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# AN EVOLUTION OF THE VACANCY CONCENTRATION IN THE ISING MAGNETIC.

## II. The Correlation between Vacancies

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Эволюция концентрации вакансий в изинговом магнетике. Учет корреляций между вакансиями

Рассматривается поведение концентрации вакансий в изинговом магнетике при учете корреляционных эффектов. Используются основные идеи суперпозиционного расщепления и формула скейлинга для корреляционных функций $\langle\sigma_f\rangle$, $\langle\sigma_f\sigma_k\rangle$. Получается уравнение для концентрации вакансий $C_v$. В этом случае показан эффект "подавления" концентрации вакансий.

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Gavrilenko G.M., Morozova S.K., Fedjanin V.K. E17 - 10973

An Evolution of the Vacancy Concentration in the Ising Magnetic. II. The Correlation between Vacancies

The behaviour of vacancy concentration in the Ising magnetic is considered when the correlation effects have been taken into account. In the approximation of the superpositional decoupling and scaling formulae for the correlation functions $\langle\sigma_f\rangle$, $\langle\hat{\sigma}_f\hat{\sigma}_k\rangle$ the equation for vacancy concentration $C_v$ is obtained. In this case the effect of vacancy concentration "suppression" is shown.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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In the last paper [1] the authors analyzed the behaviour of the vacancy concentration in the Ising magnetic under the assumption that $\tau \gtrsim z^{-1}$ ( $\tau = \left|1-\frac{T_c}{T}\right|$ ), $z$ is the number of the nearest neighbours ( $z \le 10$). The correlation between the vacancies may not be taken into account in this case. But for $\tau \to 0$ we are in the region when $\tau < z^{-1}$, and the correlation radius $R_c \sim \tau^{-\nu}$ is bigger than the mean distance between the vacancies $r_v \sim C^{-1/d}$ ( $d$ is the dimension) the system is in the region of the phase transition, and the correlation between the vacancies should be taken into consideration correctly. It is the aim of our study. Since $\nu d = 2$ [2] our results are valid for temperatures $\tau \ge C^{1/d\nu} = \sqrt{C}$ (supposing that $\tau < z^{-1}$, i.e. the constraint $z^{-1} > \sqrt{C}$ is rather reasonable since $z^{-1} \sim 0.1$ and $C \sim 1$). In the region $\tau < \sqrt{C}$ the main parameter of the problem is the mean distance between the impurities ($\equiv$ vacancies), that can change the phase transition character (the second order phase transition turns to the first order one). The means of the analysis of this situation are not clear, and we limit ourselves to the case

$$C^{1/d\nu} \lesssim \tau \lesssim z^{-1} . \quad (1)$$

We use the basic ideas of the superpositional decoupling and scaling-formulae /2/ for deriving an equation for $C(\beta)$.

In this case it is natural to generalize the formula of the paper /1/ by the following approximation for the free energy change:

$$\delta F = -\theta \ln \langle \prod_{i=1}^{N_1} \hat{\vartheta}(i) \rangle \Rightarrow -\theta \ln \left\{ \langle \hat{\vartheta} \rangle_0^{N_1} \frac{\langle \hat{n}_1 \hat{n}_2 \rangle_0^{N_1 - 1}}{\bar{n}_1^{N_1-1} \cdot \bar{n}_2^{N_1-1}} \right\} \quad (2)$$

The notation is from ref. /1/. Formula (2) can be justified as follows:

$$\langle \hat{\vartheta}(1) \cdot \hat{\vartheta}(2) \cdots \hat{\vartheta}(N_1) \rangle_0 \equiv \langle \tilde{\hat{\vartheta}}(1) \cdot \hat{n}_1^2 \hat{n}_2^2 \tilde{\vartheta}(2) \cdots \rangle_0 \Rightarrow \quad (3)$$

$$\frac{\langle \tilde{\hat{\vartheta}}(1) \hat{n}_{g_1} \rangle_0 \langle \hat{n}_{g_1}(1) \hat{n}_{g_1}(2) \rangle_0 \langle \hat{n}_{g_2} \tilde{\hat{\vartheta}}(2) \ldots \rangle_0}{\bar{n}_1 \cdot \bar{n}_2} \Rightarrow$$

$$\frac{\langle \hat{\vartheta}(1) \rangle_0 \langle \hat{n}_1 \hat{n}_2 \rangle_0 \langle \tilde{\hat{\vartheta}}(2) n_{g_3}(2) \rangle_0 \langle \hat{n}_2 \hat{n}_3 \rangle_0 \langle n_{g_3}(3) \tilde{\hat{\vartheta}}(3) \ldots \rangle_0}{\bar{n}_1 \cdot \bar{n}_2 \cdot \bar{n}_3}$$

here $\hat{n}_{g_K}(K-1)$ is the particle number operator of the site near the $(K-1)$-vacancy; the last one is the nearest to the $K$-vacancy. As we postulate the random distribution of the vacancies, the distance between them is $z_v \sim C^{-1/3}$ and

$$\langle \hat{n}_1 \hat{n}_2 \rangle_0 = \langle \hat{n}_2 \hat{n}_3 \rangle_0 = \cdots = \langle \hat{n}_K \hat{n}_{K+1} \rangle_0 = \cdots \quad (4)$$

where the indices $1, 2, 3, K, K+1$ - number of vacancies. These simple considerations and (3) validate eq. (2). The total energy of the system in the region (1) is given by the formula:



$$F_{tot} = F_0 + N_v \delta E - \theta N_v \ln \frac{N!}{N_v!(N-N_v)!} + \quad (5)$$
$$\mathcal{E}_s N_v - \theta N_v \ln \langle N(v) \rangle_0 - \theta (N_v - 1) \times$$
$$\times \ln \langle \hat{n}_1 \hat{n}_2 \rangle_0 + 2\theta (N_v - 1) \ln \bar{n} .$$

It transforms to the corresponding expression for $F_{tot}$ in paper /1/ if the correlations between the vacancies are not taken into consideration: $\langle \hat{n}_1 \hat{n}_2 \rangle \Rightarrow \langle \hat{n}_1 \rangle \langle \hat{n}_2 \rangle = \bar{n}^2$.

