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METHOD OF QUASI-AVERAGES FOR METASTABLE AND MIXED SYSTEMS

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There exists several modifications of the method of quasi-averages serving for separating thermodynamic states corresponding to pure absolutely stable phases. Bogolubov[1] has formulated the method of sources connected with the introduction into a Hamiltonian of infinitesimal fields. One can also define quasi-averages breaking the commutation relations[2] for field operators. A review of these and other methods is given in ref.[3]

To separate pure metastable states, one can use the saddle-point method for the statistical sum, fixing an extremum bearing on a relative (not absolute) minimum[4]. Here and in what follows we mean the thermodynamics of metastable states leaving aside the questions connected with their dynamics[5]. Classification, stability and other mathematical aspects of describing metastable states have been thoroughly analyzed by Sewell[6].

Besides pure states there exist heterophase ones that might correspond to absolutely stable as well as to metastable systems[7-9]. After a renormalization procedure[10,11] quasi-equilibrium heterophase systems are presentable as a mixture of different thermodynamic phases. For example, it can be the mixture of solid- and liquidlike phases[12-14], superconducting and normal[15], ferromagnetic and paramagnetic ones[16-18]. Such heterophase systems have a number of peculiarities[19], letting to explain many thermodynamic anomalies observed in some matters, e.g. maxima[20] and jumps[21] in the specific heat below the Curie point.

When dealing with the description of heterophase systems it is extremely important to separate in a correct way the phases needed. This can be done by imposing additional conditions on the Green functions[22] or combining the procedures of spontaneous break and restoration of symmetry[23]. In the paper[11] one more method of quasi-overaging has been formulated, based on a construction of a Hamiltonian that leads to the free energy explicitly containing order parameters. Then the separation of different phases is realized by postulating the corresponding properties of these order parameters. The most known type of Hamiltonians, leading to an explicit dependence of the free energy on order parameters, is the class of Hamiltonians with a long-range interaction.

In the present paper the method of separating phases by means of order parameters[11] is applied to a one-dimensional modified Ising model, containing the short - as well as long-range interactions. The low dimensionality allows one to solve the model exactly and the presence of the long-range interaction securės the existence of the ferromagnet - paramagnet phase transition. In such a way the model considered differs from the usual Ising model by two principal peculiarities: 1) the presence of two kinds of interactions, the ferromagnetic long-range interaction and a short-range interaction whose sign can vary; 2) taking account of heterophase states including absolutely stable as well as metastable states. These peculiarities lead to a quite nontrivial thermodynamics of the model.

Let on a chain, whose lattice sites are enumerated by i =1,2 ... N, the variables $s_i = \pm 1$ be given, the interaction

$$\mathcal{J}_{ij} = \nu \mathcal{J}_s \delta_{i+1,j} + (1-\nu)\frac{\mathcal{J}_\ell}{N} \qquad (\nu \le 1) \tag{1}$$

containing besides the nearest-neighbour interaction (first term) the long-rang part (second term) too. To take into consideration heterophase states, we construct, following the general theory[7-10], the Hamiltonian

$$H(\nu) = H_1(\nu) \oplus H_2(\nu) , \tag{2}$$

in which

$$H_\alpha(\nu) = w_\alpha^2 \left(\frac{N}{2} U - \frac{1}{4}\sum_{ij} \mathcal{J}_{ij} s_i s_j \right) ; \tag{3}$$

α = 1 corresponds to ferromagnetic and α = 2 to paramagnetic phase, that is the additional conditions of averaging are imposed:

$$\langle s_i \rangle_{H_1(\nu)} \equiv \sigma \neq 0 , \quad \langle s_i \rangle_{H_2(\nu)} \equiv 0 ; \tag{4}$$

the phase probabilities w_α are defined by the relations

$$\frac{\partial f}{\partial w_\alpha} = 0 , \quad \frac{\partial^2 f}{\partial w_\alpha^2} > 0 , \quad w_1 + w_2 = 1 , \tag{5}$$

$$f = -\lim_{N\to\infty} \frac{\Theta}{N} \ln \mathrm{Tr} \exp\left[-H(\nu)/\Theta\right] .$$

The constant U in eq.(3) plays the role of the cristalline-field constant. Under the change of ν from 0 to 1 the crossover from the long - to short-range interaction occurs.

