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Two Coupled Ising Planes: Phase Diagram and Interplanar Force

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The statistical mechanics of two Ising ferromagnetic planes coupled by a local interlayer two-spin interaction have been studied by means of a variety of calculational methods, including different mean-field approximations, Migdal–Kadanoff-type renormalization-group techniques, scaling theory, as well as numerical Monte Carlo simulation techniques. The phase diagram has been derived as a function of the interlayer coupling strength. Furthermore, various thermodynamic variables have been determined, including the interlayer correlation function, which is proportional to the interplanar force. It is found that a Migdal–Kadanoff renormalization with a decimation procedure which involves the interlayer coupling in an appropriate fashion provides an accurate description of the phase diagram and that a mean-field description provides a good description of the phase diagram and the interplanar force, except for very low interlayer coupling strengths.

KEY WORDS: Ising model; layered systems; phase diagram; interlayer coupling; mean-field theory; renormalization group; scaling theory; Monte Carlo simulation.

1. INTRODUCTION

In the absence of an exact solution to the three-dimensional Ising problem, a number of attempts to go beyond the well-known statistical mechanical solution to the two-dimensional Ising problem have been proposed for systems of coupled two-dimensional Ising planes, and all conceivable aspects of semi-infinite Ising systems have been studied by a variety of

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techniques.[1–10] Originally much of this work formed an integral part of the general study of critical phenomena and served at least two major purposes. One was to study the dimensional crossover in the critical behavior.[8] Another purpose was to produce solutions to lattice models of thin films which are finite in one dimension and infinite in the two other dimensions.[6] One of the cornerstones in this work was the development of the celebrated finite-size scaling theory,[5] which has proved so successful for deriving results valid in the thermodynamic limit from data for finite systems, e.g., as they can be obtained from computer-simulation calculations.[11]

More recently a renewed interest has arisen in the properties of coupled Ising planes, in particular the limit of two interacting planes, as a model system of interacting solid surfaces or thin films.[10] In our case, the interest is largely motivated by fundamental problems underlying the general study of forces between surfaces and questions regarding colloidal stability.[12] This study often considers materials properties of thin monomolecular organic films, such as Langmuir and Langmuir–Blodgett films or lamellar amphiphilic (e.g., lipid) bilayers.[13] The experimental study of such systems has made significant advances in recent years due to the advent of the surface force apparatus[12] and microscopic techniques like the atomic force microscope.[14,15] It is now well known that the strength of the force (and even its sign) between surfaces depends in a very critical fashion on the molecular degrees of freedom on the surfaces as well as on the nature of the medium in between the surfaces.

The fundamental physical problem in relation to the study of forces between surfaces and macroscopic bodies is, given a certain form of the direct intra- and intersurface microscopic forces, to understand the form of the resulting effective macroscopic force acting between macroscopic bodies whose surfaces are covered with molecular entities with internal degrees of freedom. The correlations in the fluctuations in these degrees of freedom within and between the layers are responsible for a thermal renormalization of the direct force between the layers, often resulting in an entropy-dominated macroscopic effective force. There are examples of systems[16] where this renormalization in the fluctuation-induced force may even change the sign of the effective macroscopic force relative to that of the microscopic force.

In the present paper we study the statistical mechanics of two coupled spin-1/2 Ising square planes which are infinite in two dimensions. The model is defined by the Hamiltonian

$$\mathscr{H} = -J_1 \sum_{\langle i,j \rangle} \sigma_i^1 \sigma_j^1 - J_2 \sum_{\langle i,j \rangle} \sigma_i^2 \sigma_j^2 - J_{12} \sum_i \sigma_i^1 \sigma_i^2 - h \sum_i (\sigma_i^1 + \sigma_i^2) \quad (1)$$

where the two first sums are over nearest-neighbor in-plane pairs in the two different planes and the third term couples pairs of opposite spins across the planes. Indices 1 and 2 refer to the two planes, and the spin variables take on the values $\sigma_i = \pm 1$. All spins are coupled ferromagnetically, $J_1 > 0$, $J_2 > 0$, $J_{12} > 0$. h is an external magnetic field. In the present paper we focus on the symmetric zero-field case ($h = 0$) with $J_1 = J_2 = J$, in which case the Hamiltonian can conveniently be written

$$-\beta \mathscr{H} = K\left(\sum_{\langle i,j \rangle} \sigma_i^1 \sigma_j^1 + \sum_{\langle i,j \rangle} \sigma_i^2 \sigma_j^2 + J_r \sum_i \sigma_i^1 \sigma_i^2 \right) \tag{2}$$

where $\beta = (k_B T)^{-1}$, $K = \beta J$, and $J_r = J_{12}/J$.

Introducing an interlayer correlation function

$$\rho_{12} = \frac{2}{N} \left\langle \sum_i \sigma_i^1 \sigma_i^2 \right\rangle \tag{3}$$

where N is the total number of sites in the two Ising planes, the differential of the generalized Gibbs potential G can be written as

$$dG = -S\, dT - N\langle \sigma \rangle\, dh - \frac{N}{2} \rho_{12}\, dJ_{12} \tag{4}$$

Assuming that the direct coupling between spins in different planes depends on interlayer distance r, as $J_{12}(r)$, the macroscopic thermodynamic force F between the two layers takes the form

$$F = -\left(\frac{\partial G(T, J_{12}, h)}{\partial r} \right)_{h,T} = -\left(\frac{\partial G}{\partial J_{12}} \right)_{h,T} \left(\frac{dJ_{12}}{dr} \right) = \frac{N}{2} \rho_{12} \left(\frac{dJ_{12}}{dr} \right) \tag{5}$$

Thus, apart from a factor depending on the details of the coupling constant and the system size, the force is determined by the interlayer correlation function.

