Renormalized Wannier functions at the border of Mott localization

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Plan

1. From atoms to metals

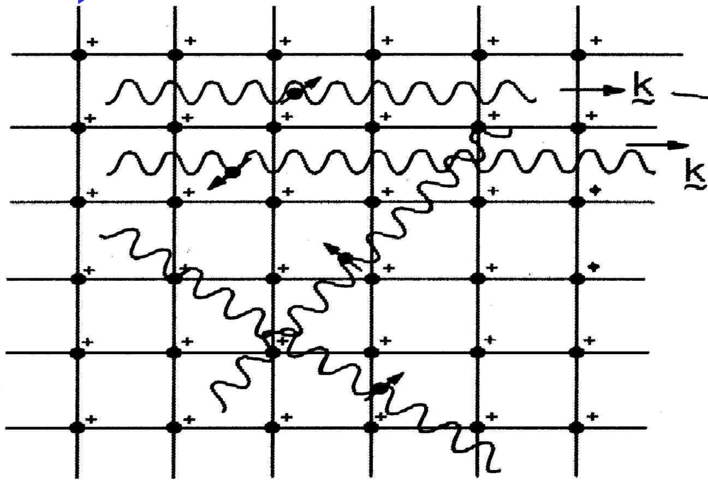
2. Wave function readjustment in the correlated electron state

3. Example: exact solution for nanosystems and Hubbard chain

4. Quantum critical behavior of the wave function (size)

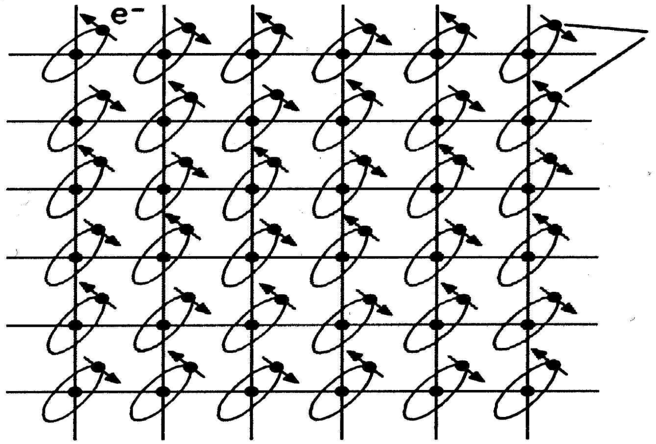
Delocalized versus localized

a) Metal

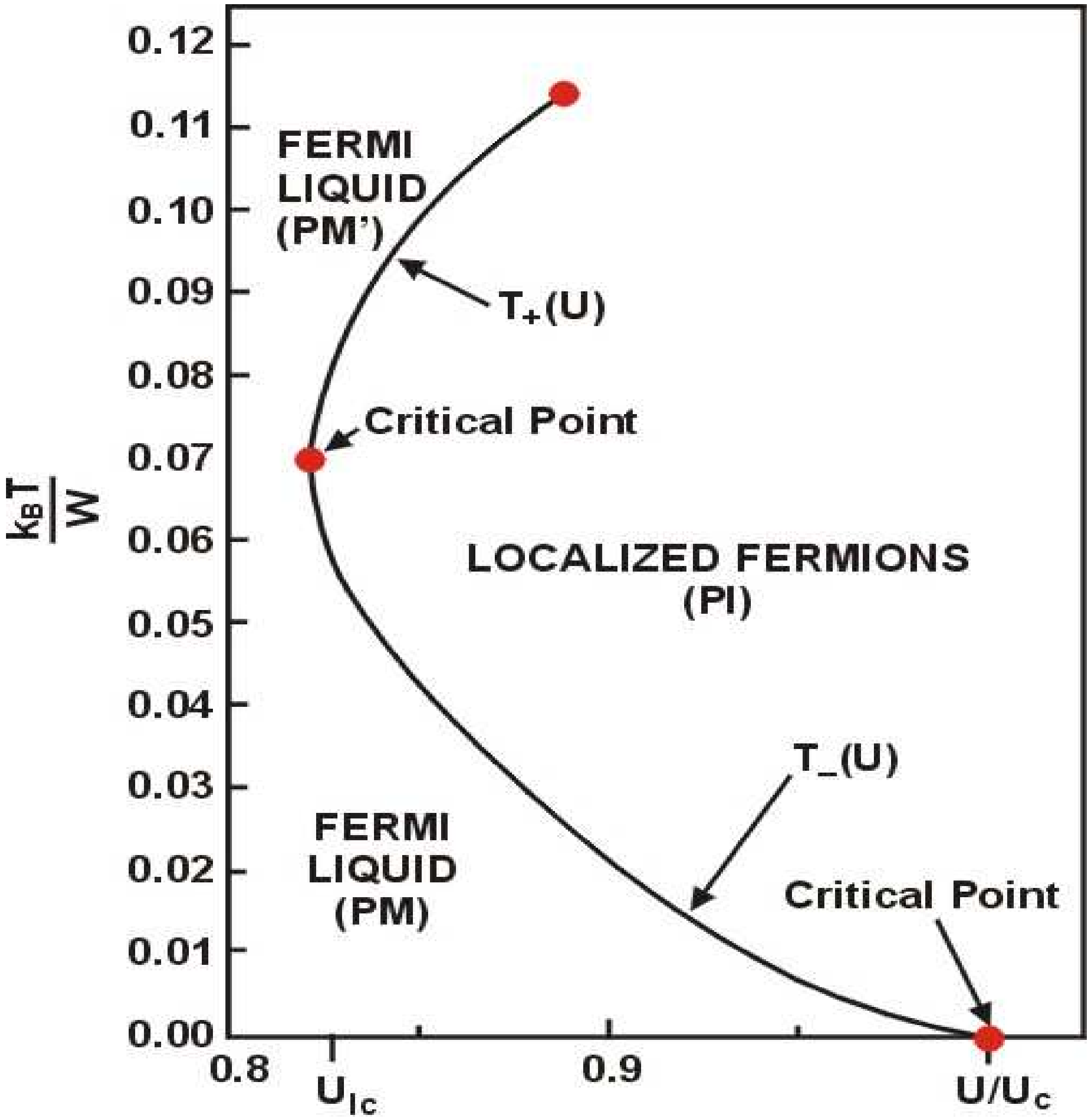


Plane waves
(Bloch states)

