

Physics of Strongly Correlated Electrons: Selected Topics

Jozef Spałek

Marian Smoluchowski Institute of Physics,
Jagiellonian University
and AGH University of Science and Technology
PL - 30-059 KRAKÓW



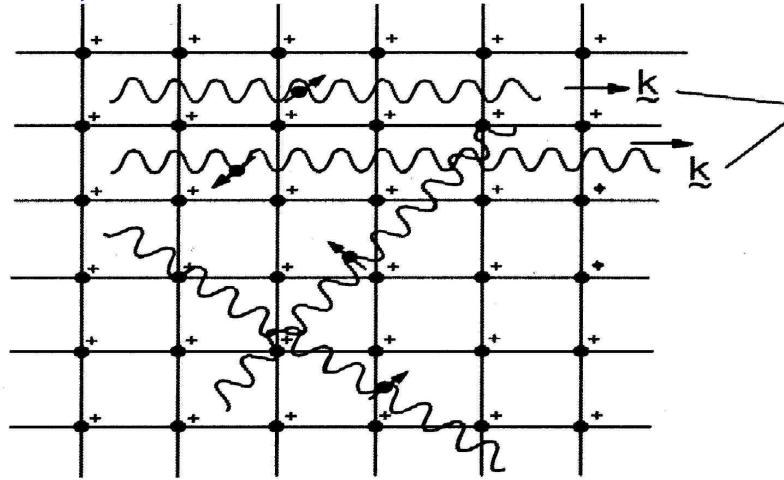
Contents

Lecture I: Metal-insulator transition at $T>0$

- 1. Elementary derivation of Gutzwiller approach,
Brinkmann-Rice criterion**
- 2. Mott criterion**
- 3. Thermodynamics of Mott transition**
- 4. 1st and 2nd quantization combined**
- 5. Critical and quantum critical behavior**
- 6. Orbitally degenerate bands**
- 7. Spin-split masses, metamagnetism**

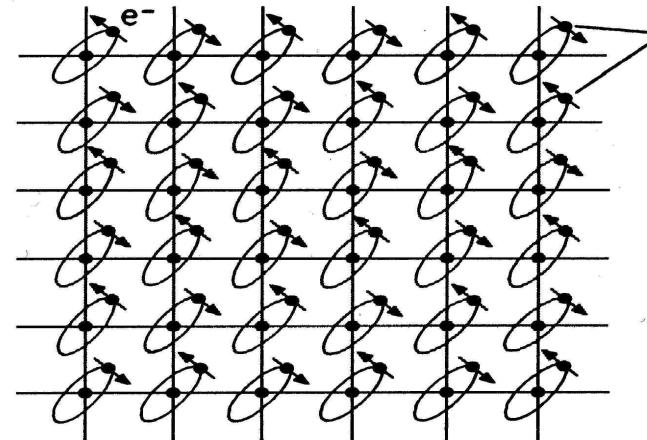
Delocalized versus localized

a) Metal



Plane waves
(Bloch states)

b) Mott-Hubbard insulator



Atomic states

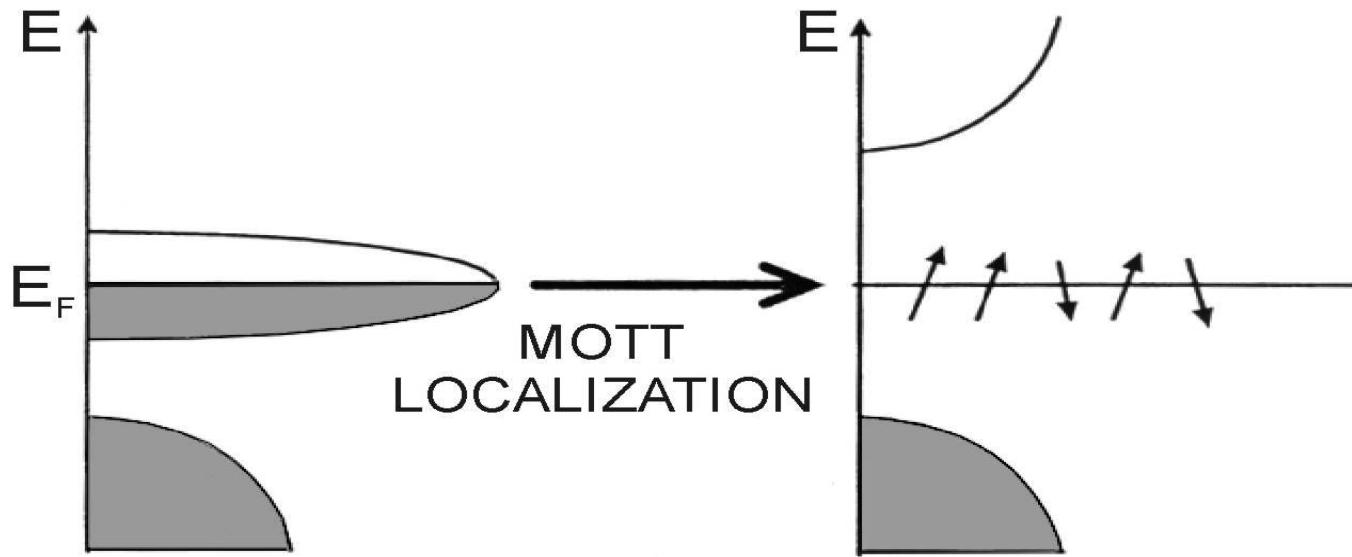
Magnetic versus superconducting

<i>4f</i>	La	Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
<i>5f</i>	Ac Th Pa U Np Pu Am Cm Cm Bk Cf Es Fm Md No Lr	
<i>3d</i>	Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn	
<i>4d</i>	Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd	
<i>5d</i>	Ba Lu Hf Ta W Re Os Ir Pt Au Hg	

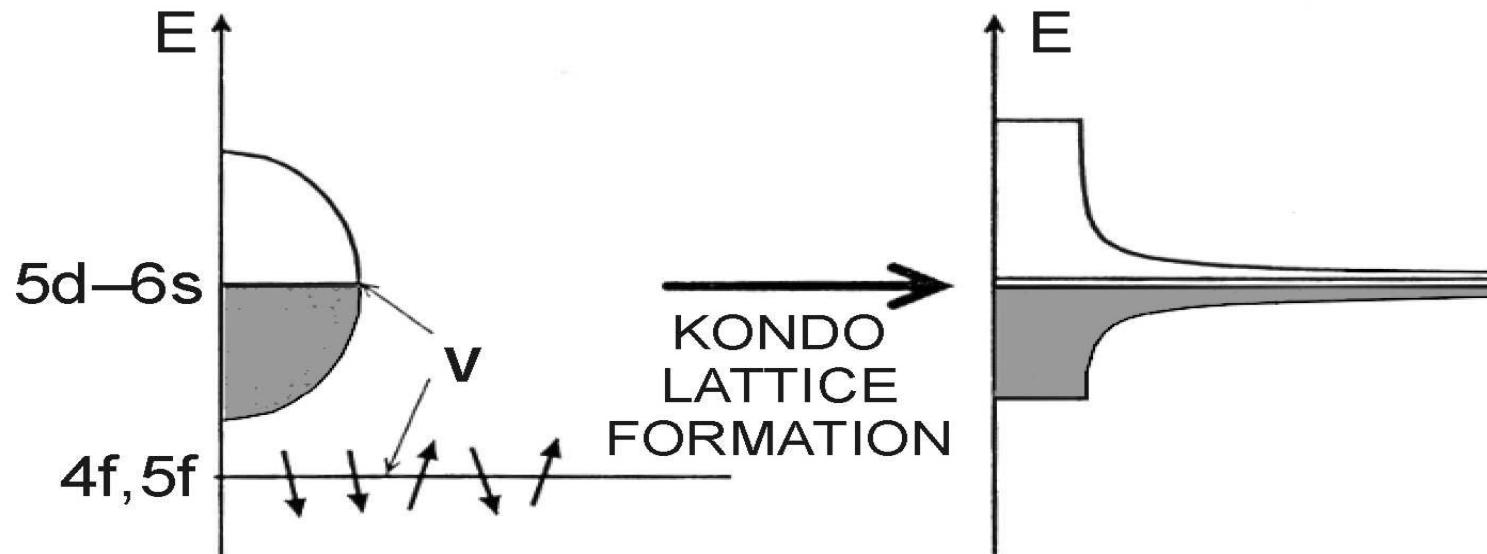
■ Magnetic

■ Superconducting

Narrow-band systems (3d)



Hybridized systems (f)



Localization criterion: Mott (Wigner)

Kinetic energy in e⁻ gas/particle

$$\overline{\epsilon} = \frac{3}{5} \epsilon_F = \frac{3}{5} \frac{\hbar^2}{2m^*} \left(3\pi^2 \frac{N}{V} \right)^{2/3} \sim \rho^{2/3}$$

Electron-electron repulsion energy/particle

$$\epsilon_{e-e} = \frac{1}{2} \frac{e^2}{\epsilon d_{e-e}} = \frac{e^2}{2\epsilon} \rho^{1/3}$$

Where the classical interparticle distance is

$$d_{e-e} = \left(\frac{V}{N} \right)^{1/3}$$

Instability of the electron gas concept if:

$$\overline{\epsilon} = \epsilon_{e-e} \quad \longrightarrow \quad \text{gas instability}$$

Note: e-e interaction dominates if $\epsilon_{e-e} > \overline{\epsilon}$, i.e. $\rho < \rho_c$

$$\underbrace{\left(\frac{\hbar^2}{m^* e^2} \epsilon \right)}_{a_B} \rho_c^{1/3} = \frac{5}{3} \frac{1}{(3\pi^2)^{2/3}} \approx 0.17$$

$a_B \rightarrow$ effective Bohr radius

$a_B \cdot \rho_c^{1/3} \approx 0.17 \sim 0.2$

Other effects \Rightarrow Fermi - sphere collaps?

In one dimension:

$a_B \rho_C \approx 1 \Rightarrow R_C \approx a_B$

Yet another Mott criterion of localization

A different derivation by Mott (1961).

Attractive potential screened by gas (Kittel,1990)

$$V(r) = -\frac{e^2}{\kappa r} \exp(-q r)$$

q is the inverse Thomas-Fermi screening length

$$q = \frac{4 m^* e^2 n_c^{1/3}}{\epsilon \hbar^2}$$

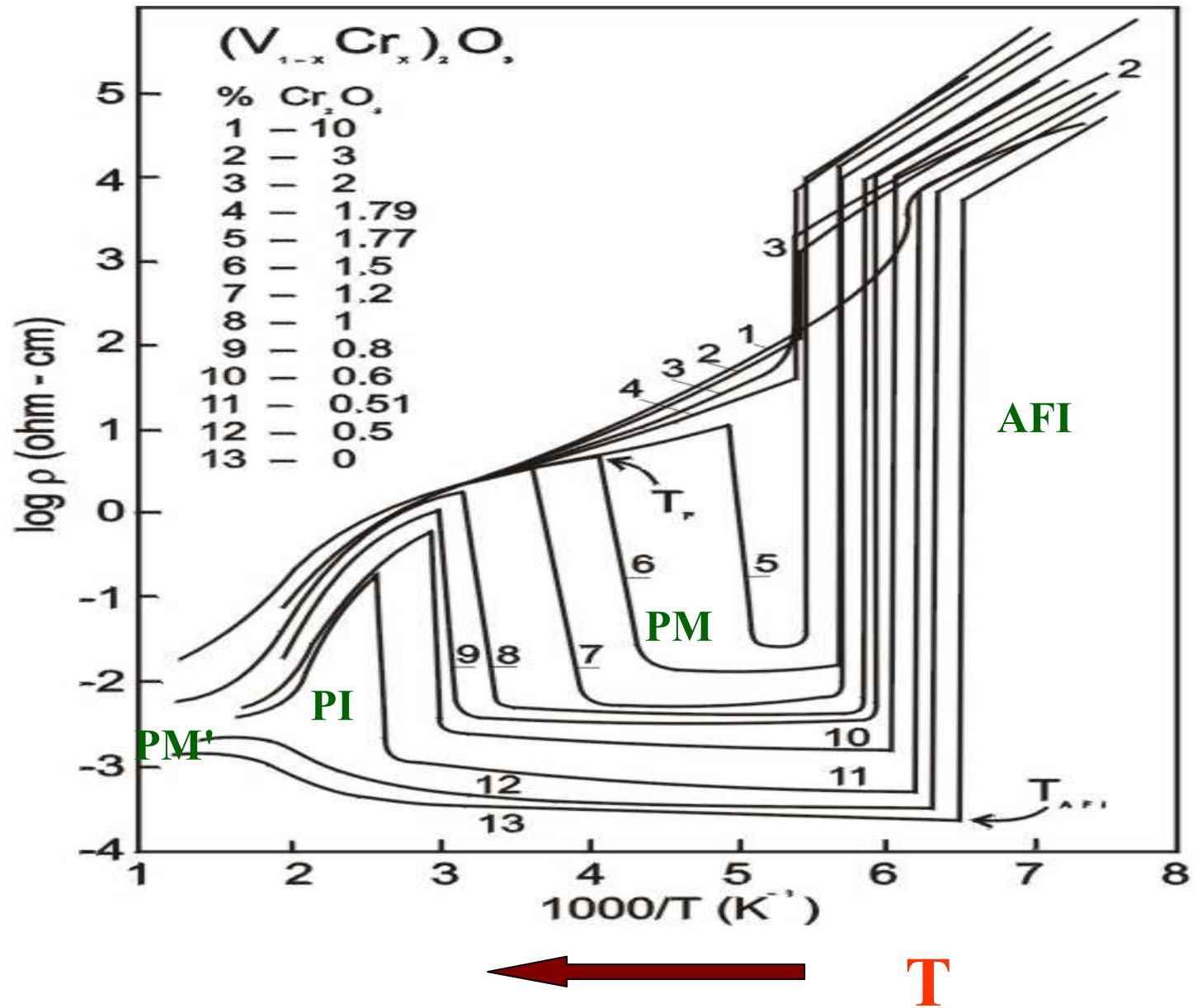
A screened potential does not lead to a bound state if (Landau, Lifshitz, 1990):

$$q > \frac{m^* e^2}{\epsilon \hbar^2} = a_B^{-1}$$

$$q^{-1} = a_B \Rightarrow n_c^{1/3} a_B = 0.25$$

First period: 1980-2000

J.S. Eur. J. Phys. 21, 511-34 (2001)



H. Kuwamoto et al., PRB 22 (1980) 2626

$$H=\epsilon_a^{\rm eff}\sum_jn_j+t\sum_{j\sigma}\left(e^{-i\phi/N}c_{j\sigma}^\dagger c_{j+1\sigma}+{\rm h.c.}\right)+U\sum_in_{i\uparrow}n_{i\downarrow}+\sum_{i<j}K_{ij}\delta n_i\delta n_j,$$

$$\delta n_i \,\equiv\, n_i - 1, \, \epsilon_a^{\rm eff} \,=\, \epsilon_a + N^{-1} \sum\nolimits_{i < j} \bigl(2/R_{ij} + K_{ij} \bigr)$$

$$t_{\langle ij\rangle}\equiv\quad t\quad\equiv\left\langle w_i\Big|H_1\Big|w_j\right\rangle$$

$$U\equiv\quad\left\langle w_i\,\,w_i\Big|V_{12}\Big|\,w_i\,\,w_i\right\rangle$$

$$K_{ij}\equiv\quad\left\langle w_i\,\,w_j\Big|V_{12}\Big|\,w_i\,\,w_j\right\rangle$$

Atomic functions

$$\Phi_i(\mathbf{r}) = \left(\pi \alpha^3 \right)^{1/2} \exp(-\alpha |\mathbf{r} - \mathbf{R}_i|)$$

$$\langle \Phi_i | \Phi_j \rangle = S_{ij}$$

Wannier functions

$$w_i(\mathbf{r}) = \sum_j \beta_{ij} \Psi_j(\mathbf{r})$$

$$\langle w_i | w_j \rangle = \delta_{ij}$$

Qualitative characteristics:

- 1) Bare band width** $W = 2z|t| ; t = \int d^3r w_i(\mathbf{r}) H_1 w_j(\mathbf{r})$
- 2) Coulomb repulsion** $U = \int d^3r d^3r' |w_i(\mathbf{r})|^2 \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |w_i(\mathbf{r}')|^2$
- $$\left(K_{ij} = \int d^3r d^3r' |w_i(\mathbf{r})|^2 \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |w_j(\mathbf{r}')|^2 \right)$$
- 3) Band filling** $n = \sum_{\sigma} \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle = \frac{1}{N} \sum_{\sigma, k \leq k_F} \langle a_{k\sigma}^\dagger a_{k\sigma} \rangle$
- (empty) $0 \leq n \leq 2$ (full)

Metallic limit:

$$U, K \ll W$$

MIT:

$$U \cong W$$

Strong correlations:

$$W \ll U$$

Physically U/W – important parameter

$$(U - K)$$

**The concept of band narrowing
(renormalization)
and
competition between band and
Coulomb energies**

Why electronic transition?

