FNP
Fundacja na rzecz Nauki Polskiej

NARODOWE CENTRUM NAUKI

# Mott Physics in Correlated Nanosystems


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**http://th-www.if.uj.edu.pl/ztms/eng/jSpalek.php**

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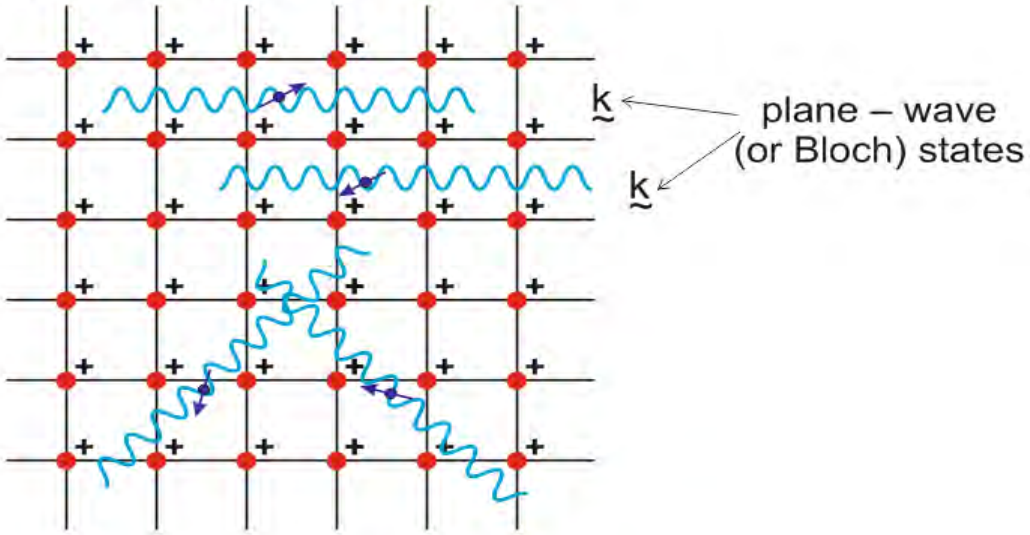
# Plan

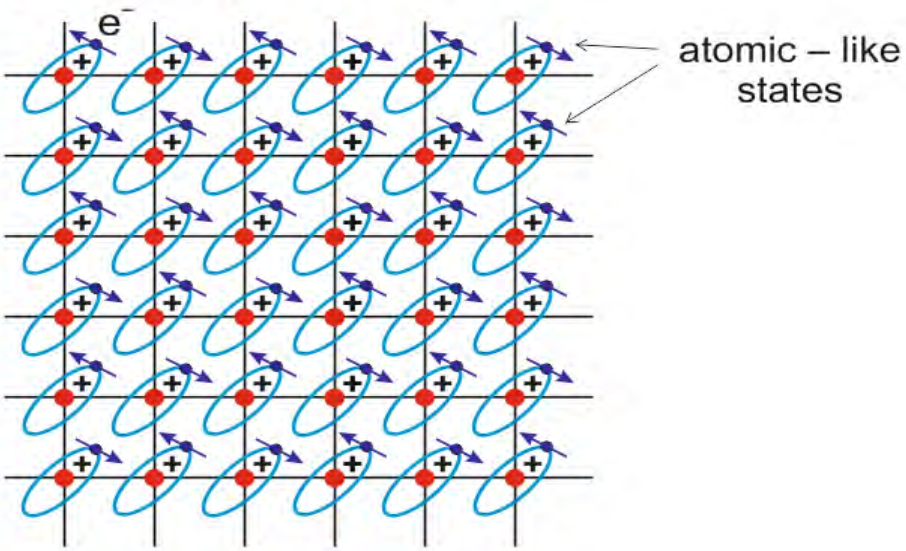
1. PART I: Strongly correlated quantum matter as such
   - Unique properties: Mott (-Hubbard) localization, spin-dependent masses of quasiparticles, high temperature superconductivity
2. PART II: Mott in correlated nanosystems
   - Selected methods: EDABI, Lanczos, VMC – results mainly
   - Unique property: Evolution of statistical distribution F-D -> local, magnetic correlations, Mott + Slater?
3. Outlook

# Localized versus delocalized

(a) Normal metal




(b) Mott insulator



# Instabilty of Fermi-gas under repulsive Coulomb int.

$$\langle T \rangle = \frac{3}{5}\frac{\hbar^2}{2m^*}\left(3\pi^2\frac{N}{V}\right)^{2/3} \sim \rho^{2/3} \qquad \rho \equiv {}^{N}/_{V}$$

**Estimate of Coulomb interaction**

$$\langle V_{12} \rangle \sim \frac{e^2}{\kappa \langle r_{12} \rangle} \qquad \langle r_{12} \rangle = \left(\frac{V}{N}\right)^{1/3} \sim \rho^{-1/3}$$

**Critical density $\rho$:**

$$\langle T \rangle = \langle V_{12} \rangle \Rightarrow \qquad \boxed{a_B \ \rho_c{}^{1/3} \sim 0.2}$$

**Mott criterion**

$\rho > \rho_c \Rightarrow$ **gas state stable (deconfinement)**

$\rho < \rho_c \Rightarrow$ **confinement**

$$a_B \equiv \frac{\hbar^2}{m^* e^2}\kappa$$ - **effective Bohr radius**

# 3. Strong correlations: Definition

$$\frac{E_G}{N} = \epsilon_a + \langle T \rangle + \langle V \rangle + \langle V_{12} \rangle \equiv E_1 + E_2$$

**Energies:** atomic kinetic potential interaction

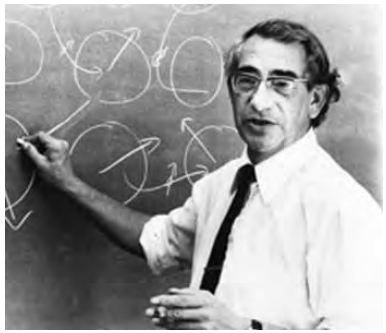
Reference energy $\epsilon_a \equiv 0$

**When:**

- $|E_1| \gg E_2$ → **fermion-gas/liquid (metallic) regime**
- $|E_1| \ll E_2$ → **strong-correlation (Mott ins.) regime (high-Tc superconducting)**
- $|E_1| \sim E_2$ → **localization (Mott-Hubbard) regime**

# Hubbard model

$$\hat{\mathcal{H}} = \sum_{ij\sigma}{}' t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \equiv \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



**Now, all fermions taken into account**

$$E_G \equiv \langle\mathcal{H}\rangle = \sum_{ij\sigma}{}' t_{ij}\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle + U\sum_{i}\underbrace{\langle\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle}_{\equiv d^2}$$

**In correlated state:** $W \equiv 2z|t| \lesssim U$

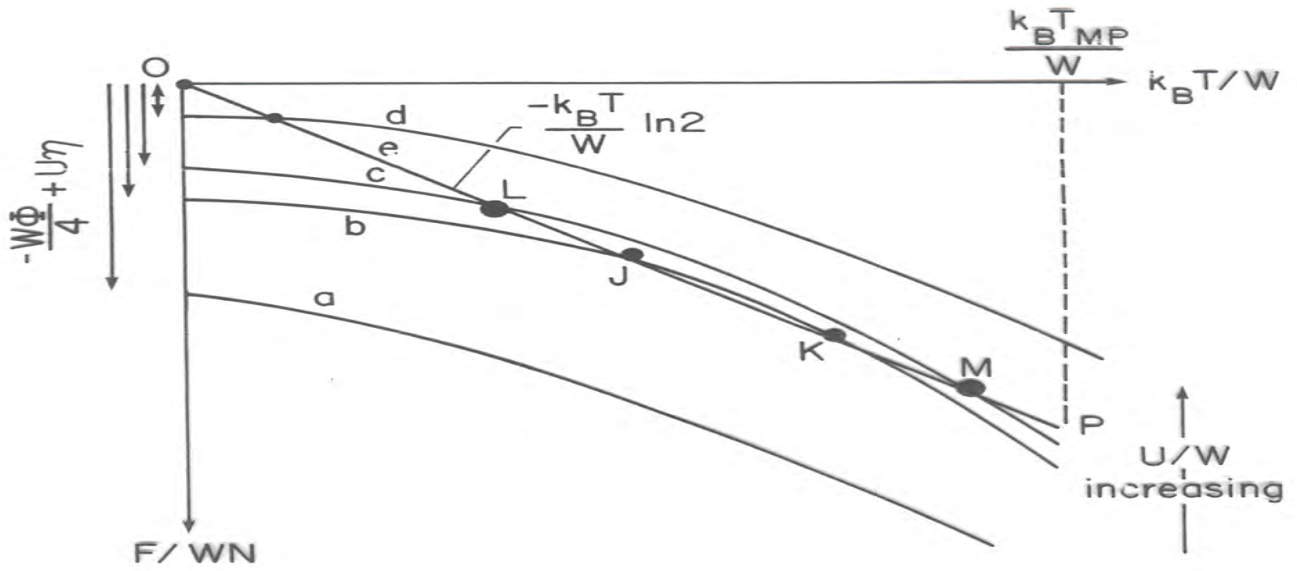
$$\left\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\right\rangle \equiv q(d^2)\left\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\right\rangle_0$$

$$F_{metal} = (1-U/U_c)^2 \bar{\epsilon} - \frac{1}{2}\frac{\gamma_0 T^2}{1-(U/U_c)^2}$$

$$F_{insulator\ (param)} = -k_B T \ln 2 \qquad (E_{ex}=0)$$

Coexistence (PM-PI): $F_{metal} = F_{insulator}$

$$k_B T_{\pm} = \frac{3\Phi_0}{2\pi^2 \rho}\left\{\ln 2 \pm \left[(\ln 2)^2 - \frac{4}{3}\pi^2 \rho |\bar{\epsilon}| \left(\frac{1-\frac{U}{U_c}}{\Phi_0}\right)^2\right]^{\frac{1}{2}}\right\}$$




*J. M. Honig & J. Spałek, A Primer to the Theory of Critical Phenomena, Elsevier (2018), chapter 16*

# $V_2O_3$: Canonical Mott-Hubbard system

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**Discontinuous Metal-Insulator Transitions and Fermi-Liquid Behavior of Correlated Electrons**

