Effect of applied magnetic field on the Mott transition: Gutzwiller ansatz with adjustment of the orbital size

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Motivation

One of the important problems in Condensed Matter Physics is the metal-insulator transition of the Mott-Hubbard type [1]. In [2] Spałek *et al.* study the quantum critical scaling of the wave function near MIT. Our aims are to investigate:

1. quantum critical behaviour of the wave function near Mott transition;
2. evaluation of the electron wave function in the strongly correlated system;
3. effect of the external magnetic field;
4. combination of first and second quantisations;

We start with the Extended Hubbard model [3]:

$$\mathcal{H} = \epsilon_a^{eff} \sum_i n_i + \sum_{i \neq j, \sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} K_{ij} \delta n_i \delta n_j - \sum_{i,\sigma} \sigma h n_{i\sigma}, \qquad (1)$$

where $h = \frac{1}{2} g \mu_B H_a$ is a reduced magnetic field.

Hamiltonian parameters

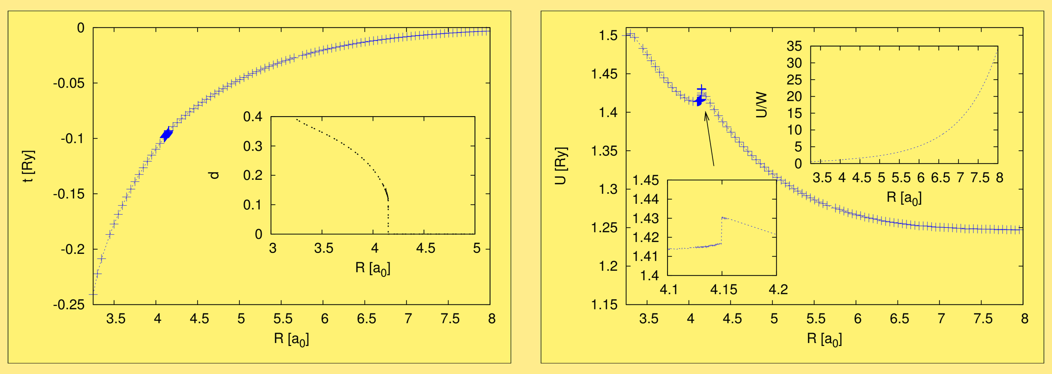

Figure 1: *left:* hopping integral t and double occupancy number d *right:* intraatomic interaction magnitude U, calculated for no magnetic field in relation with lattice size.

Methods applied

EDABI

We obtain Hamiltonian parameters by approximating Wannier orbital by series of Gaussian functions:

$$w_i(\underline{r}) = \beta \Psi_i(\underline{r}) - \gamma \sum_{j=1}^{z} \Psi_j(\underline{r}),$$
$$\Psi_i(\underline{r}) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha |\underline{r} - \underline{R_i}|} \approx \alpha^{\frac{3}{2}} \sum_{a=1}^{n} B_a \left(\frac{2\Gamma_a^2}{\pi} \right)^{\frac{3}{4}} e^{-\Gamma_a^2 |\underline{r} - \underline{R_i}|^2}. \qquad (2)$$

β and γ parameters depend explicitly on the integrals of Ψ_i functions and z is the number of nearest neighbours. Parameters B_a and Γ_a are derived by minimising energy of single atom (Hamiltonian $\mathcal{H} \overset{a.u.}{=} -\nabla^2 - \frac{2}{|\underline{r} - \underline{R_i}|}$). n is a number of Gaussian functions used for the approximation. Parameter α is found as a value minimising the ground energy. The Hamiltonian parameters are obtained by integrating:

$$t_{ij} = \langle w_i | H_1 | w_j \rangle, \quad U = \langle w_i w_i | V_{12} | w_i w_i \rangle, \ etc., \qquad (3)$$

where H_1 is the Hamiltonian for a single particle in the system, and V_{12} represents interparticle interaction.