- **Band (kinetic) energy:** $W = 1 \div 2 \text{ eV}$
- **Coulomb repulsion energy:** $U \sim \text{few eV}$
- **Thermal energy:** $k_B T \sim 10 \text{ meV}$ ($T \sim 100 \text{ K}$)
- **Why phase transition possible?** For $U \sim U_C \sim W$

$$W \rightarrow \tilde{W} = W q \leq 0.1 \text{ eV}$$

$$U \langle n_{i\uparrow} n_{i\downarrow} \rangle \sim 0.1 \text{ eV}$$

$$\frac{E_G}{N} = -\frac{q W}{4} + U \langle n_{i\uparrow} n_{i\downarrow} \rangle \sim k_B T, g \mu_B H_a, \text{disorder}$$

Canonical model: Hubbard (results):

$$\frac{E_G}{N} = \frac{\langle H \rangle}{N} = \frac{1}{N} \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} f(E_{\mathbf{k}}) + U \underbrace{\langle n_{i\uparrow} n_{i\downarrow} \rangle}_{=d^2}$$

$$\left\{ \begin{array}{l} E_{\mathbf{k}} = q(d^2) \in_{\mathbf{k}} \\ q(d^2) = 8d^2(1 - 2d^2) < 1 \end{array} \right.$$

$E_G = E_{\min} :$ **$U_C \equiv 8|\epsilon|$** :

$$\left\{ \begin{array}{l} d^2 = \frac{1}{4} \left(1 - \frac{U}{U_C} \right), \quad 8|\epsilon| = U_C \\ \frac{E_G}{N} = \left(1 - \frac{U}{U_C} \right)^2 \epsilon \\ \frac{m^*}{m_0} = \frac{1}{1 - \left(\frac{U}{U_C} \right)^2} \sim \gamma \rightarrow \infty \\ \frac{x}{\gamma} = \frac{1 + \frac{U}{2U_C}}{\left(1 + \frac{U}{U_C} \right)^2} \sim 4 \end{array} \right.$$

**Simplest model: Hubbard model at half filling ($n=1$):
classical regime for fermion systems –**

**Nonzero temperature (statistical physics):
consequences of mass renormalization, etc.**

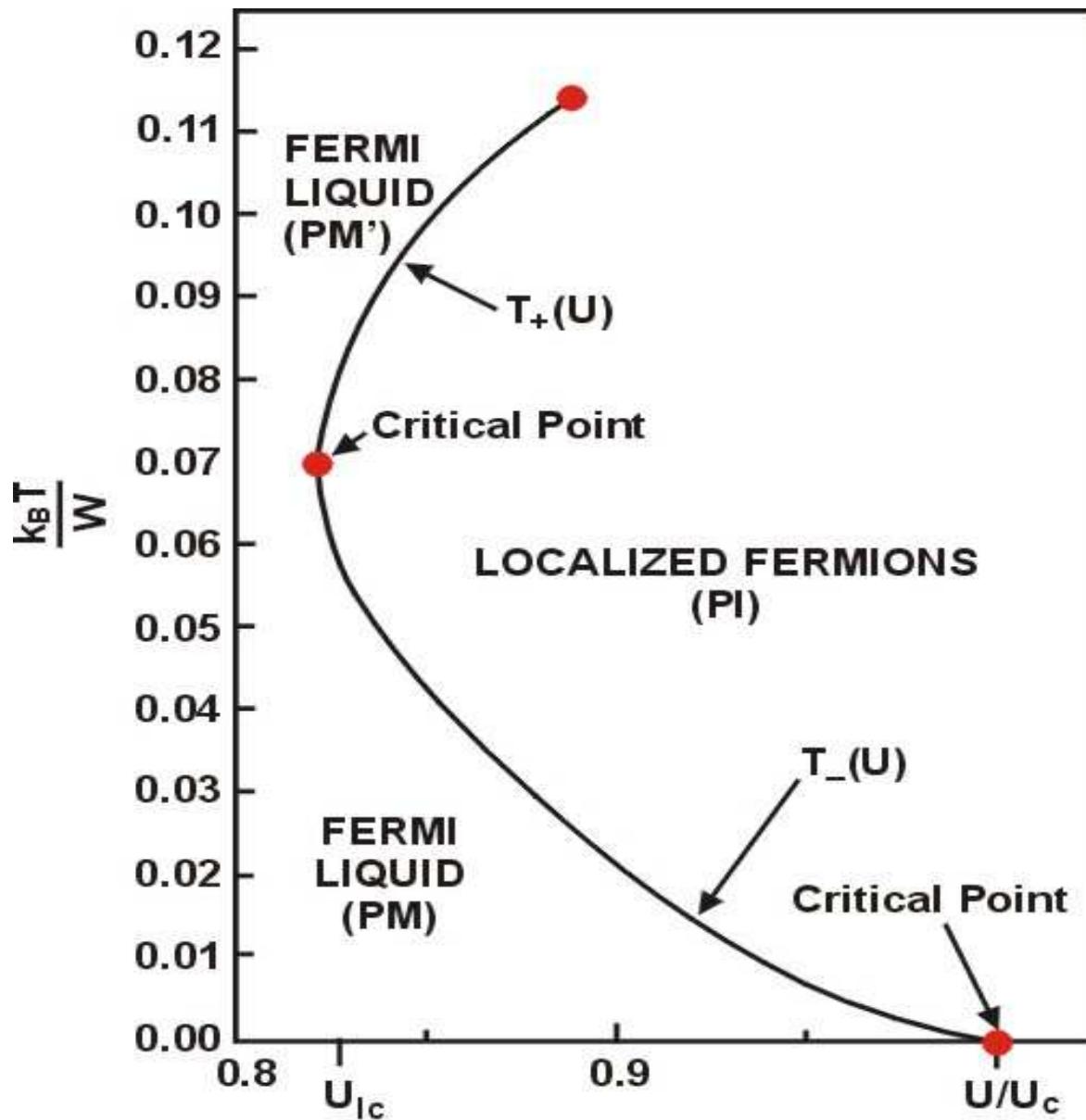
THERMODYNAMICS:

$$\left\{ \begin{array}{l} F_{\text{metal}} = \left(1 - \frac{U}{U_c}\right)^2 \quad \epsilon = -\frac{1}{2} \frac{\gamma_0 T^2}{1 - \left(\frac{U}{U_c}\right)^2} \\ F_{\text{insulator}} = -k_B T \ln 2 \quad (E_{\text{ex}} = 0) \end{array} \right.$$

Coexistence: $F_{\text{metal}} = F_{\text{insulator}}$
(PM – PI)

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

Important:
Two transitions



J. S. et al., PRL **59**, 728 (1987) – orbitally nondegenerate;
 A. Klejnberg & J. S., PRB **57**, 12 041 (1998) – degenerate.

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

J. Spalek

Department of Solid State Physics, Akademia Gorniczo-Hutnicza, Pl-30059 Krakow, Poland

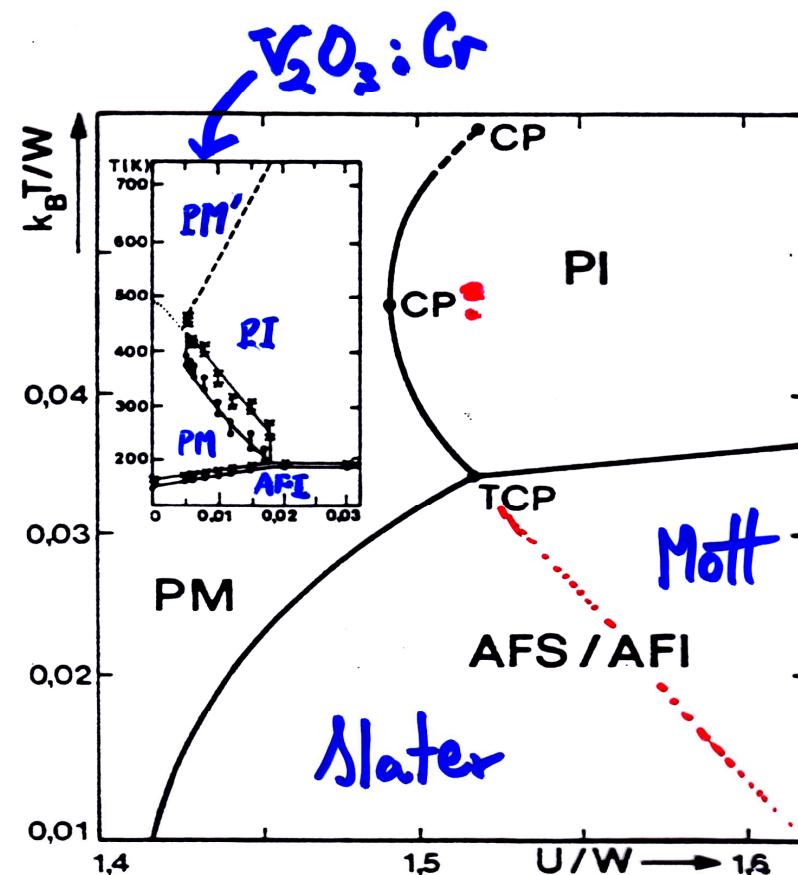
and

A. Datta and J. M. Honig

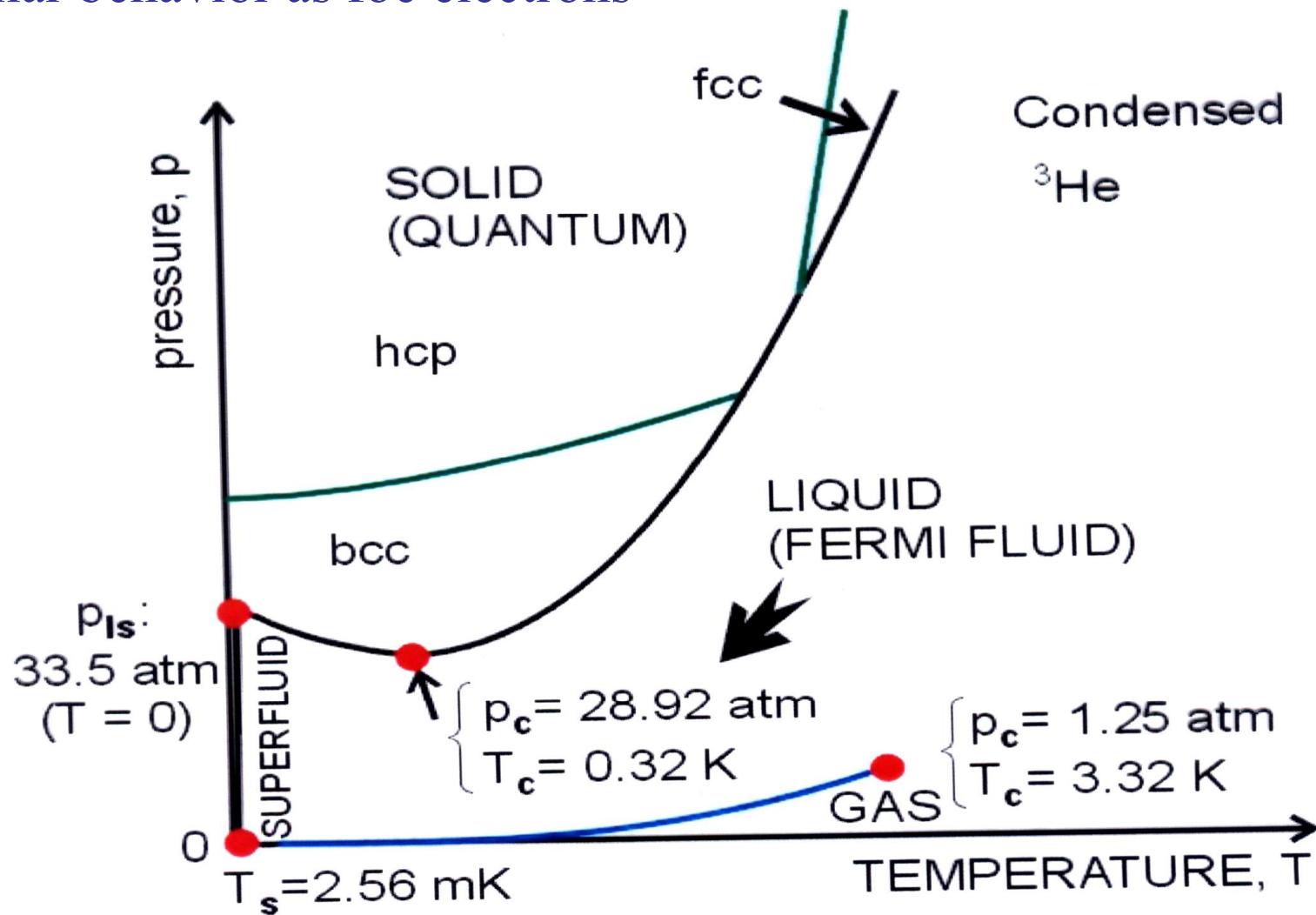
Department of Chemistry, Purdue University, West Lafayette, Indiana 47907

(Received 2 June 1986)

Cf. also Korbel et al.,
EPJ B 32, 315 (2003)



Liquid helium-3 as a continuous Mott system:
similar behavior as free electrons



J.S., in: Encycl. of Condens. Matter Phys., vol.3, 126-36 (2005)

Conclusions I:

- 1. The concept of (narrow) band narrowing-> quasiparticle-mass renormalization**
- 2. First-order MIT with critical (quantum) points**
- 3. Theory valid below U_c - in the metallic phase**
- 4. Double occupancy d as an mean-field order parameter**

Extension I: Almost localized Fermi liquid (ALFL)

Landau – Fermi liquids of fermions

For $T \rightarrow 0$

- Electrical resistivity: $\rho = \rho_0 + AT^2$

- Magnetic susceptibility: $\chi = \chi_0 + aT^2$

- Specific heat: $c_p = \gamma T + \delta T^3 \ln T / T_0$ $\gamma \propto m^*$

- Wilson ratio: $R = \chi / \chi_0 / \gamma / \gamma_0$

- Kadowaki – Woods scaling $A \sim \gamma^2$

- Quasiparticle lifetime: $\tau^{-1} = \tilde{a} \omega^2 + bT^2$

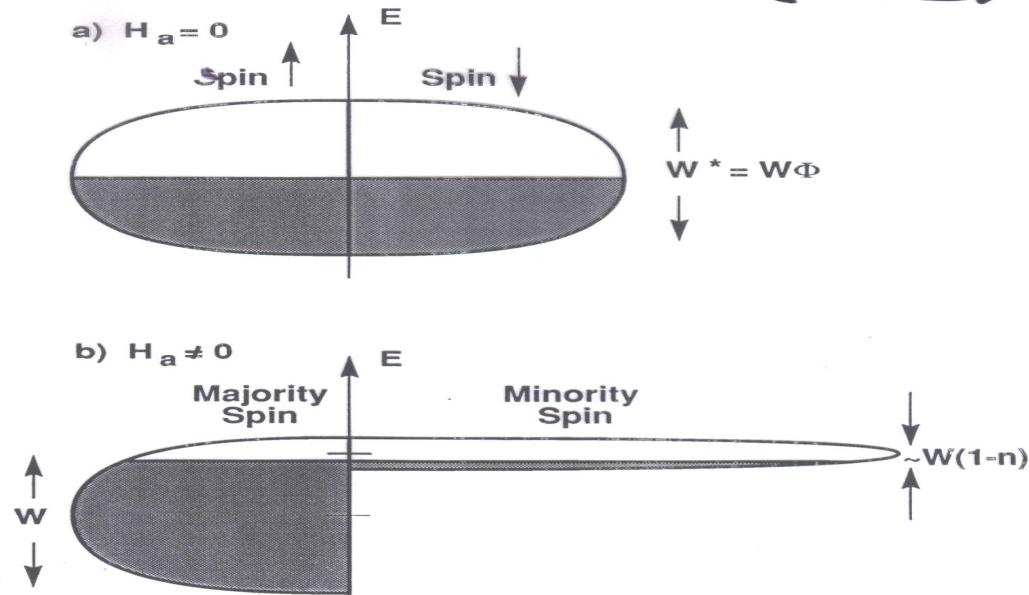
ALFL: Important novel points:

1. Concept of spin-dependent quasiparticle mass (1990 → 2005):

$$m_\sigma / m_0 = 1/Z_\sigma$$

2. Moving Cooper pair: Q nonzero
3. Discontinuous BCS – FFLO transition

D. SPIN DEPENDENT EFFECTIVE MASS $(m \neq 1)$



J. Spalek & P. Gopalan,
 Phys. Rev. Lett. (1990) 64, 2823

$$\frac{m_\sigma}{m_B} = \frac{1}{q_\sigma}$$

$$q_\sigma = \frac{1}{n_\sigma(1-n_\sigma)} \left\{ \left[(n_\sigma - d^2)(1-n_\sigma + d^2) \right]^{\frac{1}{2}} + d(n_\sigma - d^2)^{\frac{1}{2}} \right\}^2$$

$$\frac{1}{N} E_G = \frac{1}{N} \sum_{k\sigma} (q_\sigma \epsilon_k - \mu_B H_a \sigma - \mu) \bar{n}_{k\sigma} + U d^2$$

Spin-dependent masses from the de Haas-van Alphen effect

	m_{\uparrow}	m_{\downarrow}	ϕ_x
$\theta = 0^{\circ}$			
α_1	21.2 ± 0.2	94 ± 7	3.14
α_2	24.2 ± 0.4	94 ± 8	3.14
α_3	14.5 ± 0.6	30 ± 8	2.42
$\theta = 10^{\circ}$			
α_1	21.3 ± 2.4	39 ± 5	3.14
α_2	24.7 ± 3.5	50 ± 13	3.14
α_3	17.6 ± 0.8	40 ± 4	3.14

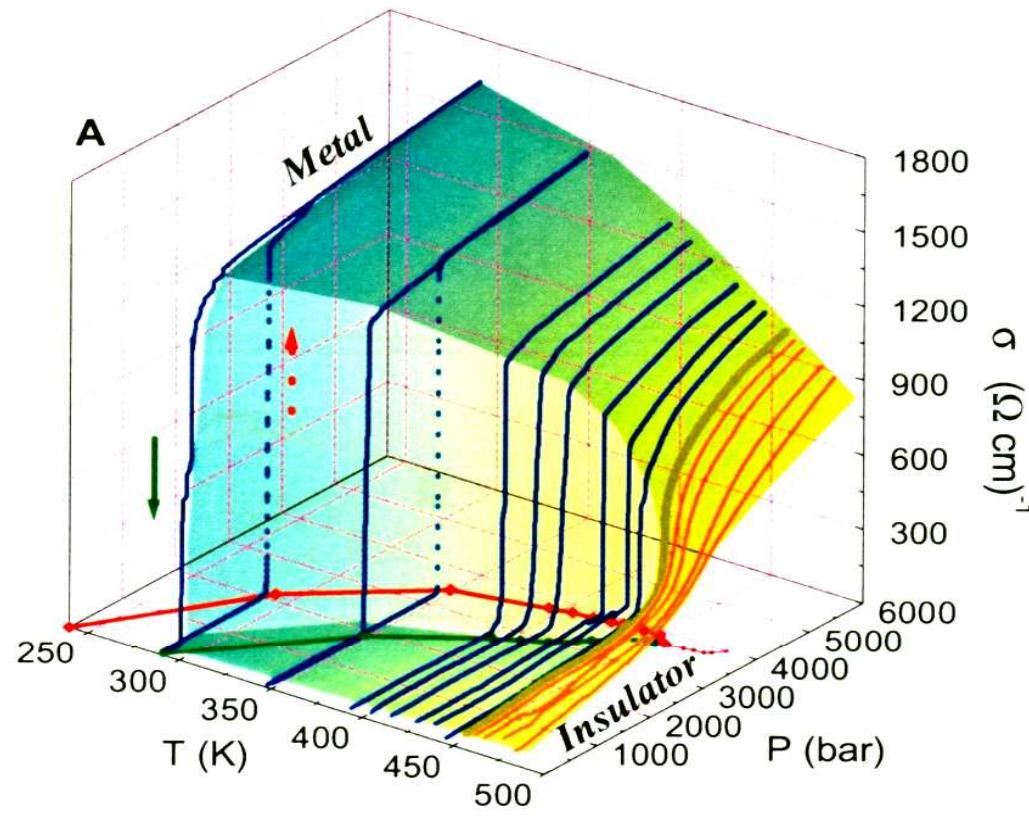
Anomalous de Haas–van Alphen Oscillations in CeCoIn₅ A. McCollam, S. R. Julian, P. M. C. Rourke, D. Aoki, and J. Flouquet

Phys. Rev. Lett., 94, 186401 (2005); Physica B (2005).