Calculating the specific free energy f one can use for the short-range part of the Hamiltonian the transfer-matrix method, while the long-range part, as is known[24], is asymptotically equivalent to the mean-field theory. As a result, we have

$$\begin{aligned} f = {} & (w^2 - w + \tfrac{1}{2}) U - w^2 \Theta (K - L\sigma^2) - \\ & - \Theta \ln\left[\cosh\varphi + 2\cosh\varphi_2 + (\sinh^2\varphi + e^{-4\varphi_1})^{1/2}\right] , \end{aligned} \tag{6}$$

where

$$w \equiv w_1 , \quad K \equiv \frac{\mathcal{J}_s \nu}{4\Theta} , \quad L \equiv \frac{\mathcal{J}_\ell (1-\nu)}{4\Theta} ,$$

$$\varphi \equiv 2\sigma w^2 L , \quad \varphi_1 \equiv w^2 K , \quad \varphi_2 \equiv (1-w)^2 K .$$

Introducing also the notation

$$u \equiv \frac{U}{\mathcal{J}_\ell} , \quad g \equiv \frac{\mathcal{J}_s}{\mathcal{J}_\ell} , \quad T \equiv \frac{\Theta}{\mathcal{J}_\ell} ,$$

for the probability of the ferromagnetic phase from the first of eq.(5) we find the equation

$$\begin{aligned} & \frac{4 g w \nu e^{-4\varphi_1}}{(\sinh^2\varphi + e^{-4\varphi_1})^{1/2}\cosh\varphi + \sinh^2\varphi + e^{-4\varphi_1}} + \\ & + u(2w-1) - 2gw\nu - 2w(1-\nu)\sigma^2 + 2g\nu(1-w)\tanh\varphi_2 = 0 . \end{aligned} \tag{7}$$

For the order parameter defined in (4) we get

$$\sigma = \frac{\sinh\varphi}{(\sinh^2\varphi + e^{-4\varphi_1})^{1/2}} . \tag{8}$$

The heterophase state is absolutely stable, if the inequalities

$$0 < w < 1 , \quad \frac{\partial^2 f}{\partial w^2} > 0 , \quad \Delta f \equiv f(1) - f(w) > 0 \tag{9}$$

are true. When only the two first inequalities are valid but the third one does not hold, the heterophase state is metastable.

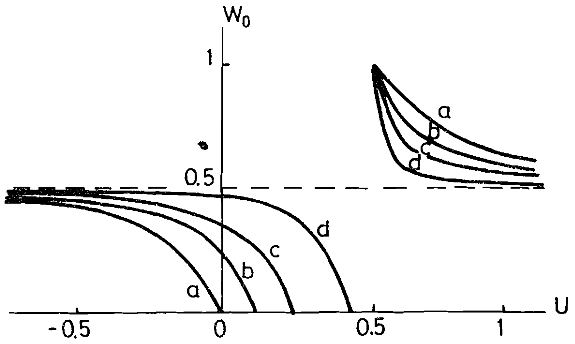
Investigate the stability of the system at $T = 0$. Then the ferromagnetic-phase probability takes the form

$$w_0 \equiv w(0) = \frac{2u - g|\nu|}{4u - 1 + \nu - g(\nu + |\nu|)} , \tag{10}$$

shown in Fig.1. In addition

$$\frac{\partial^2 f}{\partial w^2} = 2\left(4u - \nu g - 1 + \nu - |\nu| g\right),$$

$$\frac{4\Delta f}{J_\ell} = \begin{cases} \dfrac{(2u - \nu g - 1 + \nu)^2\,(4u + 2\nu g - 1 + \nu)}{(4u - 1 + \nu)^2}, & \nu < 0, \\[2ex] \dfrac{(2u - \nu g - 1 + \nu)^2}{4u - 2\nu g - 1 + \nu}, & 0 \le \nu \le 1 . \end{cases}$$



F i g. 1. The probability of the ferromagnetic phase at zero temperature for $g = 1$: a) $\nu = 0$; b) $\nu = 0.25$; c) $\nu = 0.5$; d) $\nu = 0.9$.