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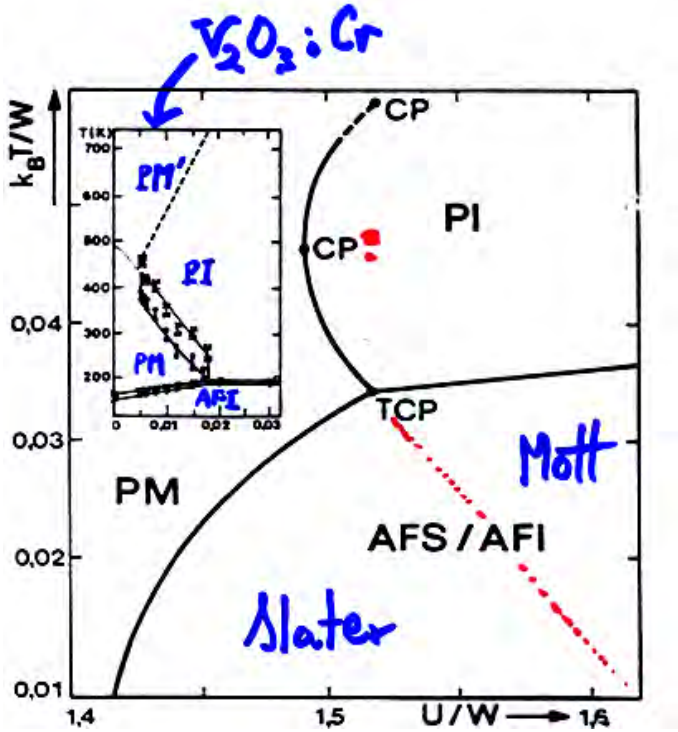
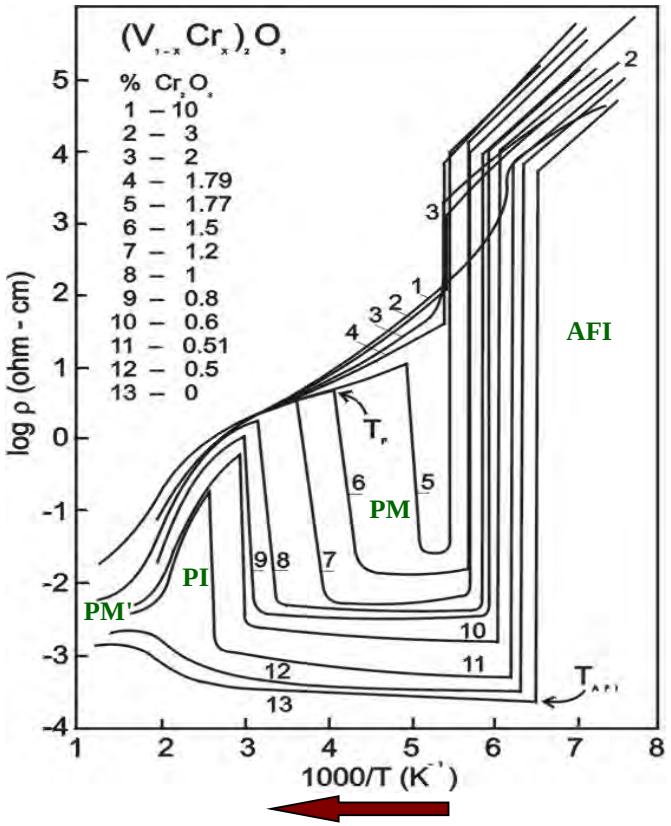
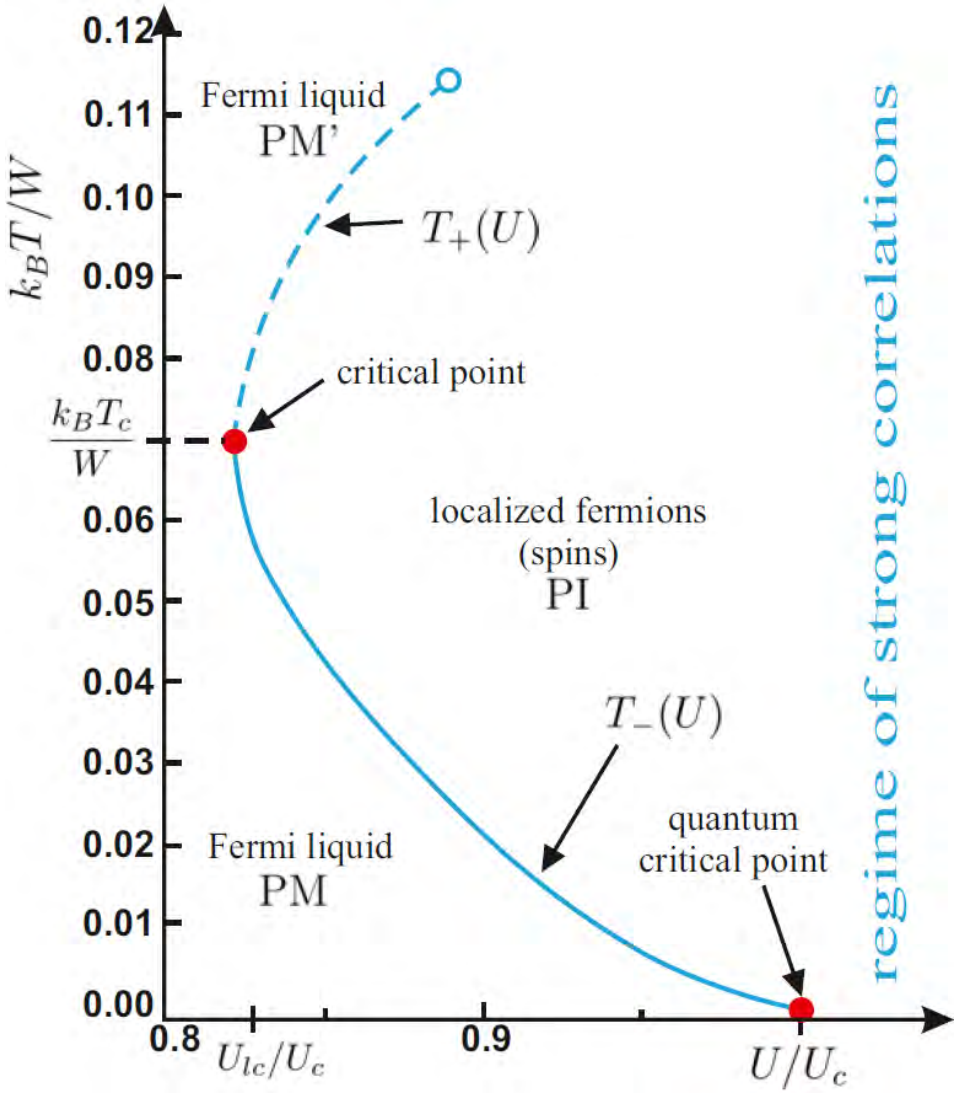
(Received 2 June 1986)




*H. Kuwamoto, J.M. Honig, and J. Appel, PRB 22 (1980) 2626*

# Mott-Hubbard *at nonzero temperature: phase diagram*



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# ON THE KINETIC EXCHANGE INTERACTIONS IN THE HUBBARD MODEL

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ABSTRACT

We use the canonical transformation method in the Hubbard model to derive the general form of the effective Hamiltonian which includes the virtual hopping from single- to double-occupied sites. The correspondence with the Anderson kinetic exchange Hamiltonian is briefly discussed.

SSPJU - 6/76
October 1976

***J. Spałek & A. M. Oleś , original derivation of the t-J model (1976)***

$$P_N \mathcal{H} P_N = P_N H P_N + U^{-1} P_N H P_0 H P_N . \qquad (15b)$$

Substituting Eq. (4c) and Eq. (4d) to Eq. (15a) and (15b), we get after some manipulations and neglecting terms connecting more than two lattice sites:

$$P_0 \mathcal{H} P_0 = t \sum_{\langle i,j\rangle,\sigma} a_{i\sigma}^{+} (1 - n_{i-\sigma}) a_{j\sigma} (1 - n_{j-\sigma}) +$$

$$+ \frac{t^2}{U} \sum_{\langle i,j\rangle,\sigma} \left[ S_i^{\sigma} S_j^{-\sigma} - n_{i\sigma} (1 - n_{i-\sigma}) n_{j-\sigma} (1 - n_{j\sigma}) \right], \qquad (16)$$

$$P_N \mathcal{H} P_N = t \sum_{\langle i,j\rangle,\sigma} a_{i\sigma}^{+} n_{i-\sigma} a_{j\sigma} n_{j-\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} +$$

$$+ \frac{t^2}{U} \sum_{\langle i,j\rangle,\sigma} n_{i\sigma} n_{i-\sigma} (1 - n_{j-\sigma}) (1 - n_{j\sigma}), \qquad (17)$$

where $S_i^{\sigma} = S_i^{\pm}$ for $\sigma = \pm 1$, respectively. The part (17) of the effective Hamiltonian does not influence the magnetic state in the case $|t| \ll U$ and $|t| \gg k_B T$ (which means that $\langle n_{i\sigma} \rangle \simeq \langle \nu_{i\sigma} \rangle$), and thus can be neglected. So the effective magnetic Hamiltonian $H_M$ can be rewritten with new operators introduced: (18)

$$b_{i\sigma} = a_{i\sigma} (1 - n_{i-\sigma}), \qquad \nu_{i\sigma} = b_{i\sigma}^{+} b_{i\sigma} ,$$

in the final form as:

$$H_M = t \sum_{\langle i,j\rangle\sigma} b_{i\sigma}^{+} b_{j\sigma} + \frac{t^2}{U} \sum_{\langle i,j\rangle,\sigma} \left[ S_i^{\sigma} S_j^{-\sigma} - \nu_{i\sigma} \nu_{j-\sigma} \right]. \qquad (19)$$

*J. Spałek & A. M. Oleś , original derivation of the t-J model (1976)*

# Fundamental concepts II: t-J model: moving pairs of spins vs. Cooper pairs

$$\mathcal{H}_{tJ} = \sum_{ij\sigma} t_{ij}\, b^{\dagger}_{i\sigma}\, b_{j\sigma} + \sum_{ij} J_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}c_1\nu_i\nu_j\right) + c_2\sum_{ijk}\frac{t_{ij}t_{jk}}{U}\left(b^{\dagger}_{i\sigma}\, S^{\bar{\sigma}}_{j}\, b_{k\bar{\sigma}} - b^{\dagger}_{i\sigma}\,\nu_{j\bar{\sigma}}\, b_{k\sigma}\right)$$

$$b^{\dagger}_{i\sigma} \equiv a^{\dagger}_{i\sigma}\left(1-n_{i\bar{\sigma}}\right),\ \ \nu_{i\sigma} \equiv n_{i\sigma}\left(1-n_{i\bar{\sigma}}\right),\ \ \nu_i \equiv \textstyle\sum_{\sigma}\nu_{i\sigma},\ \ S^{\sigma}_{i} \equiv b^{\dagger}_{i\sigma}\, b_{i\bar{\sigma}},\ \ \bar{\sigma} \equiv -\sigma$$

*original derivation: J. Spałek & A. Oleś, Physica B 86-88, 375 (1977); K. A. Chao, J. Spałek, and A. M. Oleś, J. Phys. C 10, L271 (1977); PRB 18, 3453 (1988); J.S. et al., Phys. Stat. Sol. (b) 108, 329 (1981) ; rederivation: C. Gros, R. Joynt & M. Rice, Phys. Rev. B 36, 381(1987); C. Zhang & T. M. Rice, Phys. Rev. B 37, 3759 (1988), and many others …*

