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# LOCAL FIELD METHOD FOR ISING MODEL WITH ARBITRARY INTERACTION

ЛЬВІВ

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**Метод локального поля для моделі Ізінга з довільною взаємодією**

С.І.Сороков, Р.Р.Левицький, Т.М.Верхоляк

**Анотація.** В даній роботі наближення локального поля, яке грунтується на використанні тотожності Калена, застосовано до моделі Ізінга з довільним типом взаємодії. На основі отриманих результатів проаналізовано, як характер взаємодії впливає на термодинамічні властивості моделі. Для функції розподілу локальних полів, яка пов'язана з поперечним перерізом непружного розсіяння нейтронів, отримана скінчена ширина ліній, що зумовлено далекосяжністю взаємодії.

**Local field method for Ising model with arbitrary interaction**

S.I.Sorokov, R.R.Levitskii, T.M.Verkholyak

**Abstract.** In present work local field approximation, based on Callen identities, is applied to the Ising model with arbitrary interaction. On the bases of obtained results it was analysed how the type of interaction changed the thermodynamic properties of the model. For the local field distribution function connected to inelastic-neutron-scattering cross section "Gaussian"-width of peaks has been observed.

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# 1. Introduction

Callen identity, derived in 1963 [1], proved to be very fruitful for the investigation of Ising model with the nearest neighbour interaction [2-5].The main equation for magnetization, which follows from Callen identity, contains spin correlation functions up to $(z-1)$ order, where $z$ is the number of the nearest neighbours (see, for example, [4]). The simplest approximation, which had been done by Honmura and Kaneyoshi, consists in neglecting of correlation between spin operators on different sites [2]. In paper [3] authors omitted in equation for magnetization all correlations higher than the triplet correlations and decoupled the last. Another way was chosen in [4,5]. Correlation of magnetization fluctuations were taken into account by introduction of correlation parameter $\lambda$. $\lambda$ was determined from Callen identity for correlation function in [5], and from inverse Callen identity in [4]. It can be noted that results for magnetization obtained by Honmura [5] coincide with Bethe approximation. In general, phase transition temperature for Ising model with the nearest neighbour interaction calculated in methods [5,4] is very close (up to 10%) to the exact result for square lattice and the result of high temperature expansions for cubic lattice.

It is also to the advantage of all these methods that they do not have any non-physical solutions in the region $T \leq T_c$ such as for example first order phase transition, which appear in diagrammatic technique [6].

It should be stressed that in last years some versions of this correlated effective theory are widely used for investigation of disordered Ising systems [7,8]

Mentioned above methods allow to calculate not only all thermodynamical properties but also some dynamical quantities. Thomsen et al obtained exactly inelastic-neutron-scattering cross section for honeycomb and square lattice [9].

In present work local field method is used to investigate Ising model with arbitrary form of interaction. We aim to analyse the influence of the interaction range on the local field distribution function and thermodynamic properties of the model.



# 2. A local field method for the model with arbitrary interaction

In order to develop the method we shall follow [9]. Let us consider the Hamiltonian of Ising model with arbitrary interaction

$$H = -\frac{1}{2}\sum_{i\neq j} J(R_{ij})S_iS_j - \sum_i \Gamma_i S_i, \tag{2.1}$$

where $\Gamma_i$ is external field ($\mu_B = 1$), $J(R_{ij})$ is exchange interaction, $S_i = \pm 1$ is $z$-component of spin operator.

One can single out the part in the Hamiltonian, which contains all the terms with the operator on site $k$:

$$H = -h_k S_k + H', \tag{2.2}$$

$$h_k = \sum_{j\neq k} J(R_{kj})S_j + \Gamma_k. \tag{2.3}$$

Here $H'$ does not include operators on site $k$. Then average of operator $AS_k$ ($A$ – does not contain any operator on site $k$) can be easily calculated

$$\langle AS_k\rangle = \langle A\tanh(\beta h_k)\rangle = \langle A\tanh[\beta(\sum_j J(R_{kj})S_j + \Gamma_k)]\rangle. \tag{2.4}$$

If $A = 1$, we shall get a selfconsistent equation for the magnetization

$$\langle S_k\rangle = \langle \tanh[\beta(\sum_j J(R_{kj})S_j + \Gamma_k)]\rangle, \tag{2.5}$$

obtained by Callen [1].