The critical behavior, i.e., the critical exponents, for a system consisting of a small number of Ising planes coupled by a bilinear interaction, specifically two coupled planes, is expected to be the same as that of the two-dimensional Ising model. This is so because the interlayer coupling neither breaks the spin-reversal symmetry nor introduces new symmetry elements and correlation lengths in the problem. Different types of interlayer couplings, e.g., four-spin interactions as in the Ashkin–Teller model, are required to change the critical behavior.[17] Whereas the critical exponents are not expected to be influenced by the presence of the interlayer coupling, nonuniversal properties, such as the value of the critical temperature, will be affected. In the ferromagnetic case the critical temperature will be increased by the coupling. In the limit of $J_{12}=0$ the critical temperature is that given by the Onsager solution, $K_c^{2D}=K_c(J_{12}=0)=\frac{1}{2}\ln(\sqrt{2}+1)$, whereas in the strong-coupling limit, $J_{12}\to\infty$, each pair of spins coupled across the layers will act as a single spin which is coupled to the other spins with twice the coupling strength, i.e., $K_c(J_{12}=\infty)=\frac{1}{2}K_c(J_{12}=0)$.

The system of two coupled, identical Ising planes ($J_1=J_2=J$) was first studied by Ballentine,[1] who investigated the model by high-temperature series expansions in the case of $J_{12}=J$. This work was later extended up to five layers by Allan.[2] The case of $J_{12}\neq J$ was studied by Abe[3] and Mikulinskii[4] in the context of a scaling theory valid in the limit of a weak interlayer coupling. The fully fledged finite-size scaling theory for finite-size Ising lattices ($J_r=1$) with open surfaces was introduced by Fisher and Barber in 1972[5] and later used by Binder[6] to analyze data generated by Monte Carlo simulations, and by Capehart and Fisher[8] to analyze data obtained by high-temperature series expansions. Using Landau theory, Imry[18] studied the closely related problem of weakly coupled layers with order parameters having a continuous symmetry group. More recently, Parga and Van Himbergen[9] studied the model with two and more layers by means of a Migdal–Kadanoff-style real-space renormalization scheme.

The more general case in which the layers are not forced to be identical ($J_1\neq J_2$) has also received some attention. The most complete account is that of Oitmaa and Enting,[7] who combined mean-field theory, scaling theory, and high-temperature expansions in a study of the two-layer model, thereby calculating, e.g., the variation of the critical temperature, the layer magnetizations, and the interlayer correlation function with J_{12}. Very recently, Ferrenberg and Landau[10] considered the same two-layer problem using Monte Carlo simulations and mean-field theory.

Finally, it should be noted that the case of two coupled one-dimensional Ising chains has also been considered[19] with a view to examining the simplest possible statistical mechanical model system with fluctuation-induced forces. For that system the phase diagram and the interchain force can be calculated exactly by means of transfer-matrix techniques.

Despite these efforts a number of interesting questions concerning the thermodynamics of coupled Ising planes remain unresolved. Specifically, phase diagrams are still lacking, tests of a number of proposed scaling relations have not been performed, and the question of interlayer forces has only received little attention. At the same time we feel that the theoretical description of the models can be improved in the case of, e.g., the scaling, mean-field, and approximative renormalization group approaches. In this paper we attack some of these problems for the simple case of two coupled, identical Ising planes.

The outline of the remaining part of this paper is as follows. In Section 2 we present the scaling arguments which lead to a prediction of the relationship between the critical temperature and the interlayer coupling strength, i.e., the phase diagram. Scaling relations for the dependence of the interlayer correlation function, the order parameter, and the corresponding isothermal susceptibility on the interlayer coupling strength are also presented. Two versions of a mean-field approximation for the phase diagram and the interlayer force are then put forward in Section 3. The renormalization-group approach to the phase diagram is presented in Section 4 in the form of two versions of a real-space Migdal–Kadanoff-type renormalization scheme involving two different ways of performing the decimation procedure. The results of a numerical Monte Carlo computer-simulation approach to the problem are then described in Section 5. Finally, the different approaches are discussed and compared in Section 6.

2. SCALING THEORY

In this section we will investigate the influence of the interlayer coupling strength on the thermodynamics of the two coupled Ising planes in terms of approximative scaling relations. The validity of these relations is examined by Monte Carlo simulations in Section 5. Thus, it is natural to be concerned with the form of the scaling relations both in the thermodynamic limit as well as for finite systems.

Some of the relations to be presented have already been known for some time. For instance, the relation for the shift in critical temperature was derived in refs. 3 and 4 by investigations of the asymptotic behavior of a perturbation expansion of the partition function for the complete problem and in refs. 7 and 18 by simple self-consistent (mean-field) arguments. Similarly, the relation $\langle \sigma \rangle = \phi(J_r)$ was derived from mean-field arguments in ref. 7, in which a number of other scaling relations were proposed for the general problem, $J_1 \neq J_2$. However, the unifying features of these approaches and the range of validity of the theory have not been discussed.

Basically, the above approaches involve simplifying arguments which will allow one to take advantage of the well-known scaling behavior of the two-dimensional Ising model[20,21] or, equivalently, of homogeneity relations, which are expressed in terms of the reduced temperature $t = K_c^{2D}/K - 1$ and the external field h, together with exponent relations and the particular values of the exponents. In the case of the perturbation or cumulant expansion of the (logarithm of the) partition function it is convenient to write the Hamiltonian in the form[3]

$$\begin{aligned}\mathscr{H} &= \mathscr{H}_0(1) + \mathscr{H}_0(2) + J_r \mathscr{H}_1 \\ \mathscr{H}_0(\alpha) &= -J \sum_{\langle i,j \rangle} \sigma_i^\alpha \sigma_j^\alpha - h \sum_i \sigma_i^\alpha \\ \mathscr{H}_1 &= -J \sum_i \sigma_i^1 \sigma_i^2\end{aligned} \tag{6}$$

where α is the layer index. With the free energy densities

$$g_0 = -\frac{1}{\beta N} \ln \left\{ \mathrm{Tr}_\sigma \exp \left[-\beta \sum_\alpha H_0(\alpha) \right] \right\} = -\frac{1}{\beta N} \ln Z_0$$

$$g = -\frac{1}{\beta N} \ln(\mathrm{Tr}_\sigma \, e^{-\beta H}) = -\frac{1}{\beta N} \ln Z$$

the perturbation expansion reads

$$g(t, h, J_r) = g_0(t, h) - \frac{1}{\beta N} \sum_{n=1}^{\infty} \frac{J_r^n}{n!} \langle (-\beta \mathscr{H}_1)^n \rangle_c \tag{7}$$