Condition (9) yields that the heterophase state is absolutely stable if either

$$u > \max\left\{\frac{1}{4}(1-\nu-2\nu g), \frac{1}{2}(1-\nu+\nu g)\right\}, \quad \nu < 0 , \tag{11}$$

or

$$u > \frac{1}{2}(1-\nu+\nu g), \quad \nu > 0 . \tag{12}$$

The heterophase state is metastable if either

$$\frac{1}{2}(1-\nu+\nu g) < u < \frac{1}{4}(1-\nu-2\nu g), \quad \nu < 0 , \tag{13}$$

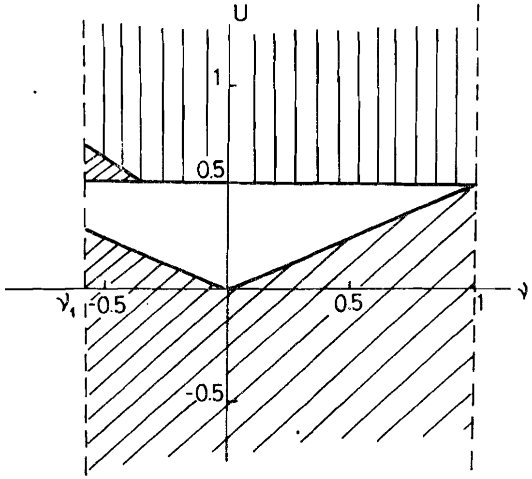
or

$$u < \frac{1}{2}\nu g , \quad \nu > 0 . \tag{14}$$

In the case when

$$\frac{1}{2}|\nu| g < u < \frac{1}{2}(1-\nu+\nu g), \tag{15}$$

the system at zero temperature is purely ferromagnetic, but beginning from the finite temperature T_n , called the nucleation temperature[21], the heterophase state becomes profitable being a mixture of ferromagnetic and paramagnetic phases. The corresponding regions of stability and metastability on the $u - \nu$ -plane are pictured in Fig. 2.



F i g. 2. Regions of stability and metastability of heterophase states at $T = 0$, $g = 1$. The vertical hatching designates the stable region, the oblique hatching shows the metastable one, the absence of any hatching between ν_1 ,and 1 corresponds to the completely ordered state.

Calculate the low-temperature asymptotes for the ferromagnetic probability

$$w \simeq w_0 \left\{ 1 - \frac{4(1-\nu+\nu g)}{4u-\nu g-1+\nu-|\nu| g} \exp\left[-\frac{w_0^2}{T}(1-\nu+4\nu g)\right] + \right.$$

$$\left. + \frac{2|\nu| g\,(2u-\nu g-1+\nu)}{(2u-|\nu| g)(4u-\nu g-1+\nu-|\nu| g)} \exp\left[-\frac{(1-w_0)^2}{T}\,2|\nu| g\right] \right\},$$

the order parameter

$$\sigma \simeq 1 - 2\exp\left[-\frac{w_0^2}{T}(1-\nu+4\nu g)\right],$$

the entropy

$$S \simeq \frac{w_0^2}{T}(1-\nu+\nu g)\exp\left[-\frac{w_0^2}{T}(1-\nu+4\nu g)\right] +$$

$$+ \frac{(1-w_0)^2}{2T}|\nu| g \exp\left[-\frac{(1-w_0)^2}{T}\,2|\nu| g\right],$$

and the heat capacity

$$C_v \simeq \frac{w_0^4}{T^2}(1-\nu+\nu g)^2 \exp\left[-\frac{w_0^2}{T}(1-\nu+4\nu g)\right] +$$

$$+ \frac{(1-w_0)^4}{4T^2}\nu^2 g^2 \exp\left[-\frac{(1-w_0)^2}{T}\,2|\nu| g\right].$$

The positivity of the specific heat indicates that the heterophase state is stable with respect to thermal fluctuations.