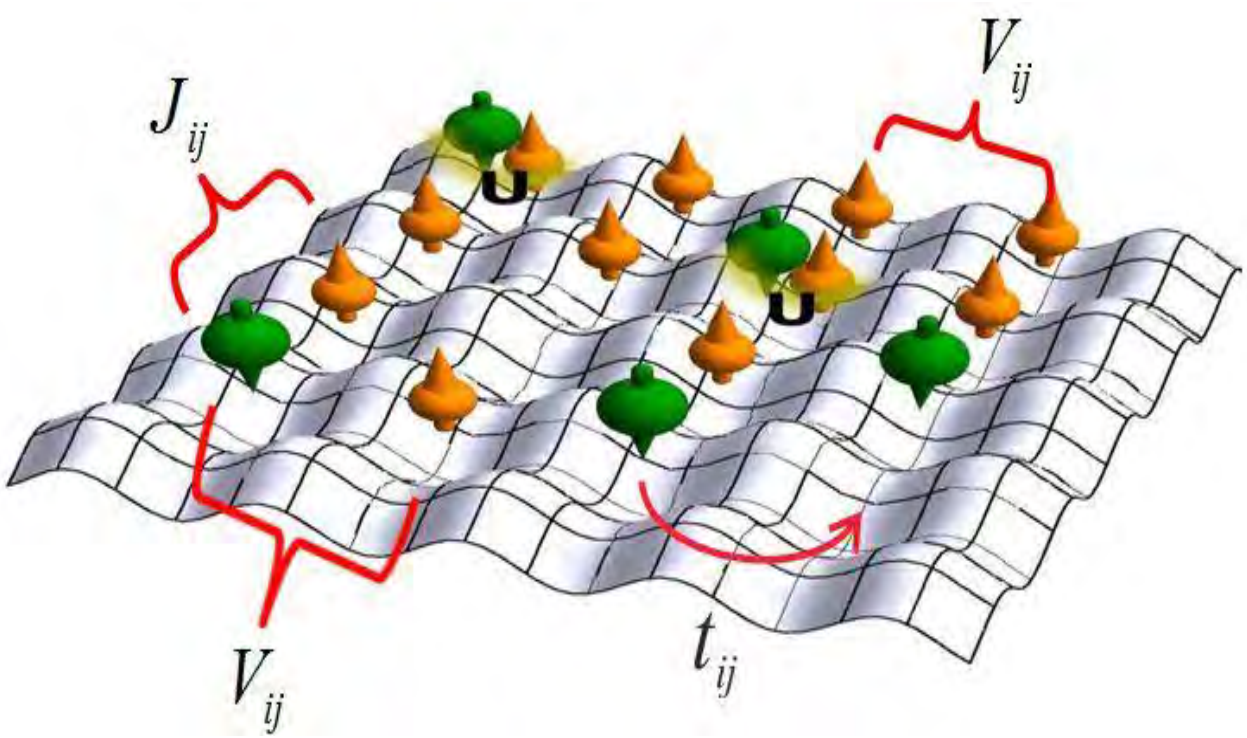
**Pairing operators:**

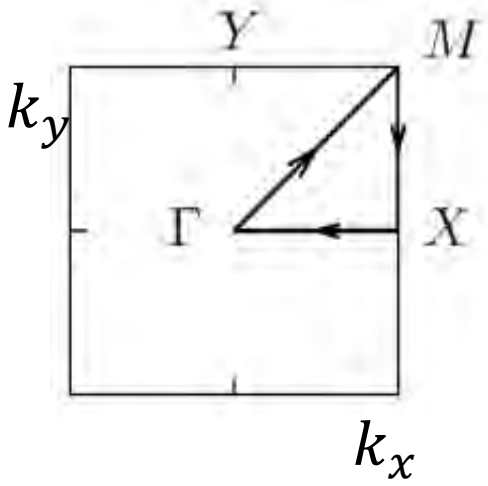
$$\begin{cases} B^{\dagger}_{ij} \equiv & \frac{1}{2}\left(b^{\dagger}_{i\uparrow}b^{\dagger}_{j\downarrow} - b^{\dagger}_{i\downarrow}b^{\dagger}_{j\uparrow},\right)\ , \\ B_{ij} \equiv & \frac{1}{2}\left(b_{i\downarrow}b_{j\uparrow} - b_{i\uparrow}b_{j\downarrow}\right) = \left(B^{\dagger}_{ij}\right)^{\dagger} \end{cases}$$

$$\mathcal{H}_{tJ} = \sum_{ij\sigma} t_{ij}\, b^{\dagger}_{i\sigma}\, b_{j\sigma} - \sum_{ijk}\frac{4t_{ij}t_{jk}}{U}B^{\dagger}_{ij}B_{kj}$$

*J.S., PRB 37, 533 (1988); didactical reviews: Acta Phys. Polon. A 111, 409 (2007); [cf. arXiv: 0706.4236]; ibid., A121, 764 (2012) [arXiv: 1202.2833]; Phil. Mag. 95,661-681 (2015) [Focus Issue: From Correlations to Unconvent. Superconductivity]*

# Theory: t-J-U-V model

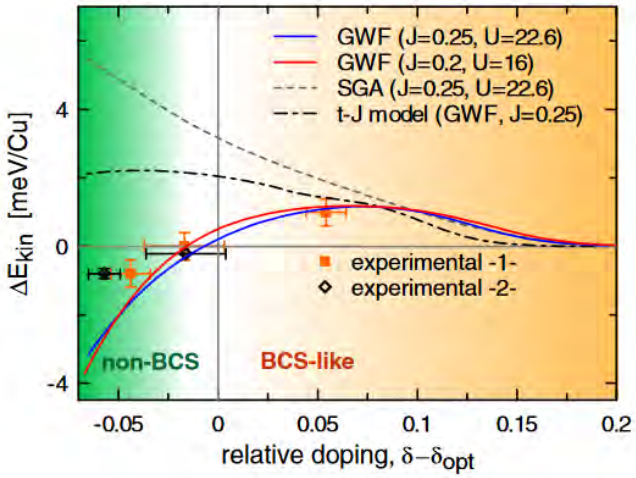


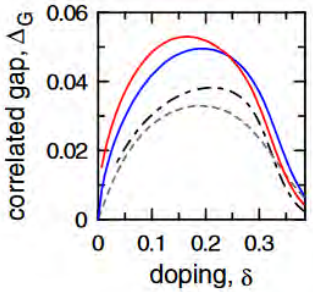



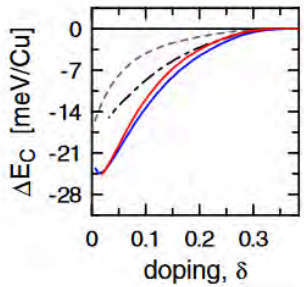

$$\hat{\mathcal{H}} = \sum_{ij\sigma}{}' t_{ij}\hat{c}^{\dagger}{}_{i\sigma}\,\hat{c}_{j\sigma} + \mathrm{U}\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{ij}{}'\left(V_{ij} - \frac{1}{4}J_{ij}\right)\hat{n}_i\hat{n}_j + \sum_{ij}{}' J_{ij}\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j$$

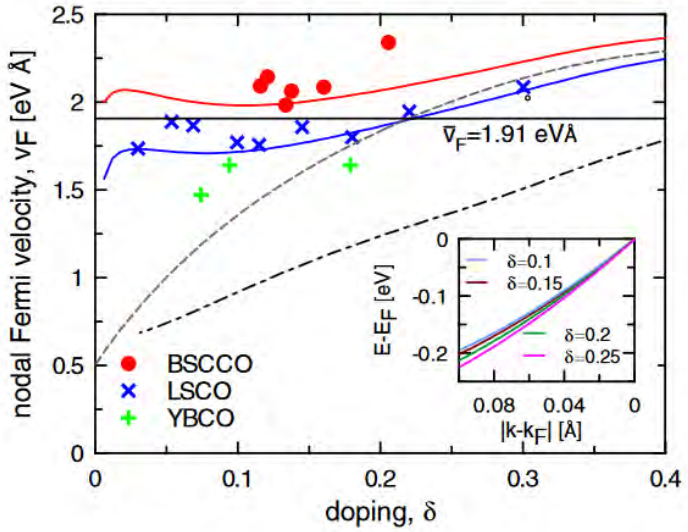
*J.S., M. Zegrodnik, & J. Kaczmarczyk, PRB 95, 024506 (2017)*

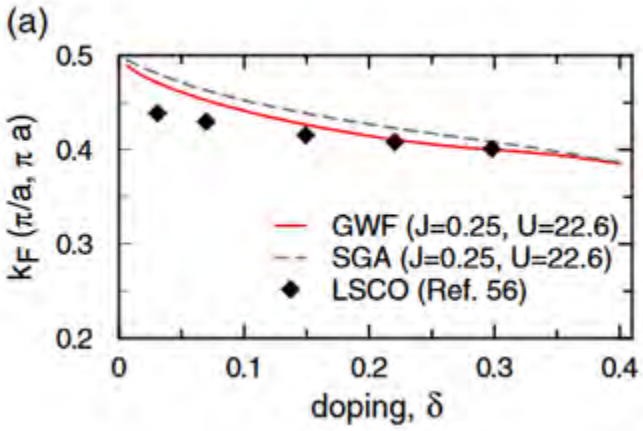
# t-J-U model: Quantitative comparison with experiment

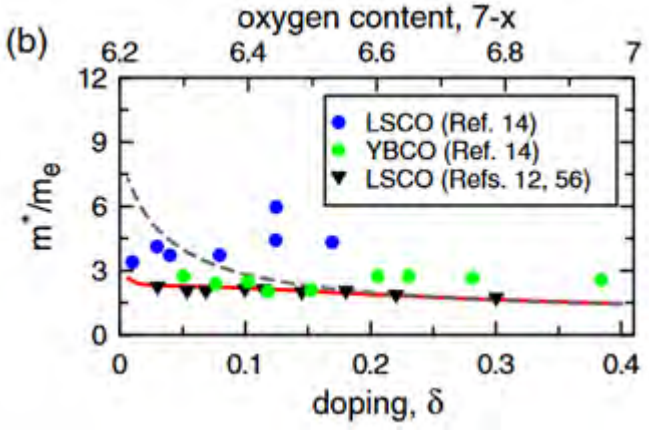


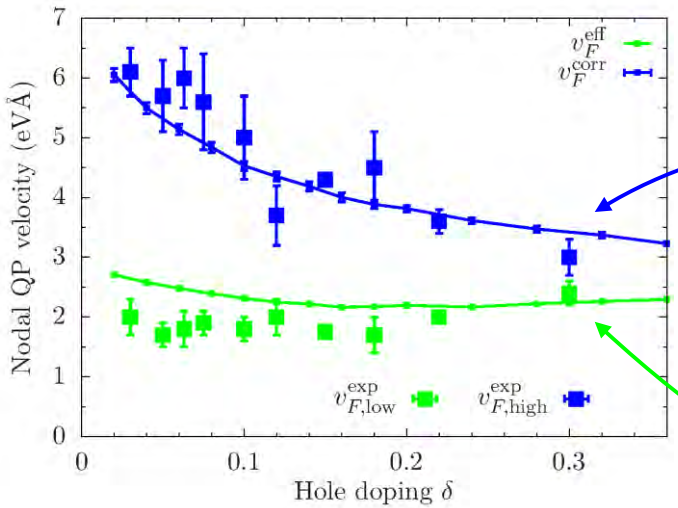



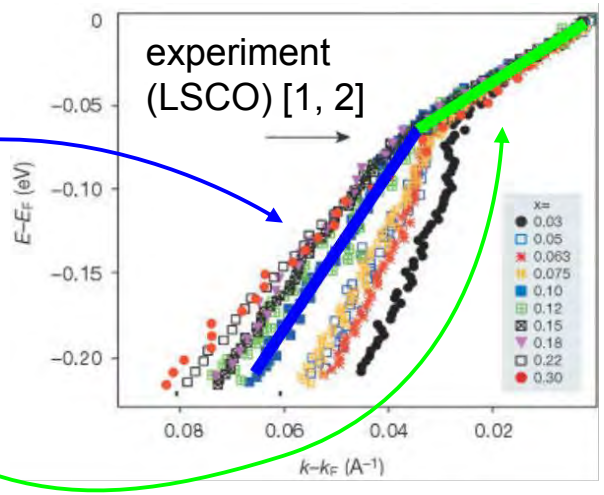

*J. S., M. Zegrodnik &J. Kaczmarczyk, PRB 95, 024506 (2017)*
*M. Zegrodnik & J. S., PRB 95, 024507 (2017)*
*M. Zegrodnik & J. S., PRB 96, 054511 (2017) …..*