In this expansion one can safely invoke the two-variable scaling hypothesis for the two-dimensional Ising model in each term of the expansion, since the cumulants $\langle (-\beta \mathscr{H}_1)^n \rangle_c$ can be rewritten as spin correlators averaged over the distribution for the decoupled Ising models. In principle, the exact asymptotic behavior close to $K_c^{2\mathrm{D}}$ is contained in this approach. However, useful generalizations can only be obtained if the exponent η is assumed to vanish.[3] By making this assumption the following form of the singular part of the free energy is obtained[3]:

$$g(t, h, J_r) = |t|^{2-\alpha} \Phi_1^\pm \left(\frac{h}{|t|^\Delta}, \frac{J_r}{|t|^\gamma} \right) \tag{8}$$

where Δ is the gap exponent and α and γ are the exponents characterizing the divergence of the zero-field heat capacity and the zero-field isothermal susceptibility, respectively. In the case of the self-consistent theory[7,18] one studies a mean-field Hamiltonian of the form

$$\begin{aligned}\mathscr{H} &= \mathscr{H}_{\mathrm{mf}}(1) + \mathscr{H}_{\mathrm{mf}}(2) \\ \mathscr{H}_{\mathrm{mf}}(\alpha) &= -J \sum_{\langle i,j \rangle} \sigma_i^\alpha \sigma_j^\alpha - \left(h + \frac{J_{12}}{2} \langle \sigma \rangle \right) \sum_{i,\alpha} \sigma_i^\alpha\end{aligned} \tag{9}$$

Basically, this is the Hamiltonian for two decoupled Ising models in an effective mean field, introduced by the decoupling $\sigma^1\sigma^2 \to \frac{1}{2}(\langle\sigma^1\rangle\sigma^2 + \langle\sigma^2\rangle\sigma^1)$ and by invoking translational invariance. Thus, close to the critical point we can, according to this theory, introduce the usual homogeneity relations in the singular part of the free energy as follows:

$$g(t, h') = g\left(t, h + \frac{J_{12}}{2}\langle\sigma\rangle\right) = |t|^{2-\alpha}\,\Phi_2^{\pm}\left(\frac{h'}{|t|^{\Delta}}\right)$$
$$= |t|^{2-\alpha}\,\Phi_2^{\pm}\left(\frac{h}{|t|^{\Delta}} + BJ\frac{J_r}{|t|^{\Delta-\beta}}\right) \qquad (10)$$

which will lead to the same scaling predictions as Eq. (8), since $\gamma = \Delta - \beta$.[21] In Eq. (10), B is a correction-to-scaling amplitude.

Now, in order to derive the scaling relations we choose Eq. (8) as the starting point. Since we expect the model to belong to the universality class of the two-dimensional Ising model, at $h = 0$ and for a fixed value of J_r, we can assume that

$$g(t, 0, J_r) = |t|^{2-\alpha}\,\Phi_1^{\pm}\left(0, \frac{J_r}{|t|^{\gamma}}\right) = \Phi_3^{\pm}\,|t'|^{2-\alpha} \qquad (11)$$

where $t' = K_c/K - 1$, K_c being the inverse critical temperature for the coupled model at J_r. Anticipating an upward shift in the critical temperature $[t' = 0,\ t(K_c) > 0]$, we write

$$\Phi_1^{+}\left(0, \frac{J_r}{t(K_c)^{\gamma}}\right) = \Phi_1^{+}(0, A^{\gamma})$$
$$t(K_c) = \frac{K_c^{2D}}{K_c} - 1 \equiv \tau_0 = AJ_r^{1/\gamma} \qquad (12)$$

where A^{γ} is the argument of Φ_1^{+} which makes Φ_1^{+} vanish. This is the scaling form for the shift in critical temperature.

Furthermore, by using Eq. (8) and the definitions

$$\langle\sigma\rangle = -\left(\frac{\partial g}{\partial h}\right)_{t, J_r}, \qquad \chi_T = -\left(\frac{\partial^2 g}{\partial h^2}\right)_{t, J_r}, \qquad \rho_{12} = -\left(\frac{\partial g}{\partial J_r}\right)_{t, h} \qquad (13)$$

standard manipulations lead to, e.g.,

$$\langle\sigma\rangle = |t|^{\beta}\,\phi_1^{\pm}\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}\right) = J_r^{\beta/\gamma}\phi_2^{\pm}\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}\right) \qquad (14)$$

and at $h=0$ and $t=0_-$ one eventually obtains

$$\begin{aligned} \langle\sigma\rangle &\sim J_r^{\beta/\gamma} \sim J_r^{1/(\delta-1)} \sim J_r^{1/14} \\ \chi_T &\sim J_r^{-\gamma/\gamma} \sim J_r^{-1} \\ \rho_{12} &\sim J_r^{2\beta/\gamma} \sim J_r^{2/(\delta-1)} \sim J_r^{1/7} \end{aligned} \tag{15}$$

where we have used the exact exponent values for the two-dimensional Ising model, $\beta=1/8$, $\gamma=7/4$, and $\delta=15$. These relations could also quite easily be obtained from Eq. (10) using the relation $\langle\sigma\rangle \sim h^{1/\delta}$ and invoking $\rho_{12}=\langle\sigma\rangle^2$, which is consistent with the mean-field ideas used in Eq. (9).

To facilitate a quantitative check of the proposed scaling relations we will formulate finite-size scaling versions of the relations (15). Clearly, the formulation will follow the same lines as those used to derive Eqs. (12) and (14). The additional requirement for the formulation is the scaling form for the correlation length ξ

$$\xi = |t|^{-\nu}\, \Psi_1^{\pm}\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}\right) = J_r^{-\nu/\gamma}\Psi_2^{\pm}\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}\right) \tag{16}$$

and the finite-size scaling hypothesis for the free energy:

$$\begin{aligned} g = g(t, h, J_r, l^{-1}) &= |t|^{2-\alpha}\, \Phi_4\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}, \frac{\xi}{l}\right) \\ &= |t|^{2-\alpha}\, \Phi_5\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}, \frac{J_r^{-\nu/\gamma}}{l}\right) \end{aligned} \tag{17}$$

where l is a characteristic length scale for the system. Again, standard methods are used to derive, e.g.,

$$\langle\sigma\rangle_l = |t|^{\beta}\, \phi_1\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}, \frac{J_r^{-\nu/\gamma}}{l}\right) = l^{-\beta/\nu}\phi_2\left(\frac{h}{|t|^{\Delta}}, \frac{J_r}{|t|^{\gamma}}, \frac{J_r^{-\nu/\gamma}}{l}\right) \tag{18}$$

