma} P'_\gamma|\Psi_0\rangle = c_{\gamma\sigma}|\Psi'_\gamma\rangle$.

Renormalization scheme

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un-projected Hilbert space	Hubbard Hamiltonian

$\Downarrow$ canonical transformation $e^{iS} H e^{-iS}$ $\Downarrow$

projected Hilbert space	t-J Hamiltonian

$\Downarrow$ Gutzwiller renormalization g $\Downarrow$

pre-projected Hilbert space	renormalized Hamiltonian

$$\frac{\langle \Psi | H_{t-J} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \frac{\langle \Psi_0 | H_{t-J}^{(renor)} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$H_{t-J}^{(renor)} = g_t T_e + g_s J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$g_t = \frac{1-n}{1-n/2}, \qquad g_s = \frac{1}{(1-n/2)^2}$$

RMFT scenario - Renormalization scheme

- Hubbard Hamiltonian:

$$H = -t\sum_{ij\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

- $\Longrightarrow$ canonical transformation $e^{iS}He^{-iS} \Longrightarrow$

- t-J Hamiltonian:

$$H_{t-J} = \hat{P}_G[-t\sum_{ij\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_{ij} J\hat{S}_i\cdot\hat{S}_j]\hat{P}_G$$

- $\Longrightarrow$ GA renormalization factors g_t and $g_S \Longrightarrow$

- t-J renormalized Hamiltonian:

$$\tilde{H}_{t-J} = -g_t t\sum_{ij\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + \sum_{ij} g_S J\hat{S}_i\cdot\hat{S}_j$$

with $\frac{\langle\psi|H_{t-J}|\psi\rangle}{\langle\psi|\psi\rangle} \sim \frac{\langle\psi_0|\tilde{H}_{t-J}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}$

Decoupling Scheme $\Longrightarrow$ BCS $|\psi_0\rangle = \prod_k(u_k + v_k c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow})|0\rangle$.

The Gutzwiller Approximation (GA)

Expectation values: $\frac{\langle \Psi'_\gamma | \hat{O} | \Psi'_\gamma \rangle}{\langle \Psi'_\gamma | \Psi'_\gamma \rangle}$

- **Gutzwiller Approximation (GA)**

$$\frac{\langle \Psi'_\gamma | \hat{O} | \Psi'_\gamma \rangle}{\langle \Psi'_\gamma | \Psi'_\gamma \rangle} = g'_\gamma \frac{\langle \Psi_0 | \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

- **Variational Monte Carlo (VMC)**

$$\frac{\langle \Psi'_\gamma | \hat{O} | \Psi'_\gamma \rangle}{\langle \Psi'_\gamma | \Psi'_\gamma \rangle} = \sum_x O_x \bar{P_x}$$

Variational Monte Carlo (VMC) method

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Variational Monte Carlo (VMC): numerical approach to compute *"exact"* expectation values over correlated wave functions:

$$\frac{\langle \Psi'_\gamma | \hat{O} | \Psi'_\gamma \rangle}{\langle \Psi'_\gamma | \Psi'_\gamma \rangle} = \sum_x O_x \bar{P}_x$$

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

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

Variational Monte Carlo (VMC) method

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Monte Carlo sampling of the configuration $|x\rangle$ shall fulfil two conditions.

- Does a stationary $\bar{P}_x$ exist?

  Yes thanks to the

  Detailed Balance: The number of processes corresponding to the transition $|x\rangle \to |x'\rangle$ shall be compensated by the number of processes in the reverse sense $|x'\rangle \to |x\rangle$:

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

- Starting from an arbitrary P_x, will the sampling converge to the stationary $\bar{P}_x$?

  Yes thanks to the

  Ergodicity: Any configuration can be reached from the initial one via a sufficiently large number of steps [iterations of the Markov chain].

  [Unicity of the $\bar{P}_x$]

Variational Monte Carlo (VMC) method

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Standard Detailed Balance:

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

$$\bar{P}_x \mathcal{P}_{x\to x'} p_{ij} = \mathcal{P}_{x'\to x} p_{ji} \bar{P}_{x'}$$

$p_{ij} = p_{ji}$: probability to select two sites i and j for hopping or spin-flip processes in the transition $x \to x'$.

$p_{ij} = p$: equiprobability to select two sites i and j.

Our Detailed Balance for large lattices with a reservoir site γ:

$$\bar{P}_x \mathcal{P}_{x\to x'} \tilde{p}_{ij} = \mathcal{P}_{x'\to x} \tilde{p}_{ji} \bar{P}_{x'}$$

$$\tilde{p}_{ij} = \theta(r-\alpha) p_{ij} + [1-\theta(r-\alpha)] p_{\gamma j} \quad ; \quad r, \alpha \in [0,1].$$

r: random number extracted in each step of the stochastic process.

This will allow to accumulate more statistics for the computations of intensive quantities for the reservoir site, such as its double occupancy d_γ.