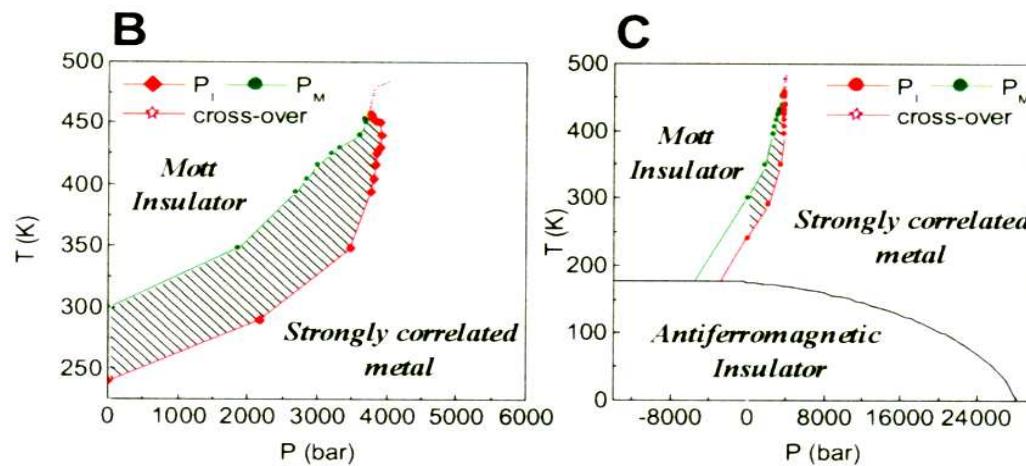
See also: I. Sheikin, et al., Phys. Rev. B 67, 094420 (2003)

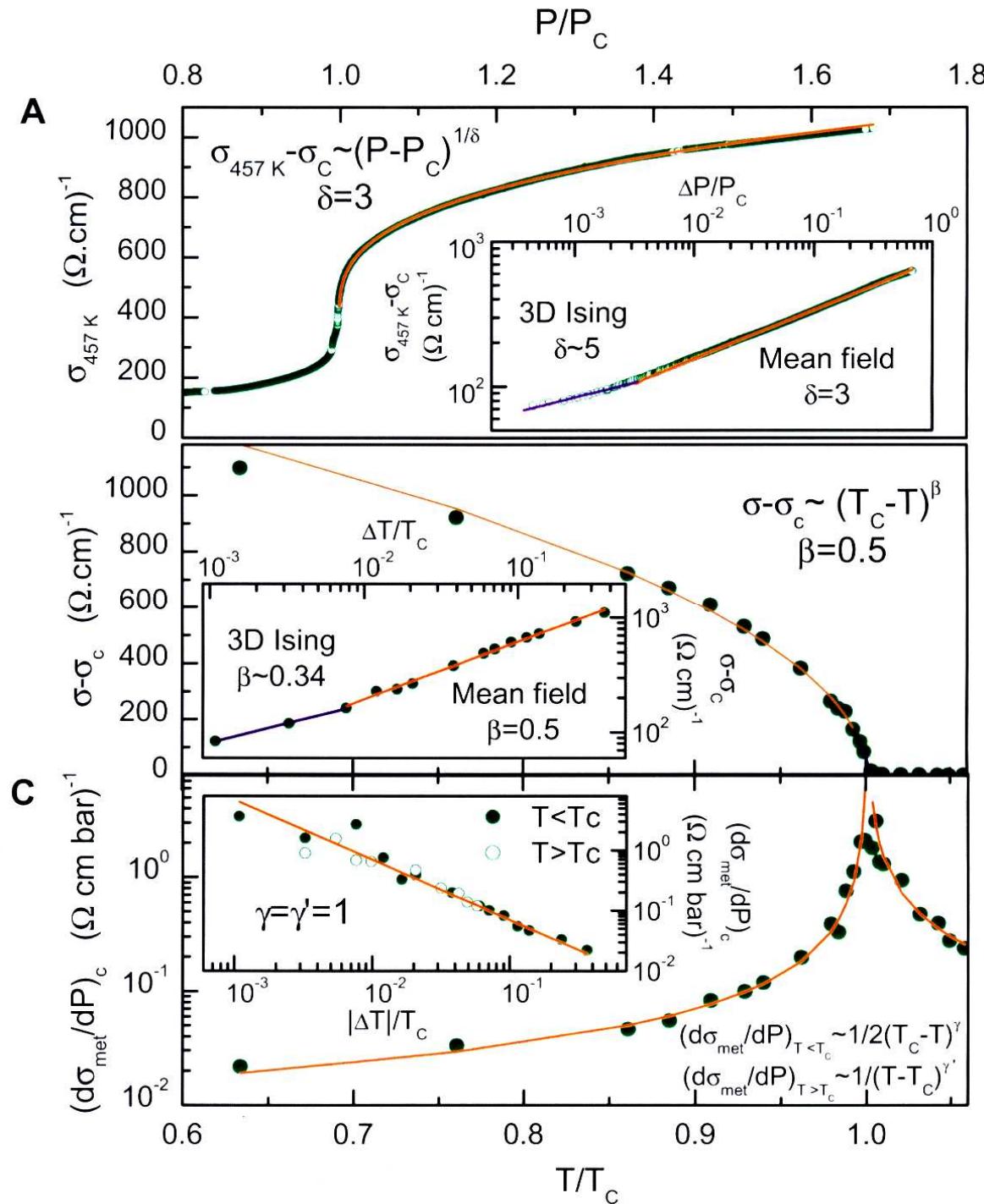
Extension II: (Classical) critical behavior

P. Limelette et al.,
Science 302, 89-92 (2003)

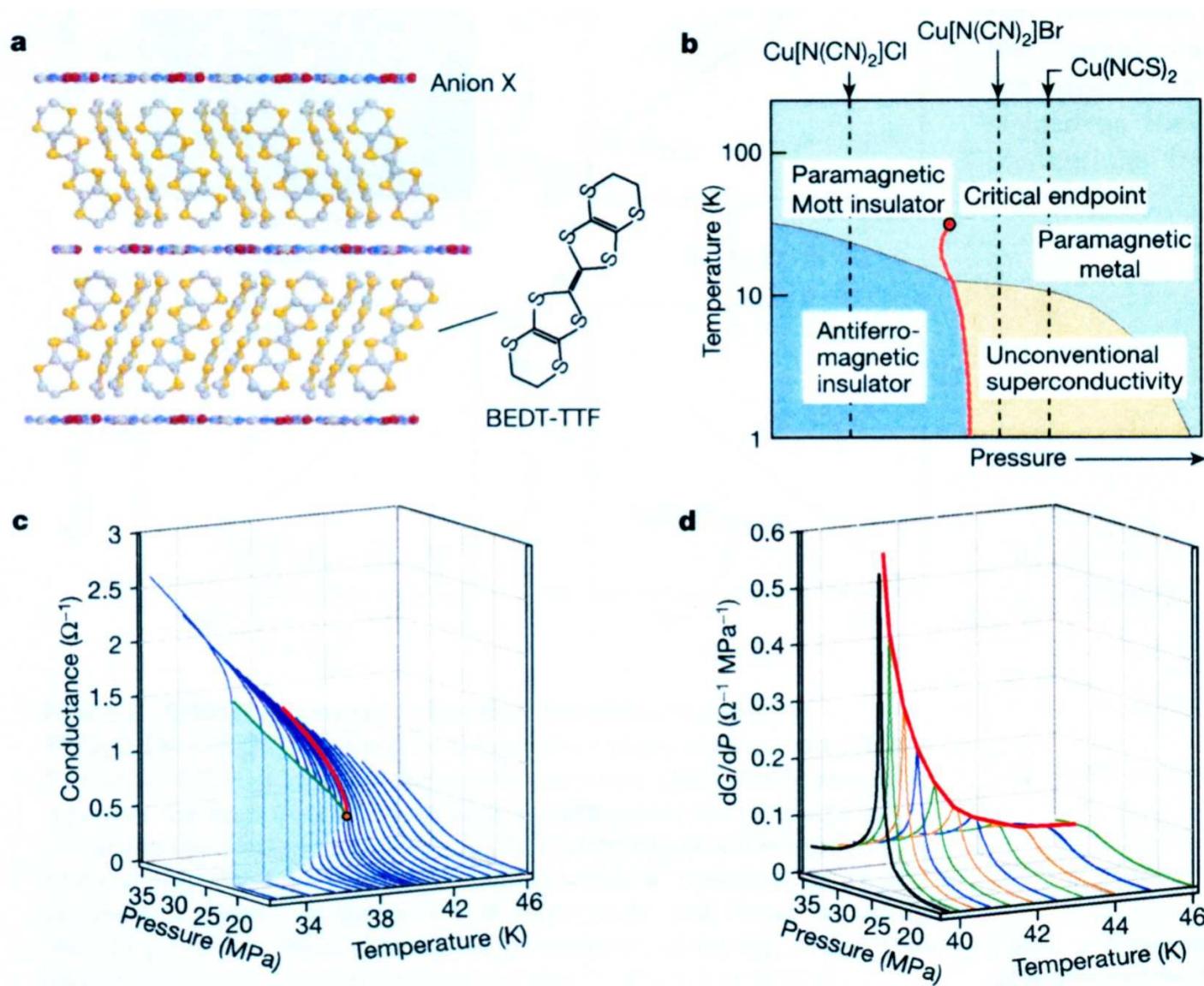


$\text{V}_2\text{O}_3:\text{Cr}$

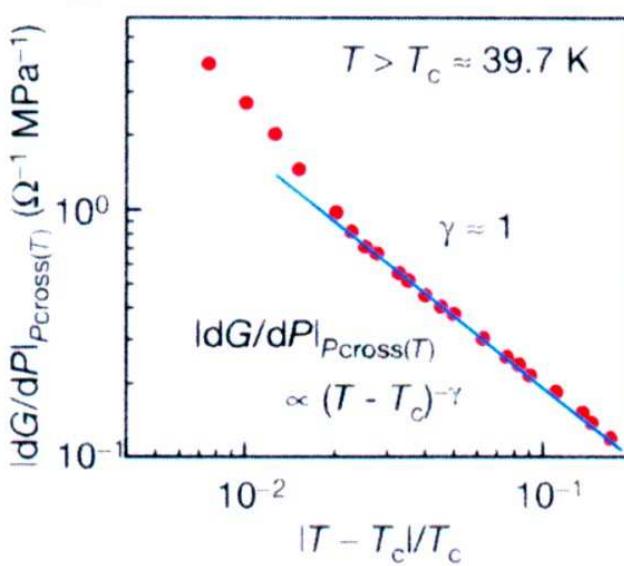
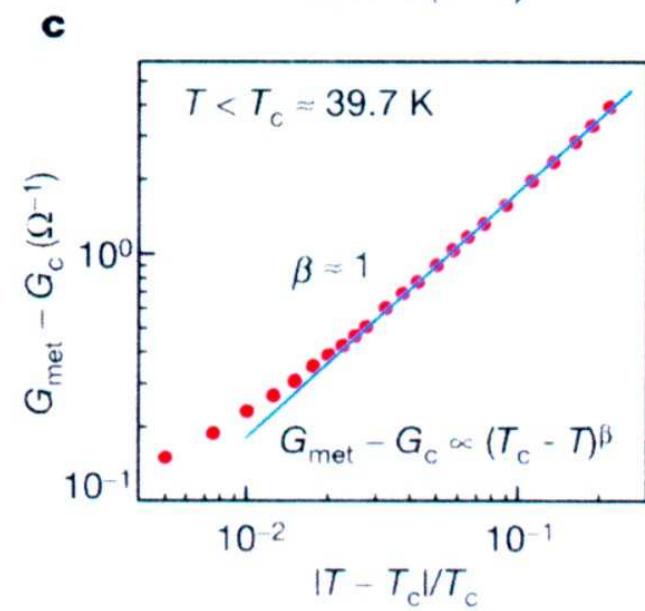
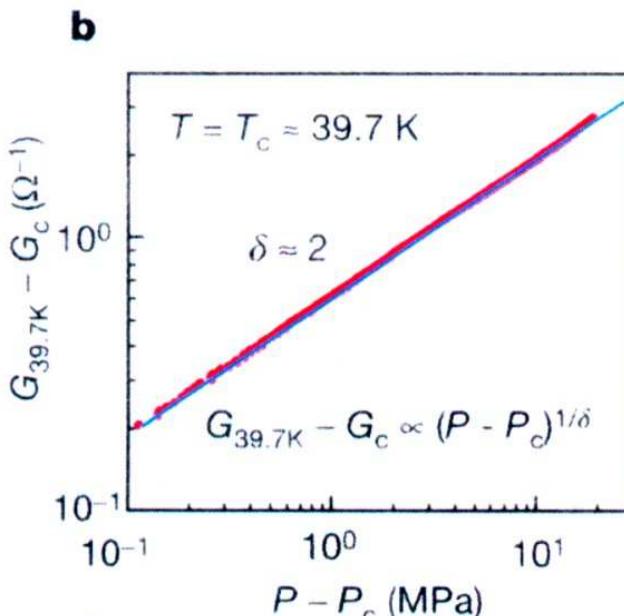
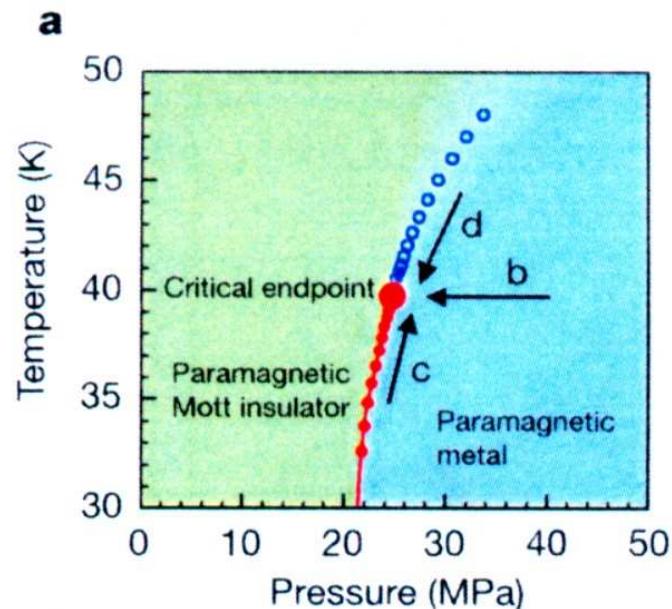