Statistically-consistent Gutzwiller Approximation

To minimise α for each considered system we have to obtain its ground energy. It was proven [4] that Gutzwiller Approximation not always results in finding the lowest energy. For such a purpose we minimise functional $\mathcal{F}$ with two additional molecular fields λ_m and λ_n, coupled with m and n respectively:

$$\mathcal{F}^{(SGA)} = -\frac{1}{\beta} \sum_{\underline{k}\sigma} \log\left(1 + e^{-\beta E_{\underline{k}\sigma}^{(SGA)}}\right) + \Lambda \left(\lambda_n n + \lambda_m m + U d^2\right). \qquad (4)$$

General Properties

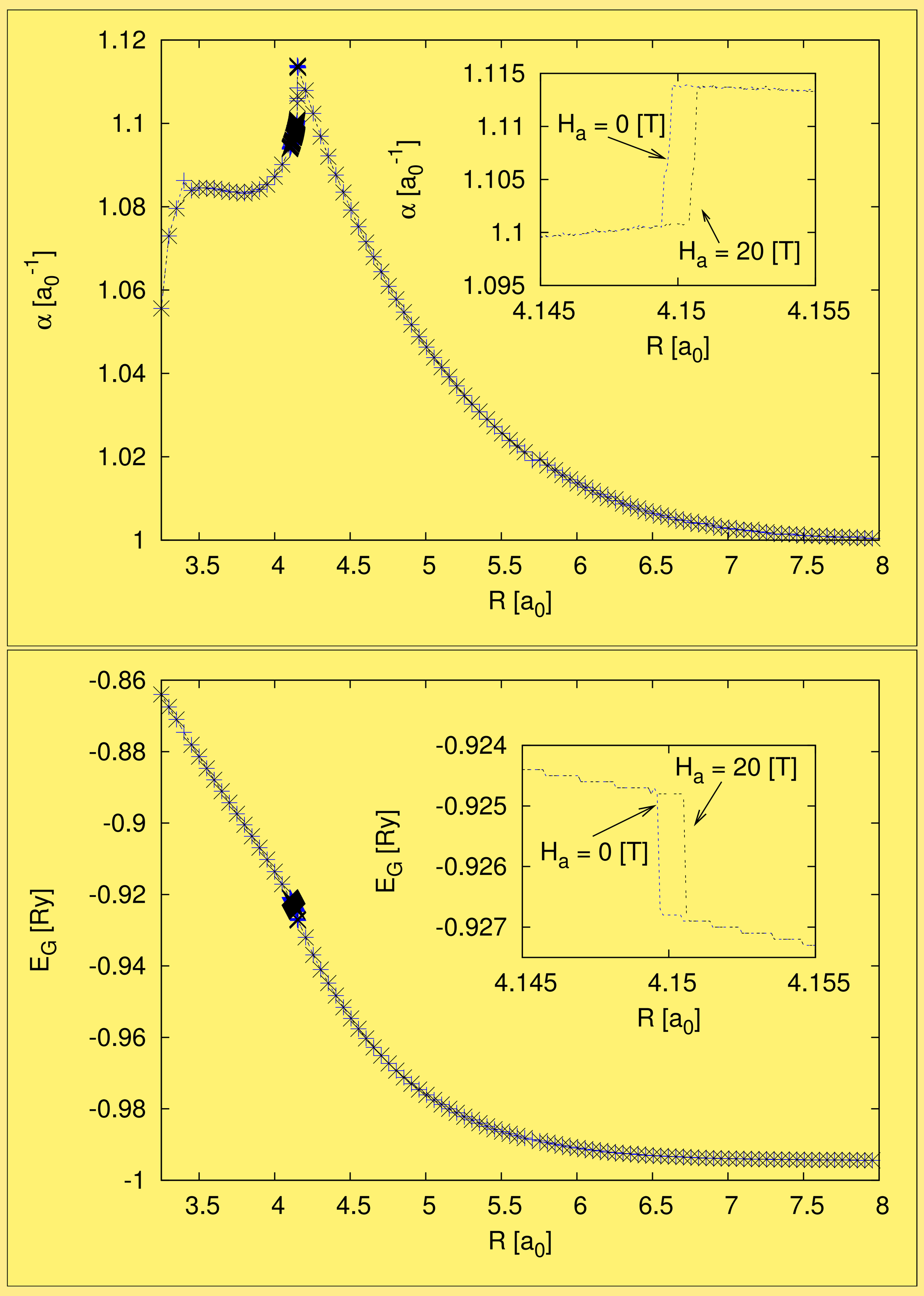

Figure 2: *top:* α parameter *bottom:* ground energy E_G in relation with lattice size R for two different magnitudes of magnetic field; magnified shows the delay of MIT transition