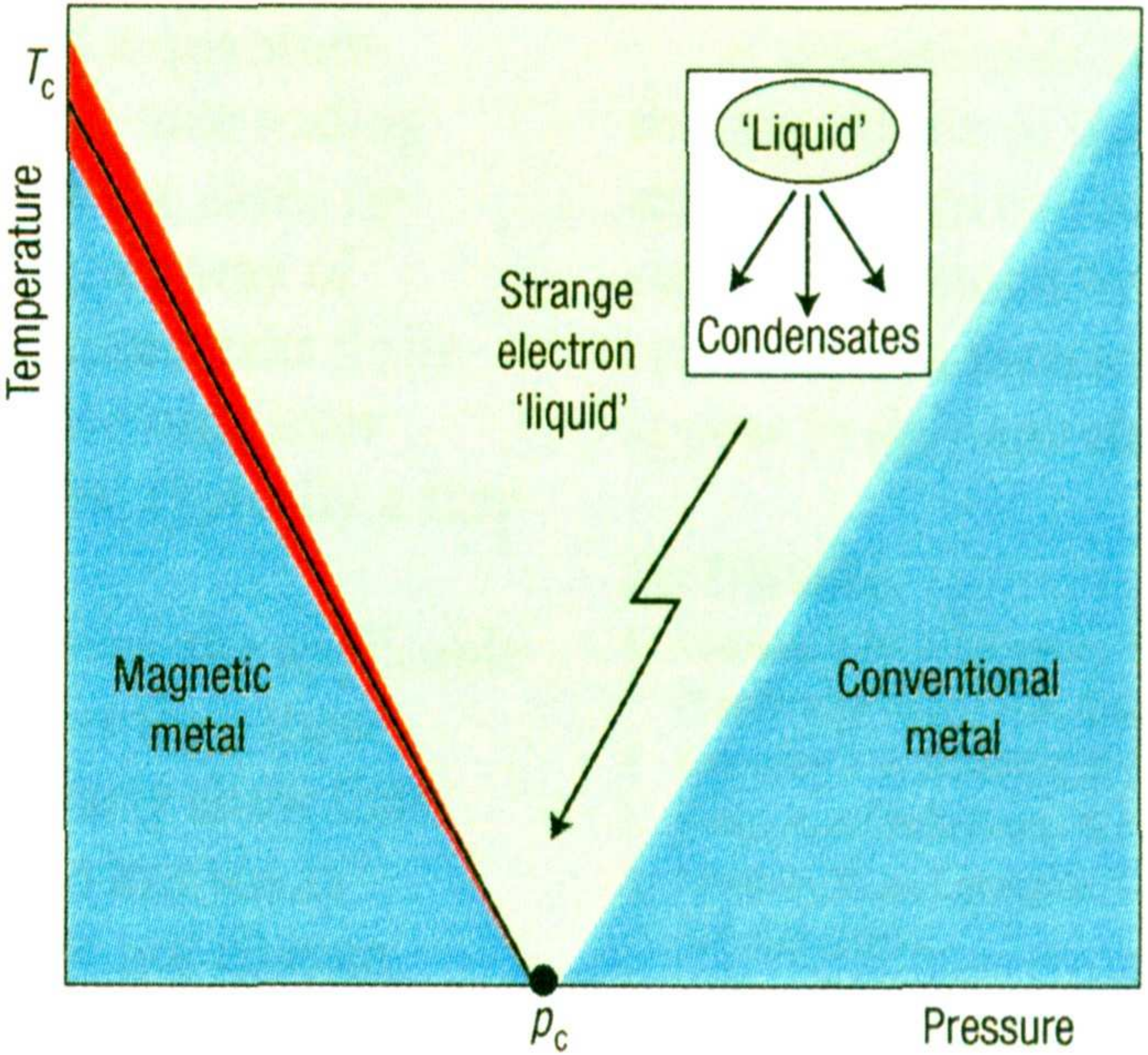
b) Mott-Hubbard insulator



Atomic states



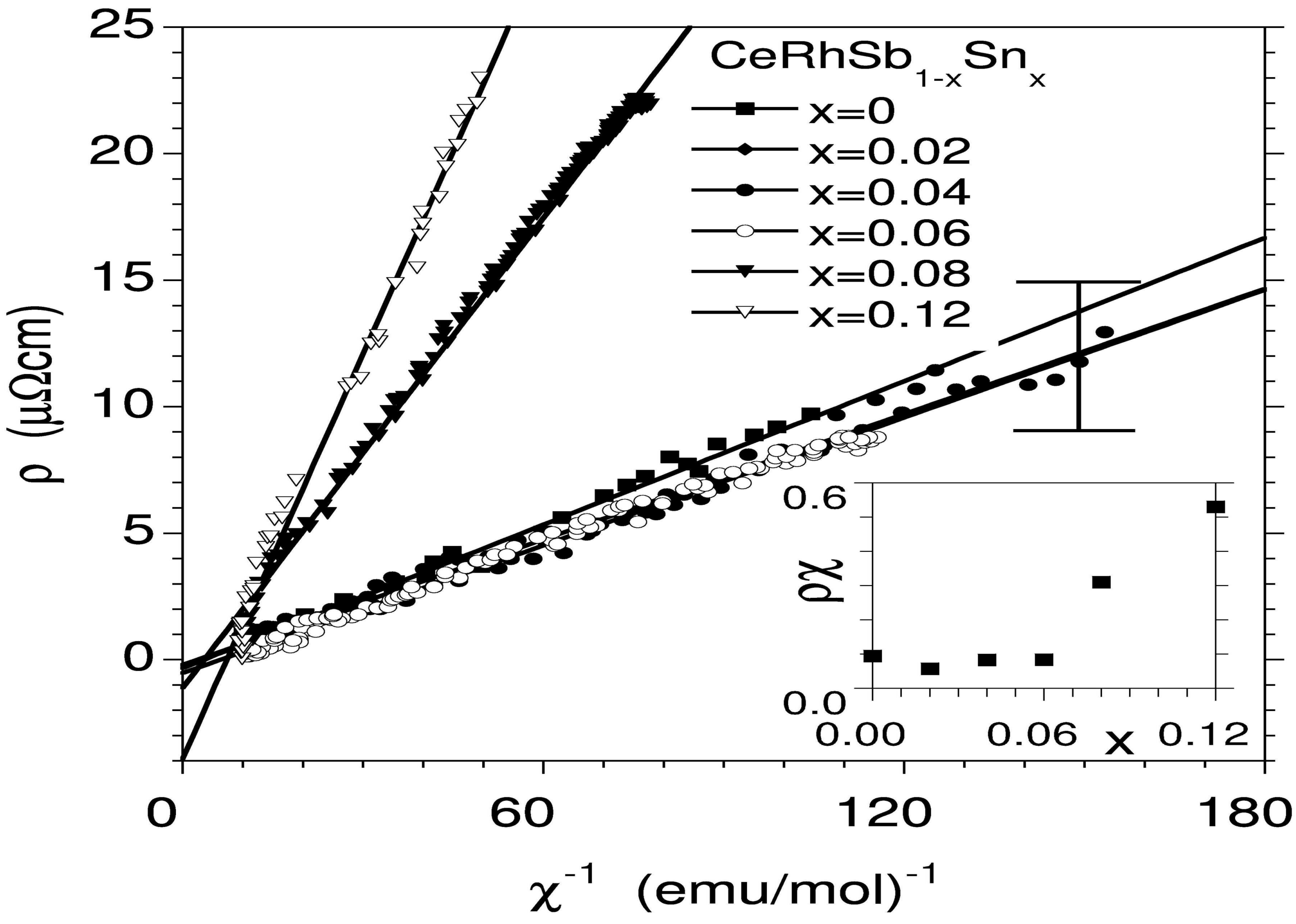
J. S. et al., PRL **59**, 728 (1987) – orbitally nondegenerate;
A. Klejnberg & J. S., PRB **57**, 12 041 (1998) – degenerate.



G. Lonzarich, Nature (2005)

Universal scaling

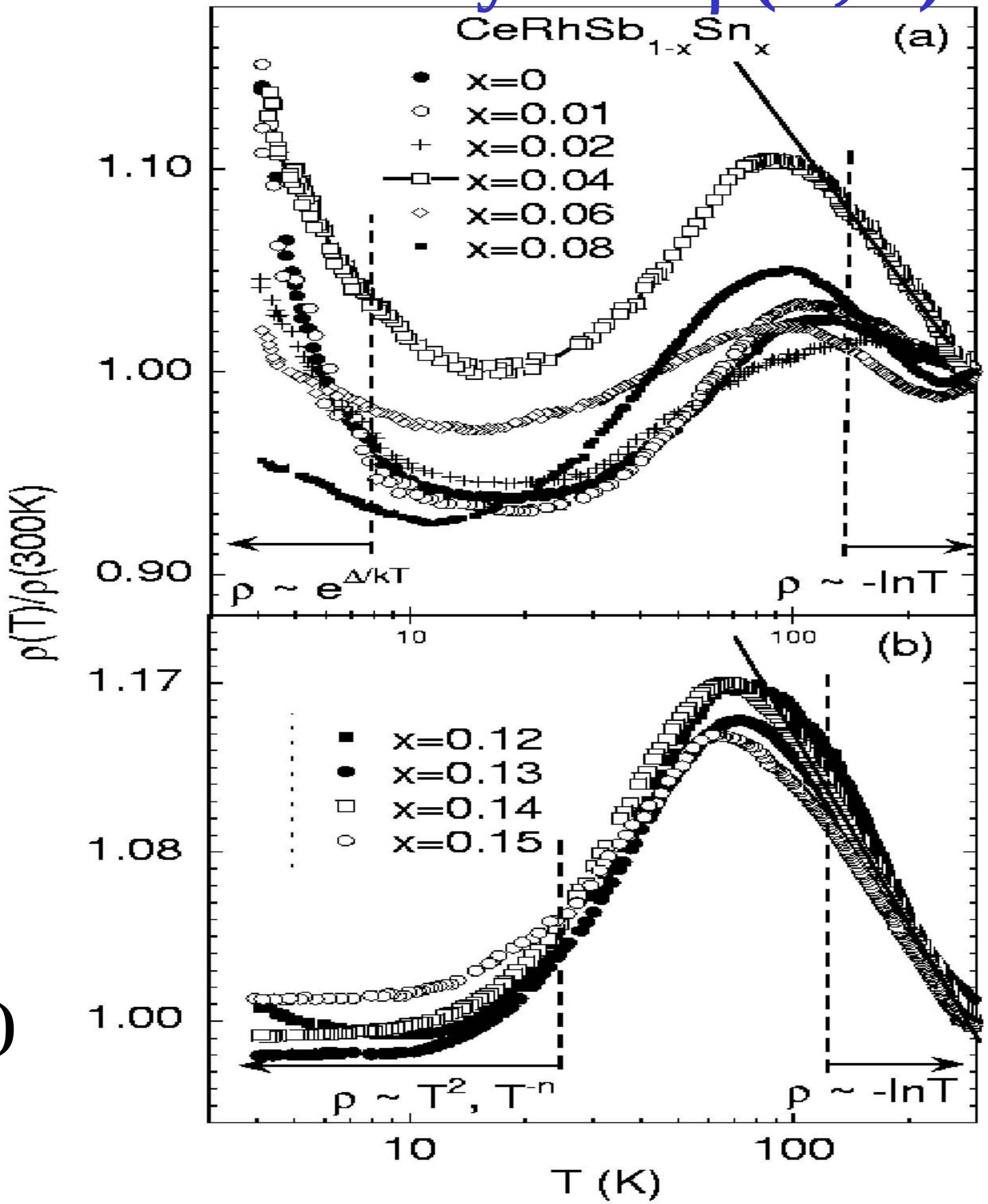
resistivity →



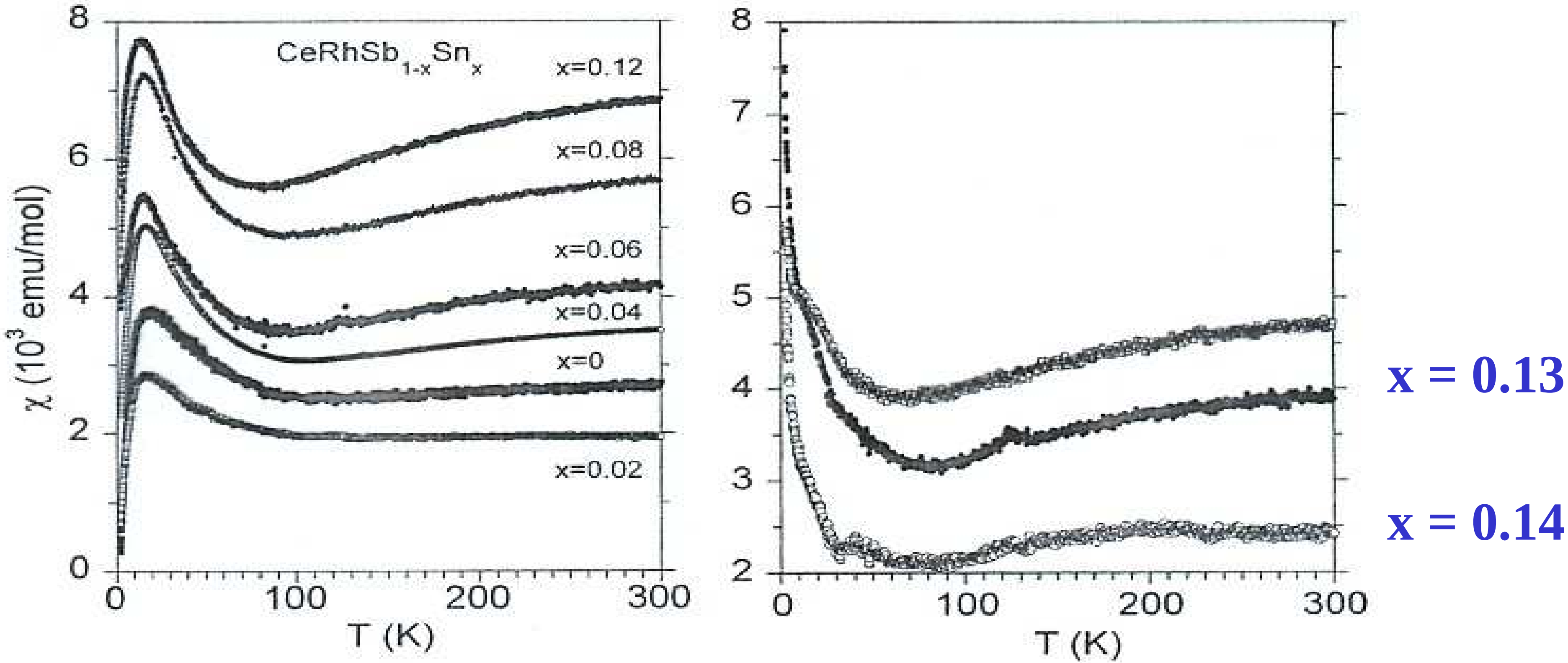
inverse susceptibility →

(A. Ślebarski, JS, PRL (2005)

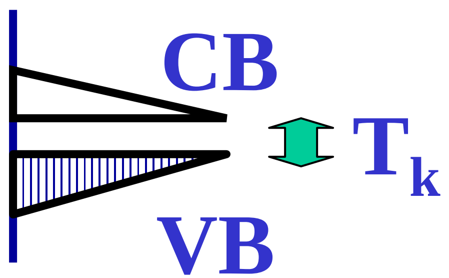
Resistivity data ρ(T; x)