Analyze now the critical behaviour of the model. For the critical temperature, when $\sigma = 0$, eq.(8) gives

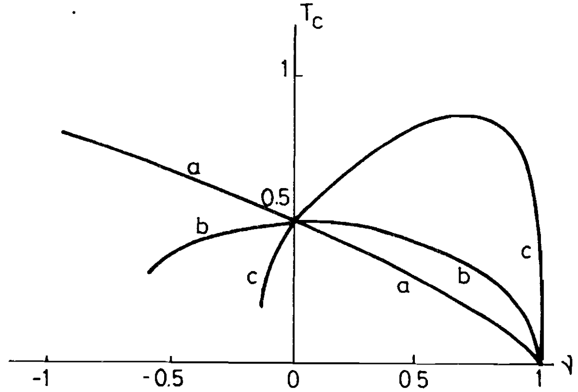
$$T_c = \frac{1-\nu}{8}\exp\left(\frac{\nu g}{2T_c}\right). \tag{16}$$

As follows from (16), there exists a negative value of the crossover parameter $\nu = \nu_1$,

$$\nu_1 = -\frac{1}{eg-1} \qquad (eg > 1), \tag{17}$$

such that for $\nu < \nu_1$ the ferromagnetic state is impossible at all temperatures. And vice versa, for $g \le e^{-1} = 0.3679$ a positive solution for T_c is available at any ν. The existence of the limiting value (17) is quite explainable. Really, negative values of ν correspond to the antiferromagnetic character of the short-range interaction. The presence of an interaction having an opposite sign in comparison with the ferromagnetic long-range interaction surves as a disordering factor. The onset of a ferromagnetic order is possible only if the disordering short-range interaction is not too large. One might adduce several other examples when an ordering in a system occurs only if some limiting relation between competing interactions takes place. Remind here only one example[25] having to do with the criterion of ferromagnetism in models with intermediate valency[26-28].

The crossover behaviour of T_c for various g is given in Fig.3.



F i g. 3. The dependence of the critical temperature on the crossover parameter: a) $g = 0.1$; b) $g = 1$; c) $g = 5$.

It is interesting that this crossover for $g > 1$ is nonmonotonic: between the value $T_c = 0.5$ corresponding to the mean-field theory and $T_c = 0$ bearing on the short-range interaction there occurs a maximum at the point

$$T_{max} = \frac{g}{8(1+\ln g)}, \qquad \nu_{max} = \frac{\ln g}{1+\ln g}.$$

Expanding thermodynamic functions in powers at $\tau \equiv (T-T_c)/T_c$ to the left of the critical temperature, we obtain the asymptote for the ferromagnetic probability

$$w-\frac{1}{2}\simeq\begin{cases}A_w(-\tau)\,, & u\neq u_0\,,\\ (-\tau)^{1/2}\,, & u=u_0\,,\end{cases}$$

where

$$A_w=\frac{2(1-\nu)(1+2K_c)^2}{(u-t)(1-4L_c^2/3)-4(1-\nu)(1+2K_c)^2}\,,$$

$$u_0=t+\frac{4(1-\nu)(1+2K_c)^2}{1-4L_c^2/3}\,,\quad t=\frac{1+16K_cL_c-4L_c^2}{(1+4L_c)^2}\,.$$