One can introduce a distribution function $P_k(h)$ for local magnetic field on site $k$:

$$P_k(h) = \langle \delta(h - h_k)\rangle. \tag{2.6}$$

The equation (2.5) can be rewritten in an integral form:

$$\langle S_k\rangle = \int_{-\infty}^{\infty} \tanh(\beta h)P_k(h)dh \tag{2.7}$$

When we take $A = \frac{1}{2}(h_k + \Gamma_k)$, we shall obtain internal energy from the identity (2.4)

$$E_k = -\frac{1}{2}\langle (h_k + \Gamma_k)S_k\rangle = -\frac{1}{2}\int_{-\infty}^{\infty} h\tanh(\beta h)P_k(h)dh - \frac{1}{2}\Gamma_k\langle S_k\rangle \tag{2.8}$$

Further we shall consider only ferromagnetic case $J(R_{ij}) > 0$ and uniform external field $\Gamma_i = \Gamma$. Thus the local field distribution function will be uniform too ($P(h) = P_k(h)$). Therefore, magnetization $m$ and internal energy $E$ averaged over the whole lattice can be determined by (2.7) and (2.8).

Formulae (2.6) - (2.8) show that $P(h)$ determines completely all the thermodynamic functions of the model. Moreover, some dynamic properties can be obtained with the help of $P(h)$, for example, inelastic-neutron-scattering cross section [9]:

$$S(k,w) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} e^{-iwt}\sum_{i,j}\exp[ikR_{ij}]\langle S_i^x S_j^x(t)\rangle = \frac{N}{2}\frac{P(\omega/2)+P(-\omega/2)}{1+\exp(-\beta\omega)}. \quad (2.9)$$

## 3. Calculation of the local field distribution function

Although we have obtained exact expressions (2.7)-(2.8), the function $P(h)$ is unknown. It may be calculated by using Fourier representation of $\delta$-function:

$$P(h) = P_k(h) = \langle\delta(h-h_k)\rangle = \langle\frac{1}{2\pi}\int_{-\infty}^{\infty} d\zeta e^{i\zeta(h-h_k)}\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\zeta\ \mathrm{e}^{i\zeta h} M_\Gamma(\zeta). \quad (3.1)$$

where

$$M_\Gamma(\zeta)=\langle e^{-i\zeta h_k}\rangle=\mathrm{e}^{-i\zeta\Gamma}M(\zeta)=\mathrm{e}^{-i\zeta\Gamma}\exp\left\{\ln\langle\prod_j e^{-i\zeta J(R_{kj})S_j}\rangle\right\}. \quad (3.2)$$

The simplest approximation $\langle\prod_j e^{-i\zeta J(R_{kj})S_j}\rangle \approx \prod_j\langle e^{-i\zeta J(R_{kj})S_i}\rangle$ gives the following result for $M(\zeta)$:

$$M(\zeta) = \exp\{\sum_j \ln[\cos(\zeta J(R_{kj})) - i\langle S_j\rangle\sin(\zeta J(R_{kj}))]\} = \prod_j[\cos(\zeta J(R_{kj})) - i\langle S_j\rangle\sin(\zeta J(R_{kj}))]. \quad (3.3)$$



For the numerical investigation in case of isotropic interaction it is worth doing sum over coordination spheres:

$$M(\zeta) = \exp\{\sum_{n=1}^{\infty} z_n\ln[\cos(\zeta J(R_n)) - i\langle S_j\rangle\sin(\zeta J(R_n))]\} = \prod_{n=1}^{\infty}[\cos(\zeta J(R_{kj})) - i\langle S_j\rangle\sin(\zeta J(R_n))]^{z_n}, \quad (3.4)$$

where $z_n$ is a number of sites in n-th coordination sphere and $R_n$ is its radius.