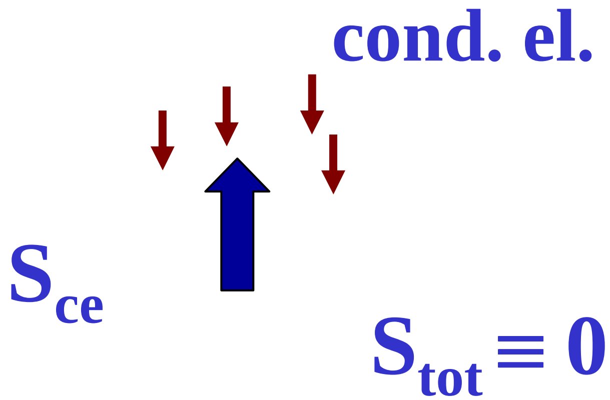
A.Ś. & J.S.
PRL (2005)

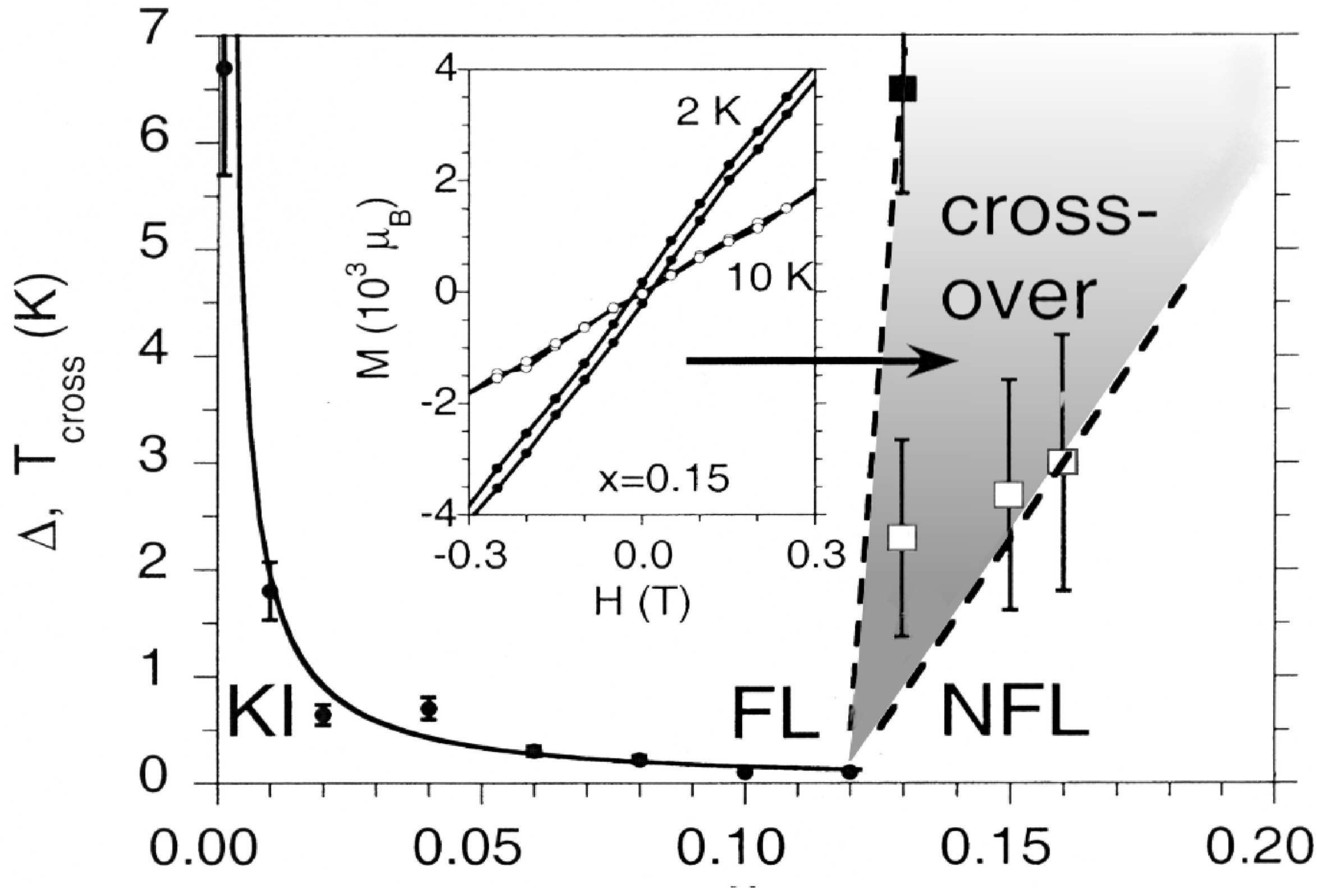


$\chi \to 0$ for $T \to 0$



or else:

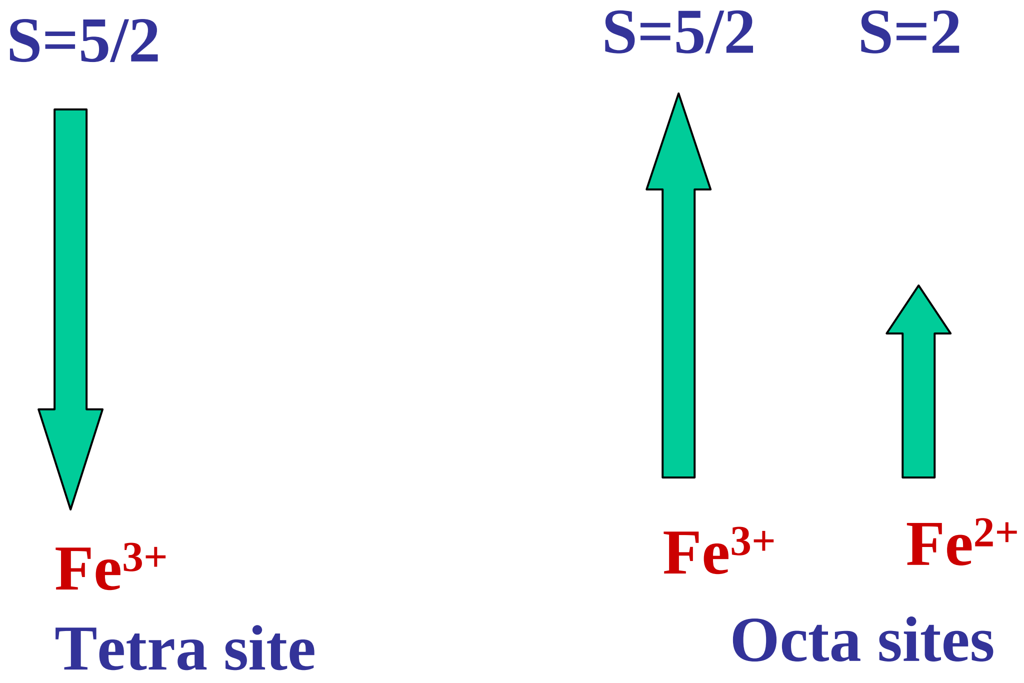




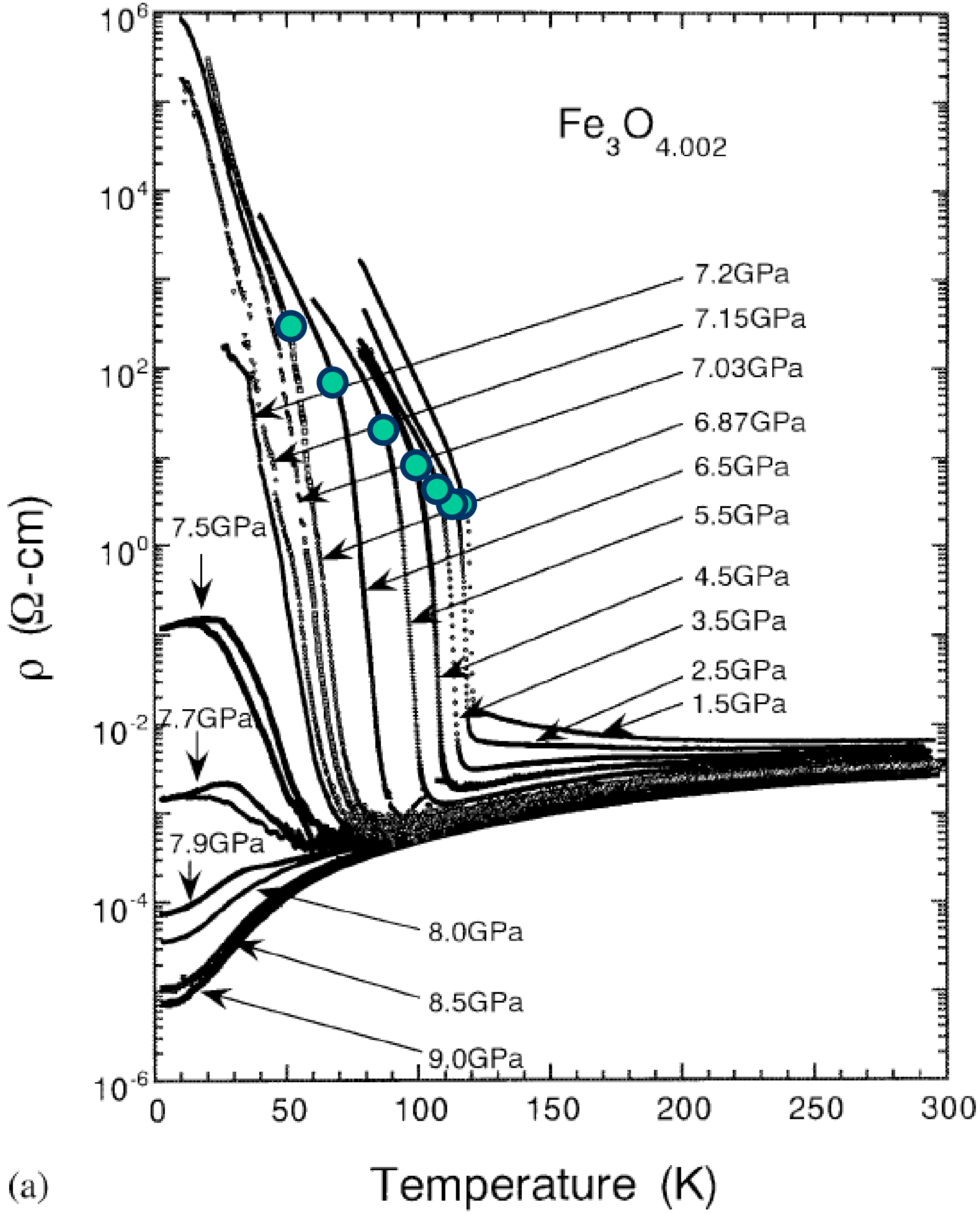
7
6
5
4
3
2
1
0
0.00
0.05
0.10
0.15
0.20
Δ, T_{cross} (K)
KI
FL
NFL
cross-over
4
2
0
-2
-4
-0.3
0.0
0.3
M (10^3 μ_B)
H (T)
2 K
10 K
x=0.15