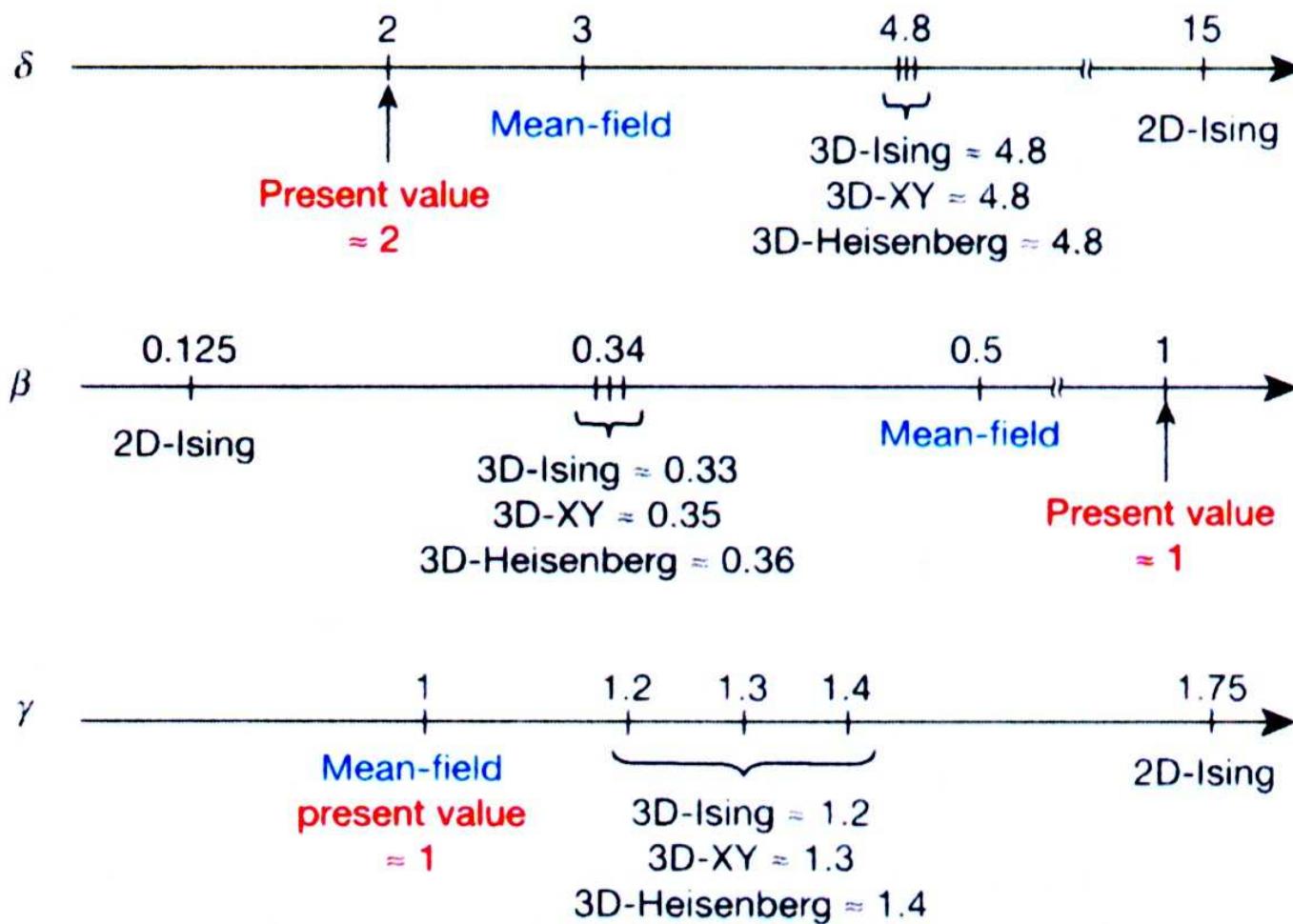


Critical point for 2D system: organic metal a novel behavior



F. Kagawa et al., Nature 436, 534 (2005)





Critical point in magnetic system:

NiSSe system

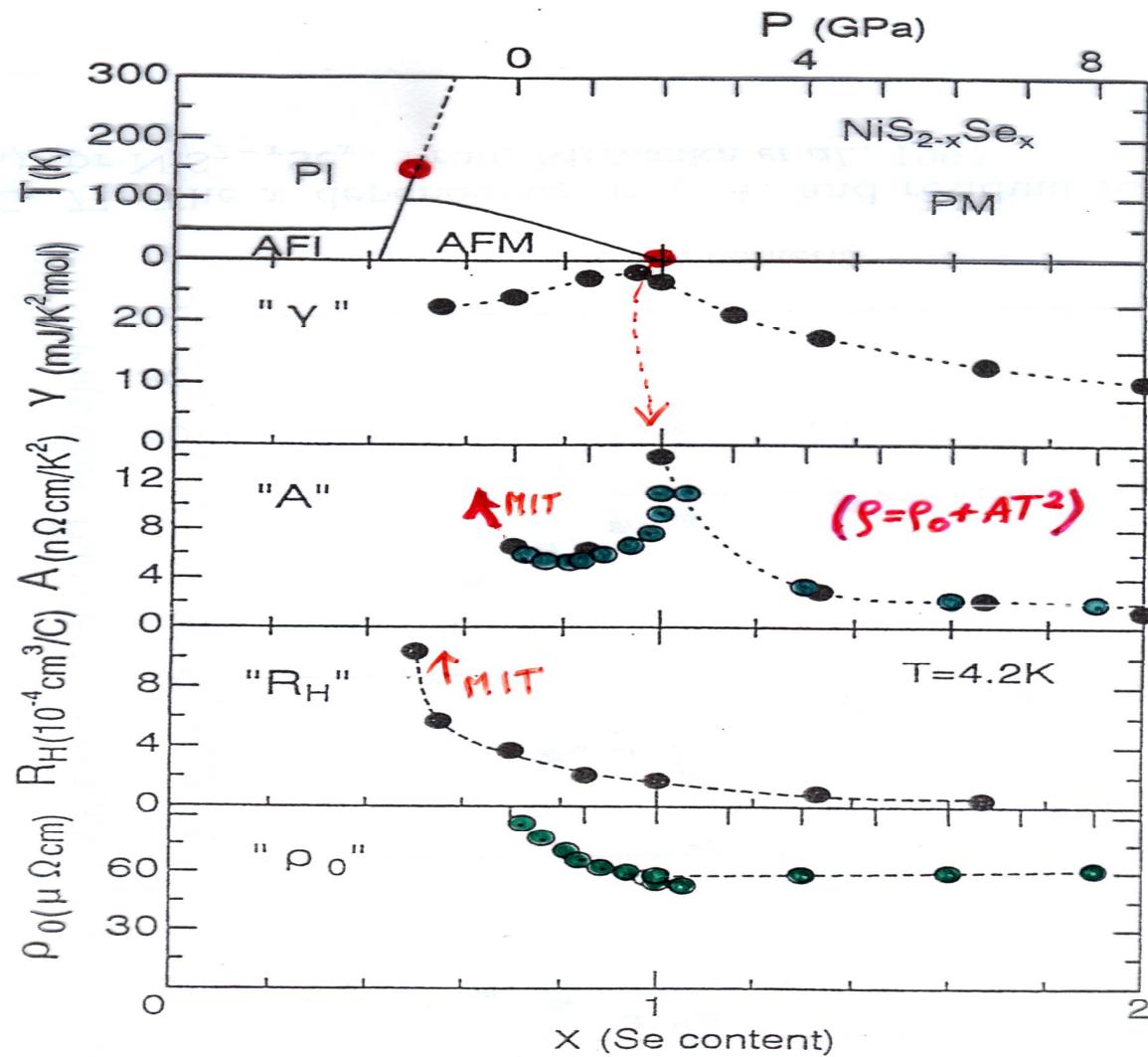


FIG. 77. The x dependence of χ , A , and residual resistivity (ρ_0) for $\text{NiS}_{2-x}\text{Se}_x$. From Miyasaka *et al.*, 1997.

Imada/Fujimori/Tokura, RMP
(1992)

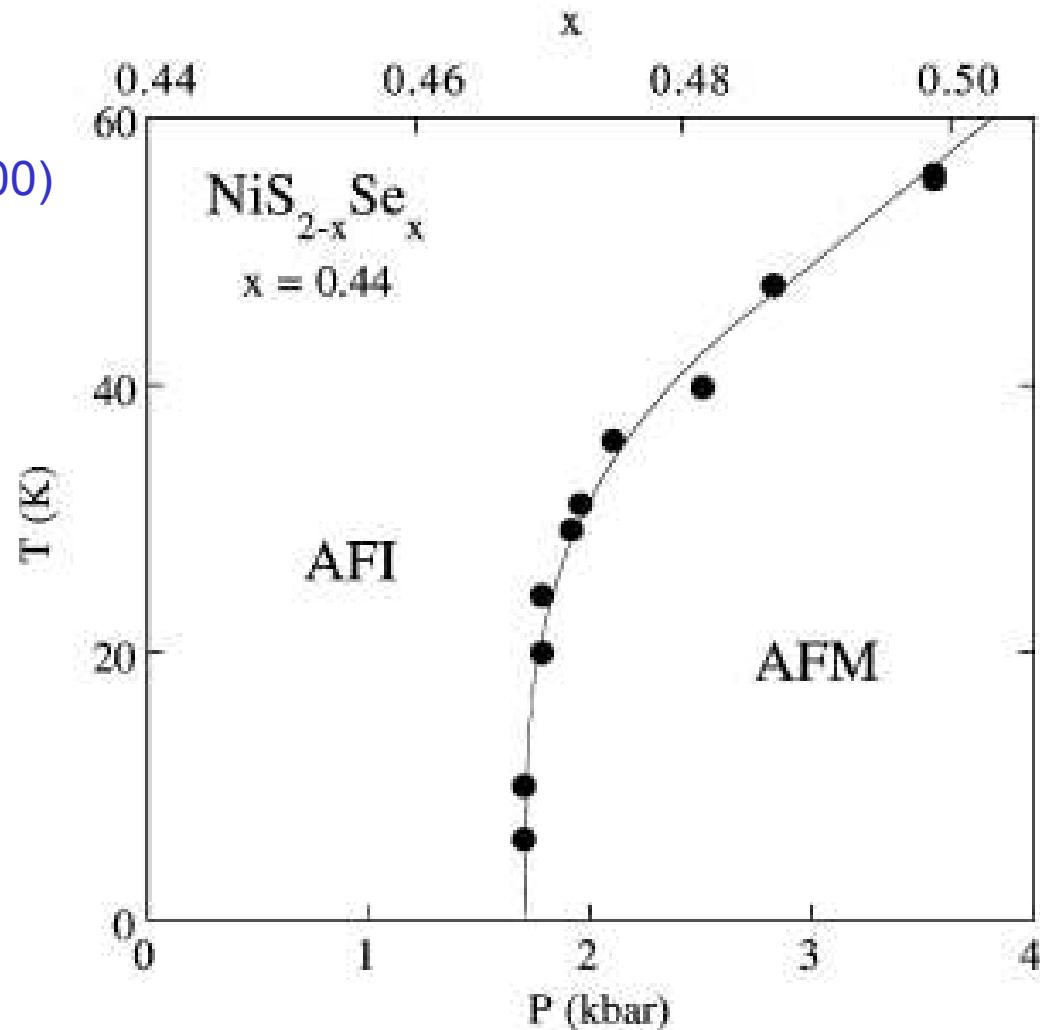


FIG. 1. Pressure-temperature phase diagram for crystals of $\text{NiS}_{1.56}\text{Se}_{0.44}$. The critical pressure for the $T = 0$ metal-insulator transition is less than 2 kbar. Each kbar of external pressure corresponds to a chemical pressure $\Delta x = 0.017$. AFI = antiferromagnetic insulator; AFM = antiferromagnetic metal.

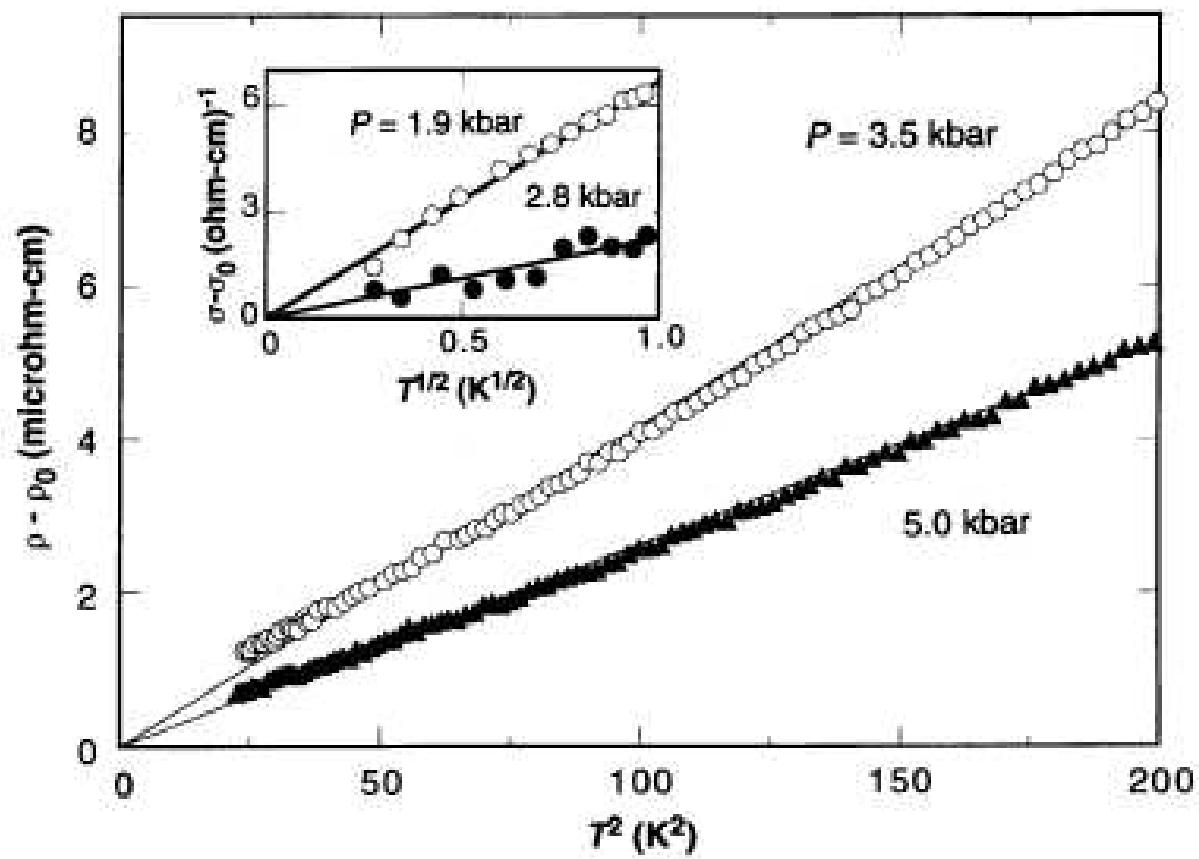


Fig. 2. The large T^2 dependence of the resistivity ρ with slope increasing at the approach to the MI transition indicates a greatly enhanced electronic effective mass. Inset: The effective mass enhancement is revealed as well by the changing slope of the $T^{1/2}$ dependence of the conductivity σ for $T < 1$ K, characteristic of electron-electron interactions in the presence of disorder.

A. Husmann et al., Science 274, 1875 (1996)

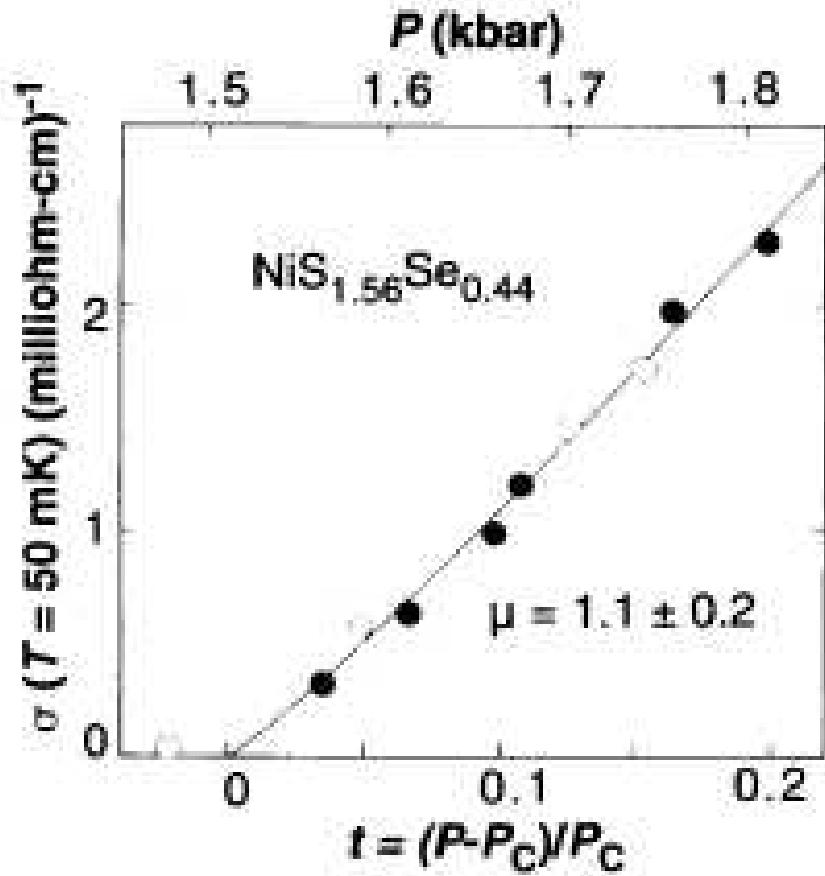


Fig. 1. The $T \rightarrow 0$ conductivity σ_0 as a function of reduced pressure t for two crystals with $P_c = 1.51$ kbar (filled circles) and $P_c = 1.67$ kbar (open circles) at the MI transition. The conductivity falls smoothly to zero, $\sigma_0 \sim t^\mu$, where 1 (millionohm-cm) $^{-1}$ is of order the Mott conductivity.