The analytical result for the local field distribution function is known only for one-dimensional model with interaction $2^{-r}$ and $T\to\infty$ (when $m = 0$, and $< S_iS_k >= 0$) [10]. In this case we can use the famous formula for product

$$\prod_{n=1}^{\infty}\cos(\zeta J2^{-n}) = \frac{\sin(\zeta J)}{\zeta J}.$$

Then, if we take into account that each coordination sphere has two sites, we shall get the following result for $M(\zeta) = \left[\frac{\sin(\zeta J)}{\zeta J}\right]^2$. After inverse Fourier transformation the expression for local field distribution density is

$$P(h) = \begin{cases} 2J-|h| & , \quad |h|<2J \\ 0 & , \quad |h|>2J \end{cases}$$

For the approximate calculation $M(\zeta)$ we single out the terms in (3.4), which correspond to the nearest-neighbour interaction and other expand in the vicinity of $\zeta$ up to second order of $\zeta$. After inverse Fourier transformation one obtains the following result:

$$P(h) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\zeta \mathrm{e}^{i\zeta(h-\Gamma_k)}M(\zeta) = \frac{1}{2^z\sqrt{2\pi J'^2(0)(1-m^2)}} \times\sum_{n=0}^{z} C_z^n(1-m)^n(1+m)^{z-n}\exp\left\{-\frac{(h-h_n')^2}{2J'^2(0)(1-m^2)}\right\}, \quad (3.5)$$

where $h_n' = \Gamma + J_1(z-2n) + mJ'(0)$, $\sum_{R\neq R_{n.n.}} J(R) = J'(0)$, $\sum_{R\neq R_{n.n.}} J^2(R) = J'^2(0)$.

Formula (3.9) shows that $P(h)$ has (z+1) peaks in the points $h = h_n'$ with the width $J'^2(0)(1-m^2)$. In case of the large dispersion peaks at the $h_n{}' \neq 0$ become invisible. The increase of magnetization leads to the shift of peaks on the magnitude $mJ'(0)$ as well as decreasing of the dispersion in $(1-m^2)$ times, as it can be seen from (3.9). For $m \to 1$ local field distribution function leads to the $\delta(h - J(0))$.

The numerical investigations were performed for the system with several interactions:

$$1)\ J(R) = J\mathrm{e}^{-\frac{(R-1)}{r_0}}, \tag{3.6}$$

$$2)\ J(R) = \frac{J}{R^3}, \tag{3.7}$$

$$3)\ J(R) = \frac{J}{R^6}. \tag{3.8}$$

On the Figs.1-3 local field distribution function $P(h)$ is depicted for the interaction (3.6). It is known that $P(h)$ is the set of $\delta$-like peaks in points $J(z-2n)$ ($z$ is the number of the nearest neighbours, n=0,...z) for the Ising model with the nearest neighbour interaction, and has Gaussian-like form for the long-range interaction. Figs.1-3 show that the change of the interaction type with the help of $r_0$ in (3.6) influence the local field distribution function $P(h)$ strongly. In Fig.4 the results of the estimation (3.5) are compared to the numerical computation (3.4) for the interaction (3.6). One can see that for the cubic lattice approximation (3.5) is almost good for all $r_0$, but it does not reflect the fine structure near very small $r_0$. Local field distribution function $P(h)$ for the interaction (3.7) and (3.8) is depicted in Fig.5. We tried to choose such values of $r_0$ that the function $P(h)$ for the interactions $\frac{1}{R^3}$ and $\exp\frac{R-1}{r_0}$, $\frac{1}{R^6}$ and $\exp\frac{R-1}{r_0}$ were as close as possible to each other. As the result the local field distribution function for interaction $\frac{1}{R^6}$ turns round the same function for the interaction $\exp\frac{R-1}{0.2014}$. However, deviation between thermodynamic functions for these interactions will not be noticeable, because expressions for thermodynamics contain $P(h)$ only in integrals. In Fig.6 the results for $P(h)$ at $T < T_c$ (when $m \neq 0$) are depicted.

## 4. Calculation of the thermodynamic functions within local field approximation

As it is emphasized in paragraph 2, the local field distribution function determines completely thermodynamics properties of the system. The magnetization and the internal energy can be calculated with the help of (2.8)-(2.9).



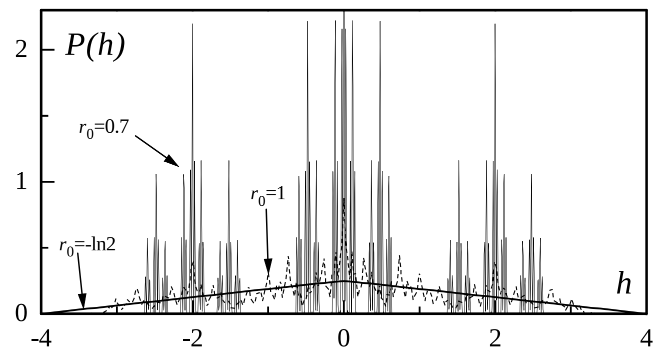


Figure 1: Local field distribution function $P(h)$ for one-dimensional lattice and the interaction $I(R) = \exp\frac{R-1}{r_0}$ for different $r_0$.