Thus, we are led to the following relations:

$$\begin{aligned} \langle\sigma\rangle_l &= l^{-\beta/\nu}\varphi_1\left(\frac{J_r^{-\nu/\gamma}}{l}\right) \\ \chi_{T,l} &= l^{\gamma/\nu}\varphi_2\left(\frac{J_r^{-\nu/\gamma}}{l}\right) \\ \rho_{12,l} &= l^{-2\beta/\nu}\varphi_3\left(\frac{J_r^{-\nu/\gamma}}{l}\right) \end{aligned} \tag{19}$$

Since the scaling relations are derived under circumstances corresponding to a mean-field description of the interlayer coupling together with an assumption of long-range correlations in the planes, we do not expect the relations to be valid for all values of the scaling variable $J_r^{-\nu/\gamma}/l$. Basically, we expect at least one crossover for high values of J_r. At high values of J_r it may be expected that the range of correlations is reduced to such an extent that the scaling hypothesis no longer applies. Furthermore, $\langle\sigma\rangle$, ρ_{12} and also τ_0 are bounded, implying that limiting values are approached at large J_r. In the limit of a very weak coupling strength the situation is less clear-cut since it is possible that the mean-field prescription $\sigma^1\sigma^2 \to \frac{1}{2}(\langle\sigma^1\rangle\,\sigma^2 + \langle\sigma^2\rangle\,\sigma^1)$ will be equivalent to replacing a one-scaling operator with a linear combination of other scaling operators in the region of strong fluctuations, which would imply a breakdown of the mean-field theory. How and to what extent the operator $\sigma^1\sigma^2$ is affected by fluctuations is hard to predict *a priori*. To complicate matters further, it should be noted that an order-of-magnitude estimate of the Ginzburg critical region t_g from a Landau expansion on the basis of Eq. (9)[18] leads to the opposite (and surprising) prediction $t_g \sim \tau_0$, implying the vanishing of the region of breakdown of mean-field theory in the low-coupling limit. This is somewhat counterintuitive, even though an expansion relying on a decoupling of layers is supposed to be exact in the limit of $J_r = 0$.

3. MEAN-FIELD THEORY

In this section we present two kinds of mean-field calculations, giving rise to approximate phase diagrams as well as determinations of the interplanar force as a function of K and J_r.

In the first approach we decouple spins corresponding to different lattice sites (i, j) within the planes. This implies that nearest-neighbor spins in different planes are not decoupled. We can regard this as an extension of the mean-field approach applied by Oitmaa and Enting,[7] where all spins are decoupled. This is obviously a crude approach, resembling the traditional mean-field description of the two-dimensional Ising model.

In the second approach, we rewrite the Hamiltonian in such a way that the interlayer correlation function can easily be treated in a mean-field manner, by regarding it as part of an effective field and incorporating this assumption into the Onsager solution of the two-dimensional Ising model. The fact that some of the variables in the problem are treated exactly in this approach is expected to give rise to a more quantitative description than the first approach.

In both cases we determine the optimum distribution by variationally minimizing the free energy with respect to the mean-field distribution by following the ideas used for multistate problems (e.g., the Potts model).[22] For a general expectation value $\langle A[p] \rangle$ regarded as a functional of the probability distribution p, we define the variational derivative as

$$\frac{\delta \langle A[p] \rangle}{\delta p_j} = \lim_{\varepsilon \to 0} \frac{\langle A[p_i + \varepsilon \delta_{ij}] \rangle - \langle A[p_i] \rangle}{\varepsilon} \tag{20}$$

which is a generalization of the definition used in ref. 20 to the discrete case.

3.1. Mean-Field Theory I

In this approach the factorization of the probability distribution and partition function in single-site factors implies that it is sufficient to consider the ith single-site term of the Hamiltonian, which can be written as

$$-\beta h_i = \left\langle \sum_{\alpha = 1,2} (2K\langle \sigma \rangle)\, \sigma_i^\alpha + J_r K \sigma_i^1 \sigma_i^2 \right\rangle \tag{21}$$

because of translational invariance. Our variational principle states that the free energy density must be minimized with respect to the single-site distribution under the constraint that the distribution is normalized. In terms of variational derivatives we write

$$\begin{aligned} -\beta \frac{\delta f}{\delta p} - \lambda &= -\beta \frac{\delta h}{\delta p} - \langle \ln p \rangle - \lambda \\ &= -\beta\phi - (1 + \ln p) - \lambda = 0 \end{aligned} \tag{22}$$

where λ is a Lagrangian multiplier. This implies that

$$p = \frac{1}{Z_0} e^{-\beta\phi} \tag{23}$$

$$Z_0 = \sum_{\sigma^\alpha} e^{-\beta\phi} \tag{24}$$

$$-\beta\phi = -\beta \frac{\delta h}{\delta p} = 4K\langle \sigma \rangle \sum_{\alpha = 1,2} \sigma^\alpha + J_r K \sigma_i^1 \sigma_i^2 \tag{25}$$

In principle these formulas contain all the relevant thermodynamic information. In particular, we have

$$\langle \sigma \rangle = \frac{\sinh(8K\langle \sigma \rangle)}{\cosh(8K\langle \sigma \rangle) + e^{-2J_r K}} \tag{26}$$

$$\rho_{12} = \frac{\cosh(8K\langle \sigma \rangle) - e^{-2J_r K}}{\cosh(8K\langle \sigma \rangle) + e^{-2J_r K}} \tag{27}$$

By expanding for $\langle\sigma\rangle \to 0$ and $K \to K_c$ we obtain

$$J_{r,c} = \frac{-\ln(8K_c - 1)}{2K_c} \tag{28}$$

This is a closed-form expression for the mean-field I phase diagram shown in Fig. 1. We note that in this approach $K_c(J_r = 0) = 0.25$ and $K_c(J_r \to \infty) = 0.125$, indicating a systematic overestimation of the critical temperature. On the other hand, the behavior confirms our expectation that the critical temperature should be doubled as $J_r \to \infty$.