Extension III:
Correlations + wave function
renormalization (2008-9)

Single-particle
Schrödinger eq.

$$\sum_j H_{ij} w_j(\mathbf{r}) = \epsilon_i w_i(\mathbf{r})$$

Single-particle basis

$$\{w_i(\mathbf{r})\}$$

Field operators

$$\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r})$$

Diagonalization
in the Fock space

$$H = |\Psi_0\rangle E_G \langle \Psi_0| + \dots$$

Ground-state energy

$$E_G = \langle \Psi_0 | H | \Psi_0 \rangle$$

Single-particle
basis optimization

$$\{w_i^{\text{ren}}(\mathbf{r})\}$$

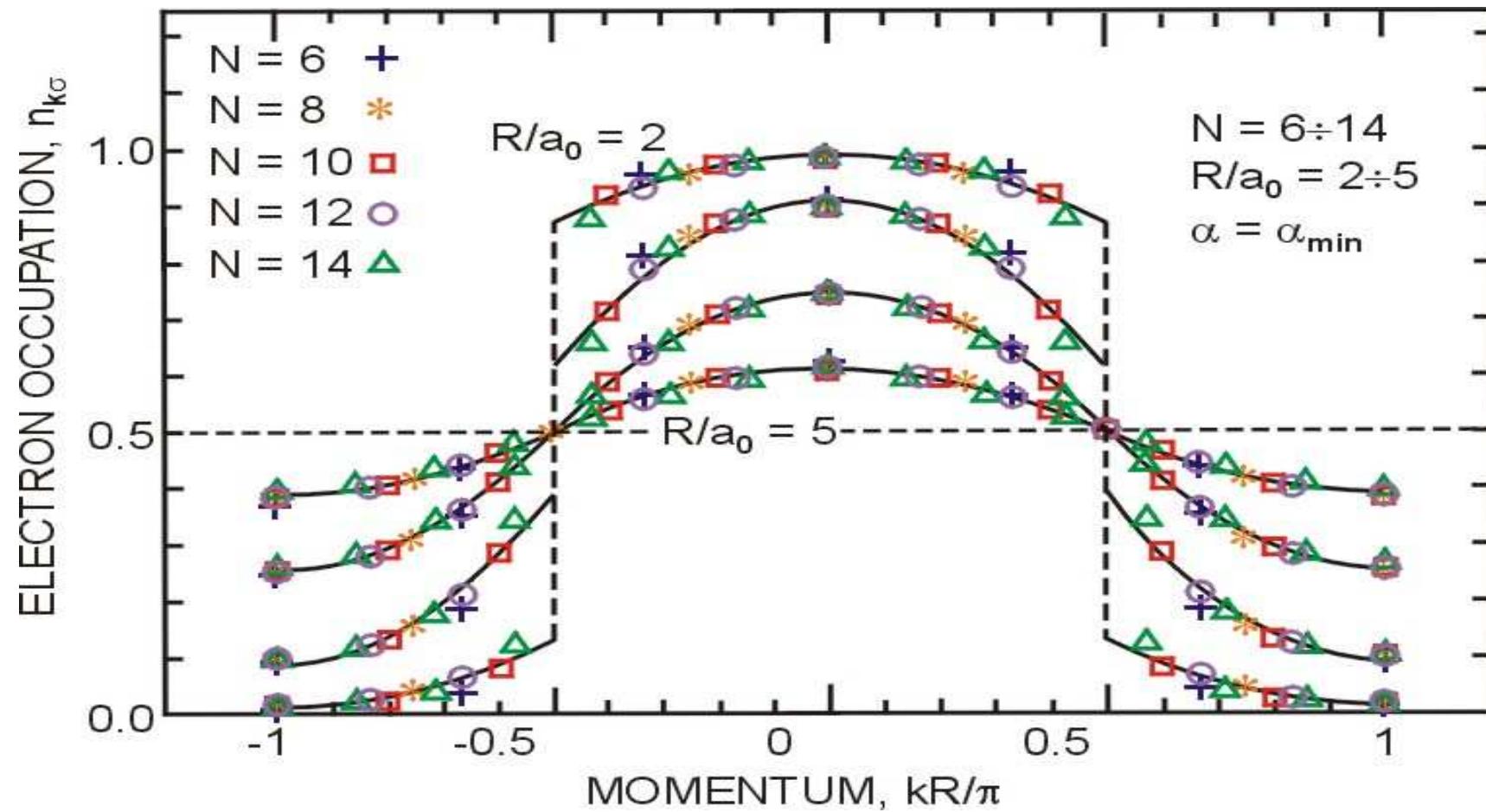
$$\hat{\Psi}^{\text{ren}}(\mathbf{r}), (\hat{\Psi}^{\text{ren}})^\dagger(\mathbf{r})$$

$$\Psi_0^{\text{ren}}(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

*Renormalized N-particle
wavefunction*

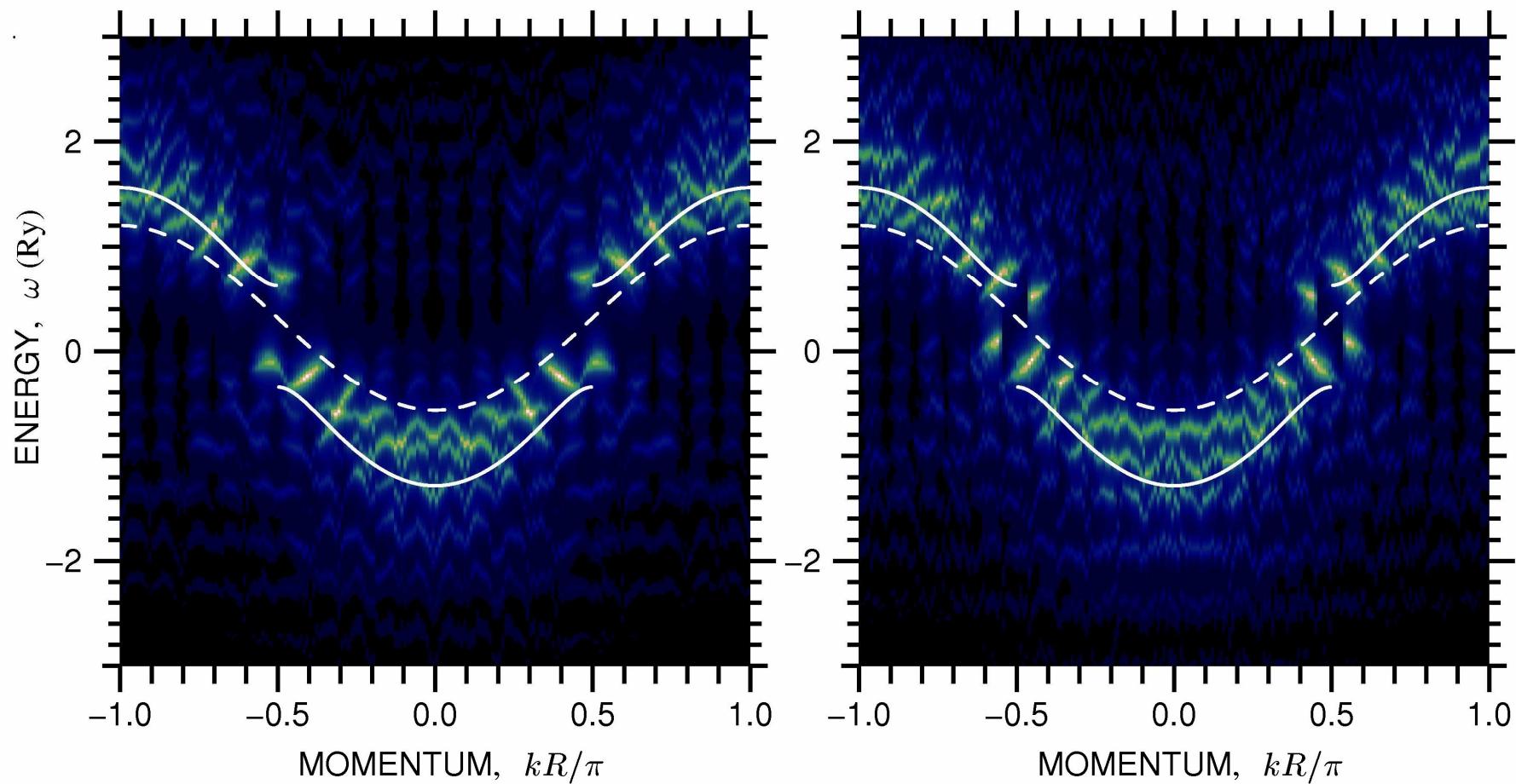
**EDABI: J. Spałek, R. Podsiadły, W. Wójcik, and A. Rycerz,
Phys.Rev. B 61, 15676 (2000); → (2001-2007);
J. Kurzyk et al. (2008-9)**

Momentum distribution: Fermi-Dirac vs continuous

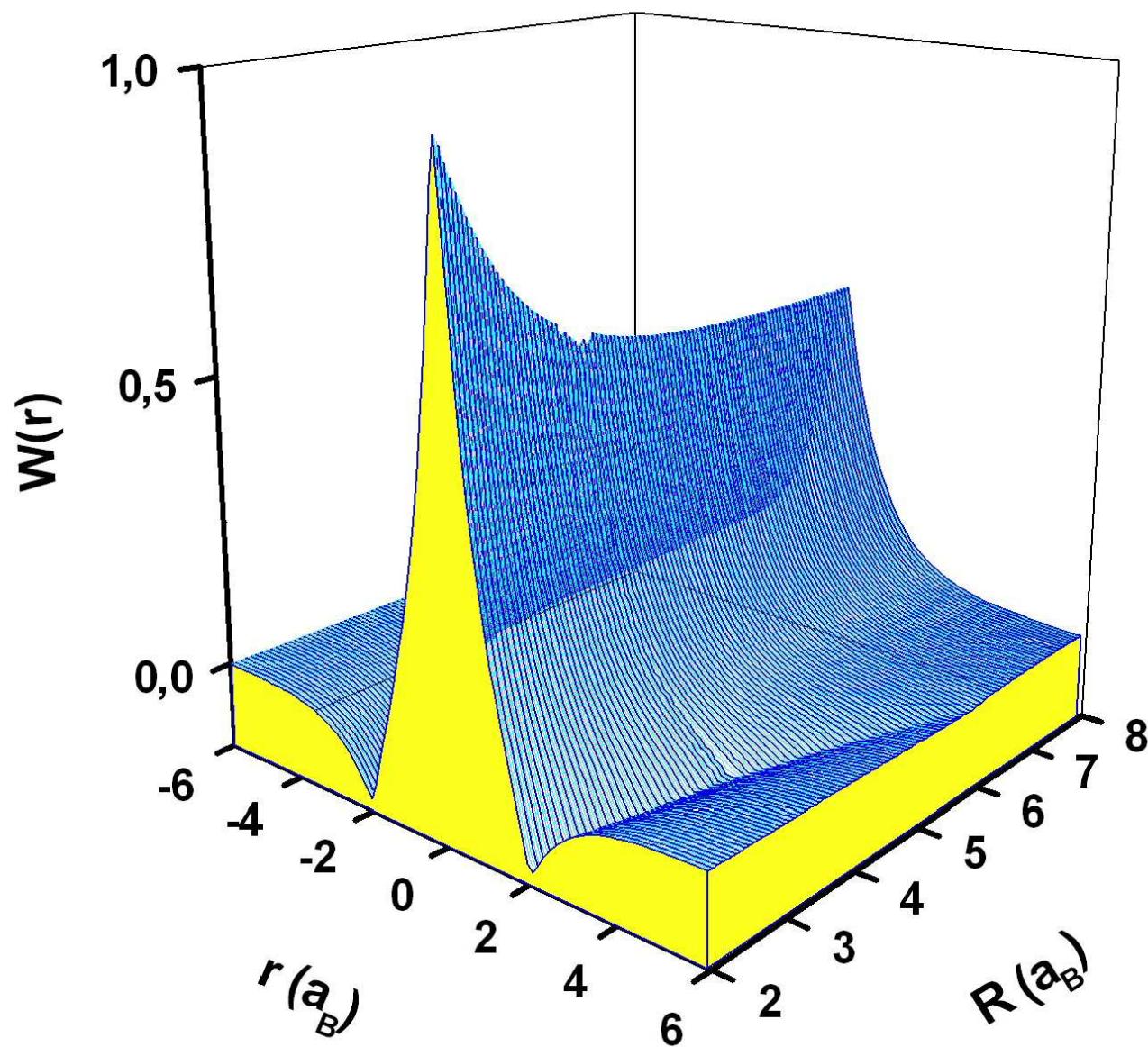


J. S. & A. Rycerz, PRB-R (2001);
J.S., in Encyclopedia of Condensed Matter Physics,
Elsevier, vol. 3, pp. 126-136 (2005)

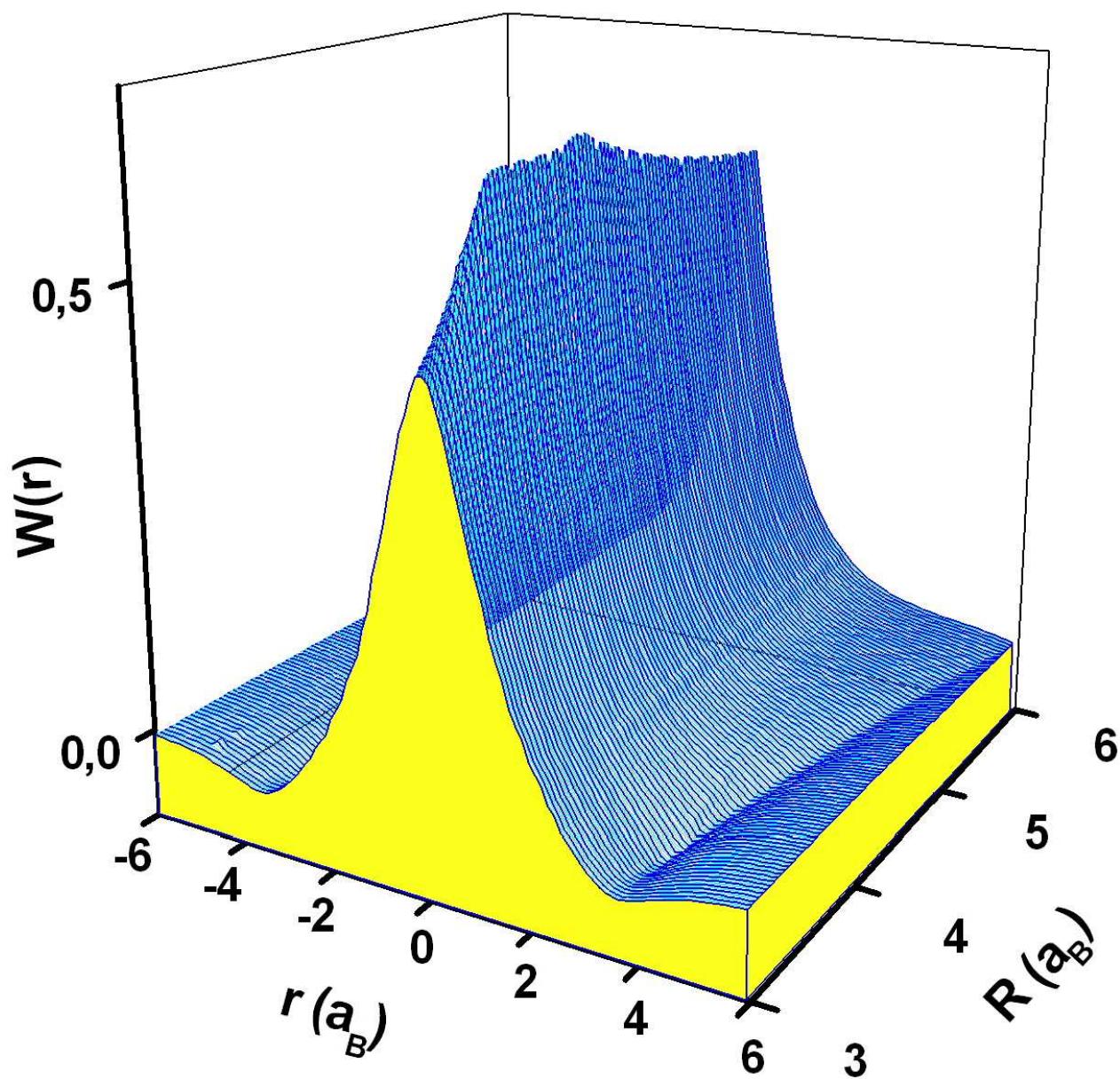
Renormalized band energies: even and odd