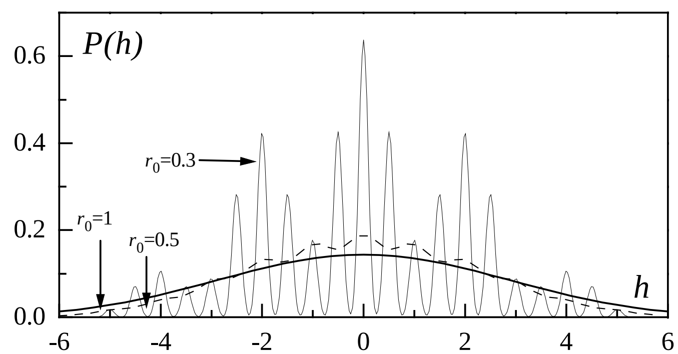


Figure 2: Local field distribution function $P(h)$ for a square lattice and the interaction $I(R) = \exp\frac{R-1}{r_0}$ for different $r_0$.

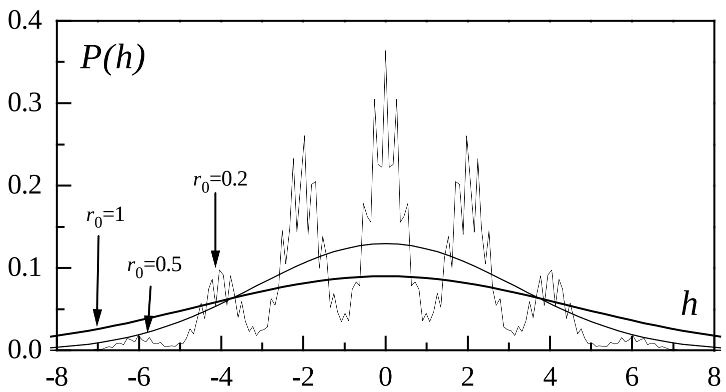


Figure 3: Local field distribution function $P(h)$ for a cubic lattice and the interaction $I(R) = \exp\frac{R-1}{r_0}$ for different $r_0$.

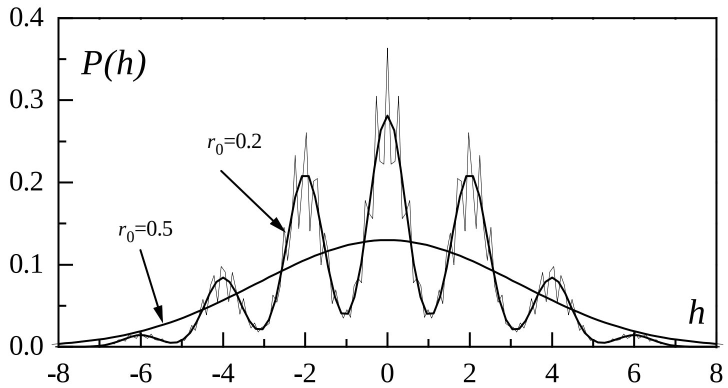


Figure 4: Local field distribution function $P(h)$ for a cubic lattice and the interaction $I(R) = \exp\frac{R-1}{r_0}$ for $r_0 = 0.2,\ 0.5$ obtained by (3.4) (thin line) and by formula (3.5) (thick line).