Detailed characteristics at MIT

Calculations were performed on 96-thread node at *ATOMIN Cluster* at Marian Smoluchowski Institute of Physics, for SC 3D crystal (hence $z = 6$). For optimising complexity $STO-3G$ basis (3 Gaussian per Ψ_i) was chosen. Alternative $STO-7G$ would slightly improve accuracy but the average execution time would be increased by the factor of 30.

Characteristics of the model

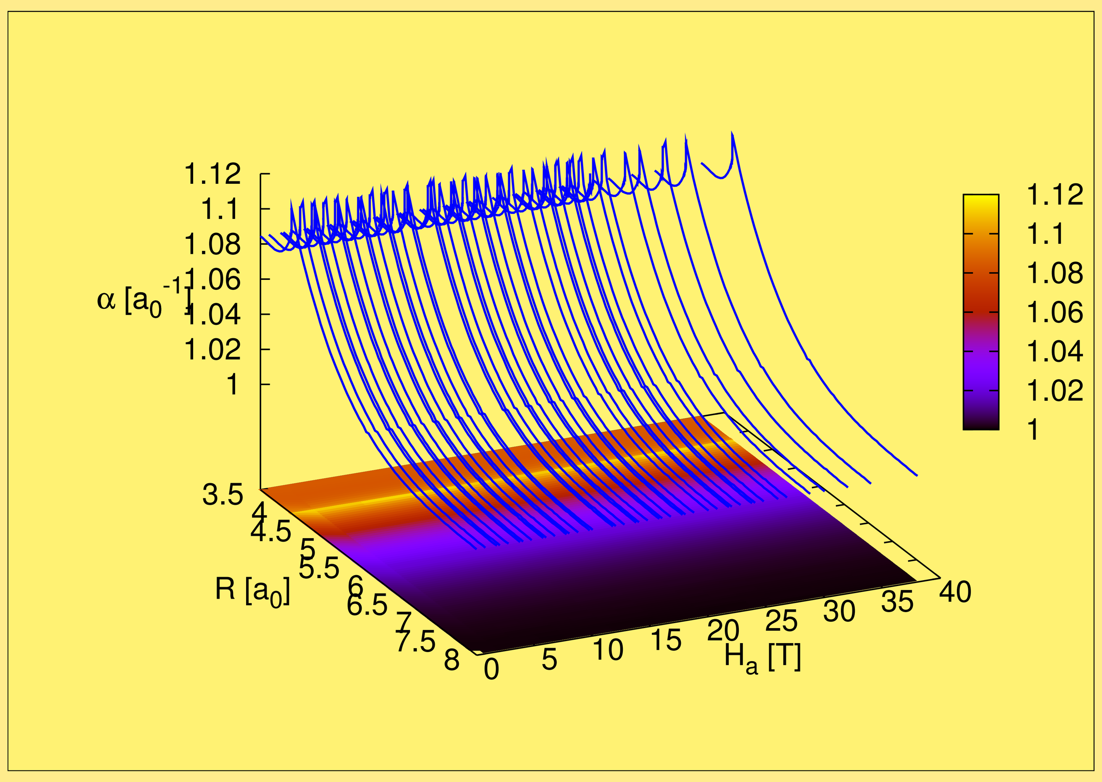

Figure 3: a density plot of $\alpha[R, H_a]$; the change of value with magnetic field is irrelevant.