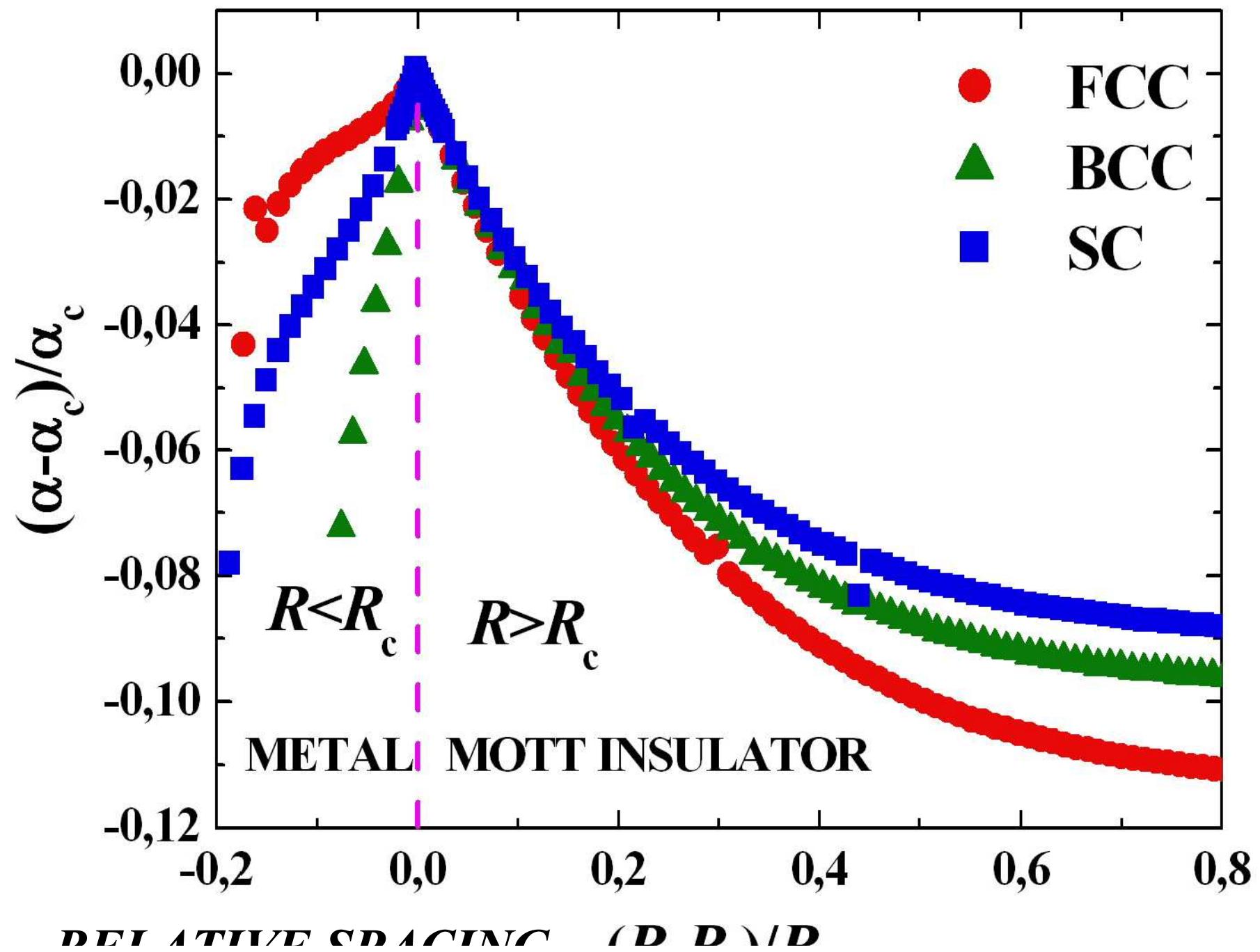


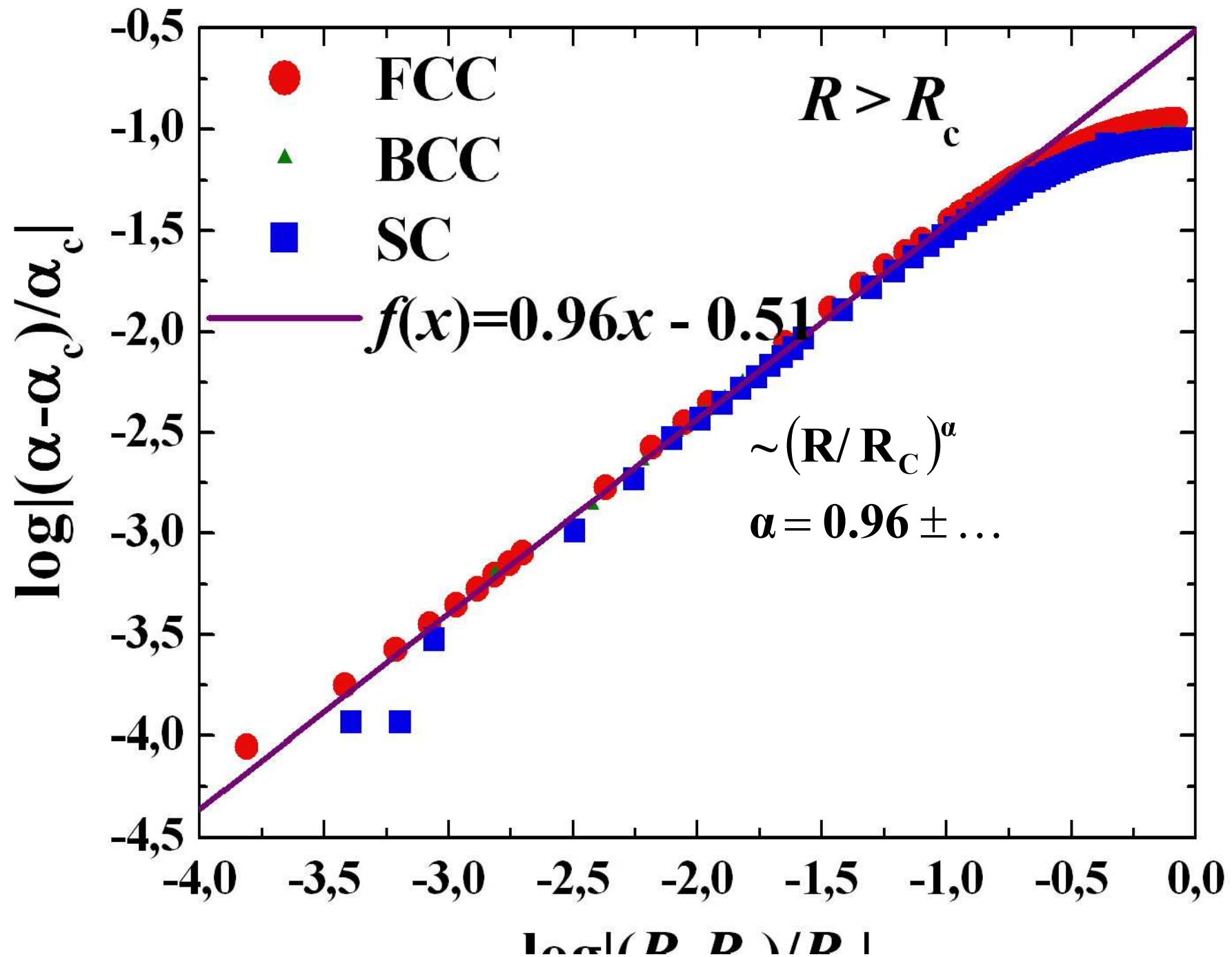
Square lattice

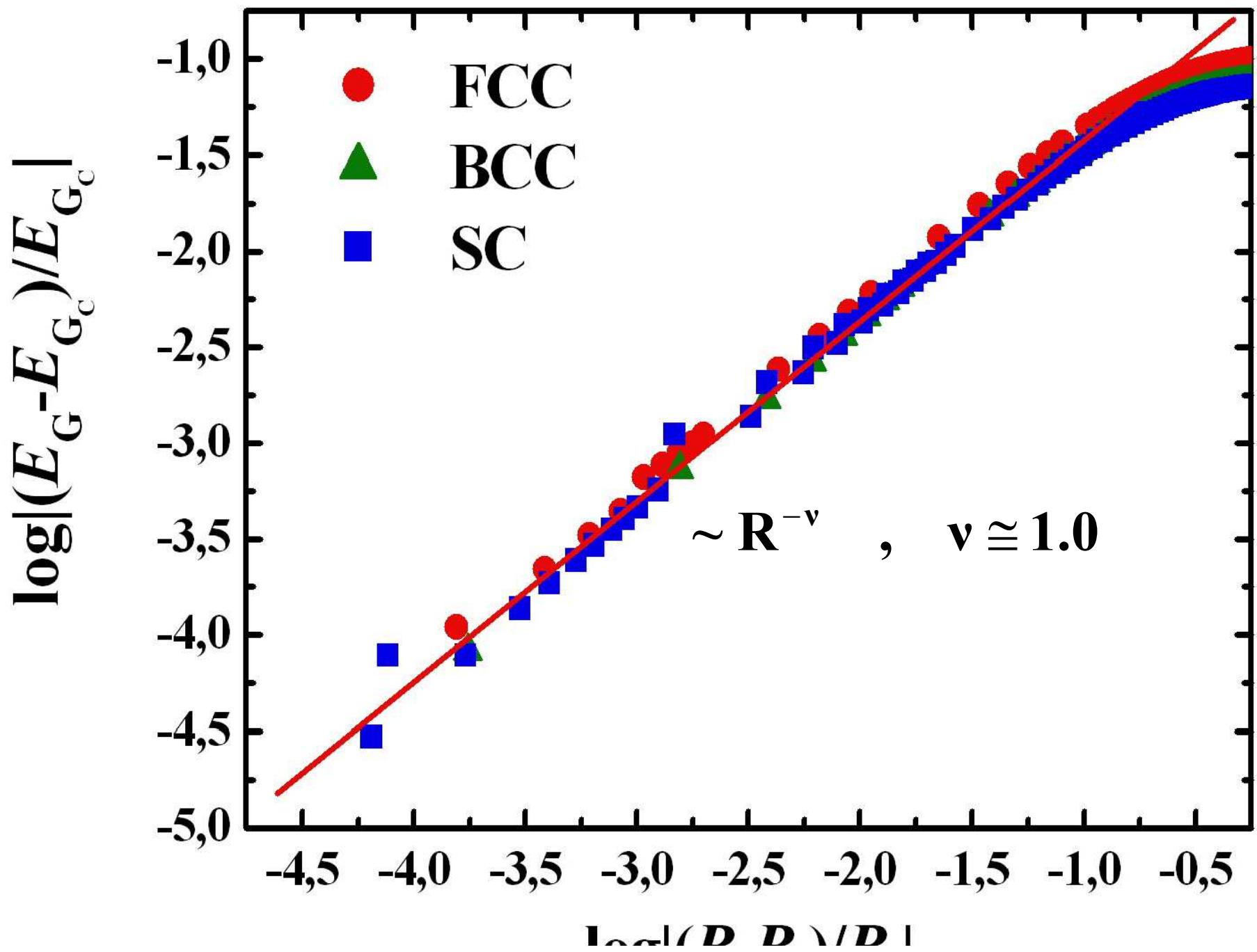


Simple Cubic lattice









Microscopic parameters at the critical point for GA solutions and for the lattices considered

Struct.	α / a_0	R_C / a_0	$(U/W)_C$
CH	1.021	3.288	2.547
SQ	1.051	3.622	1.621
TR	1.054	3.569	1.318
SC	1.099	4.236	1.337
BCC	1.109	4.384	1.080
FCC	1.128	4.351	0.880

Conclusions II:

Wave function renormalization +
Two-particle correlations
combined

Extension IV: Orbitally degenerate model

$$H_1 = \frac{1}{2}U \sum_i n_i^2 - J \sum_i \mathbf{S}_i^2 + \frac{1}{4}J \sum_{il} n_{il}^2 - J \sum_{il} (\mathbf{S}_{il}^z)^2$$

E.M. Goerlich et al. (2009)

l = 1,..., L - the orbital index

Hubbard-Stratonowich transformation

$$\exp \left\{ \frac{\hat{\alpha}^2}{2} \right\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{x^2}{2} \pm \hat{\alpha}x \right\}$$

To be continued ...

Supplement: Infinite Hubbard chain vs. nanochain

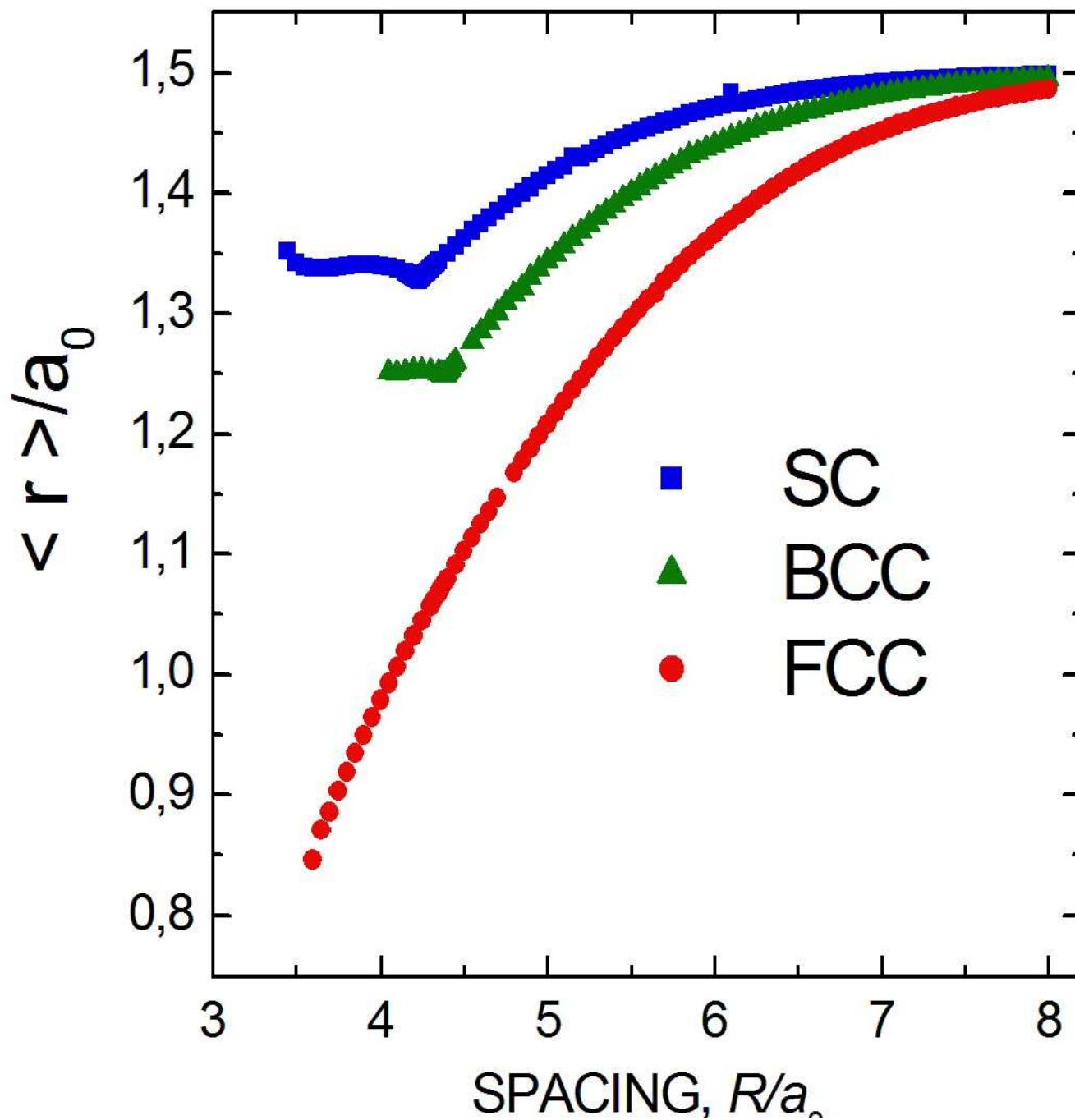
Ground state energy functional:

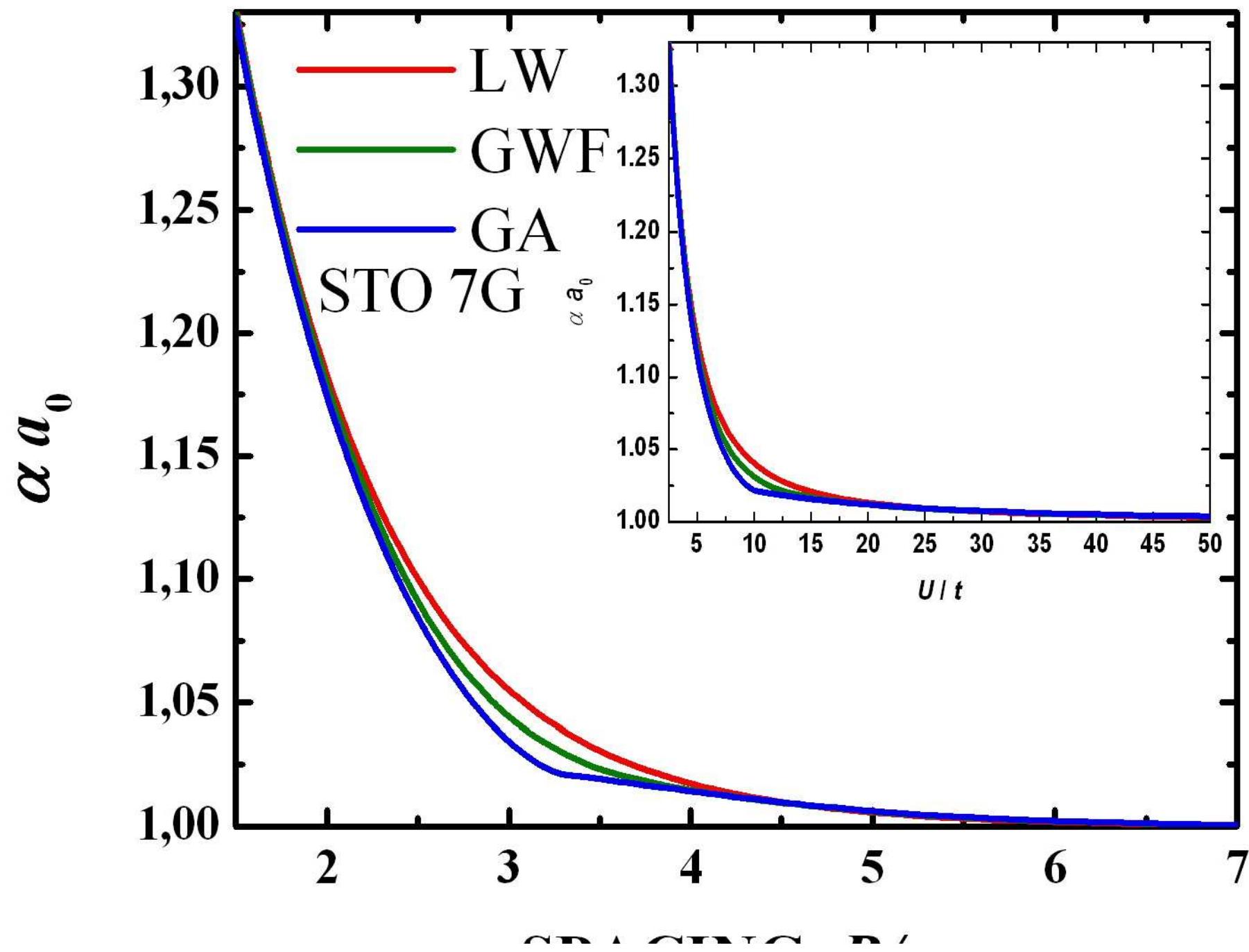
$$\frac{E}{N} = \epsilon_a^{\text{eff}} - 4t \int_0^\infty \frac{J_0(\omega)J_1(\omega)}{\omega [1 + \exp(\omega U / 2t)]} d\omega$$