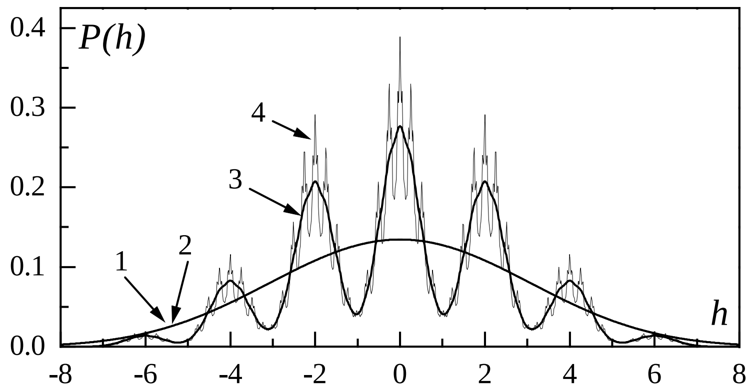


Figure 5: Local field distribution function $P(h)$ for a cubic lattice and the interactions: 1 - $I(R) = \frac{1}{R^3}$, 2 - $I(R) = \exp\frac{R-1}{0.4475}$, 3 - $I(R) = \frac{1}{R^6}$,4 - $I(R) = \exp\frac{R-1}{0.2014}$.

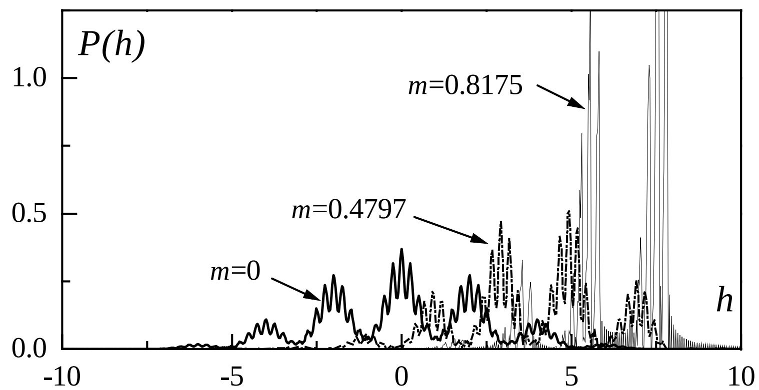


Figure 6: Local field distribution function $P(h)$ for a cubic lattice and the exchange interaction $I(R) = \exp\frac{R-1}{0.2}$ for different temperatures: $T > T_c$ $(m = 0)$, $T = 0.78I(0)$ $(m = 0.4797)$, $T = 0.64I(0)$ $(m = 0.8175)$.

For the numerical investigation it is more convenient to use $M_\Gamma(\zeta)$ instead of $P(h)$ in expressions (2.8)-(2.9). After some transformations one can get the following formula for magnetization:

$$m = \int_{-\infty}^{+\infty} d\zeta M_\Gamma(\zeta)\phi(\zeta), \tag{4.1}$$

where $\phi(\zeta)$ is Fourier representation of $\tanh(\beta h)$:

$$\phi(\zeta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dh \tanh(\beta h) \mathrm{e}^{i\zeta h} = \frac{iT}{2\sinh\frac{\pi\zeta T}{2}}. \tag{4.2}$$

Similarly, the expression (2.8) for internal energy can be rewritten as follows:

$$E = \frac{i}{2}\int_{-\infty}^{+\infty} d\zeta\phi'(\zeta)[M(\zeta) - M(0)]. \tag{4.3}$$

When we take the derivative of (4.1) over external field $\Gamma$, we shall get the equation for static susceptibility that has the following solution:

$$\chi = \frac{\partial m}{\partial\Gamma} = \frac{\int_{-\infty}^{+\infty} d\zeta(-i\zeta)\phi(\zeta)M(\zeta)}{1 - \int_{-\infty}^{+\infty} d\zeta\phi(\zeta)\frac{\partial M(\zeta)}{\partial m}}. \tag{4.4}$$

Due to the definition (3.5), one can show that

$$\frac{\partial M(\zeta)}{\partial m} = iM(\zeta)\sum_j \frac{\sin(\zeta J(R_{kj}))}{\cos(\zeta J(R_{kj})) - im\sin(\zeta J(R_{kj}))}. \tag{4.5}$$

We see from (4.4) that static susceptibility diverges, when

$$\int_{-\infty}^{+\infty} d\zeta\phi(\zeta)\frac{\partial M(\zeta)}{\partial m} = 1. \tag{4.6}$$