For the order parameter one has the asymptote

$$\sigma\simeq\begin{cases}A_\sigma(-\tau)^{1/2}\,, & u\neq u_0\,,\\ (-\tau)^{1/4}\,, & u=u_0\,,\end{cases}$$

in which the critical amplitude A_σ is given by the expression

$$A_\sigma^2=\frac{2(u-t)(1+2K_c)}{(u-t)(1-4L_c^2/3)-4(1-\nu)(1+2K_c)^2}\,.$$

The quantity A_σ^2 as a function of the crossover parameter is depicted in Fig. 4, where ν_2 is defined by the equation

$$(1-\nu_2)^2=12\,T_c^2\,. \qquad (18)$$

The specific heat jump

$$\Delta C_v\equiv\lim_{T\to T_c-0}C_v-\lim_{T\to T_c+0}C_v=A_\sigma(1+2K_c)L_c$$

and the value of the heat capacity to the right of the critical point

$$C_v^c\equiv\lim_{T\to T_c+0}C_v=\frac{16K_c^2L_c}{(1+L_c/2)^2}$$

are shown in Fig. 5 and Fig. 6, respectively.

Antiferromagnetic character of the short-range interaction and the presence of heterophase fluctuations can break the second-order

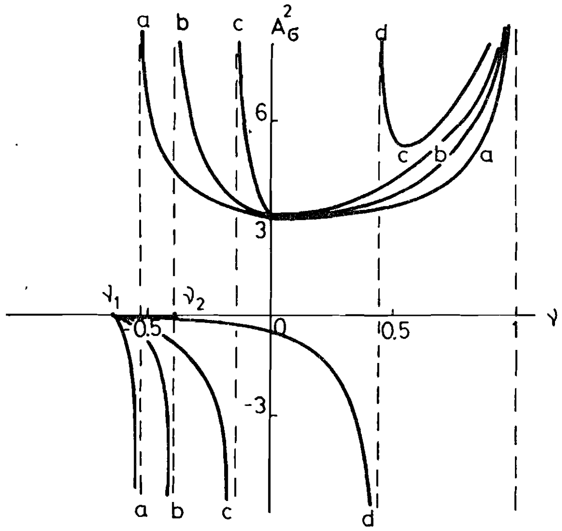


Fig. 4. The crossover behaviour of the critical amplitude squared A_σ^2 for g = 1: a) u = -5; b) u = $\pm\infty$; c) u = 5; d) u = 1.

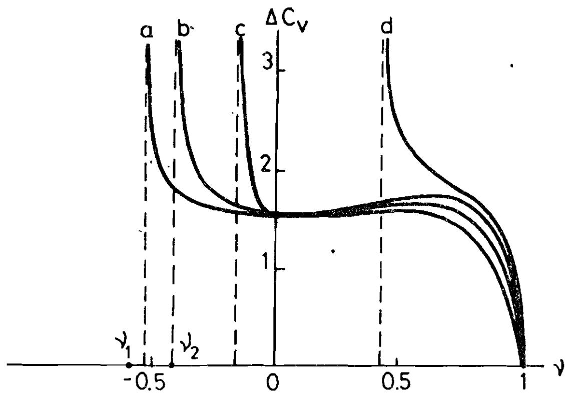
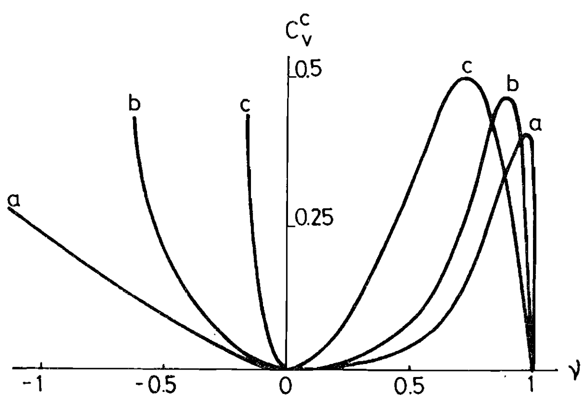


Fig. 5. The specific-heat jump at the critical point for g = 1: a) u = -5; b) u = $\pm\infty$; c) u = 5; d) u = 1.