II. Metallization of magnetite

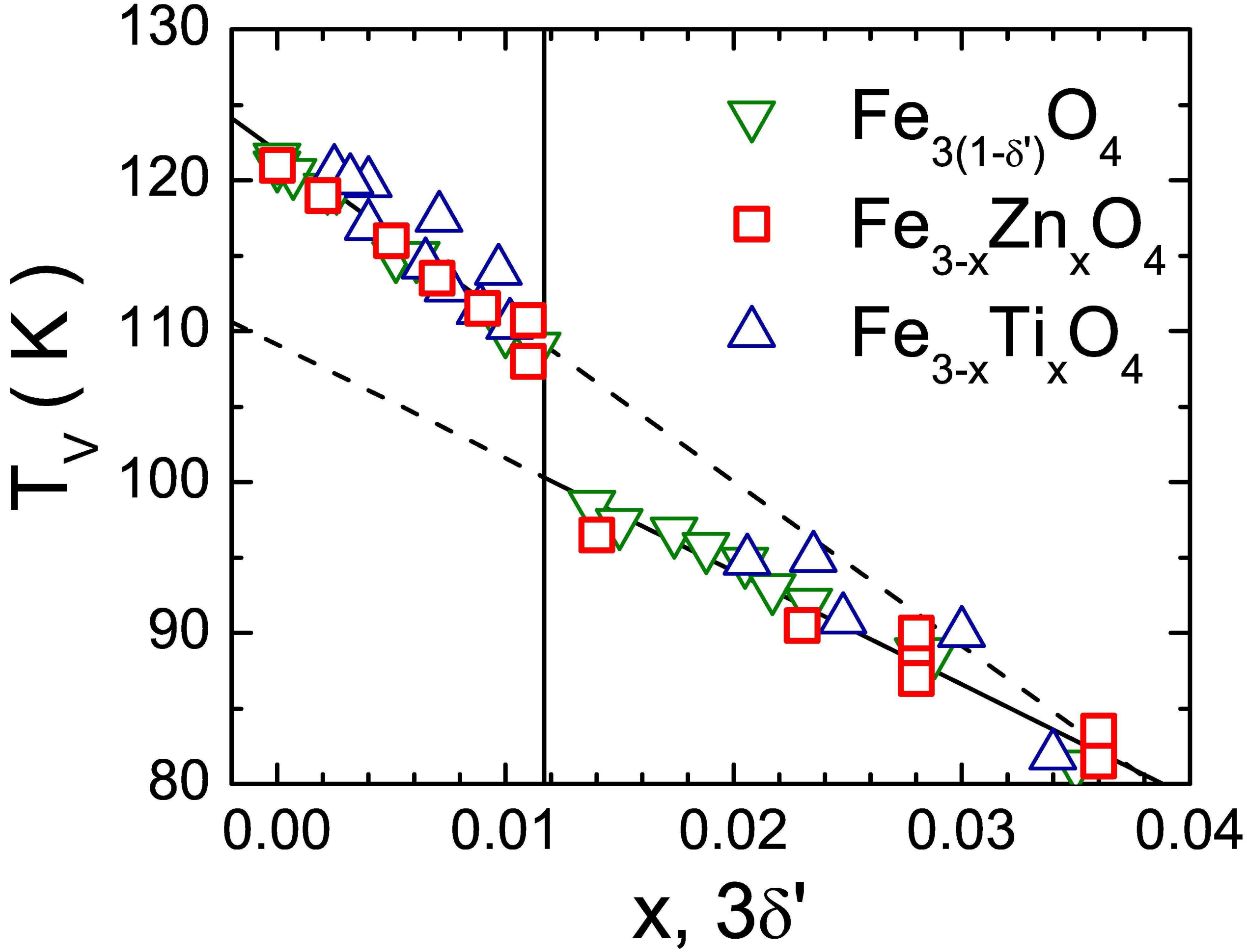
- **Ferrimagnetic material:**
  T_C=860 K, M=4.1 Bohr magnetons



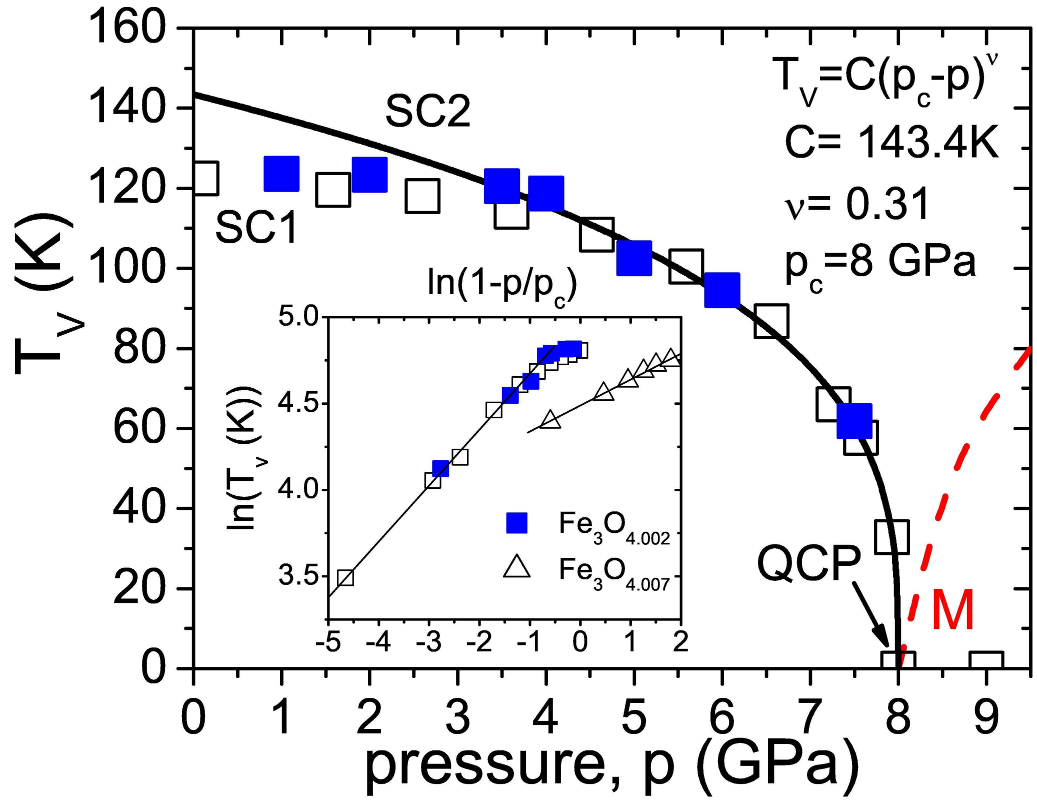
- **Verwey transition: T_V = 122 K ± 1 K**
  (at p = 0)



N. Mori et al. (a)
Physica B, 2002



Z. Kąkol, A. Kozłowski, Z. Tarnawski,…J.M. Honig



J.S., A. Kozłowski, Z. Tarnawski, Z.Kąkol,, Y.Fukami, F.Ono, R. Zach, L.J. Spałek, and J.M. Honig,
Phys. Rev.B 78, 100401 (R) (2008)

Localization criterion: Mott

Kinetic energy in e⁻ gas/particle

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

$$\in_{e-e} = \frac{1}{2}\frac{e^2}{\varepsilon d_{e-e}} = \frac{e^2}{2\varepsilon}\rho^{1/3}$$

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

$\overline{\in} = \in_{e-e}$ ⟶ **gas instability**

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

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

$\Rightarrow$ Fermi - sphere collapse

In one dimension:

$$\mathbf{a_B \rho_C \cong 1 \Rightarrow R_C \cong a_B}$$

Microscopic many-particle Hamiltonian for a nanosystem

(for extended system no phase factor in t)

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

$$\delta n_i \equiv n_i - 1, \ \epsilon_a^{\text{eff}} = \epsilon_a + N^{-1} \textstyle\sum_{i<j} (2/R_{ij} + K_{ij})$$

The microscopic parameters t, U, K should be calculated together with the H diagonalization -> wave function optimization in the correlated state

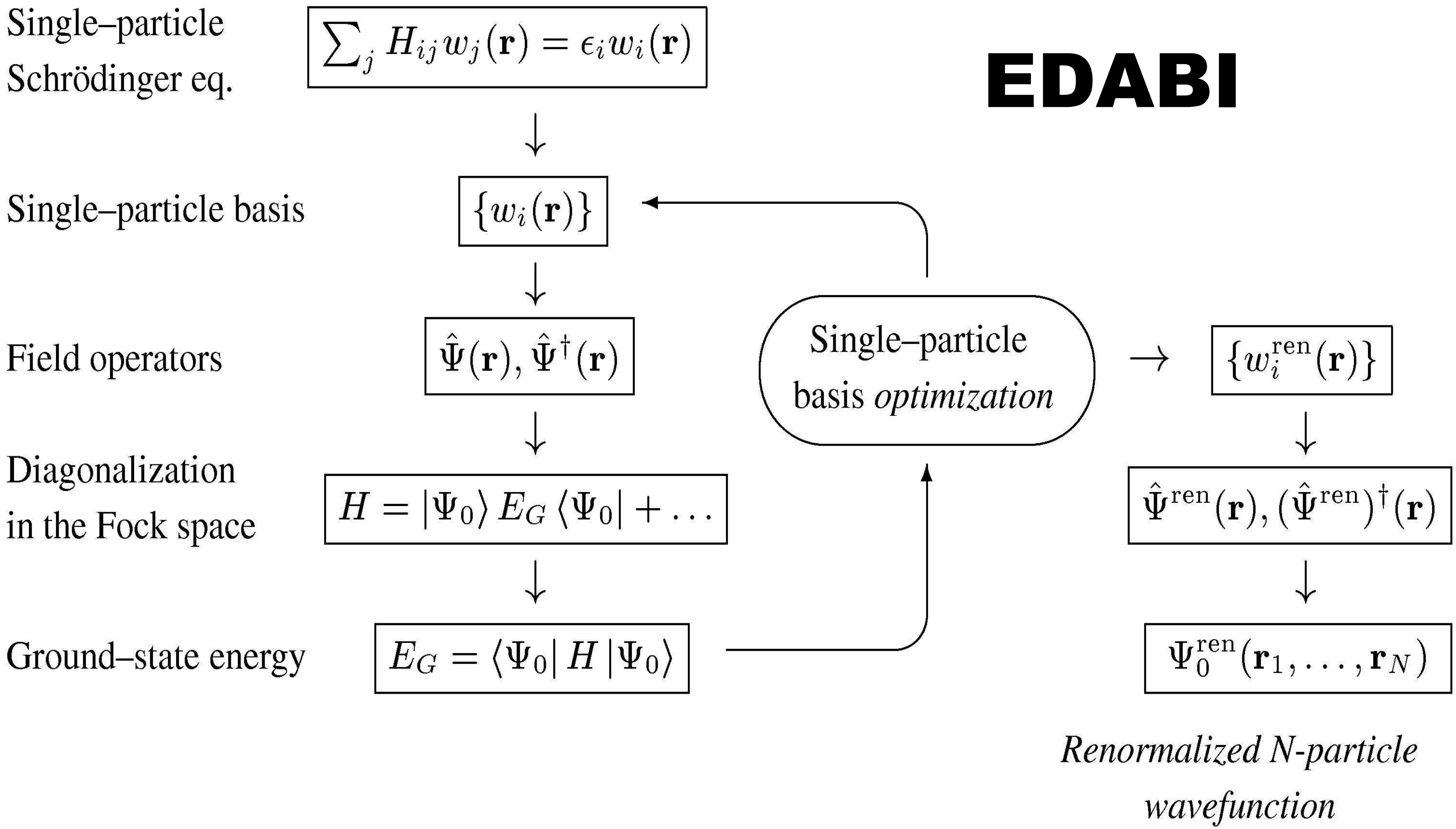
The main ingredient:

interelectronic correlations and wave function treated on the same footing

The main result:

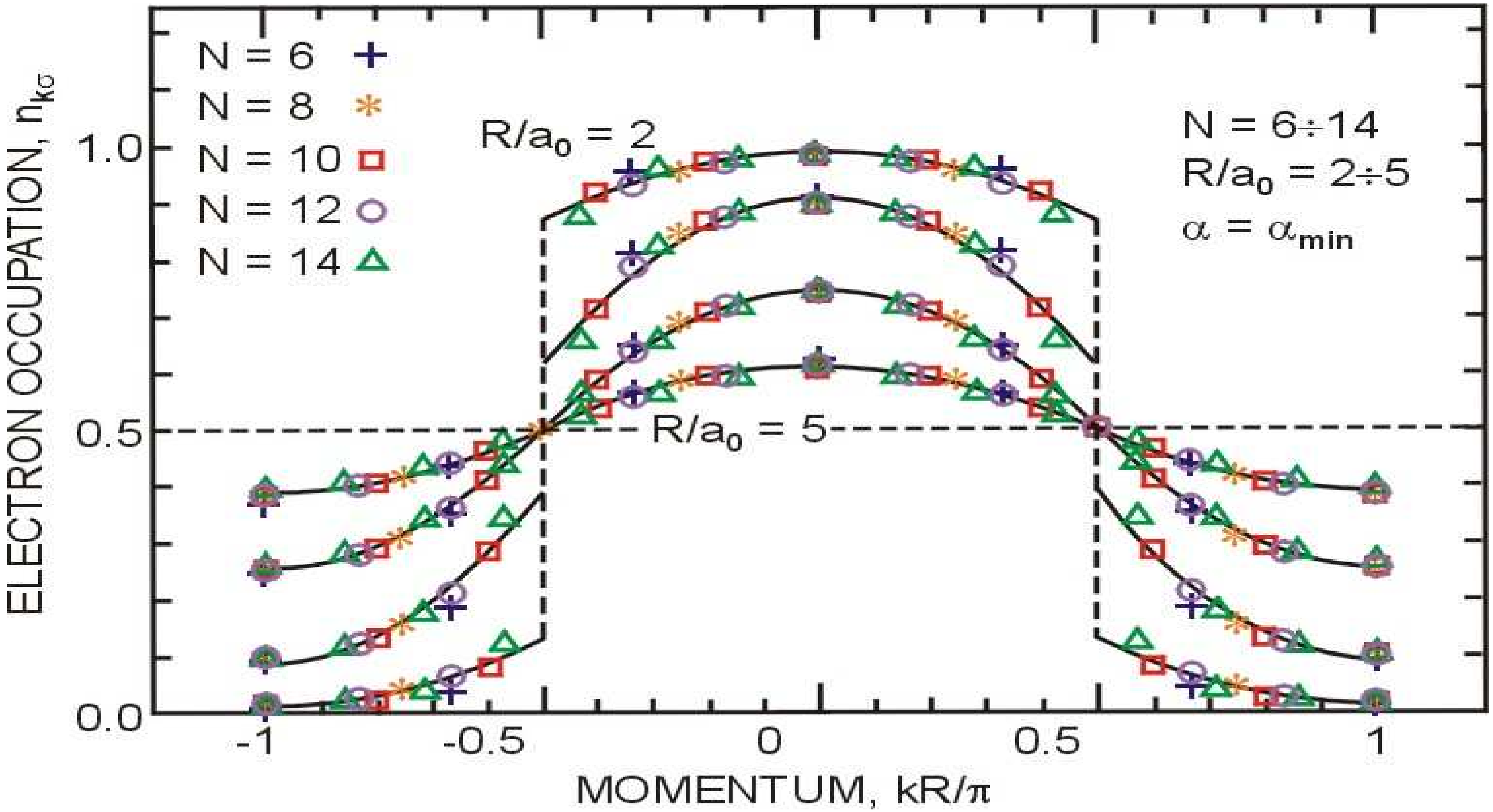
evolution of the many-atom system as a function of interatomic spacing

EDABI



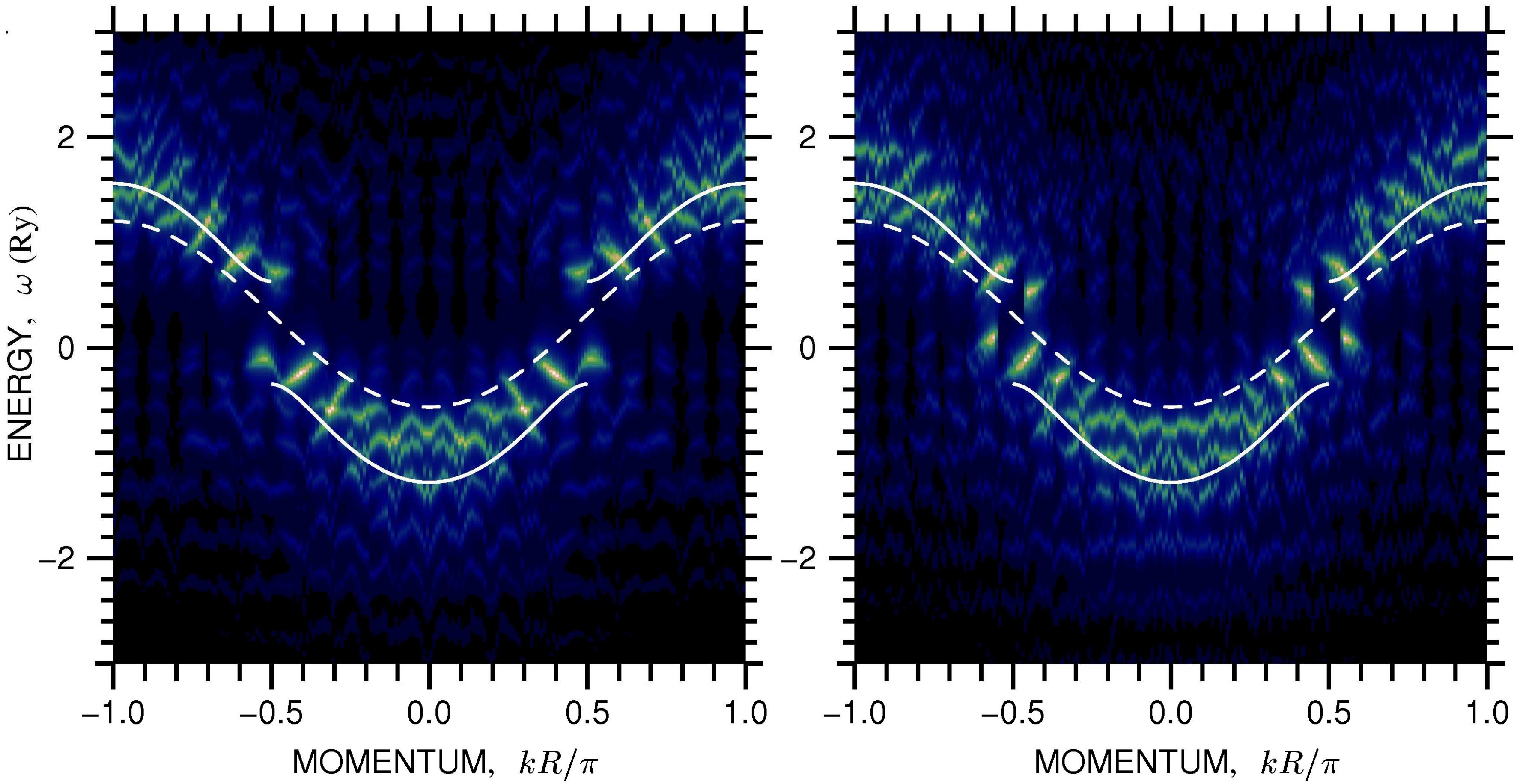
J. Spałek, R. Podsiadły, W. Wójcik, and A. Rycerz, Phys.Rev. B 61, 15676 (2000);PRB (2001-2002)

Momentum distribution:Fermi-Dirac vs continuous



J. S. & A. Rycerz, PRB-R (2001-2004); review: 2007; Didactical: J.S., in Encyclopedia of Condensed Matter Physics, Elsevier, vol. 3, pp. 126-136 (2005)

Renormalized band energies: even and odd



Extended systems : EDABI
D=1

Supplement: Infinite Hubbard chain vs. nanochain

Ground state energy functional:

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

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

Periodic bound cond.