For $K \leqslant K_c$ we get the following relations for the interlayer correlation function:

$$\rho_{12}(K \leqslant K_c, J_r) = \tanh(J_r K) \approx J_r K + \mathcal{O}((J_r K)^3) \tag{29}$$

$$\rho_{12}(K = K_c, J_{r,c}) = \frac{1}{4K_c} - 1 \tag{30}$$

while ρ_{12} must be determined numerically for $K > K_c$. The formulas in Eqs. (29) and (30) indicate that ρ_{12} increases linearly for small values of $J_r K$. Furthermore, in this mean-field picture the possible singular behavior of ρ_{12} in the critical region must solely come from singularities in the order parameter $\langle\sigma\rangle$.

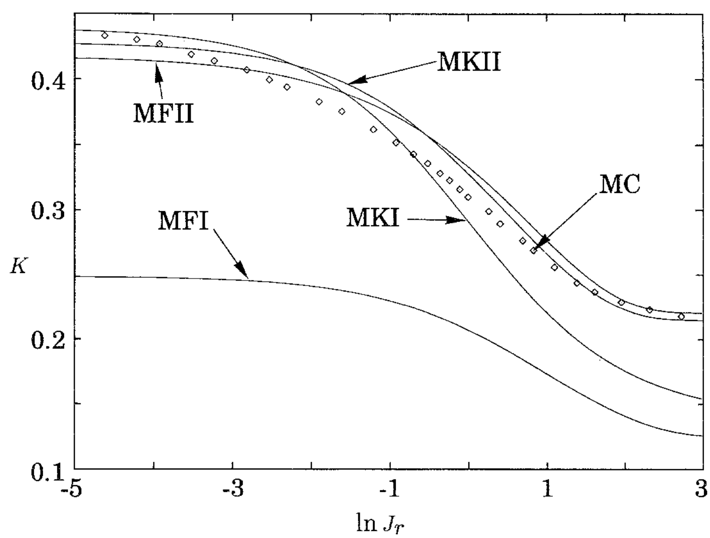

Fig. 1. Phase diagram, K vs. $\ln(J_r)$, obtained for the ferromagnetically coupled Ising bilayer system by using MC data and various theoretical approaches. In this semilogarithmic plot the extremely weak coupling strengths $J_r < 0.01$ are not represented.

3.2. Mean-Field Theory II

Let us reformulate the Hamiltonian as follows:

$$-\beta\mathscr{H} = K\left(\sum_{\langle i,j\rangle} \sigma_i^1\sigma_j^1 + \sum_{\langle i,j\rangle} \sigma_i^2\sigma_j^2 + J_r \sum_i \sigma_i^1\sigma_i^2\right) \tag{31}$$

$$= K\left(\sum_{\langle i,j\rangle} \sigma_i\sigma_j \cdot (s_i s_j + 1) + J_r \sum_i s_i\right) \tag{32}$$

where we have introduced the new spin variables

$$s_i = \sigma_i^1\sigma_i^2, \qquad \sigma_i = \sigma_i^1 \tag{33}$$

In terms of these variables the interlayer correlation function is simply $\rho_{12} = \langle s_i\rangle = \langle s\rangle$ because of translational invariance. We will now formulate a mean-field approach, based on two assumptions, namely that the total probability distribution can be factorized into a product of an s- and a σ-dependent distribution and that we can treat the s distribution in a single-site approximation. This implies that the average value of the Hamiltonian can be written as

$$\langle -\beta\mathscr{H}\rangle_s = (1 + \langle s\rangle_s^2) K \sum_{\langle i,j\rangle} \sigma_i\sigma_j + \frac{N}{2} J_r K \langle s\rangle_s = -\beta\mathscr{H}_{\mathrm{mf}} \tag{34}$$

$$\langle -\beta\mathscr{H}\rangle_{s,\sigma} = (1 + \langle s\rangle_s^2)\left\langle K \sum_{\langle i,j\rangle} \sigma_i\sigma_j\right\rangle_\sigma + \frac{N}{2} J_r K \langle s\rangle_s \tag{35}$$

where the subscripts s and σ refer to the individual s- and σ-dependent distributions. The σ-dependent average has the form of minus the average dimensionless internal energy for a two-dimensional Ising model evaluated at K. It follows from Eq. (34) that the mean-field model is equivalent to a different Ising model with a new coupling constant and a displaced zero point of the internal energy. From this fact we immediately conclude that the critical point can be determined as

$$K_c'(\rho_{12}) = K_c[1 + (\rho_{12,c})^2] = \tfrac{1}{2}\ln(1 + \sqrt{2}) \tag{36}$$

where $g_{12,c}$ refers to the optimal distribution, which is determined by the same variational principle as in the previous section. Applying this technique, we obtain

$$-\beta\phi = -\beta\frac{\delta h}{\delta p_s} = [2\rho_{12}\langle -\beta h(K)\rangle_\sigma + J_r K]\, s_j \tag{37}$$

$$Z_0 = \sum_{s_j = \pm 1} e^{-\beta\phi} = 2\cosh[2\rho_{12}\langle -\beta h(K)\rangle_\sigma + J_r K] \tag{38}$$

$$\rho_{12} = \tanh[2\rho_{12}\langle -\beta h(K)\rangle_\sigma + J_r K] \tag{39}$$

where $\langle -\beta h(K)\rangle_\sigma$ is minus the average dimensionless internal energy for the two-dimensional Ising model, evaluated at the inverse temperature K. This can be obtained from the Onsager solution by numerical evaluation.[20] Inverting Eq. (39) and combining this with Eq. (36), we obtain an expression for the phase diagram in closed form as

$$J_{r,c} = \frac{1}{2K_c}\left[\ln\left(\frac{1+\rho_{12,c}}{1-\rho_{12,c}}\right) - 4\rho_{12,c}\langle -\beta h(K_c)\rangle_\sigma\right] \tag{40}$$

$$\rho_{12,c} = \left[\frac{\frac{1}{2}\ln(1+\sqrt{2})}{K_c} - 1\right]^{1/2} \tag{41}$$