Minimizing (5) with respect to $N_v$ and neglecting the terms of an order of $O(1/N)$, $O(1/N_v)$, $O(1)$, we obtain the following equation for $C(\beta)$:

$$C = \tilde{z}(x,z) \frac{\langle \hat{n}_1 \hat{n}_2 \rangle_0}{\bar{n}^2} C_0 , \quad \tilde{z} = \langle \hat{\vartheta}(v) \rangle_0 e^{-\beta \delta F_s} , \quad C_0 = e^{-\beta E_v} . \quad (6)$$

Considering that

$$\langle \hat{n}_f \rangle = \frac{1}{2} - \langle \hat{\sigma}_f \rangle , \quad \langle \hat{n}_f \hat{n}_K \rangle = \frac{1}{4} - \langle \hat{\sigma}_f \rangle + \langle \hat{\sigma}_f \hat{\sigma}_K \rangle \quad (7)$$

and using for $\langle \hat{\sigma}_f \rangle$ and $\langle \hat{\sigma}_f \hat{\sigma}_K \rangle$ the scaling formula for zero magnetic field /2/

$$\langle \hat{\sigma}_f \rangle = \tau^{\beta_0} f_1(0) , \quad \langle \hat{\sigma}_K \hat{\sigma}_f \rangle = |f-K|^{-2X_\sigma} f_2 \left( \frac{|f-K|}{\tau^{-\nu}} \right) \quad (8)$$

we obtain the following equation for $C(\beta)$:

$$C = \tilde{z}(x,z) \left[ 1 - \tau^{\beta_0} f_1(0) + \left( \frac{4\pi}{3} C \right)^{\frac{2X_\sigma}{3}} f_2 (\tau^{\nu} C^{1/3}) \right] \left[ \frac{1}{2} - \tau^{\beta_0} f_1(0) \right] C_0 \quad (9)$$

We have use the fact that the mean distance between the vacancies is $z_v = |f-K| = \left( \frac{4\pi}{3} C \right)^{-1}$, $\beta_0, X_\sigma, \nu$, are the corresponding critical exponents [2]. Note that $f_2(x) \simeq 1$ for $x \leq 1$ and rapidly decreases for $x \to \infty$, $f_1(0) \sim 1$, $2x_6 = \frac{9}{\sqrt{d}} \sim 1$, $\beta_0 \sim \frac{1}{3}$. As the calculation of $\langle \hat{\vartheta}(v) \rangle_0$ in the region (1) (formally the expression for $\langle \hat{\vartheta}(v) \rangle_0$ is similar to the one of the paper [1]) it is necessary to use $F_K(f)$ and $\mathcal{F}_K(f)$ which are calculated in the critical region (1). They are unknown and the expression for $\xi(x,z)$ is different from the expression for $\tilde{\xi}(x,z)$ (obtained in different approximations in [1]). But these correlators are due to the short-range correlations with a radius of an order of the lattice constant $a_0$ ($a_0 \ll r_0$). We hope that the difference between $\xi(x,z)$ and $\tilde{\xi}(x,z)$ is small $\left( \langle \hat{n}_f \prod_{i=1}^{K} n_{g_i} \rangle \simeq \left(\frac{1}{2}\right)^{K+1} - (K+1)\, \tau^{\beta_0} f_1(0) + \cdots, \; K \leq z \right)$

As $C \ll 1$, $C_0 \ll 1$ up to the melting point eq. (9) can be reduced to

$$C\left(1 - 4\left(\frac{4\pi}{3} C\right)^{\frac{1}{3}}\right) = \vartheta(x,z)\left(\frac{z}{z-2}\right)^{-\frac{z x}{3}} C_0 , \quad (10)$$

where the explicit formulae for $\vartheta(x,z)$ are given in [1], $x = \beta/\beta_c$. Equation (10) can be analyzed by a computer for a wide region of the parameters $\beta$, $\mathcal{E}_v$, $z$ and for the exchange integral $I$ (see the formula for $\bar{\vartheta}$ in ref. [1]).

Obviously, in ferro-phase $C/C_0 \ll 1$ and in para-phase $C/C_0 \sim 1$ up to $\tau \simeq \sqrt{C}$, e.g. the temperature interval of changing from 1 to 0 is narrower than that occuring when we neglect the correlation effects [1].

This result for the vacancy concentration "suppression" with changing spontaneous magnetisation from its asymptotical value in the critical region ($\sigma \sim \tau^{\beta_0}$) to its asymptotical value for saturation ($\sigma \sim 1$) is quite natural. The experimental observation of this effect requires high Curie temperatures $T_c$



and low energy of the vacancy formation $\mathcal{E}_v$. It is possible to discover analogous anomalies of the magnetic physical characteristics which are connected with $C_v$ (for example, the self-diffusion coefficient).

## References


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