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

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

↓

Renormalized wave equation:

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

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

Atomic functions:

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

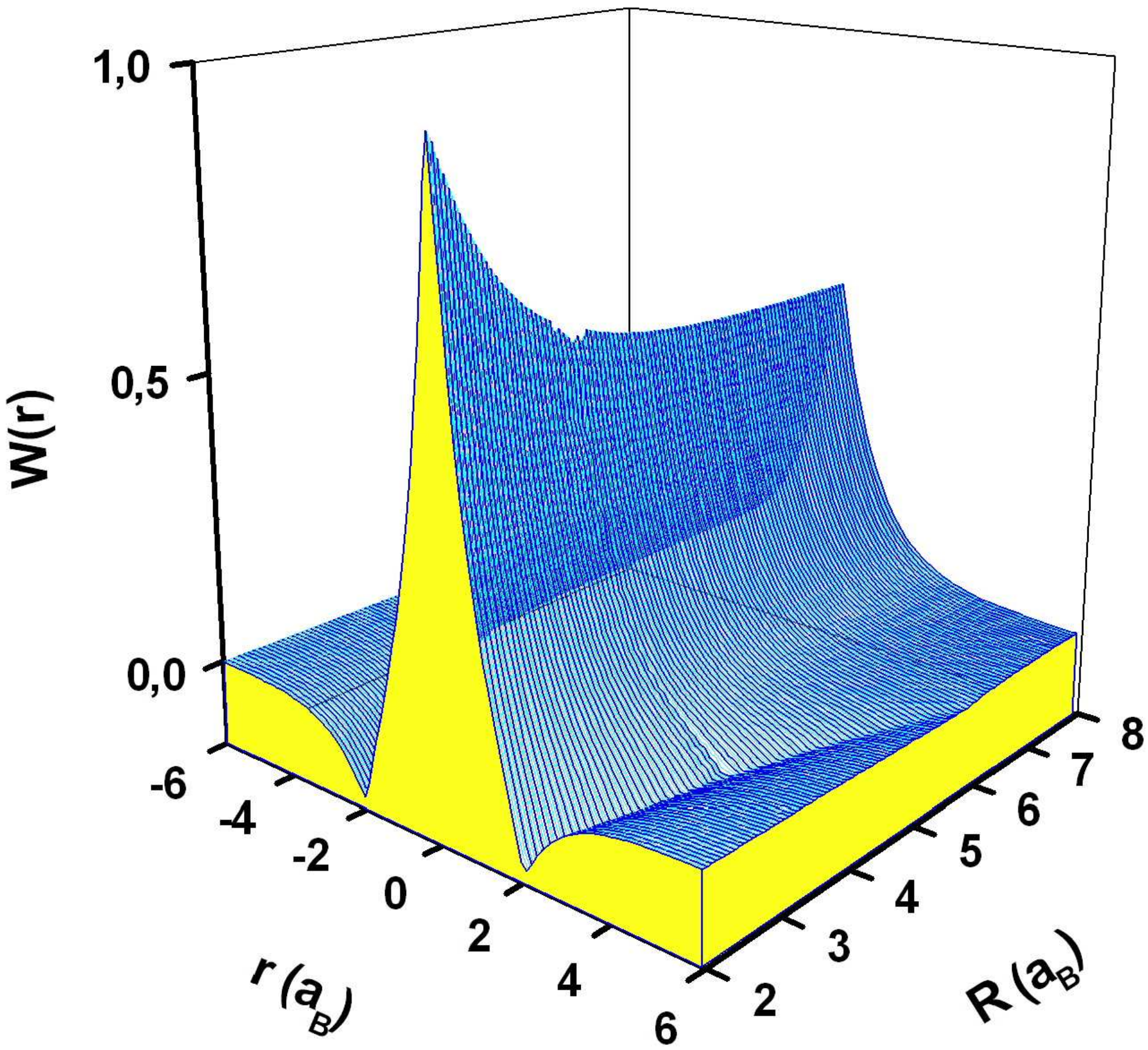
$$\left\langle \Phi_i \middle| \Phi_j \right\rangle = S_{ij}$$

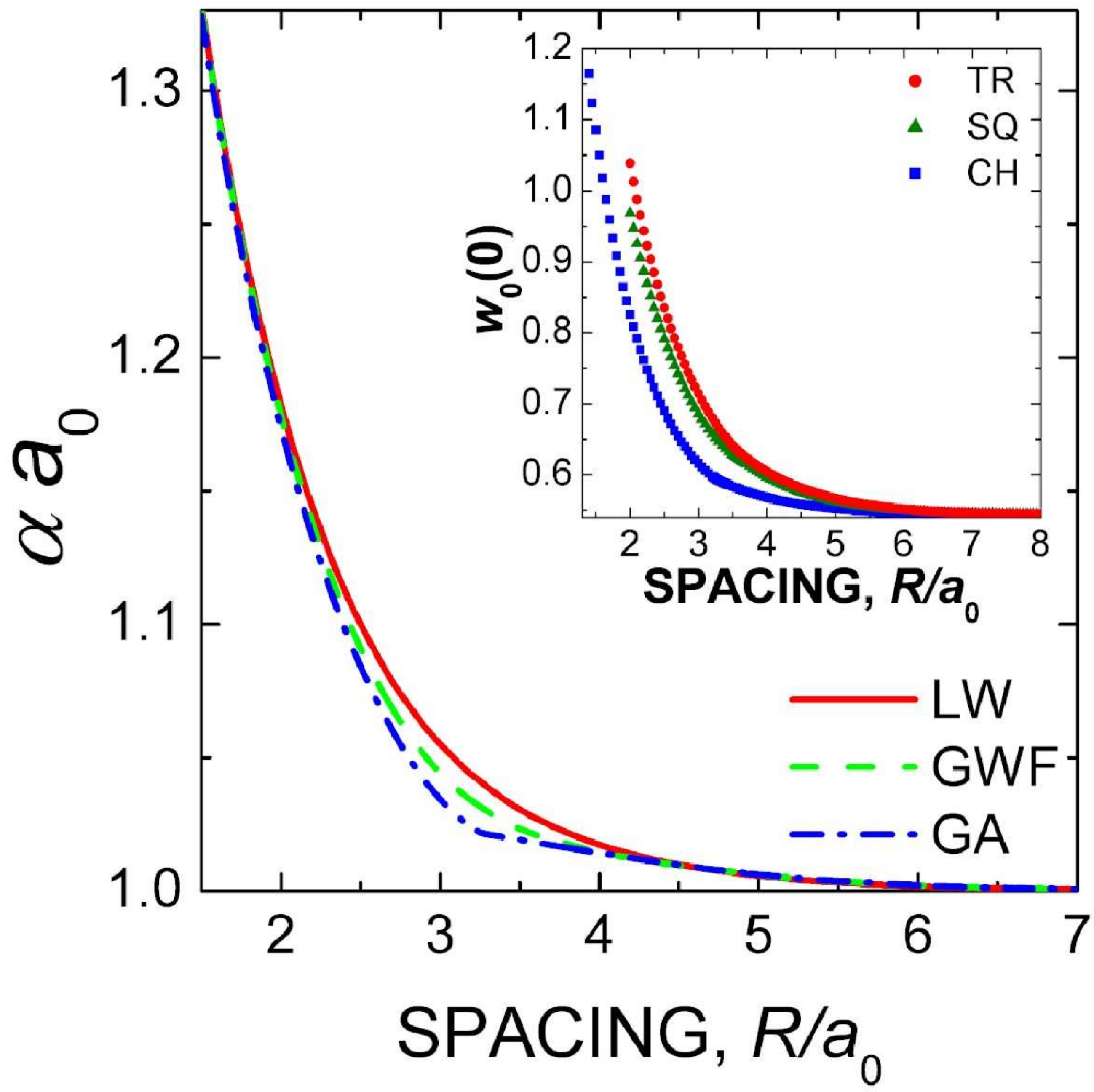
Wannier functions (wave functions):