It is equation for the phase transition temperature. Specific heat of the system is defined by thermodynamic relation $c = \frac{dU}{dT}$:

$$c = \frac{1}{2}\int_{-\infty}^{+\infty} d\zeta\left\{\left[\frac{d}{dT}i\phi'(\zeta)\right][M(\zeta - M(0)]\right\}$$
$$+\frac{1}{2}\int_{-\infty}^{+\infty} d\zeta i\phi'\frac{\partial M(\zeta)}{\partial m}\times\frac{\partial m}{\partial T} \tag{4.7}$$



Unknown function $\frac{\partial m}{\partial T}$ can be obtained similarly to static susceptibility, when we take derivative of (4.1) over $T$:

$$\frac{\partial m}{\partial T} = \frac{\int_{-\infty}^{+\infty} d\zeta\left[\frac{d}{dT}\phi(\zeta)\right]M(\zeta)}{1 - \int_{-\infty}^{+\infty} d\zeta\phi(\zeta)\frac{\partial M(\zeta)}{\partial m}}. \tag{4.8}$$

Since denominator of (4.8) turns into zero, when $T \to T_c$, specific heat diverges at the critical temperature as well as static susceptibility.

In Figs.7-9 the temperature dependence of magnetization in local field approximation is depicted for one-dimensional, square and cubic lattices. Fig.10 shows phase transition temperature $T_c/I(0)$ as a function of interaction range $r_0$ for hypercubic lattices of different dimensions. In case of $D = 1$ the phase transition temperature leads to zero when $r_0 \to 0$. Temperature dependence of inverse static susceptibility for square and cubic lattice one can see on Figs.11,12.

## 5. Conclusions

In this work local field method for the Ising model with arbitrary interaction has been developed and the local field distribution function, the magnetization and static susceptibility have been calculated for the linear, square and cubic lattices.

For interaction $\exp\frac{R-1}{r_0}$ it has been found out how $r_0$ and lattice dimensionality influence forming of fine structure. It was shown that changing of interaction type from $\frac{1}{R^6}$ to $\exp\frac{R-1}{r_0}$ lead to appearance of satellite peaks.

It should be emphasized that the approximation (3.3) neglects the dependence of local field distribution function on temperature (for $T > T_c$) and get exact results only at $T \to \infty$. In forthcoming works we intend to take into account higher correlation effects similar to how it was done in [5] for the model with the nearest neighbour interaction.

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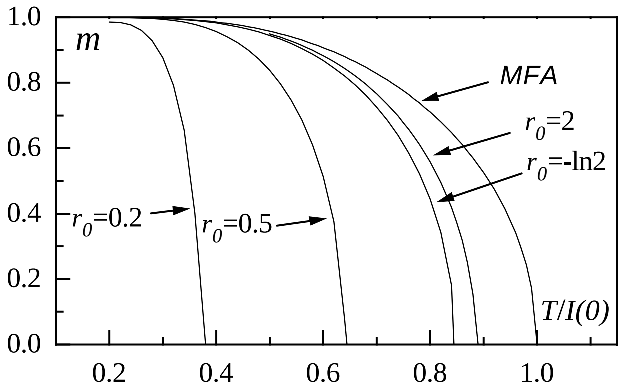


Figure 7: The magnetization $m$ of one-dimensional lattice vs. temperature $T/I(0)$ for the exchange interaction $I(R) = \exp\frac{R-1}{r_0}$.

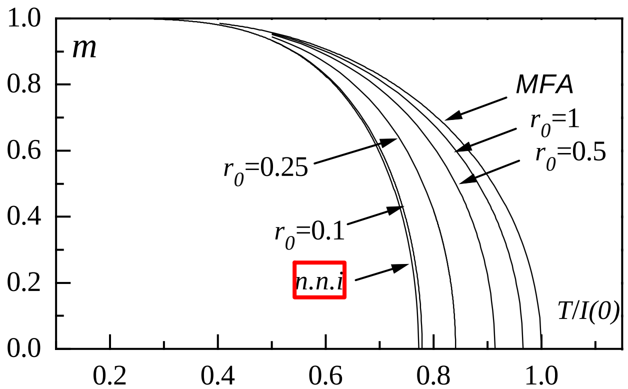


Figure 8: The magnetization $m$ of the square lattice vs. temperature $T/I(0)$ for exchange interaction $I(R) = \exp\frac{R-1}{r_0}$ (n.n.i means model with the nearest neighbour interaction).