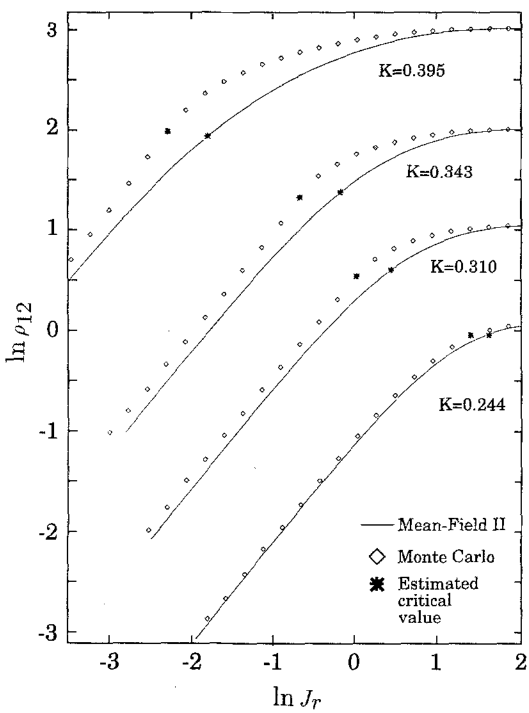

Fig. 2. ρ_{12} as a function of J_r in a double logarithmic plot displayed for four different values of K. The curves were obtained from the MFII approach and from Monte Carlo simulations on an $l = 32$ lattice. For both types of data the respective value of $\rho_{12,c}$ corresponding to the critical point is marked on the curves by an asterisk. For convenience, the different curves have been displaced vertically with $\Delta \ln \rho_{12} = 1$ relative to the one below. The values on the vertical axis correspond to $K = 0.244$.

The phase diagram obtained from the above equations is also shown in Fig. 1. Apart from the existence of bistable solutions corresponding to negative values of J_r for $0.419 \leqslant K \leqslant \frac{1}{2}\ln(1+\sqrt{2})$, a phase diagram in accordance with our expectations is obtained. In particular, $K_c \to \frac{1}{4}\ln(1+\sqrt{2})$ for $J_r \to \infty$. The peculiar behavior in the vicinity of the critical point of the two-dimensional Ising model is likely to be a consequence of the restrictive assumptions made in our mean-field approach. Regarding our model as a perturbated two-dimensional Ising model, we must expect that the mean-field approach breaks down in the vicinity of the critical point of the two-dimensional Ising model itself.

The interplanar force, Eq. (5), as a function of K and J_r can be obtained from Eq. (41). Figure 2 shows $\rho_{12}(J_r)$ for different values of K. It is seen that $\rho_{12}(J_r)$ increases linearly in a log–log plot for $J_r < J_{r,c}$. By direct evaluation, one finds a slope of value 1, which agrees well with the mean-field approach I.

4. RENORMALIZATION-GROUP CALCULATIONS

In this section, we will apply a real-space Migdal–Kadanoff-type renormalization scheme[23,24] in two different ways in order to obtain approximate phase diagrams.

In the first approach (Section 4.1) we treat the interlayer coupling as a sort of perturbation in the sense that we add step by step the interlayer couplings to the intralayer couplings during the renormalization group (RG) transformations by bond-moving procedures, so that we restrict the decimations to involve intralayer couplings only. Thus by "smearing" out the interlayer couplings we force the system to behave qualitatively like a two-dimensional Ising model from the start, and we regard the interlayer coupling only as an additional coupling strength that allows the system to enjoy an ordered state at a higher temperature than for the uncoupled two-dimensional Ising model. Hence, the fact that the interlayer coupling also forces the layers to be correlated is only taken into account indirectly. We must therefore expect that this approach works best at low interlayer coupling strengths.

In the second approach (Section 4.2) we try to account for the interlayer coupling in a more accurate way by including it in the decimation procedure. This approach involves a more complicated decimation procedure, but it must be expected that more reliable results are obtained, at least for strong interlayer couplings.

In both approaches we apply a four-step procedure, where we distinguish between the x and y directions in the Ising planes.[24,25] It is important to note that when we perform the RG transformations we shall treat the interlayer couplings and the intralayer couplings as independent couplings of different types. This means that when we renormalize the interlayer couplings, we can suppress the K dependence and treat them as if it is only J_r that varies during the transformations. In the end we shall locate fixed points in the RG equation for K, choosing different fixed values of J_r in order to obtain the phase diagram for the system. It should be noted that by treating the interlayer coupling in this way, we can regard the methods as approximate ways of implementing a Migdal–Kadanoff renormalization scheme, in the sense that the total sum of the bond strengths and the symmetry in the problem are preserved.

2.1. Migdal–Kadanoff RG I

This approach is closely related to the Migdal–Kadanoff renormalization scheme applied to the two-dimensional Ising model, involving the familiar one-dimensional decimation procedure for the Ising chain.[24] The interlayer coupling is incorporated by an additional bond-moving procedure as described in Fig. 3. We obtain the following equations:

1. Bond moving in the y direction and bond moving of interlayer couplings (Figs. 3bI and 3cI):

$$K_y' = 2K_y \tag{42}$$

$$K_x' = K_x\left(1 + \frac{J_r}{4 + J_r}\right) \tag{43}$$

$$J_r' = J_r\left(1 + \frac{J_r}{4 + J_r}\right) \tag{44}$$

2. Decimation in the x direction (Fig. 3dI):

$$\begin{aligned} K_x'' &= \tanh^{-1}[\tanh^2(K_x')] \\ &= \tanh^{-1}\left\{\tanh^2\left[K_x\left(1 + \frac{J_r}{4 + J_r}\right)\right]\right\} \end{aligned} \tag{45}$$

3. Bond moving in the x direction and bond moving of interlayer couplings (Figs. 3eI and 3fI):

$$K_x''' = 2K_x'' = 2\tanh^{-1}\left\{\tanh^2\left[K_x\left(1 + \frac{J_r}{4 + J_r}\right)\right]\right\} \tag{46}$$

$$K_y'' = K_y\left(2 + \frac{J_r'}{8 + J_r'}\right) = K_y\left(2 + \frac{J_r(1 + J_r/(4 + J_r))}{8 + J_r(1 + J_r/(4 + J_r))}\right) \tag{47}$$