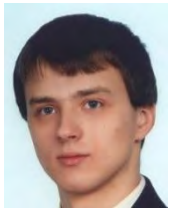
*G. Deutscher et al., Phys. Rev. B 72, 092504 (2005);*
*F. Carbonne et al., Phys. Rev. B 74, 064510 (2006);*
*H.J.A. Molegraaf et al., Science 295, 2239 (2002);*
*A.A. Kordyuk et al., Phys. Rev. B 71, 214513 (2005);*
*S.V. Borisenko et al., Phys. Rev. Lett. 96, 117004 (2006)*

# k-DE-GWF: nodal properties of quasiparticles (Hubbard model, SC)

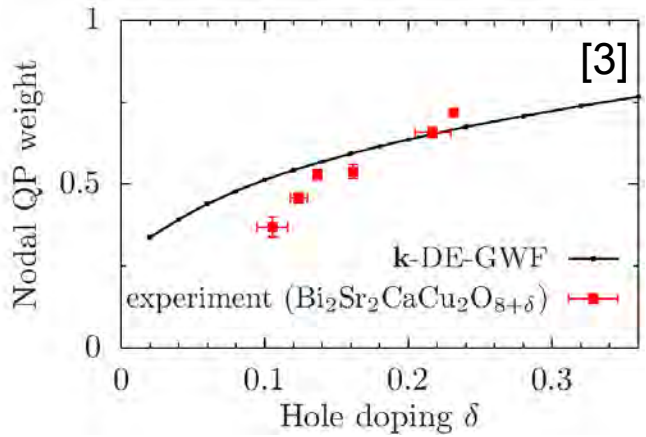
## Two „Fermi" velocities in the nodal direction



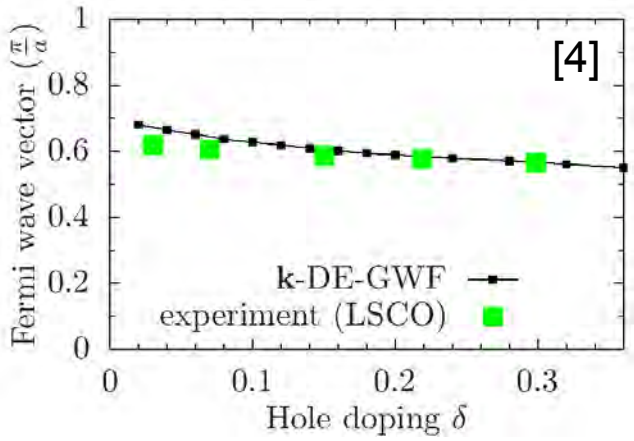



## quasiparticle weight




## Fermi wavevector




$$\epsilon_k - \mu = v_F(k - k_F)$$

*M. Fidrysiak et al., JPCM, 30, 475602 (2018) pp. 1-22*


[1] Experiment: *X. J. Zhou et al., Nature 423, 398 (2003).*
[2] Experimental data elaboration: *K. Matsuyama et al., Phys. Rev. B 95, 165435 (2017).*
[3] Experiment: *P. D. Johnson et al., Phys. Rev. Lett. 87, 177007 (2001); M. Randeria et al., Phys. Rev. B 69, 144509 (2004).*
[4] Experiment: *M. Hashimoto et al., Phys. Rev. B 77, 094516 (2008).*

# PART II: Mott features in nano

# EDABI: Fundamental concept

**Starting Hamiltonian in 2nd quantization**

$$\hat{\mathcal{H}} = \sum_{\sigma} \int d^3r\, \hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r}) \mathcal{H}_1(\mathbf{r}) \hat{\Psi}_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d^3r\, d^3r'\, \hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r}) \hat{\Psi}^{\dagger}_{\sigma'}(\boldsymbol{r'}) V(\mathbf{r}-\boldsymbol{r'}) \hat{\Psi}^{\dagger}_{\sigma'}(\boldsymbol{r'}) \hat{\Psi}_{\sigma}(\mathbf{r})$$

**Wannier basis (single-band, incomplete):**

$$\hat{\Psi}_{\sigma}(\mathbf{r}) \equiv \sum \varphi_{i\sigma}(\mathbf{r})\, \hat{a}_{i\sigma}$$

**Explicite form in particle language**

$$\hat{\mathcal{H}} = \sum_{ij\sigma} t_{ij} \hat{a}^{\dagger}_{i\sigma}\, \hat{a}_{j\sigma} + \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} V_{ijkl}\, \hat{a}^{\dagger}_{i\sigma}\, \hat{a}^{\dagger}_{j\sigma'}\, \hat{a}_{l\sigma'}\, \hat{a}_{k\sigma}$$

**where parameters – with hidden single-particle wave function**

$$t_{ij} \equiv \langle \varphi_{i\sigma} | \mathcal{H}_1 | \varphi_{j\sigma} \rangle \quad \text{and} \quad V_{ijkl} = \langle \varphi_i \varphi_j | V | \varphi_k \varphi_l \rangle$$

# EDABI: Renormalized wave equation

**Define functional**

$$E\{w_i(\mathbf{r})\} \equiv E_G\{w_i(\mathbf{r})\} - \mu N - \sum_{i \geqslant j} \lambda_{ij} \left( \int d^3\mathbf{r}\, w_i^*(\mathbf{r})\, w_j(\mathbf{r}) - \delta_{ij} \right)$$

**where**

$$N = \sum_\sigma \int d^3\mathbf{r} \left\langle \hat{\Psi}_\sigma^\dagger(\mathbf{r}) \hat{\Psi}_\sigma(\mathbf{r}) \right\rangle = \sum_{ij\sigma} \int d^3\mathbf{r}\, w_i^*(\mathbf{r})\, w_j(\mathbf{r}) \left\langle \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} \right\rangle$$

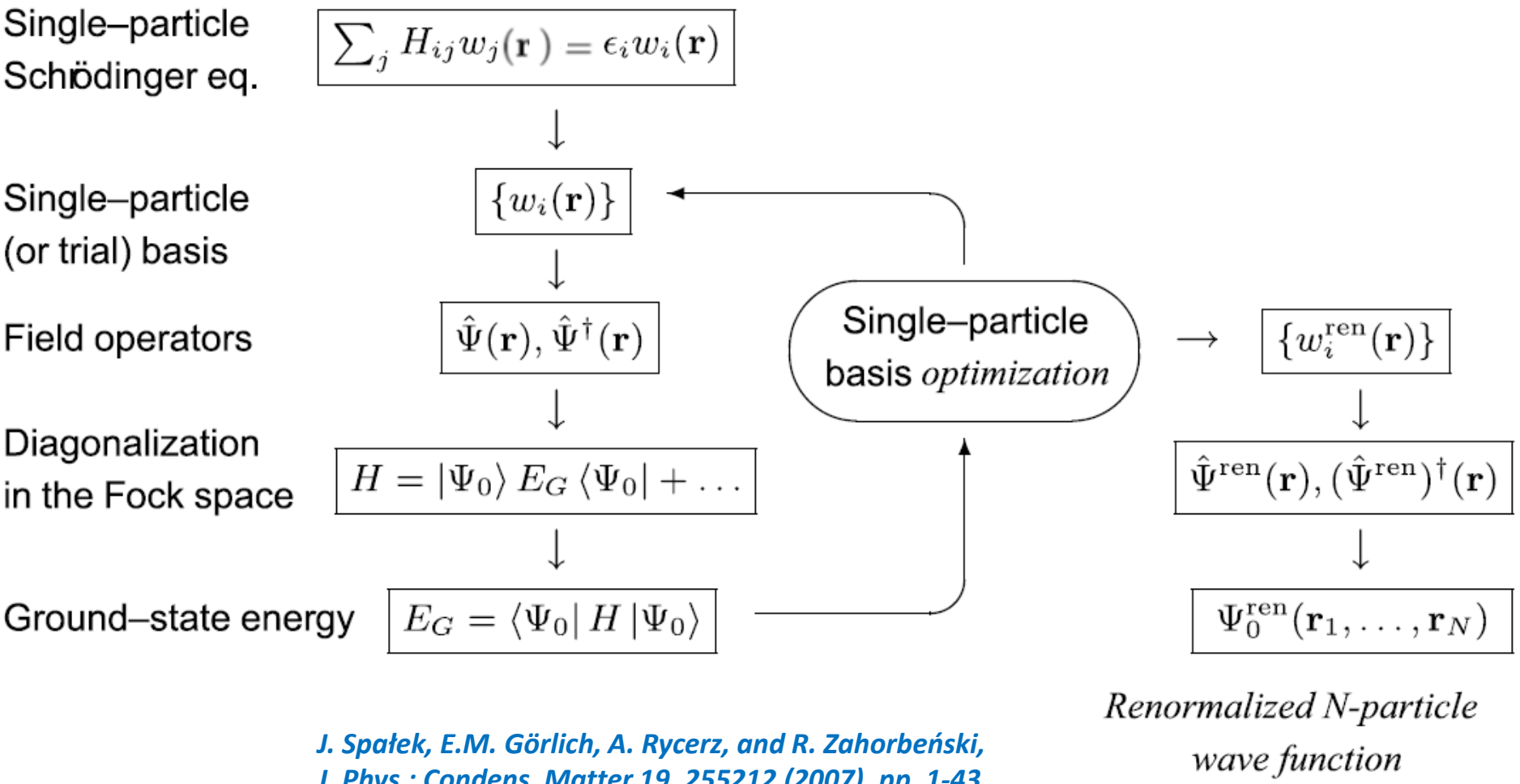
**Euler variational equation for renormalized Wannier wave function (in correlated state)**

$$\frac{\delta(E_G - \mu N)}{\delta w_i^*(\mathbf{r})} - \nabla \frac{\delta(E_G - \mu N)}{\delta(\nabla w_i^*(\mathbf{r}))} - \sum_{i \geqslant j} \lambda_{ij}\, w_j(\mathbf{r}) = 0$$