F i g. 6. The specific heat at the critical point from the right depending on the crossover parameter: a) $g = 0.1$; b) $g = 1$; c) $g = 5$.

phase transition to the first-order one. The region of first-order phase transition is defined by the inequalities

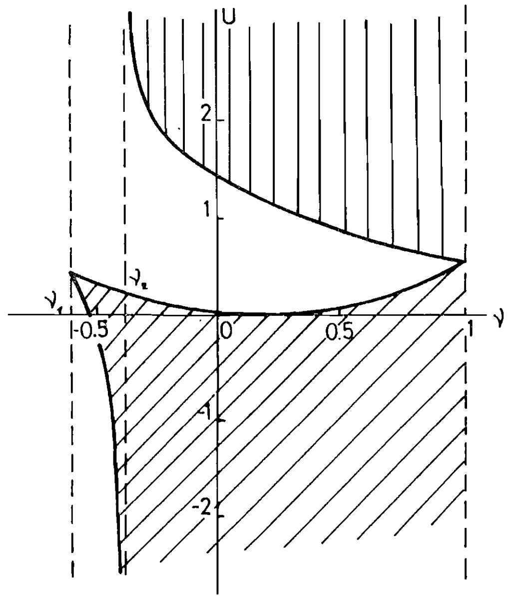
$$t < u < t + \frac{4(1-\nu)(1+2K_c)^2}{1-4L_c^2/3}, \quad \nu > \nu_2, \tag{19}$$

or

$$t < u < t - \frac{4(1-\nu)(1+2K_c)^2}{|1-4L_c^2/3|}, \quad \nu_1 < \nu < \nu_2. \tag{20}$$

The change of a trsnsition order in the $u-\nu$ -plane is illustrated in Fig. 7.

The most interesting properties of the model considered, from our point of view, are, firstly, the existence of a strongly nonmonotonic dependence of the critical temperature and critical amplitudes on the crossover parameter ν , and, secondly, the possibility for the phase transition to be of both the orders. Quite nontrivial properties of the model and their large variety depending on a relation between the Hamiltonian parameters make it probable to apply the model to the interpretation of experimental data for various quasi-one-dimensional magnets[29].



F i g. 7. Regions of phase transitions in the heterophase system. The vertical hatching corresponds to the second-order transition in the stable system, the oblique hatching shows the second-order transition in the metastable system, the region without hatching in the interval $\nu_1 \leq \nu \leq 1$ means the first-order transition.

We have considered here a classical model, but as is evident, it can be without difficulties generalized to the quantum case. There are, however, reasons[30] to suspect that the behaviour of analogous quantum models will be qualitatively the same.

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Кислинский В.Б., Юкалов В.И. E17-86-535
Метод квазисредних для метастабильных и смешанных систем

Рассмотрен метод определения квазисредних, позволяющий описывать наряду со стабильными фазами также метастабильные фазы и смеси нескольких фаз. Метод иллюстрируется на примере одномерной гетерофазной модели Изинга со взаимодействием, аддитивно включающем как взаимодействие ближайших соседей, так и дальнодействие. Выяснено, что критическая температура и критические амплитуды нелинейно и, вообще говоря, немонотонно зависят от кроссоверного параметра, характеризующего переход от близкодействующей к дальнодействующей модели. Род фазового перехода ферромагнетик-парамагнетик может изменяться со второго на первый в зависимости от соотношения между обменным интегралом, кроссоверным параметром и константой кристаллического поля.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Kislinsky V.B., Yukalov V.I. E17-86-535
Method of Quasi-Averages for Metastable and Mixed Systems

A method of defining quasi-averages is considered giving the possibility for describing besides stable phase the metastable ones as well as mixtures of several phases. The method is illustrated by the one-dimensional heterophase Ising model with additive short - and long-range interactions. It is found that the critical temperature and critical amplitudes are nonlinear and, generally speaking, are nonmonotonic with respect to a crossover parameter characterizing the crossing from the short-range to long-range model. The ferromagnet-paramagnet phase transition can change its order from second to first depending on the relation between the exchange integral, crossover parameter and crystalline-field constant.

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

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