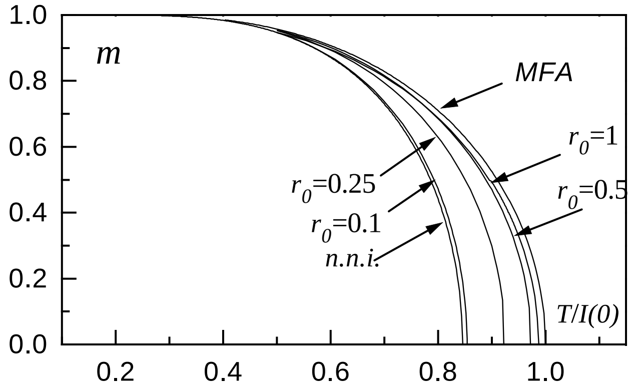


Figure 9: The magnetization $m$ of a cubic lattice vs. temperature $T/I(0)$ for the exchange interaction $I(R) = \exp\frac{R-1}{r_0}$ (n.n.i means model with the nearest neighbour interaction).

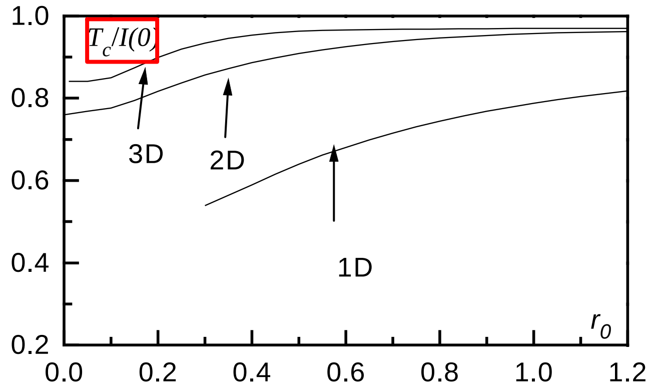


Figure 10: Phase transition temperature of Ising model vs. interaction range $r_0$ for $I(R) = \exp\frac{R-1}{r_0}$ and hypercubic lattices of different dimensions.

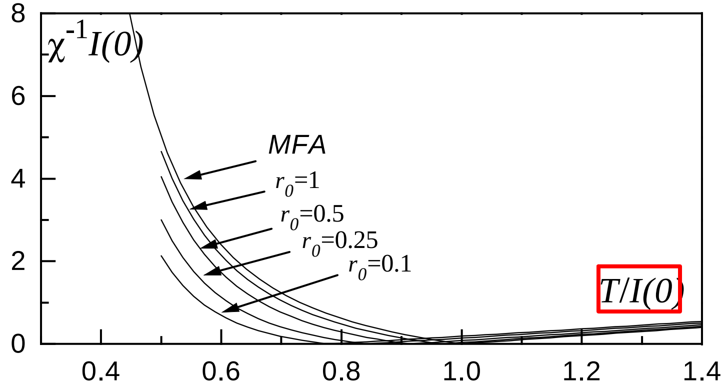


Figure 11: The inverse static susceptibility $I(0)/\chi_{zz}$ of a square lattice vs. temperature $T/I(0)$ for the exchange interaction $I(R) = \exp \frac{R-1}{r_0}$.

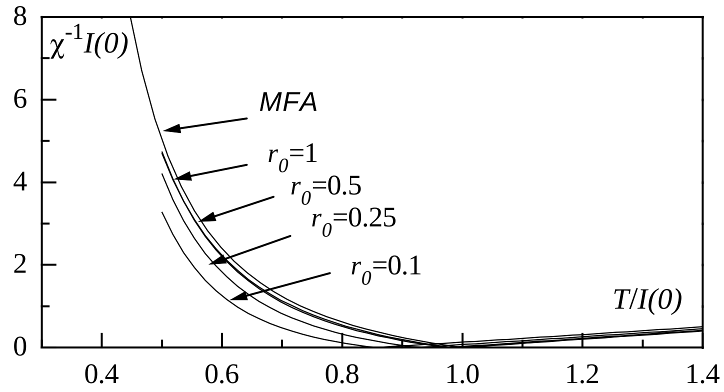


Figure 12: The inverse static susceptibility $I(0)/\chi_{zz}$ of a cubic lattice vs. temperature $T/I(0)$ for the exchange interaction $I(R) = \exp \frac{R-1}{r_0}$.



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