**Output: Renormalized Wannier function, explicit form of ground-state energy …**

**NOTE: No double counting of interaction whatsoever**

# Flowchart of EDABI calculations




*J. Spałek, E.M. Görlich, A. Rycerz, and R. Zahorbeński, J. Phys.: Condens. Matter 19, 255212 (2007), pp. 1-43 (Mott Centennial Symposium, Cambridge)*

# EDABI: Example of He atom

**Define field operator**

$$\hat{\Psi}(\mathbf{r}) = \Phi_{\uparrow}(\mathbf{r})\hat{a}_{\uparrow} + \Phi_{\downarrow}(\mathbf{r})\hat{a}_{\downarrow}$$

**Hamiltonian in the 2nd quantization**

$$H = \varepsilon_a(\hat{n}_{\uparrow} + \hat{n}_{\downarrow}) + U\hat{n}_{\uparrow}\hat{n}_{\downarrow}$$

where $\hat{n}_{\sigma} = \hat{a}^{\dagger}_{\sigma}\hat{a}_{\sigma}$, whereas

$$\varepsilon_a = \langle \Phi_{\sigma} | H_1 | \Phi_{\sigma} \rangle,$$

and

$$U = \langle \Phi_{\sigma}\Phi_{\overline{\sigma}} | V | \Phi_{\overline{\sigma}}\Phi_{\sigma} \rangle$$

are the matrix elements of the single-particle part defined as

$$H_1 = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{\kappa_0 r_1} - \frac{2e^2}{\kappa_0 r_2} \overset{a.u.}{\equiv} -\nabla_1^2 - \nabla_2^2 - \frac{4}{r_1} - \frac{4}{r_2}$$

$1s$-type Slater orbitals for the He atom

$$\Phi_{\sigma}(\mathbf{r}) = (\alpha^3/\pi)^{1/2}\exp(-\alpha r)\chi_{\sigma}$$

# He atom: renormalized wave equation

**Ground state energy for fixed No. of electrons**

$$E\{\Phi_\sigma(\mathbf{r})\} = \sum_\sigma \int d^3r \Phi^*_\sigma(\mathbf{r}) H_1(\mathbf{r}) \Phi_\sigma(\mathbf{r}) + \frac{1}{2} \sum_\sigma \int d^3r d^3r' |\Phi_\sigma(\mathbf{r})|^2 V_{12}(\mathbf{r}-\mathbf{r}') |\Phi_{\overline{\sigma}}(\mathbf{r})|^2$$

**Renormalized wave equation of the unrestricted Hartree form**

$$\left(\nabla^2 - \frac{2e^2}{\kappa_0 r}\right) \Phi_\sigma(\mathbf{r}) + \Phi_\sigma(\mathbf{r}) \int d^2r' \frac{e^2}{\kappa_0 |\mathbf{r}-\mathbf{r}'|} |\Phi_{\overline{\sigma}}(\mathbf{r}')|^2 = \lambda \Phi_\sigma(\mathbf{r})$$

**Optimized Bohr-orbit radii:**

| | $a_{1s}$ | $a_{2s}$ | $a_{2p}$ | $S$ | $E_G$ (Ry) |
|---|---|---|---|---|---|
| H | 1 | 2 | 2 | 0 | -1 |
| $H^-$ | 0.9696 | 1.6485 | 1.017 | -0.1 | -1.0487 |
| He | 0.4274 | 0.5731 | 0.4068 | -0.272 | -5.79404 |
| $He^-$ | 1.831 | 1.1416 | 0.4354 | -0.781 | -5.10058 |
| Li | 0.3725 | 1.066 | 0.2521 | 0.15 | -14.8334 |
| $Be^+$ | 0.2708 | 0.683 | 0.1829 | 0.109 | -28.5286 |

# Example II: $H_2$ molecule

**Hamiltonian**

$$\mathcal{H} = \sum_{i\sigma} \varepsilon_i \hat{n}_{i\sigma} + t \sum_{\sigma} \left( \hat{a}^{\dagger}_{2\sigma} \hat{a}_{1\sigma} + \hat{a}^{\dagger}_{1\sigma} \hat{a}_{2\sigma} \right) + \sum_{i=1}^{5} U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} K_{ij} \hat{n}_i \hat{n}_j$$
$$- \frac{1}{2} \sum_{i \neq j} J_{ij} \left( \mathbf{S_i} \cdot \mathbf{S_j} - \frac{1}{2} \hat{n}_i \hat{n}_j \right) + \sum_{i \neq j} J_{ij} \hat{a}^{\dagger}_{i\uparrow} \hat{a}^{\dagger}_{i\downarrow} \hat{a}_{j\downarrow} \hat{a}_{j\uparrow} + \sum_{i \neq j \sigma} V_{ij} \hat{n}_{i\bar{\sigma}} \hat{a}^{\dagger}_{i\sigma} \hat{a}_{j\sigma}.$$

$$E_G \equiv \lambda_5 = 2\varepsilon_a + \frac{1}{2}(U+K) + J - \frac{1}{2}\Big( (U-K)^2 + 16(t+V)^2 \Big)^{1/2}$$

$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \frac{1}{\sqrt{2}} \langle 0 | \hat{\Psi}(\mathbf{r}_1) \hat{\Psi}(\mathbf{r}_2) | G \rangle$$

**Ground-state two-particle wave function:**

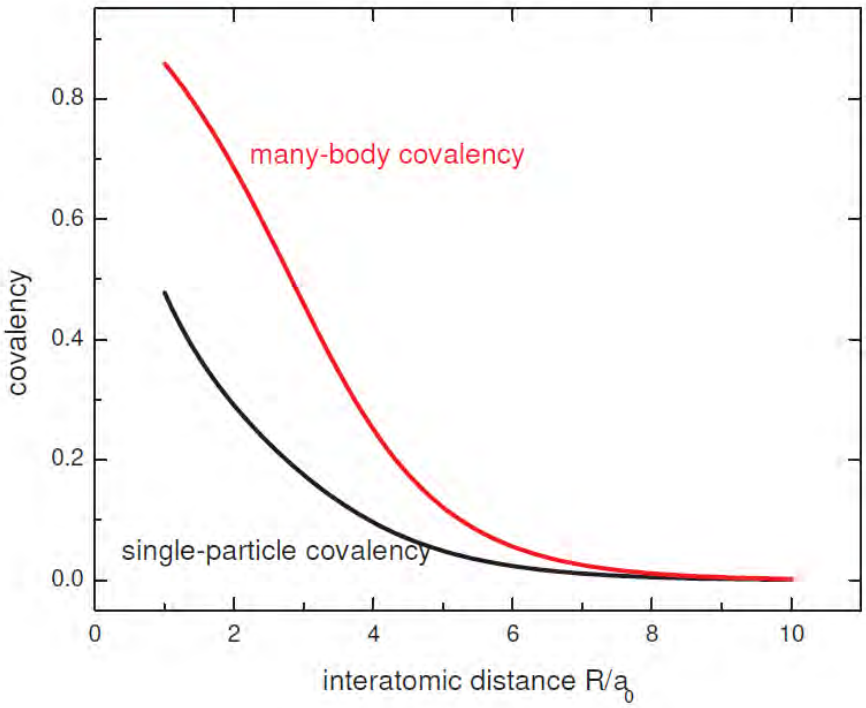
$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2) = \frac{2(t+V)}{\sqrt{2D(D-U+K)}} \Phi_c(\mathbf{r}_1, \mathbf{r}_2) - \frac{1}{2} \sqrt{\frac{D-U+K}{2D}} \Phi_i(\mathbf{r}_1, \mathbf{r}_2)$$

$$D \equiv \left( (U-K)^2 + 16(t+V)^2 \right)^{1/2}$$

$$\Phi_c(\mathbf{r}_1, \mathbf{r}_2) = \Big( w_1(\mathbf{r}_1) w_2(\mathbf{r}_2) + w_1(\mathbf{r}_2) w_2(\mathbf{r}_1) \Big) \Big( \chi_{\uparrow}(\mathbf{r}_1) \chi_{\downarrow}(\mathbf{r}_2) - \chi_{\downarrow}(\mathbf{r}_1) \chi_{\uparrow}(\mathbf{r}_2) \Big)$$

$$\Phi_i(\mathbf{r}_1, \mathbf{r}_2) = \Big( w_1(\mathbf{r}_1) w_1(\mathbf{r}_2) + w_2(\mathbf{r}_1) w_2(\mathbf{r}_2) \Big) \Big( \chi_{\uparrow}(\mathbf{r}_1) \chi_{\downarrow}(\mathbf{r}_2) - \chi_{\downarrow}(\mathbf{r}_1) \chi_{\uparrow}(\mathbf{r}_2) \Big)$$