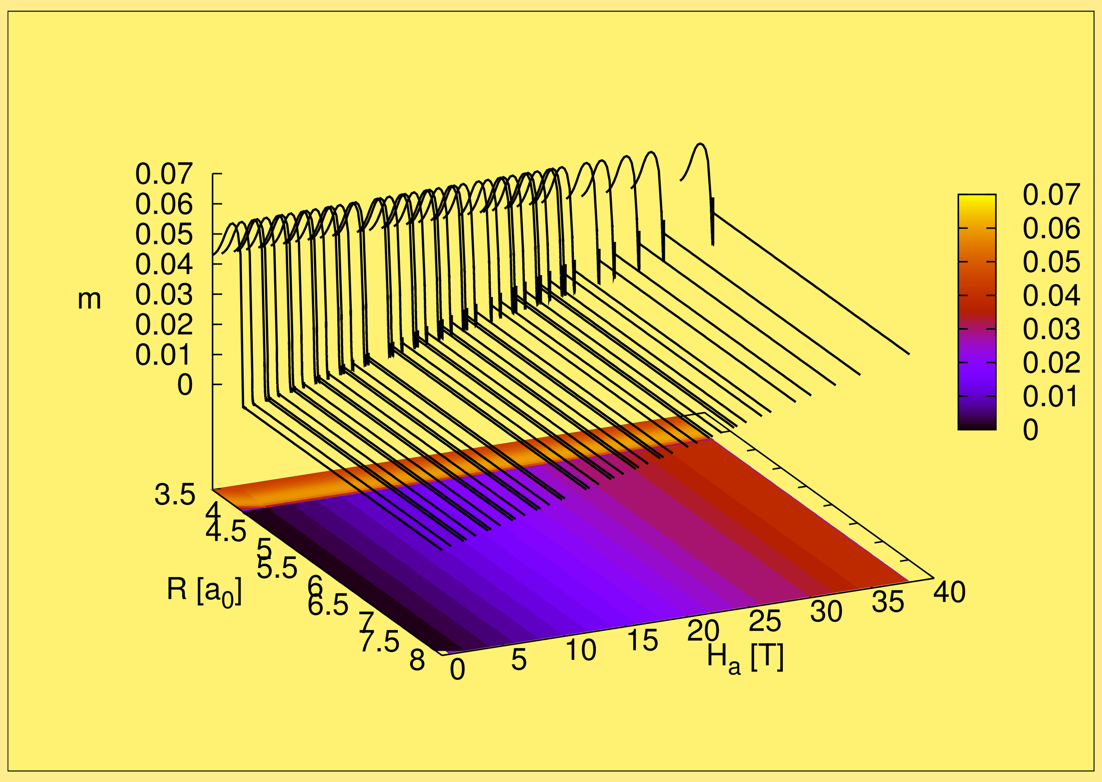

Figure 4: a density plot of $m[R, H_a]$; the change of value in metal state is relevant (shown on figure 7).