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

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

Square lattice

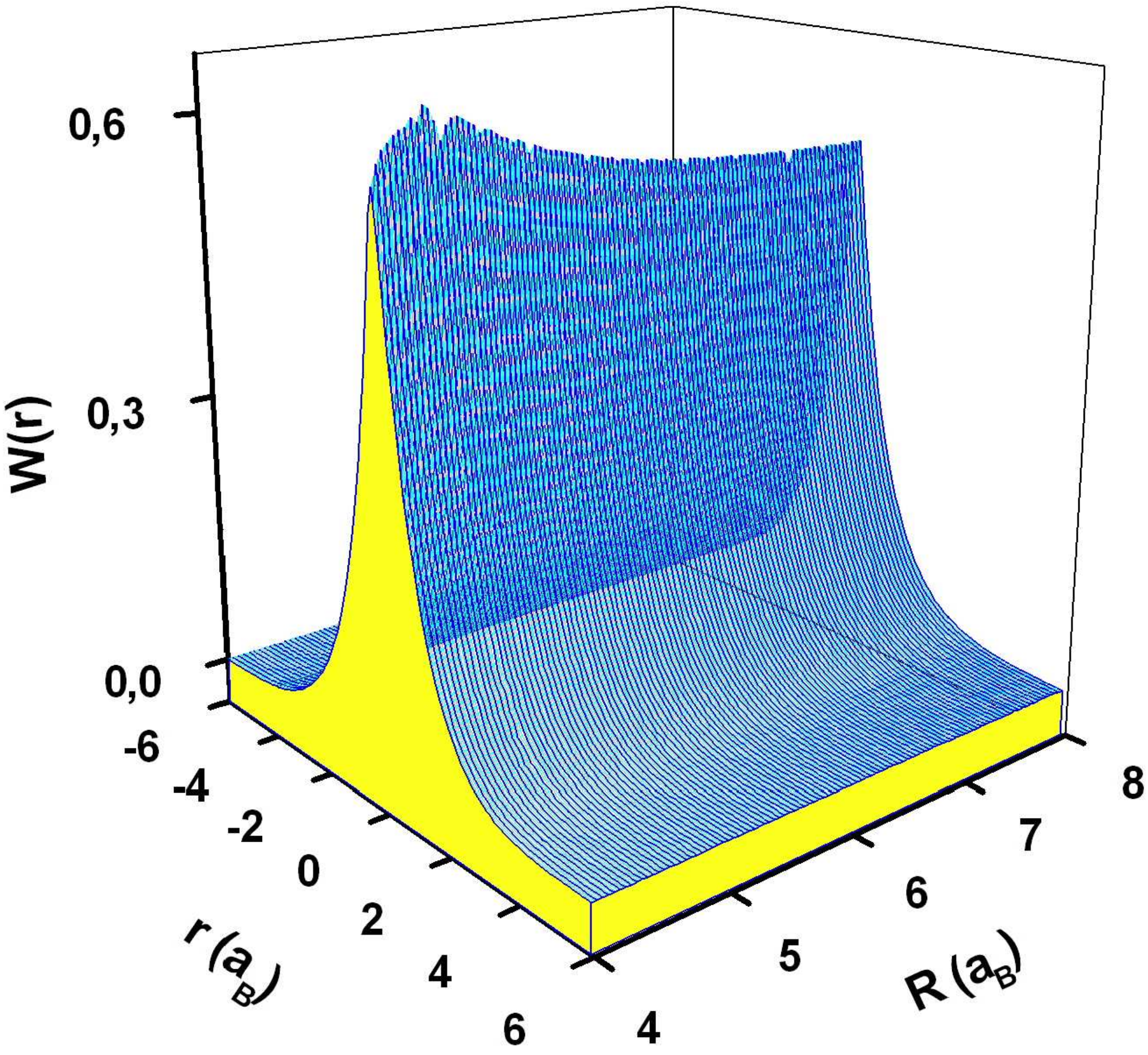


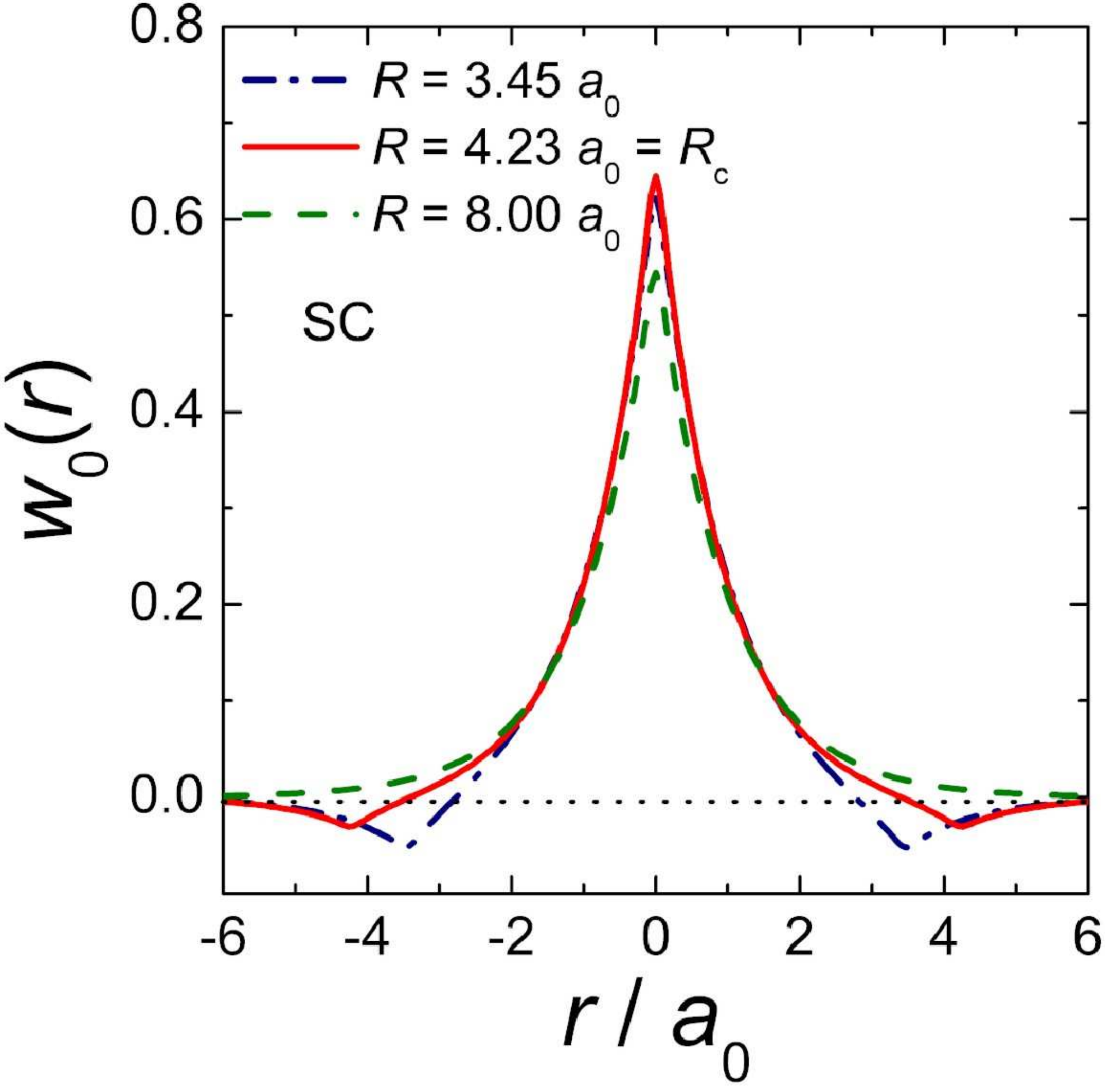


1.3
1.2
1.1
1.0
2
3
4
5
6
7
α a0
SPACING, R/a0
LW
GWF
GA
1.2
1.1
1.0
0.9
0.8
0.7
0.6
2
3
4
5
6
7
8
w0(0)
SPACING, R/a0
TR
SQ
CH