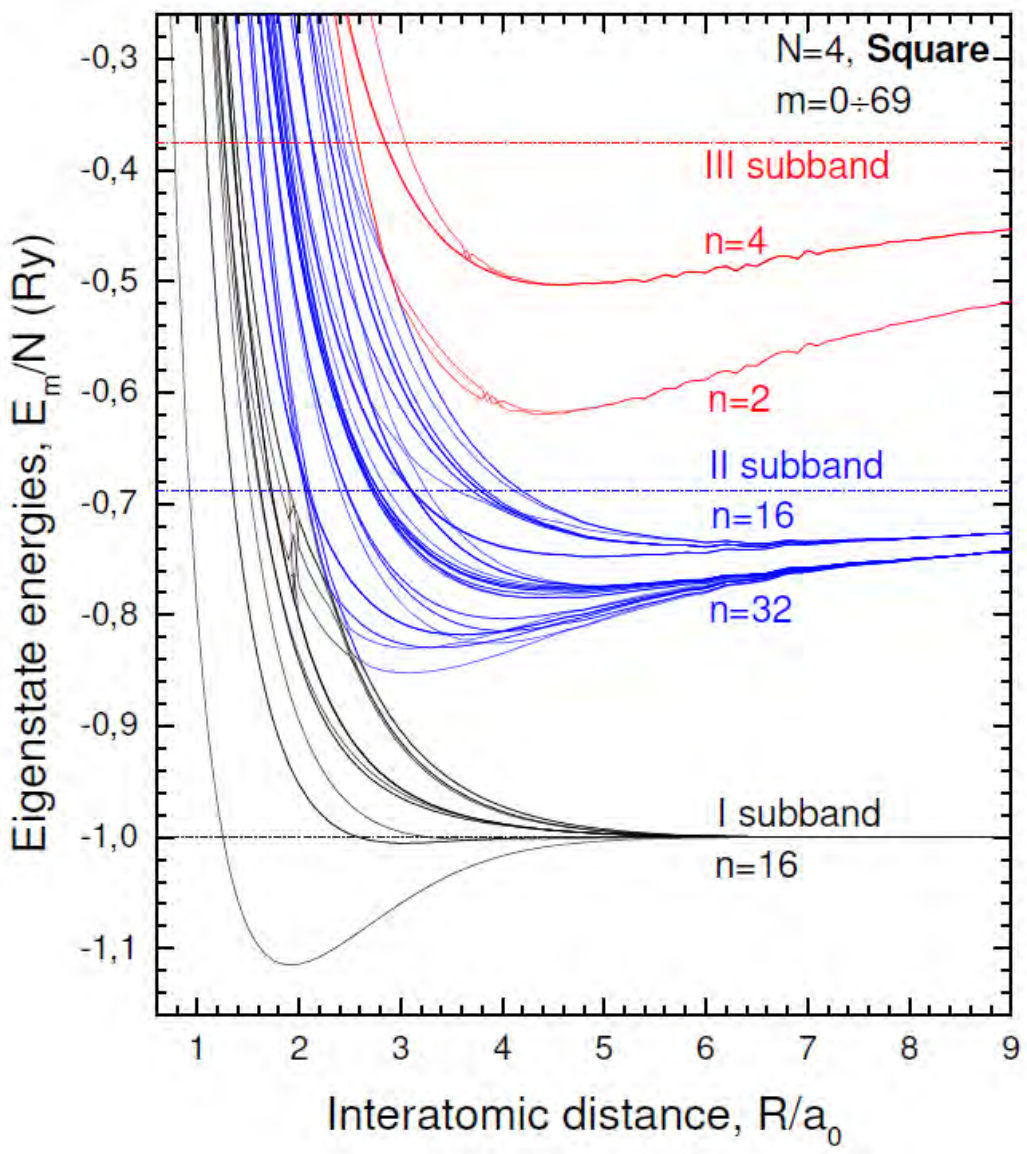
# Many-particle vs. single-part. bonding



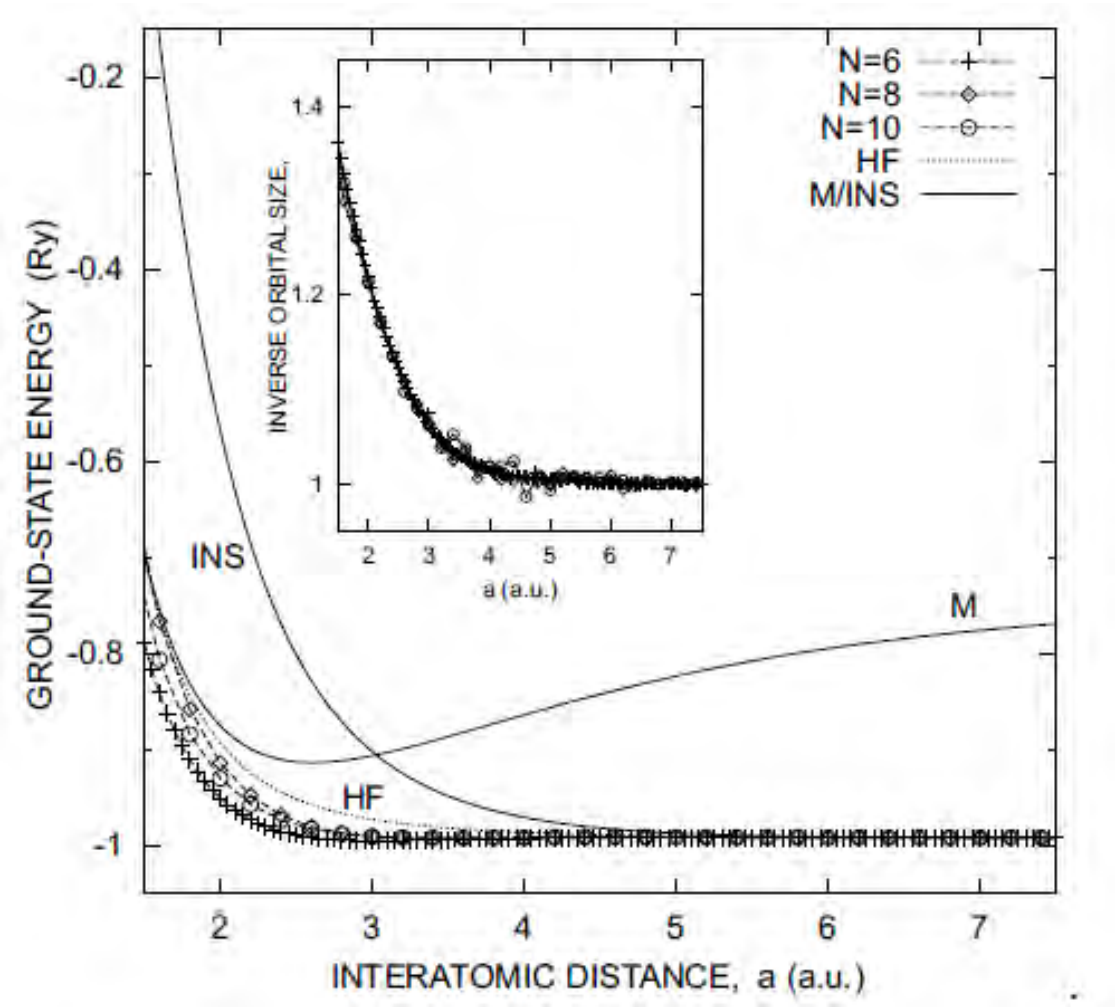

$$w_i(\mathbf{r}) = \beta\left(\Phi_i(\mathbf{r}) - \gamma\Phi_j(\mathbf{r})\right)$$