Further characteristics

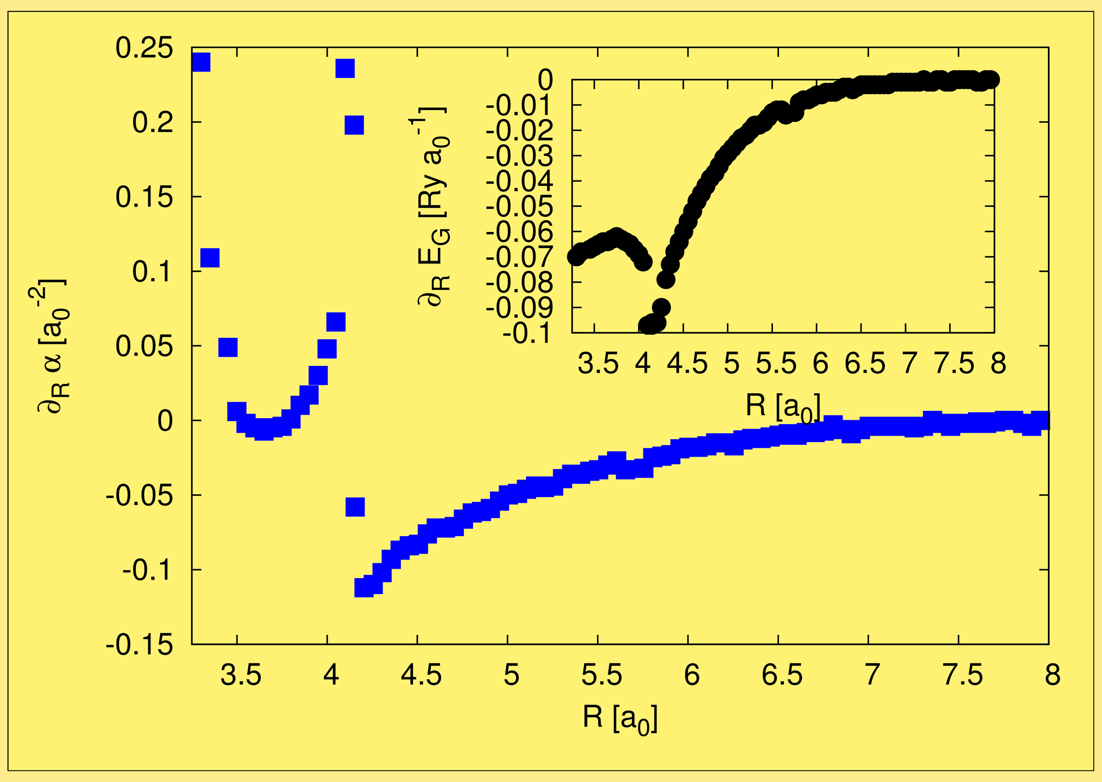

Figure 5: Derivative $\frac{\partial \alpha}{\partial R}$ has a discontinuity at the critical point. At the moment it is also observable for derivative $\frac{\partial E}{\partial R}$ (upper right). More precise calculation are on their way.