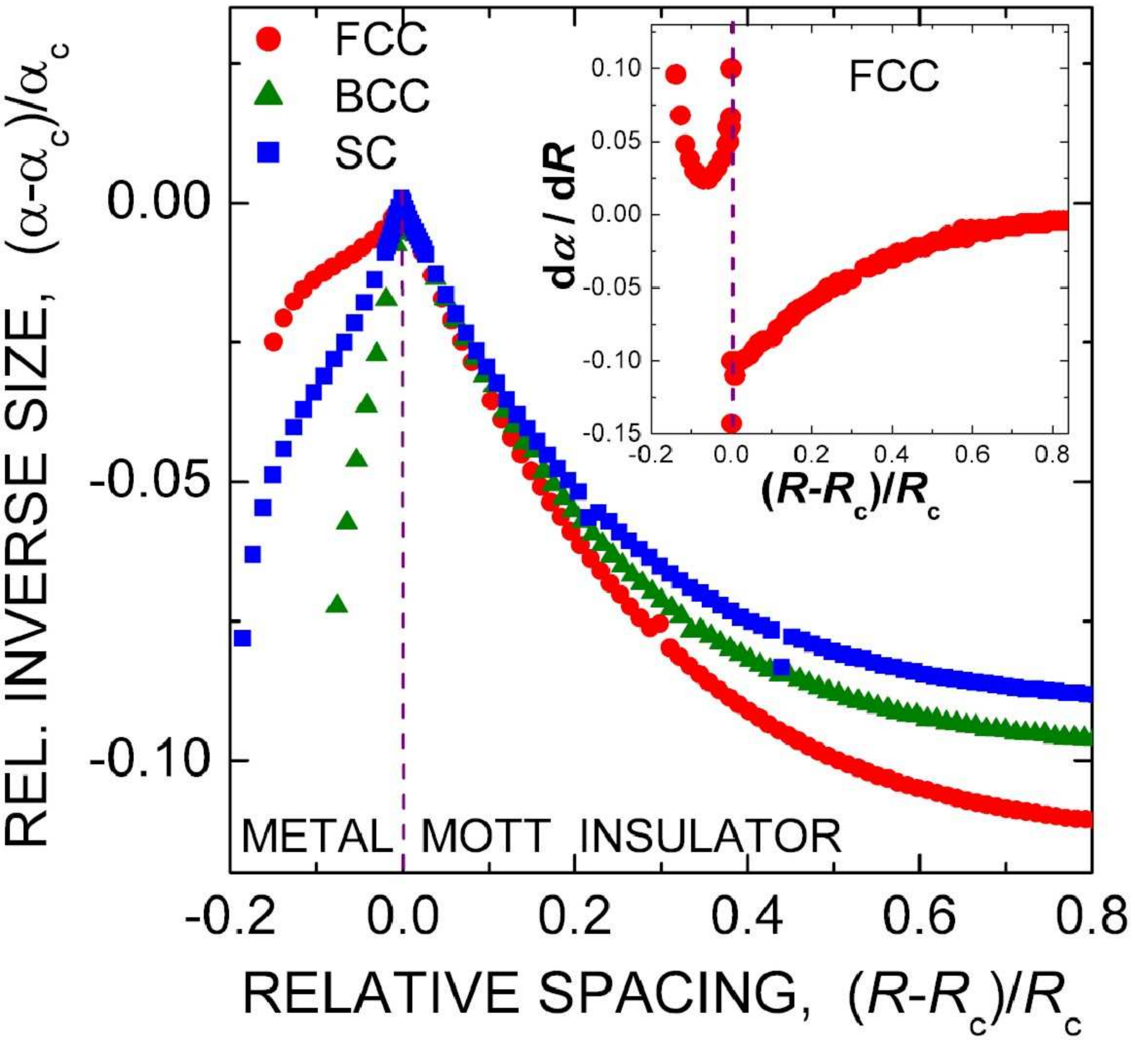
3 Dimensions: Gutzwiller approach

Body Centered Cubic lattice

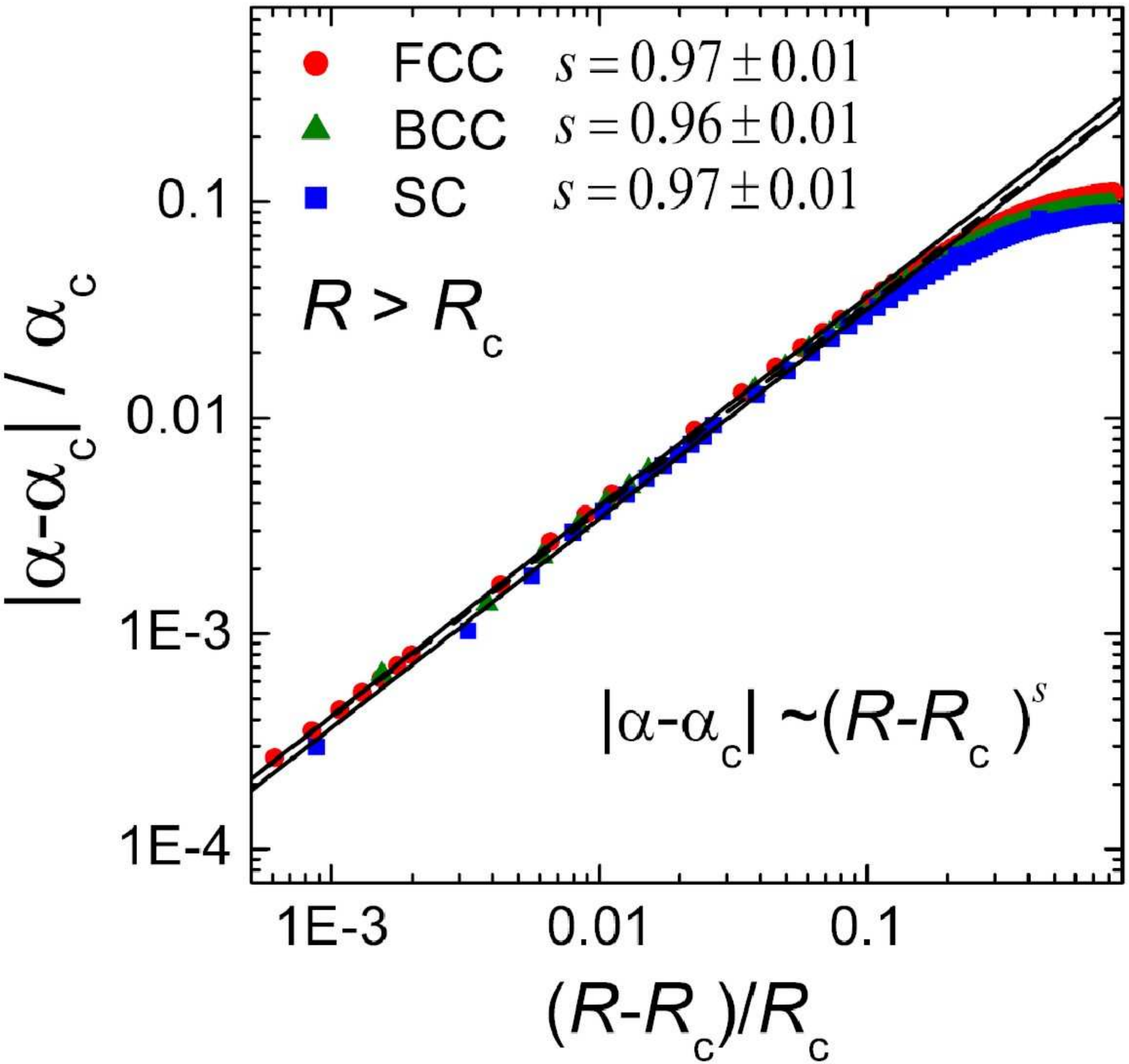




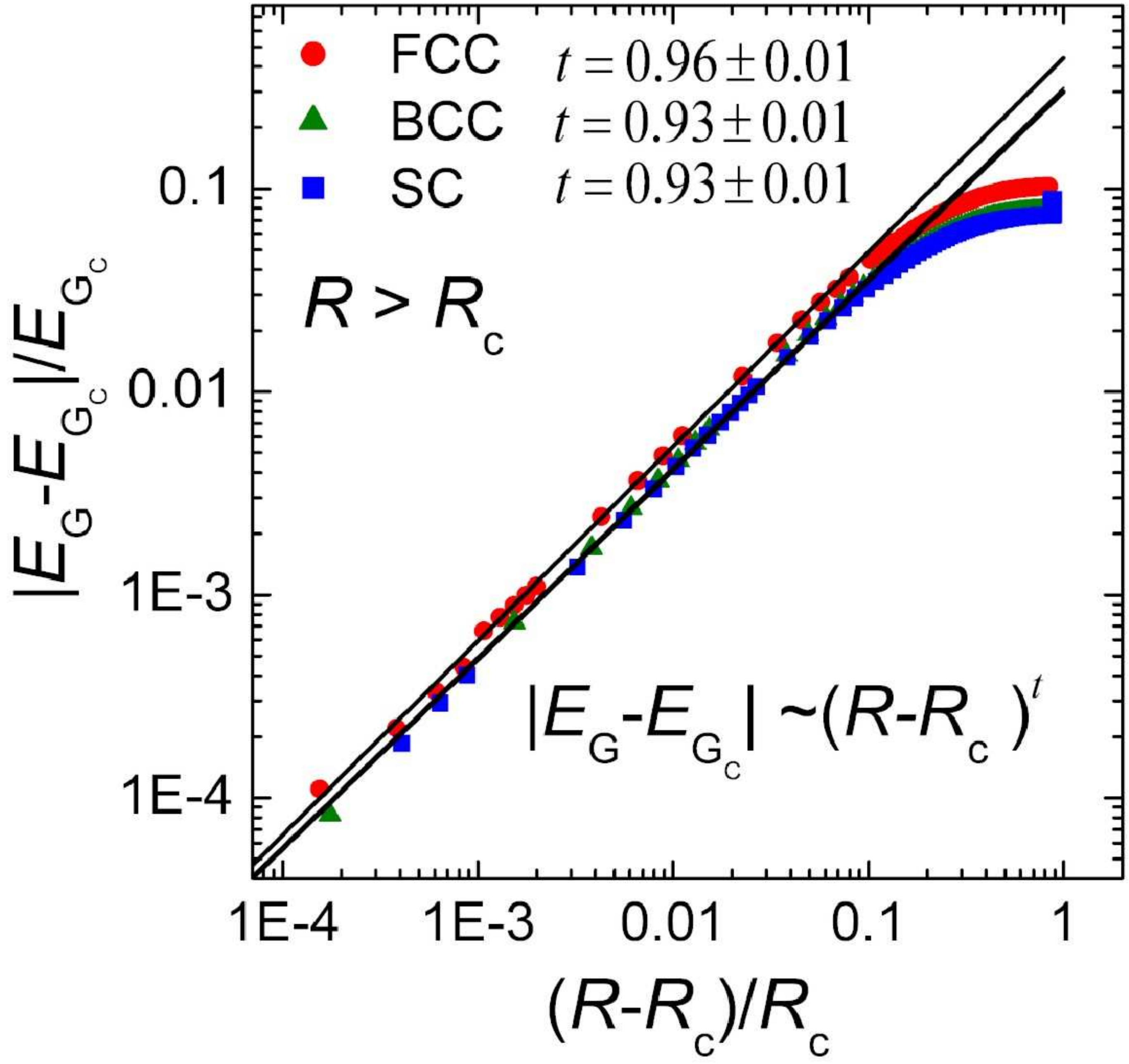
0.8
0.6
0.4
0.2
0.0
R = 3.45 a_0
R = 4.23 a_0 = R_c
R = 8.00 a_0
SC
$w_0(r)$
-6
-4
-2
0
2
4
6
r / a_0



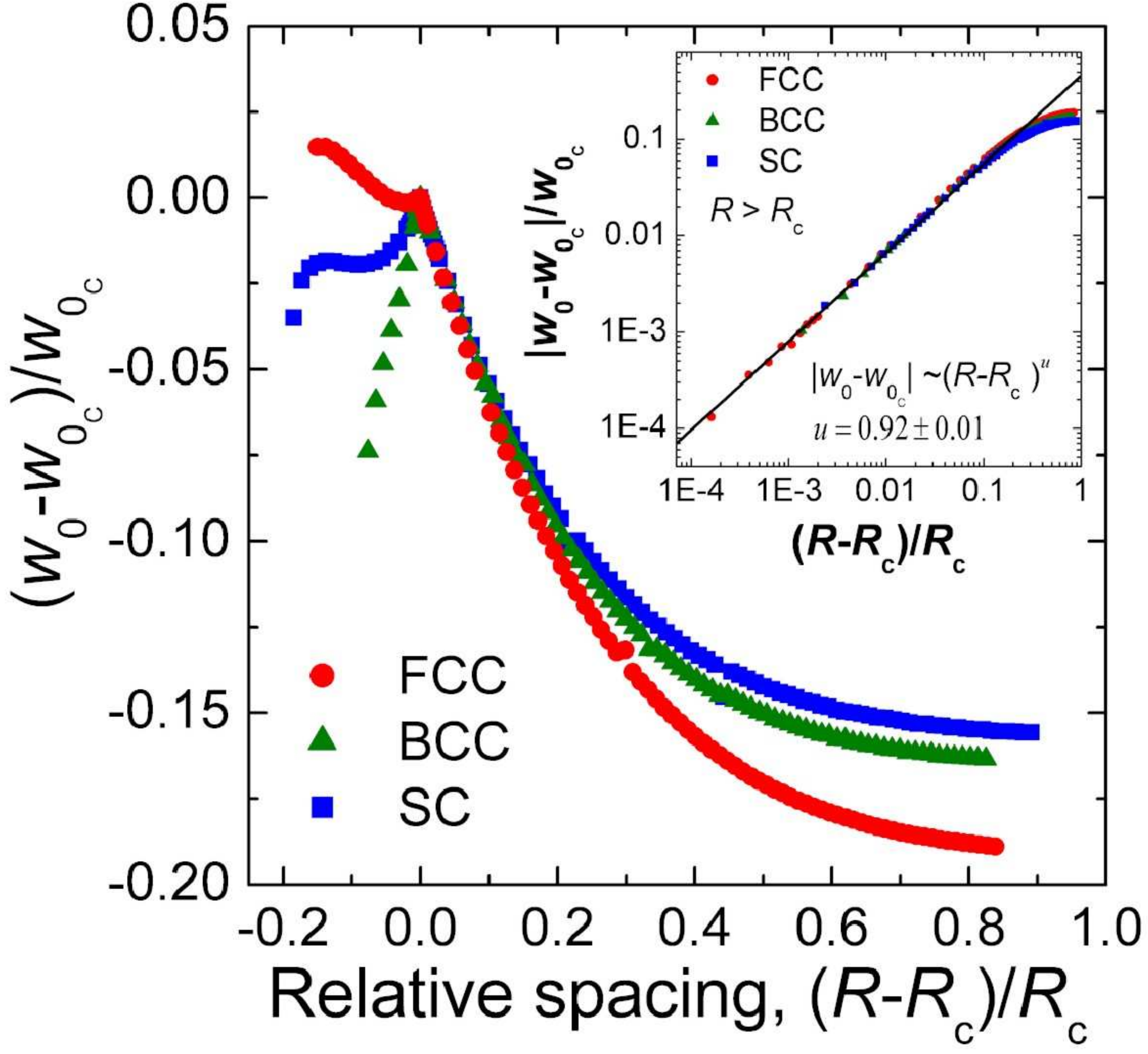
REL. INVERSE SIZE, $(\alpha-\alpha_c)/\alpha_c$
0.00
-0.05
-0.10
FCC
BCC
SC
METAL
MOTT INSULATOR
-0.2
0.0
0.2
0.4
0.6
0.8
RELATIVE SPACING, $(R-R_c)/R_c$
FCC
$d\alpha$ / dR
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.2
0.0
0.2
0.4
0.6
0.8
$(R-R_c)/R_c$



FCC $s = 0.97 \pm 0.01$
BCC $s = 0.96 \pm 0.01$
SC $s = 0.97 \pm 0.01$
$R > R_c$
$|\alpha - \alpha_c| \sim (R - R_c)^s$
$|\alpha - \alpha_c| / \alpha_c$
$(R - R_c)/R_c$
0.1
0.01
1E-3
1E-4
1E-3
0.01
0.1



FCC
BCC
SC
$t = 0.96 \pm 0.01$
$t = 0.93 \pm 0.01$
$t = 0.93 \pm 0.01$
$R > R_c$
$|E_G - E_{G_c}| \sim (R - R_c)^t$
$|E_G - E_{G_c}|/E_{G_c}$
$(R - R_c)/R_c$
0.1
0.01
1E-3
1E-4
1E-4
1E-3
0.01
0.1
1



0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
$(w_0 - w_{0_c})/w_{0_c}$
Relative spacing, $(R-R_c)/R_c$
FCC
BCC
SC
FCC
BCC
SC
$R > R_c$
$|w_0 - w_{0_c}|/w_{0_c}$
$(R-R_c)/R_c$
$|w_0 - w_{0_c}| \sim (R-R_c)^u$
$u = 0.92 \pm 0.01$
0.1
0.01
1E-3
1E-4
1E-4
1E-3
0.01
0.1
1

Outlook

1. **Method allows for study of the electron state evolution as a funtion of interatomic spacing**
2. **The evolution of the wave function in the correlated state through the Mott threshold:**
   from atoms to solid state (or vice versa)
3. **Scaling and critical behavior of the wave function and a critical behavior**

4. **Future: Bose Hubbard**
   d-orbitals