$\gamma$ **- single particle covalency**

# Square of hydrogen atoms: Hubbard subbands

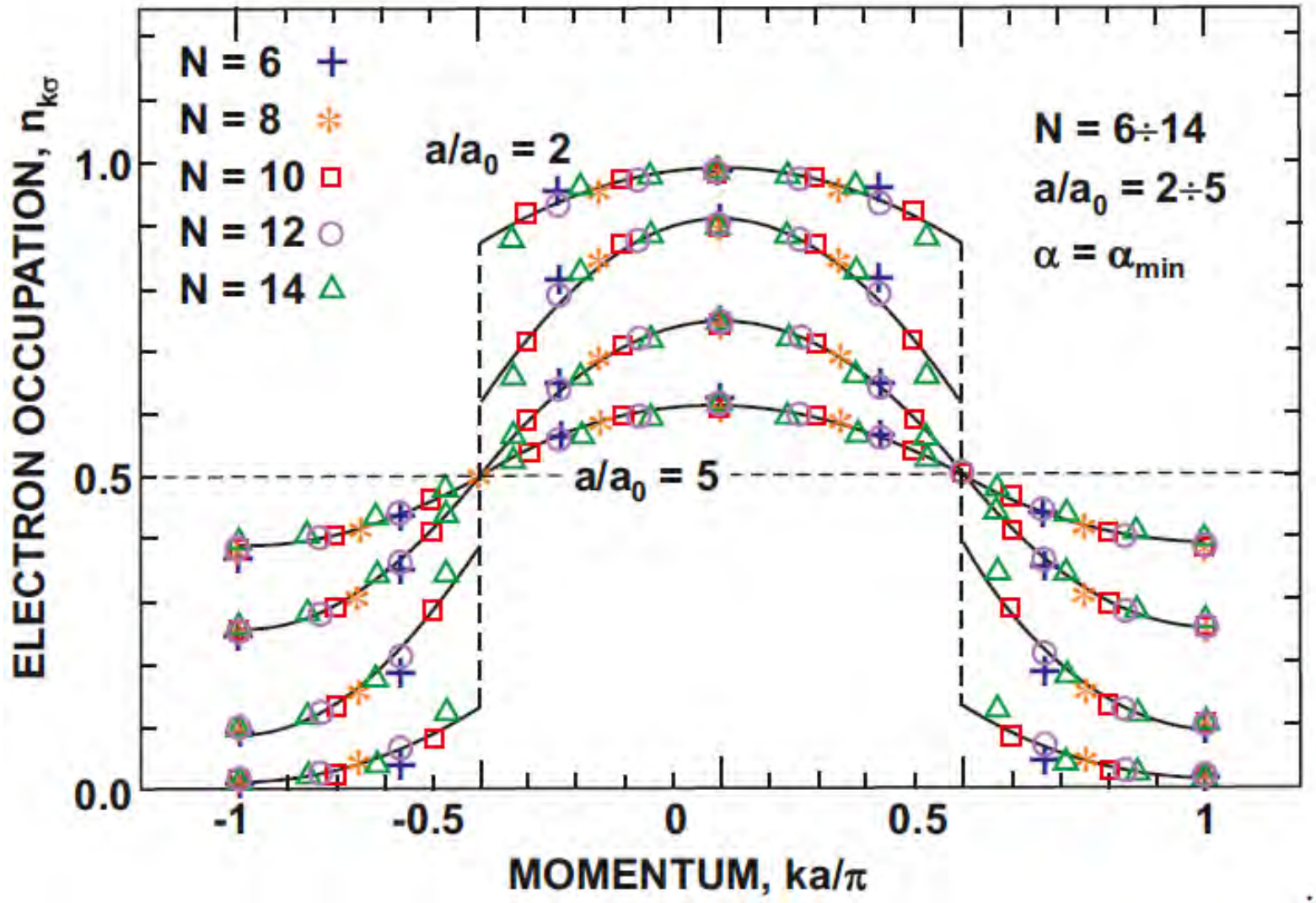


# Hydrogen chain of N atoms

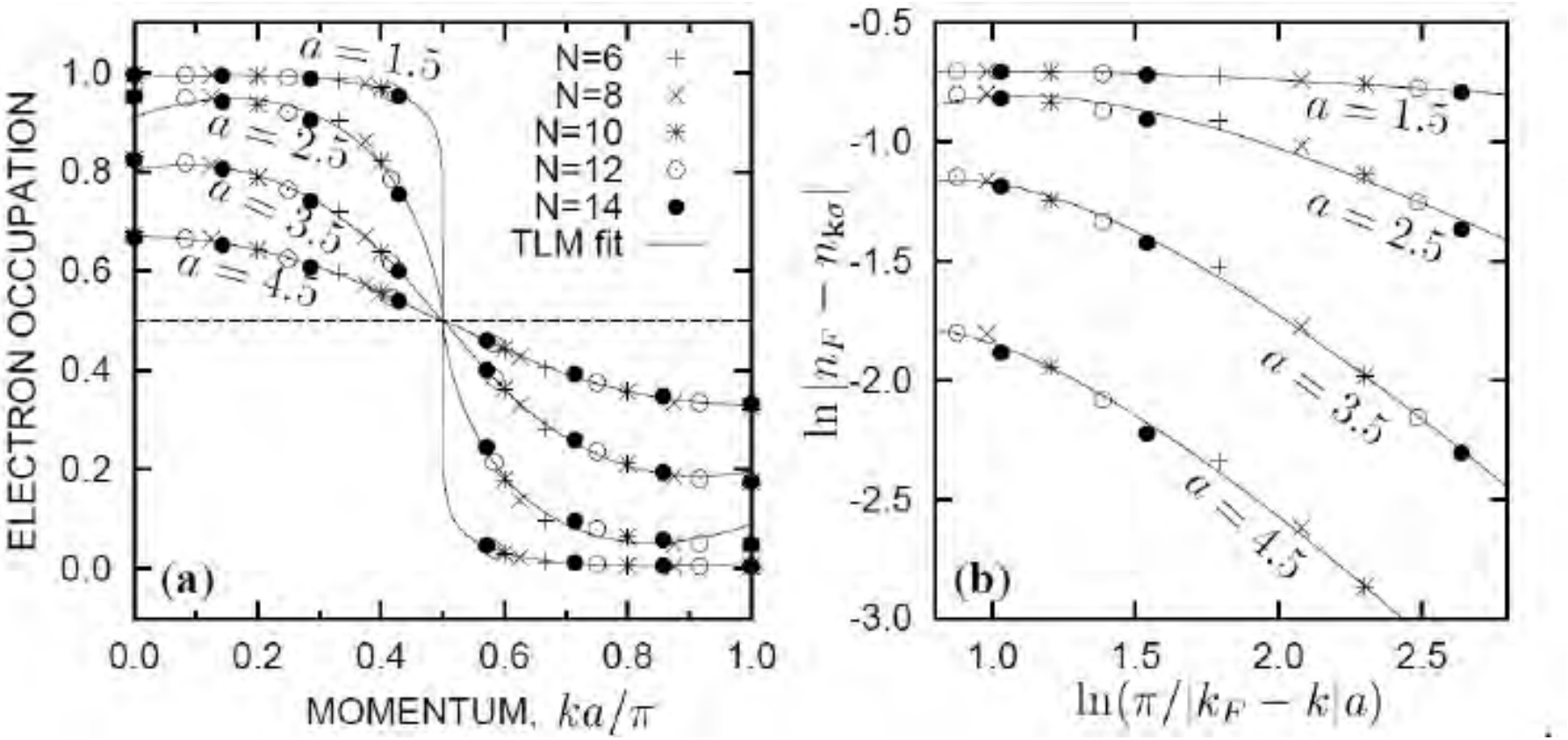



*A. Rycerz, Ph.D. Thesis, Jagiellonian University, Kraków (unpublished)*

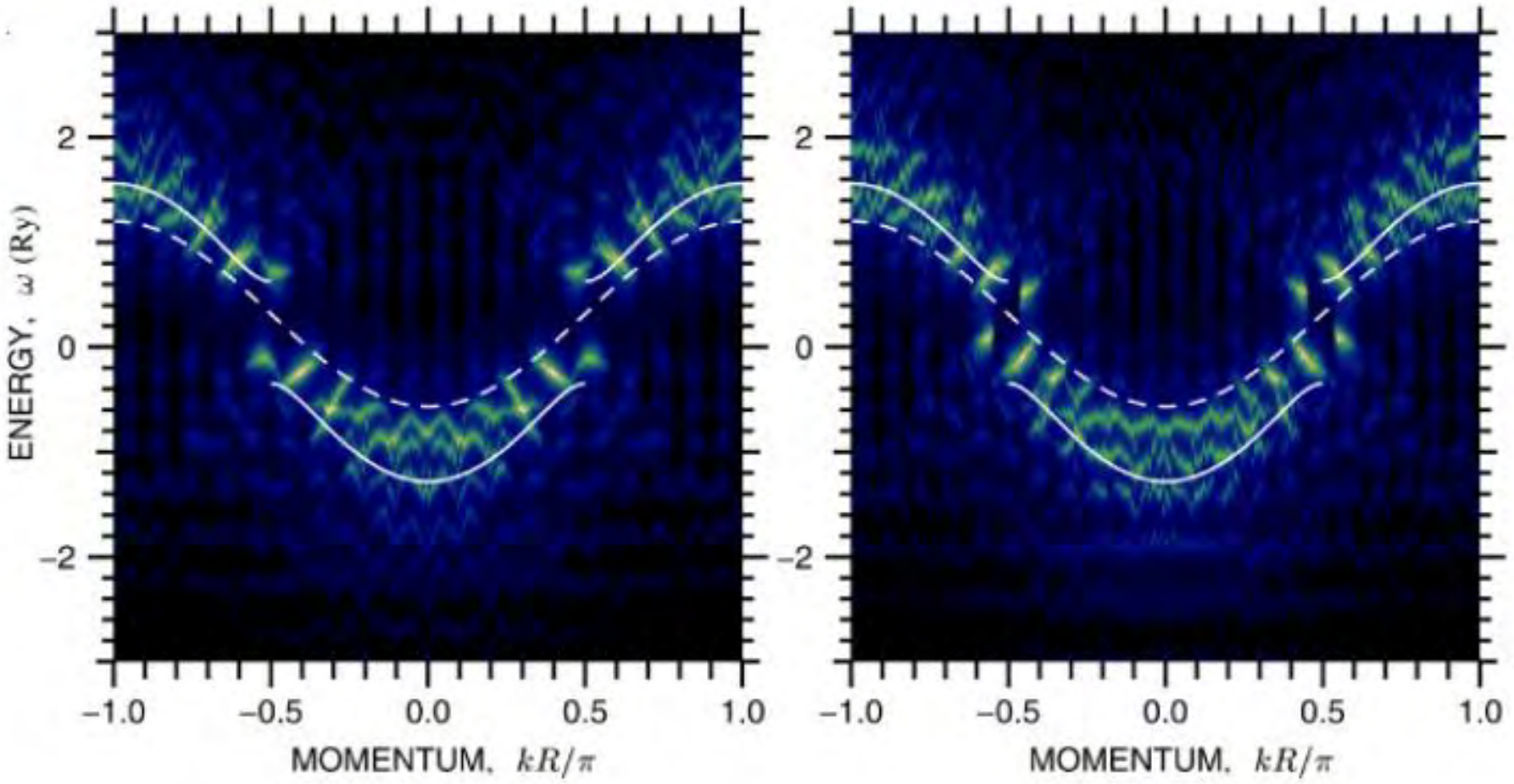
# Statistical distribution: From F-D to localized