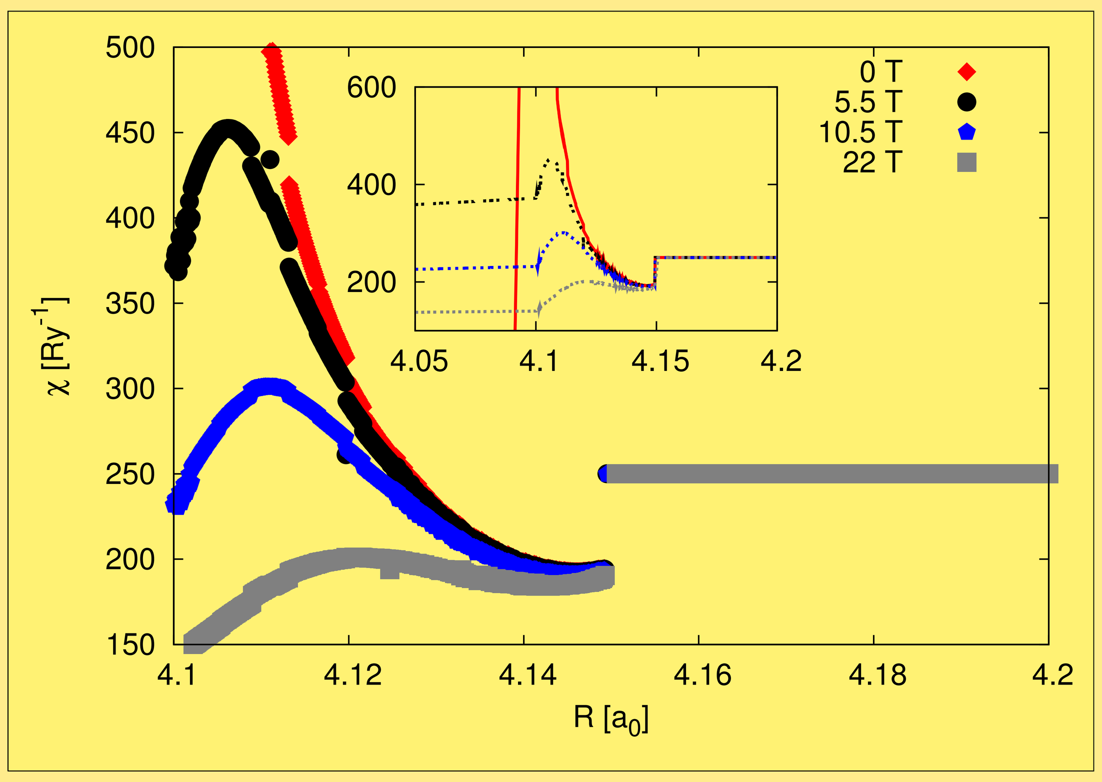

Figure 6: magnetic susceptibility $\chi = \frac{\partial m}{\partial h}$ for different values of external magnetic field; metal-insulator transition clearly shown.

Conclusions

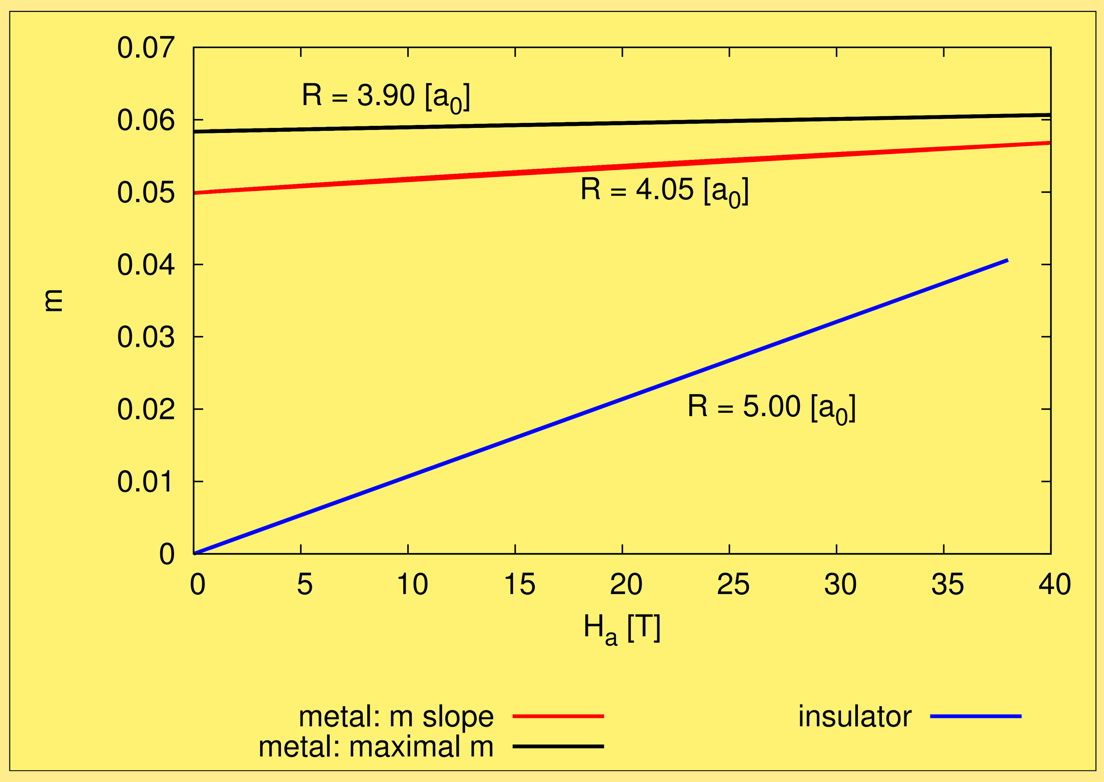

Figure 7: intersections of Figure 4 for three different lattice sizes, cutting magnetisation on the maximum, on the slope just before and after the phase transition

Our calculations reproduce the results in [2] with extension of the study of the influence of magnetic field.

Obtained data suggest that the critical behaviour of function size ($\propto \alpha^{-1}$) though it influences the ground state energy, can still be considered physical (more accurate calculation required to investigate ground energy near MIT - Figure 5).

The behaviour of susceptibility (Figure 6), especially before the critical point is a starting point for new calculations exchanging existing lattice with two separate ones.

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References

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