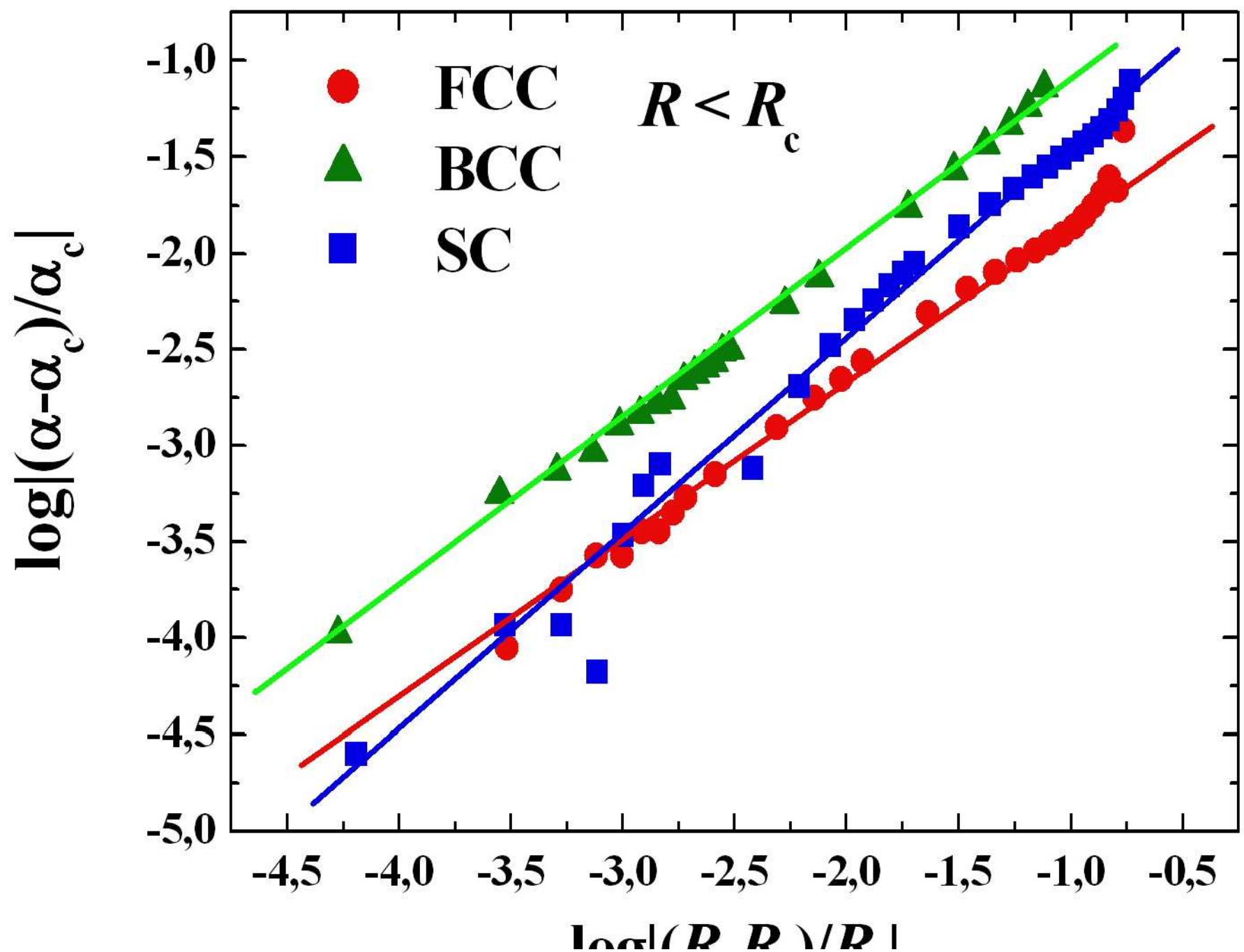
$$\delta n_i \equiv 1 - n_i \equiv 0$$



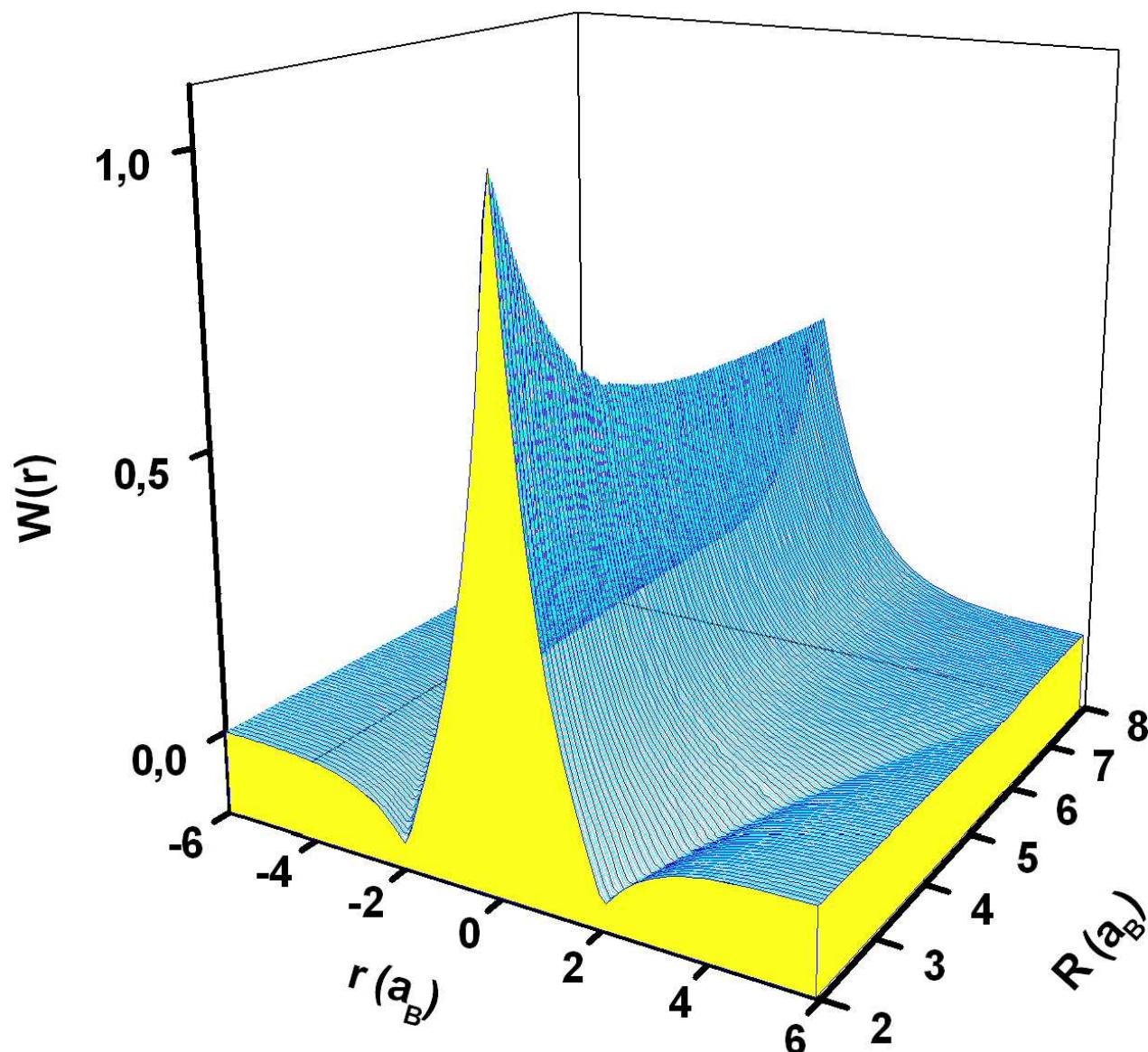
Periodic bound cond.



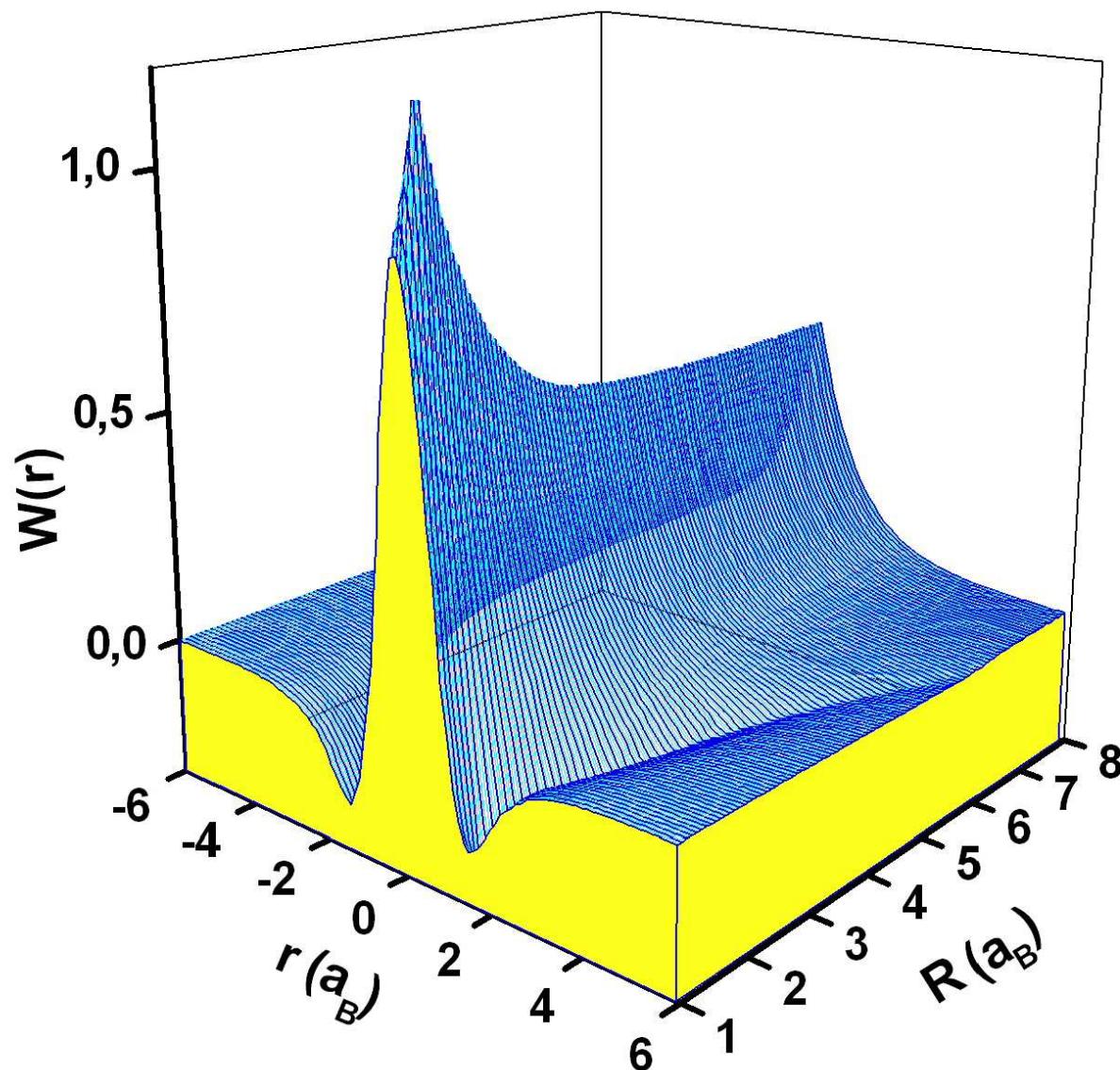




Triangle lattice



Chain



$$t = \langle w_i | H_1 | w_j \rangle$$

$$U = \langle w_i^2 | V_{12} | w_i^2 \rangle$$



Renormalized wave equation:

$$\frac{\delta(E - \mu N_e)}{\delta w_i^*(\mathbf{r})} - \nabla \cdot \frac{\delta(E - \mu N_e)}{\delta(\nabla w_i^*(\mathbf{r}))} = \sum_{i \geq j} \lambda_{ij} w_j(\mathbf{r})$$

**Adjustable Slater or STO-3G
basis forms a trial Wannier
function obtained variationally**

Collaboration

Jan Kurzyk – Tech. Univ., Krakow

Robert Podsiadły – Jag. Univ., Krakow

Włodek Wójcik – Tech. Univ., Krakow

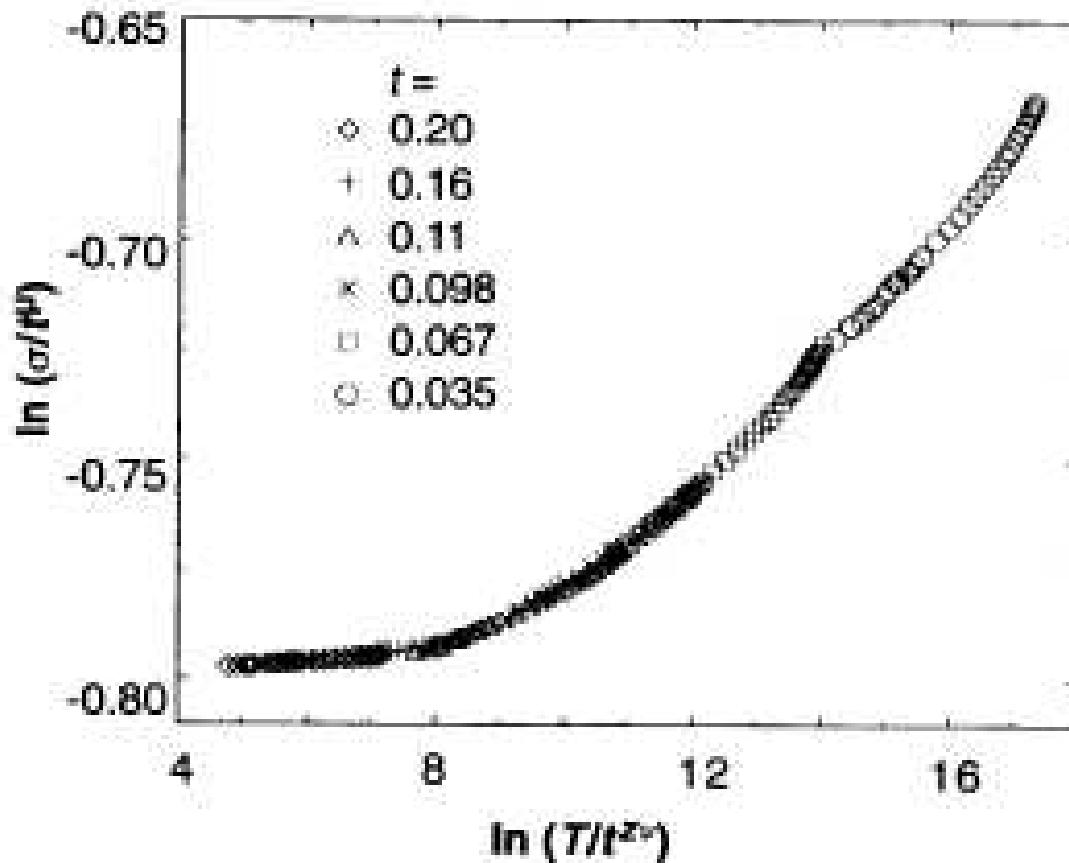


Fig. 4. Dynamical scaling curve for the six closest reduced pressures t to the $T = 0$ Mott-Hubbard MI transition. The ability to collapse the data onto a universal curve reflects the measurable influence of the quantum critical point.

$$[(\Phi_i)_{\sigma\sigma'}]=\left(\begin{array}{cc} \imath\eta_i+v_i^z & v_i^- \\ v_i^+ & \imath\eta_i-v_i^z \end{array}\right)$$

$$N=N(U,J,L)=\frac{1}{4U}+\frac{L}{2J}-\frac{\left(\frac{1}{4U}-\frac{L}{2J}\right)^2}{\frac{1}{4U}+\frac{L}{2J}}=\frac{2L}{J+2LU}\sim\frac{1}{U}$$

$$V=V(U,J,L)=\frac{1}{2J}-\frac{1}{2J(1+L)}=\frac{L}{2J}$$

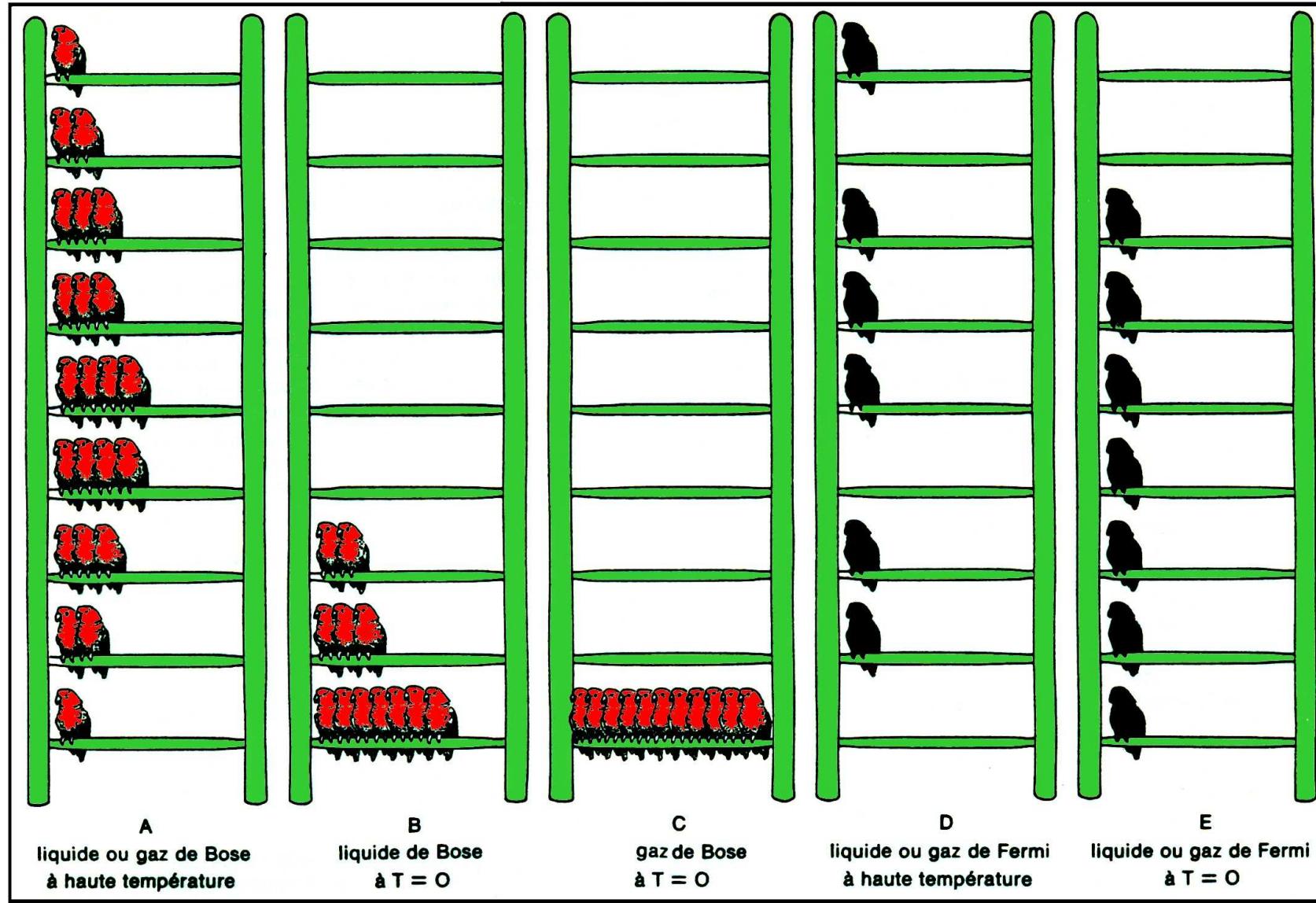
$$\begin{aligned} Z = & \int D[\bar{a},a]_k \int d\eta d^3v \exp \left\{ -\frac{\beta}{2} \sum_n \left(N\eta^2 + Vv^2 \right) \right\} \\ & \times \exp \left\{ - \sum_{klmn} \left(\bar{a}_{kln\uparrow}, \bar{a}_{kln\downarrow} \right) \left((-\imath\omega_n + \epsilon_k - \mu)\delta_{mn} \mathbf{1} + \hat{\Phi}_{m-n} \right) \begin{pmatrix} a_{klm\uparrow} \\ a_{klm\downarrow} \end{pmatrix} \right\} \end{aligned}$$

$$\begin{aligned} Z &= \exp \left\{ -\frac{1}{2}\beta(N\eta_0^2 + Vv_0^2) + \underbrace{2\ln(\beta v_0)}_* + \sum_{kn} \ln [\beta^2(\epsilon_k - \mu + \imath\eta_0 + \imath\omega_n)^2 - \beta^2 v_0^2] \right\} \\ &= \exp \{-S_{eff}\} \end{aligned}$$