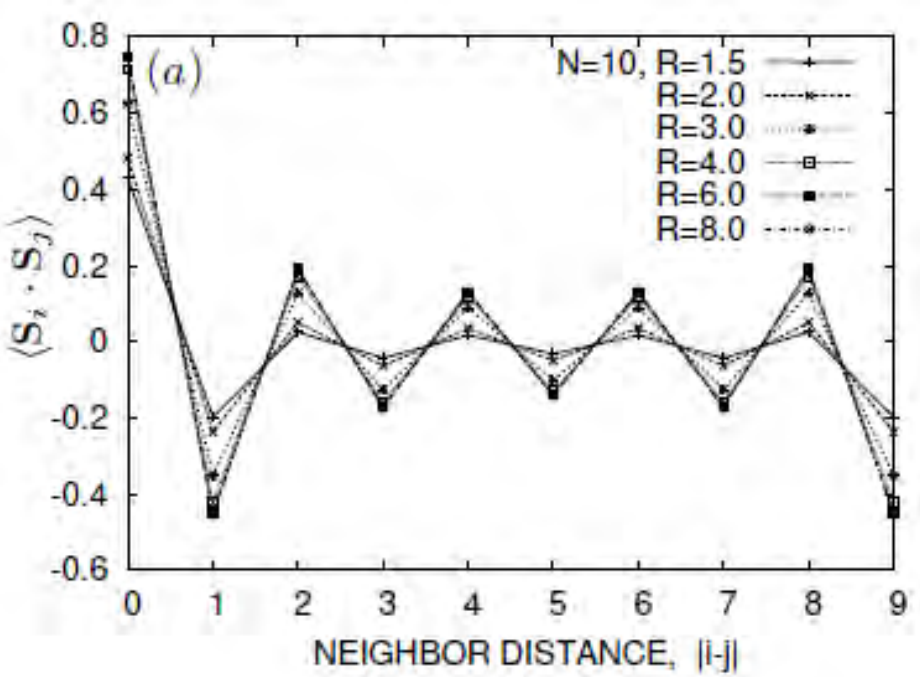
# Luttinger-liquid fit

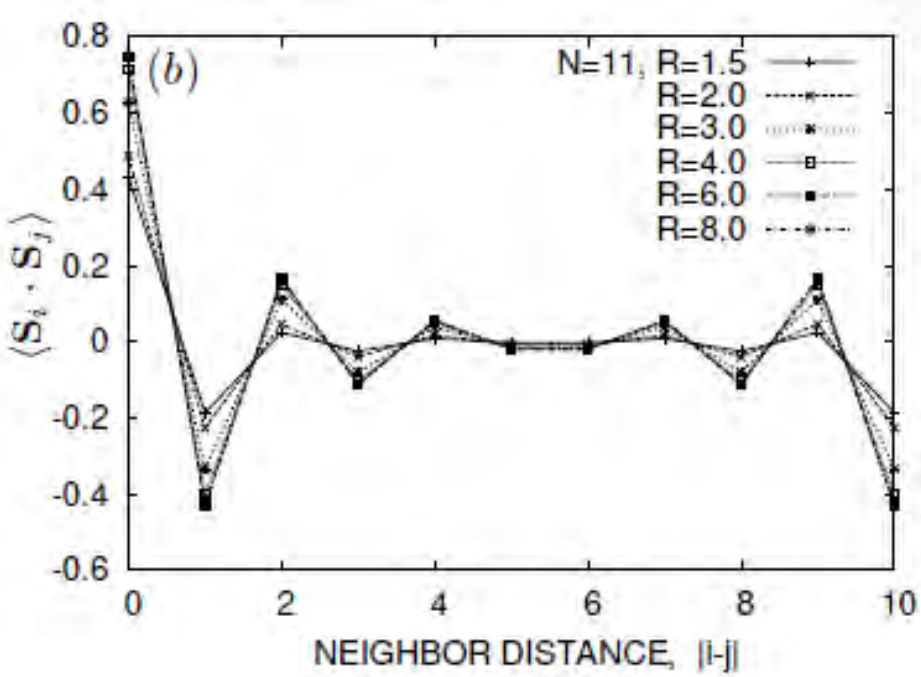


# Renormalized electronic structure

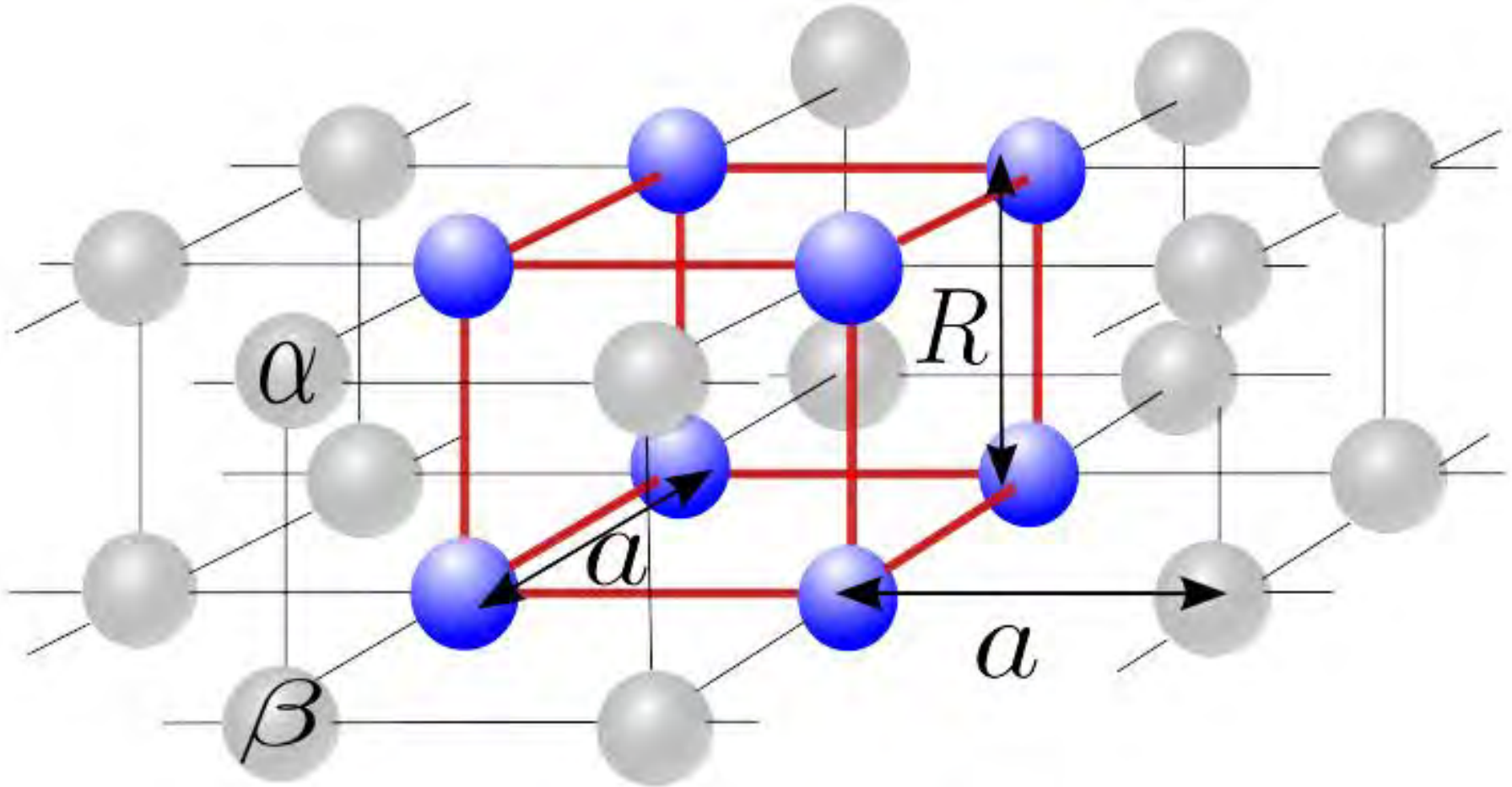


# Spin-spin correlation function

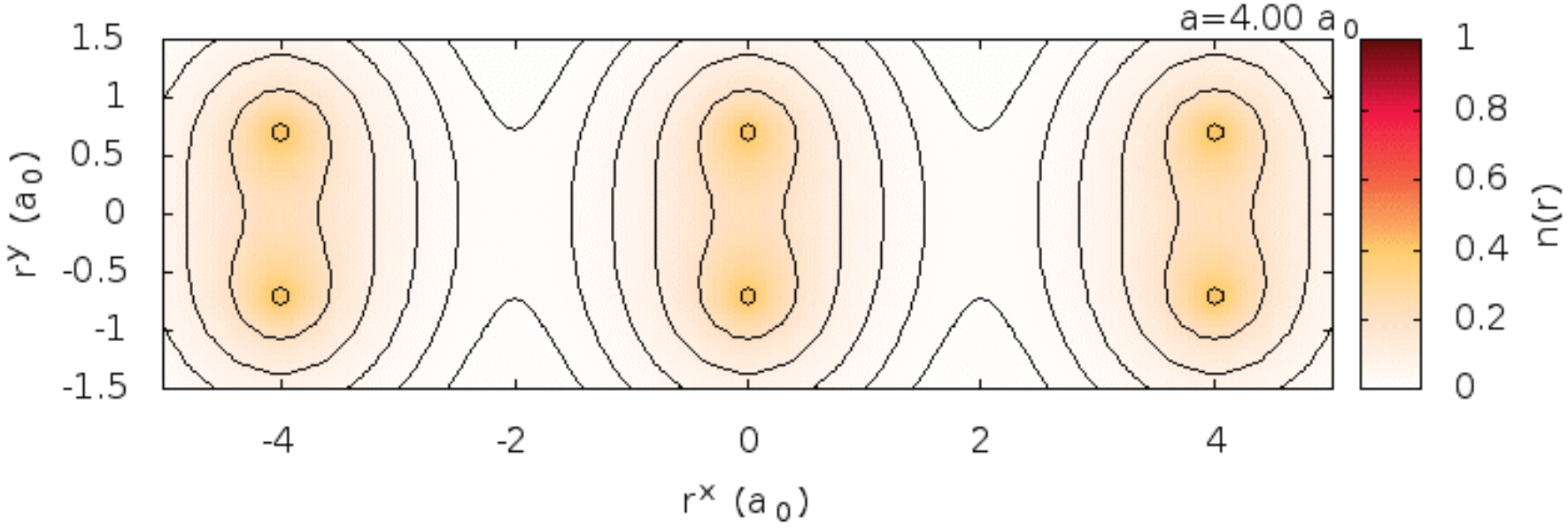


# Stack of hydrogen molecules

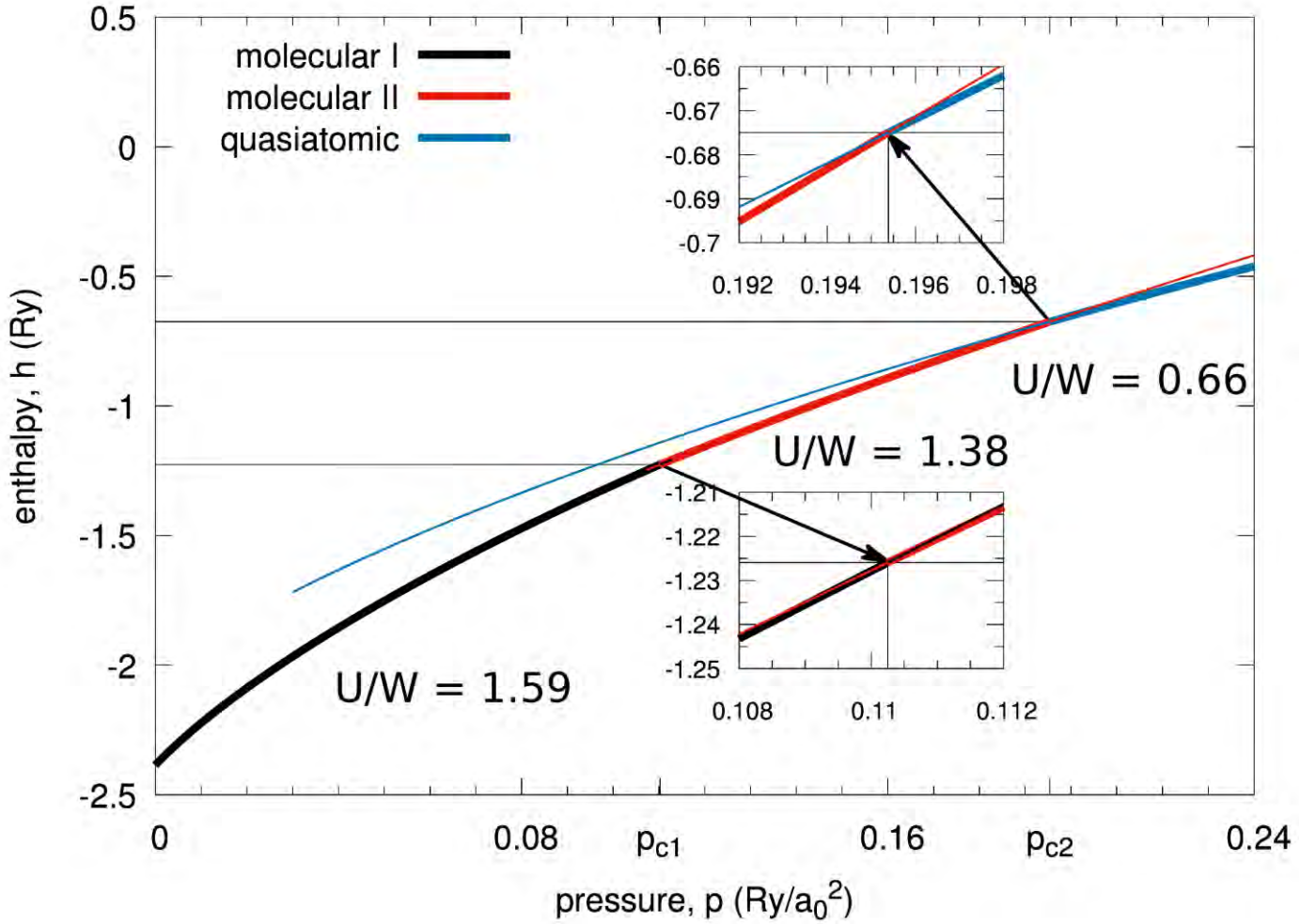


# wodór molekularny → atomowy: $H_2$ → 2H




*A. Biborski, A. Kądzielawa & JS, Comp. Phys. Comm. 197,7-16 (2015);*
*A. P. Kądzielawa, A. Biborski & JS, Phys. Rev. B 92 161101(R) (2015);*
*A. Biborski, A. Kądzielawa & JS, arXiv (2017); PRB (submitted)*

# Metal-insulator transitions for $H_2$ stack




*A. Biborski, A. P. Kądzielawa & J. Spałek, Phys. Rev. B 96, 085101 (2017), pp. 1-14.*

# Outlook

- Strongly correlated electrons encompass limiting situation of condensed matter physics, with unique (thermo)dynamic properties
- EDABI as a method making the theory of correlated systems complete – **calculations of microscopic parameters and electronic structure within a single approach**, without double counting. **So far**, EDABI computable for simple original orbital structures. Can serve as a reference method for testing approxiamte solutions.
- **EDABI: Evolution of properties in correlated state are discussed as a function of lattice parameter, not only vs. model parameters**
- Hubbard model Lieb-Wu solution with calculation of U and t for arbitrary lattice spacing has been implemented with EDABI (please ask, if you are interested)