Extension III: Effective Landau-Hertz functional

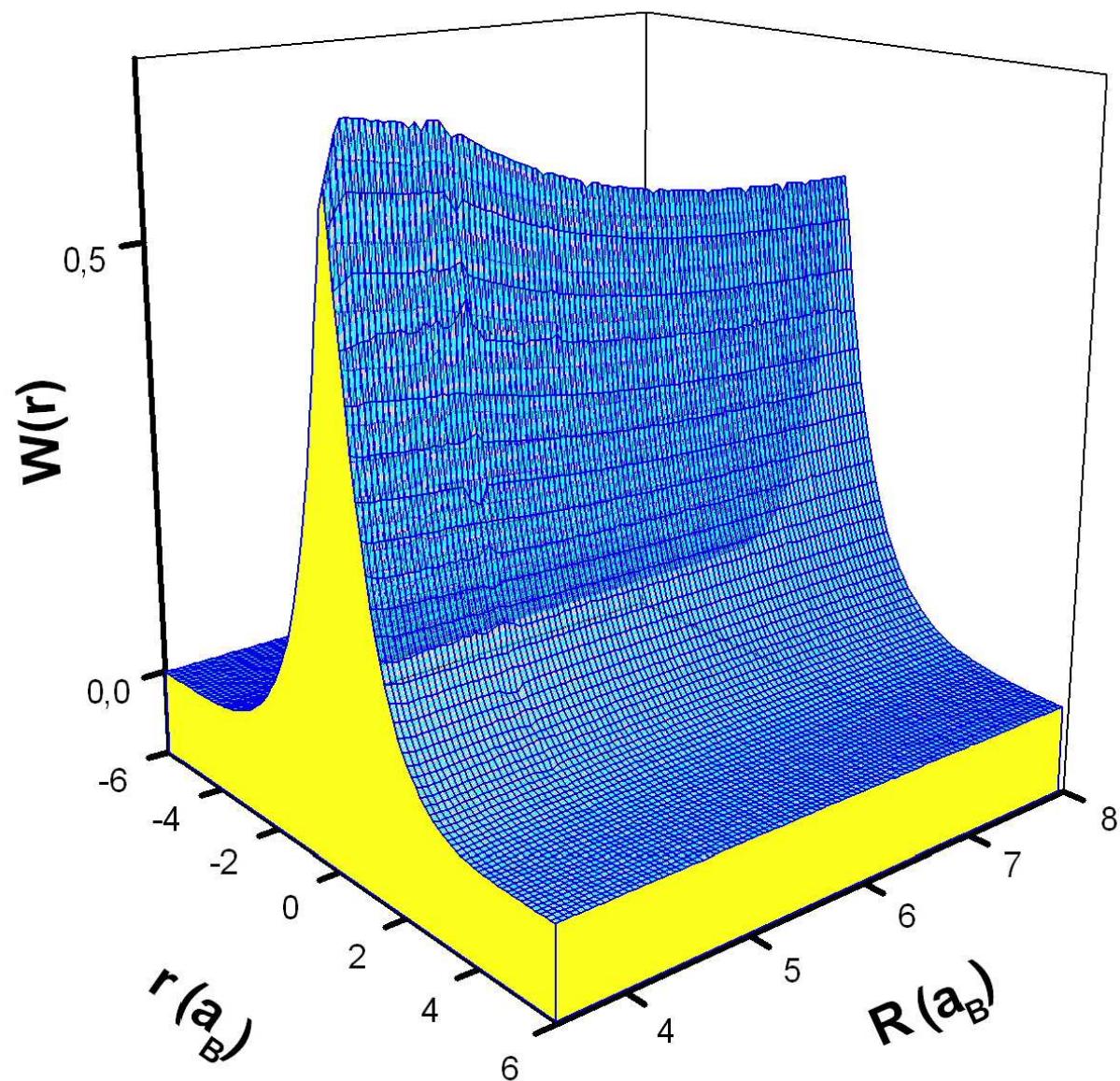
$$\Omega_{\text{eff}} =$$

$$\Omega_{\text{free}} + (N/2 + LC_0)\eta^2 + (V/2 - LC_0)v^2 + L\beta^2 C_1(\eta^4 + v^4 - 6\eta^2 v^2)$$

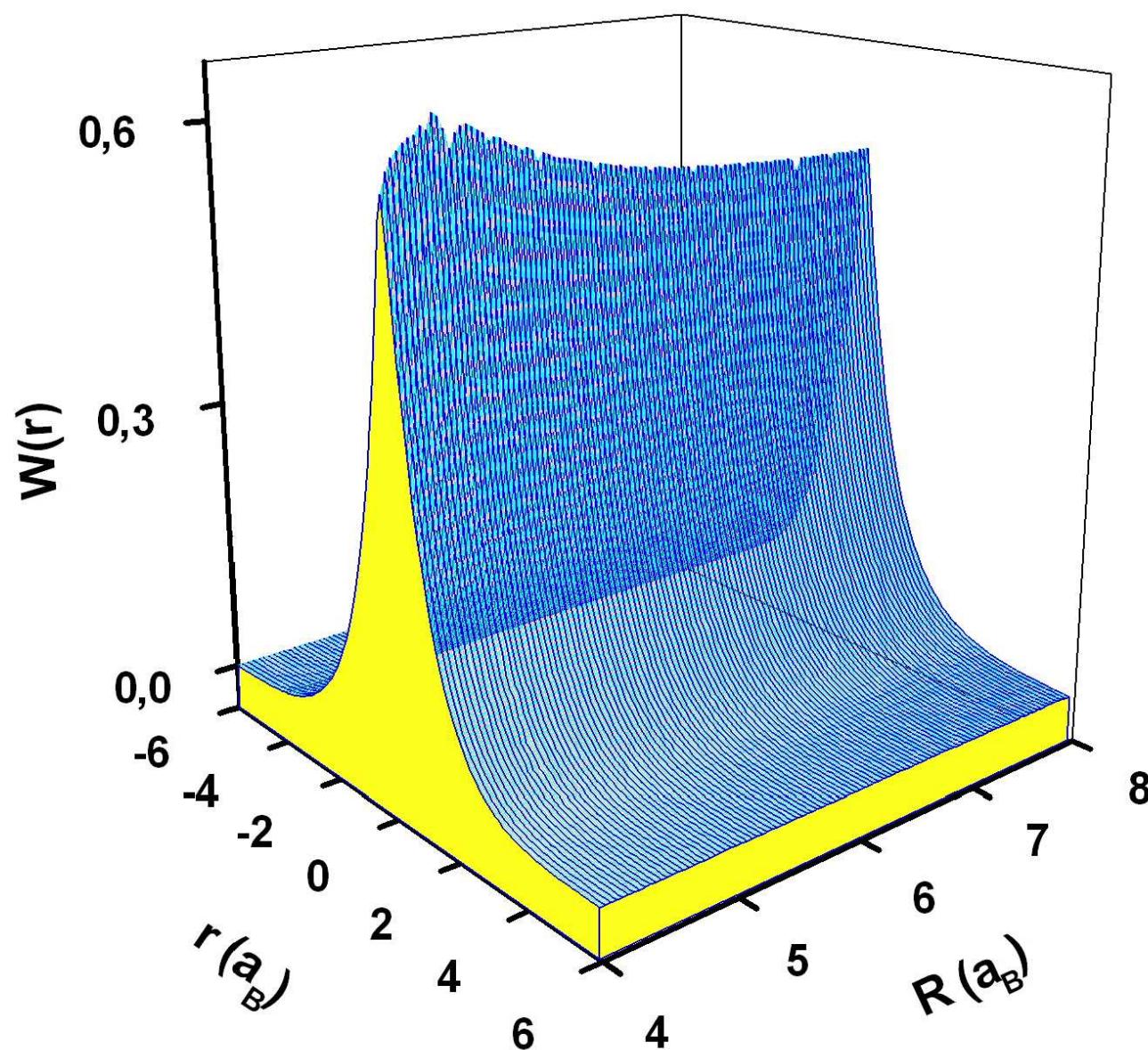


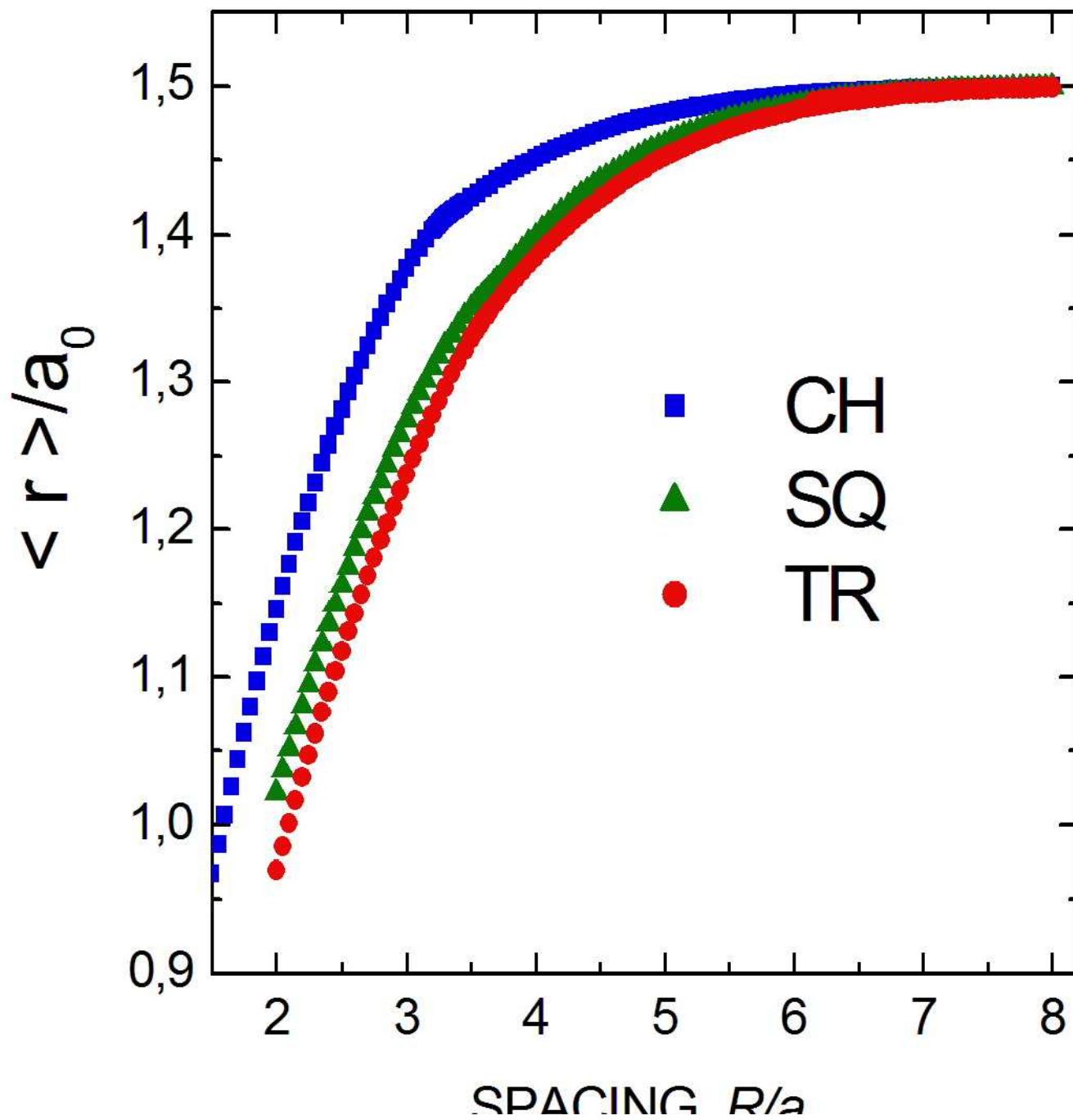
S. Balibar, La Recherche

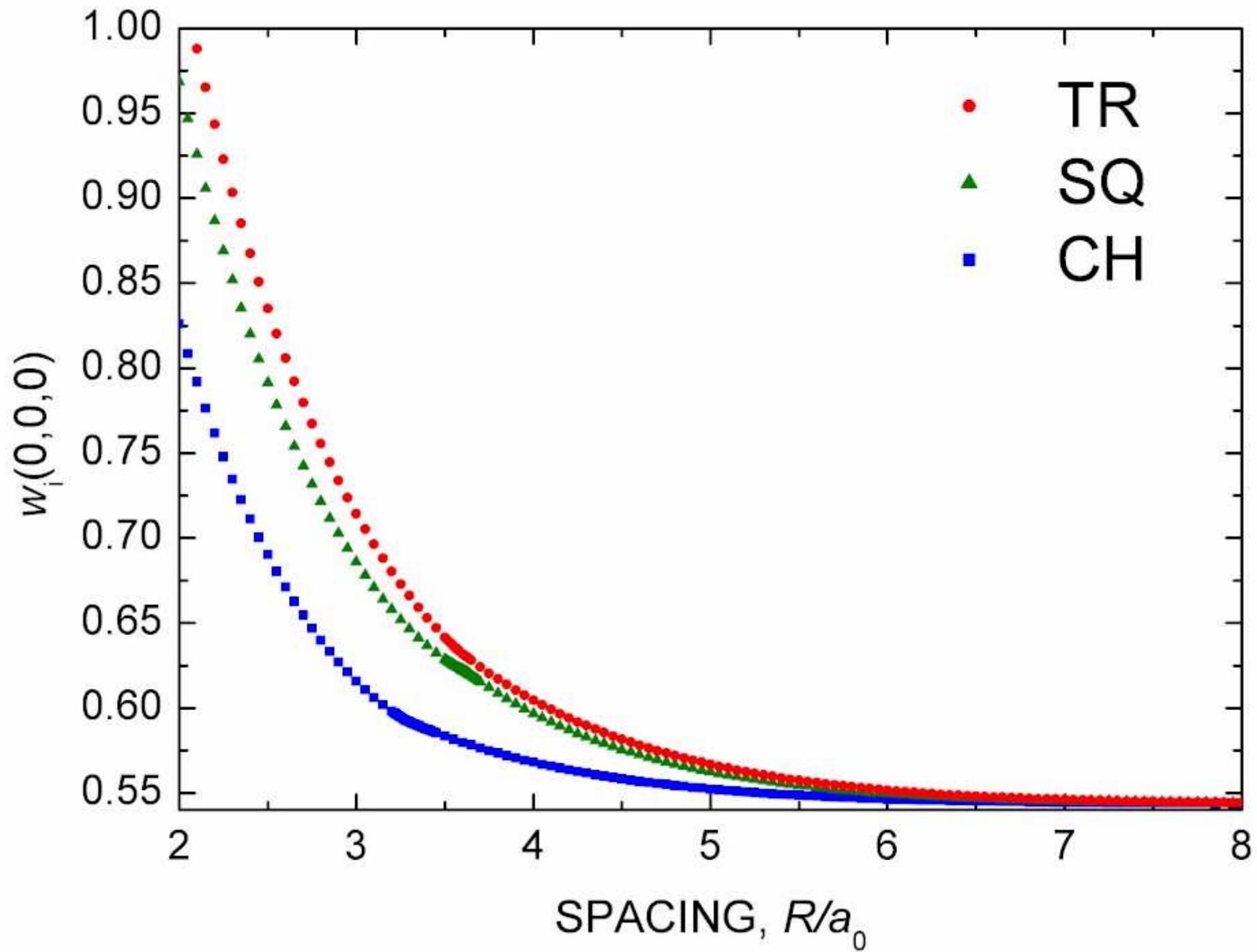
Face Centered Cubic lattice



Body Centered Cubic lattice







Contents

Part II: Real space pairing and d-wave superconductivity

- 1. Derivation of t-J model from the Hubbard model**
- 2. Real-space pairing operators vs. magnetism**
- 3. Mean-field solution(s)**
- 4. Interorbital pairing: heavy fermions**
- 5. Spin-triplet pairing(?)**