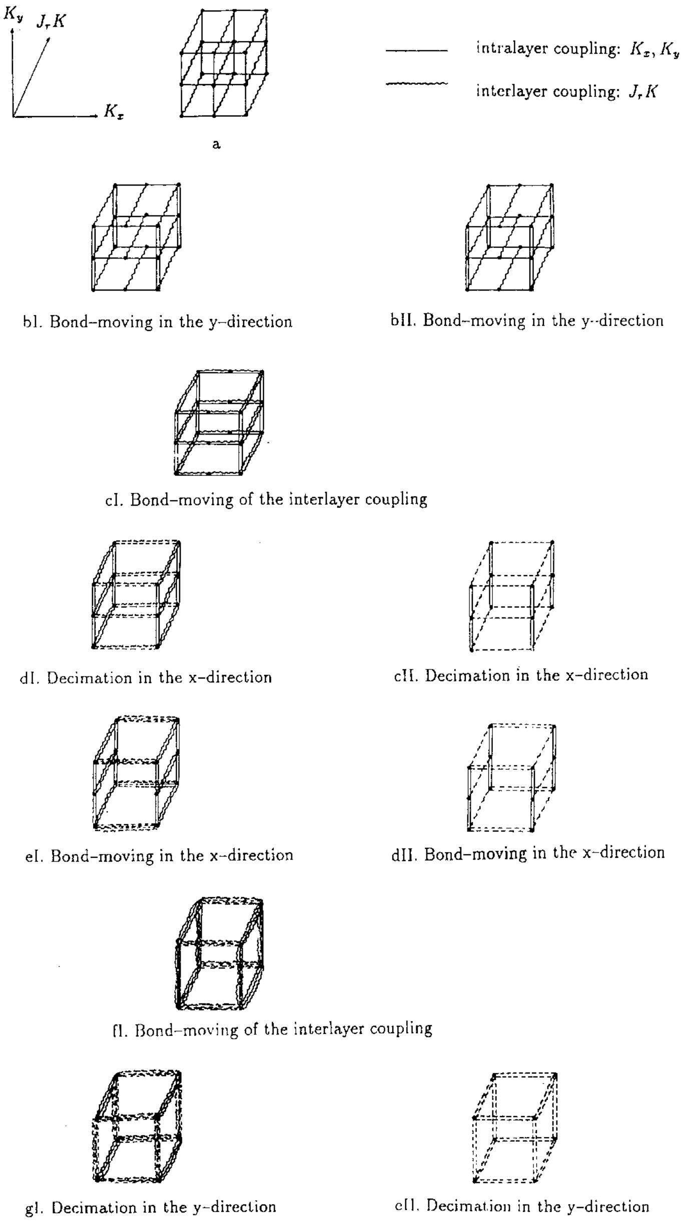

Fig. 3. The steps in the decimation procedure applied in the RG calculations. MKI (left panel) involves a successive introduction of the interlayer coupling in the planes (cI, eI), while MKII (right panel) involves a more traditional decimation (four-step procedures).

4. Decimation in the y direction (Fig. 3gI):

$$K_y''' = \tanh^{-1}\left\{\tanh^2\left[K_y\left(2+\frac{J_r(1+J_r/(4+J_r))}{8+J_r(1+J_r/(4+J_r))}\right)\right]\right\} \tag{48}$$

We have now completed the RG transformation for $\lambda = 2$ (corresponding to an increase in the lattice constant by a factor 2). The above equations can be generalized to arbitrry λ to obtain

$$R^\lambda(K_x) = \lambda \tanh^{-1}\left\{\tanh^\lambda\left[K_x\left(1+\frac{(\lambda-1)\,J_r}{2\lambda+J_r}\right)\right]\right\} \tag{49}$$

$$R^\lambda(K_y) = \tanh^{-1}\left\{\tanh^\lambda \times\left[K_y\left(\lambda+\frac{(\lambda-1)\,J_r(1+(\lambda-1)J_r/(2\lambda+J_r))}{2\lambda^2+J_r(1+(\lambda-1)J_r/(2\lambda+J_r))}\right)\right]\right\} \tag{50}$$

Expanding these two equations around $\lambda = 1$ to first order we get in both cases

$$R^\lambda(K) = K + (\lambda-1)\left[K\left(1+\frac{J_r}{2+J_r}\right) + \sinh K \cosh K \ln(\tanh K)\right] \tag{51}$$

which justifies putting $K_x = K_y = K$. We can now find K_c for a given value of $J_r = J_{r,c}$ by solving the equation

$$K_c\left(1+\frac{J_{r,c}}{2+J_{r,c}}\right) + \sinh K_c \cosh K_c \ln(\tanh K_c) = 0 \tag{52}$$

By rearranging we obtain an analytical equation for $J_{r,c}$ as a function of K_c:

$$J_{r,c} = -2\,\frac{K_c + \sinh K_c \cosh K_c \ln(\tanh K_c)}{2K_c + \sinh K_c \cosh K_c \ln(\tanh K_c)} \tag{53}$$

The phase diagram described by Eq. (53) is shown in Fig. 1. We notice that $K_c(J_r = 0) = \frac{1}{2}\ln(1+\sqrt{2})$, which is exact, whereas $K_c(J_r \to \infty) \approx 0.140$, implying that this approach overestimates the critical temperature in the strong-coupling limit.

4.2. Migdal–Kadanoff RG II

This approach follows the same general pattern as the one above, with the exception that instead of adding the interlayer couplings to the intralayer couplings, we involve them in the decimation procedure (see Figs. 3bII–3eII). This requires that we apply a special decimation procedure corresponding to the decimation of two opposite spins in two coupled Ising chains. We start with the one-dimensional Hamiltonian [compare with Eq. (2)]

$$-\beta\mathscr{H} = K\sum_{i=1}^{N}\left[\sigma_i^1\sigma_{i+1}^1 + \sigma_i^2\sigma_{i+1}^2 + \tfrac{1}{2}J_r(\sigma_i^1\sigma_i^2 + \sigma_{i+1}^1\sigma_{i+1}^2)\right] \tag{54}$$

and define spins μ to be situated at every second σ site along the chains. After some algebra we obtain the following renormalized Hamiltonian:

$$\begin{aligned}-\beta\mathscr{H} = \sum_{i=1}^{N/2} & (\tfrac{3}{4}A + \tfrac{1}{2}B + \tfrac{1}{4}D) + (\tfrac{1}{4}D - \tfrac{1}{4}A)(\mu_i^1\mu_{i+1}^1 + \mu_i^2\mu_{i+1}^2)\\ & + \tfrac{1}{4}C(\mu_i^1\mu_{i+1}^2 + \mu_i^2\mu_{i+1}^1) + (\tfrac{1}{2}J_rK + \tfrac{1}{4}C)(\mu_i^1\mu_i^2 + \mu_{i+1}^1\mu_{i+1}^2)\\ & + (\tfrac{1}{4}D - \tfrac{1}{4}A - \tfrac{1}{2}B)(\mu_i^1\mu_{i+1}^1\mu_i^2\mu_{i+1}^2)\end{aligned} \tag{55}$$

where

$$\begin{aligned}A &= \ln[4\cosh(J_rK)]\\ B &= \ln[\cosh(2K)]\\ C &= \frac{1}{2}\ln\{4[2\cosh(2J_rK)\cosh(4K) + 1 + \cosh^2(4K)]\}\\ D &= \frac{1}{2}\ln\frac{e^{2J_rK}\cosh(4K) + 1}{e^{2J_rK} + \cosh(4K)}\end{aligned}$$

The renormalized Hamiltonian involves two kinds of new couplings. There is a four-spin coupling as in the Ashkin–Teller model, which we choose to truncate, since it introduces a nontrivial and hard to handle coupling type into the problem. We also get a two-spin coupling between next-nearest neighbors across the chains. Qualitatively, after a large number of renormalizations this kind of coupling will be connecting spins at a large distance with respect to the original chain, and therefore it does not seem unreasonable to add this coupling strength to the intralayer couplings. In fact, when we apply the Migdal–Kadanoff renormalization scheme, we can regard this as an additional bond-moving process. If instead one chooses either to add it to the interlayer couplings or to truncate it, the predicted phase diagram will suffer from the problem that the transition temperature is unbounded in the strong-coupling limit. With the above approximations, the decimation equations for the Ising chains become

$$R^2(K) = \frac{1}{4} D - \frac{1}{4} A + \frac{1}{4} C = \frac{1}{4} \ln \frac{e^{2J_r K} \cosh(4K) + 1}{e^{2J_r K} + 1} \tag{56}$$

$$R^2(J_r) = J_r + \frac{1}{4} \ln \frac{e^{2J_r K} \cosh(4K) + 1}{e^{2J_r K} + \cosh(4K)} \tag{57}$$

Following Figs. 3bII–3eII, we now perform a four-step renormalization scheme similar to the one performed in Section 4.1, where we make use of the decimation procedure described above. Since generalizations from $\lambda = 2$ to arbitrary λ have not been possible, we end up with two different equations describing the renormalization of K, corresponding to the two different directions in the planes. By averaging the two equations we get the following fixed-point equation:

$$\frac{1}{4} \ln(\Gamma) + \frac{1}{8} \ln \frac{1 + e^{2J_{r,c} K_c} \sqrt{\Gamma} \cosh(8K_c)}{1 + e^{2J_{r,c} K_c} \sqrt{\Gamma}} - K_c = 0 \tag{58}$$

where

$$\Gamma = \frac{e^{2J_{r,c} K_c} \cosh(4K_c) + 1}{e^{2J_{r,c} K_c} + \cosh(4K_c)} \tag{59}$$

This equation has to be solved numerically in order to obtain K_c as a function of $J_{r,c}$ (see Fig. 1). We notice that $K_c(J_{r,c} = 0) \approx 0.429$ and $K_c(J_{r,c} \to \infty) \approx 0.215$, which means that this approach describes the strong-coupling limit more accurately than the first approach.

It should be noted that Parga and Van Himbergen,[9] who studied finite Ising slabs, including the system of two coupled planes, used the Migdal–Kadanoff approximation scheme in a way that resembles ours. But in contrast to our approach, these authors treated the problem strictly within the Migdal–Kadanoff approximation by incorporating the additional couplings appearing in Eq. (57) in the unrenormalized Hamiltonian and instead of making a four-state procedure they performed a two-state renormalization[21] in which bond moving takes place in one step. In this way they reached a line of fixed points corresponding to nonzero values of the additional couplings except for $J_r = 0$. By projecting this line onto the (K, J_r) plane, they found a phase diagram which involves a serious overestimation of the critical temperature for all values of J_r.

5. MONTE CARLO SIMULATIONS

We have used conventional Monte Carlo computer-simulation techniques[26,27] to investigate the equilibrium behavior of the two coupled Ising planes. Specifically, we have been concerned with the determination of the phase diagram $K_c(J_r)$, the test of the scaling relations suggested in Section 2, and the determination of the behavior of the interlayer correlation function in the vicinity of the critical line $K_c(J_r)$ in the (K, J_r) plane.

The simulations were carried out using a standard Metropolis Monte Carlo method for the grand canonical ensemble (constant values of K and J_r). The elementary excitation was chosen to be a single-spin-flip process (Glauber dynamics). The calculations were performed for a number of different system sizes, $N = 2l^2$, with l ranging from 4 to 48, and with each of the two lattices subjected to periodic boundary conditions. Each simulation was initiated in the completely ordered state and $t_0 = 4 \times 10^3$ Monte Carlo steps per site (MCS) were used for equilibration. Typically, $t_1 = 10^5$ MCS were subsequently used for computing averages. For large values of the relative coupling strength J_r larger values of t_1 were chosen to circumvent the problem of an increase in the relaxation time of dynamic correlations: for $J_r = 7$, 10 we chose $t_1 = 3 \times 10^5$ MCS and for $J_r = 15$ we chose $t_1 = 6 \times 10^5$ MCS.

The basic thermal averages calculated were the size-dependent interlayer correlation function $\rho_{12,l} = \langle \sigma^1 \sigma^2 \rangle_l$, the order parameter $\langle \sigma \rangle_{l,i}$, the isothermal susceptibility $\chi_{T,l,i} = N_i K(\langle \sigma^2 \rangle_{l,i} - \langle \sigma \rangle_{l,i}^2)$, and the 4th-order cumulant $U_{l,i} = 1 - \frac{1}{3} \langle \sigma^4 \rangle_{l,i} / \langle \sigma^2 \rangle_{l,i}^2$. Here the subscript $i = 1, 2$ refers to taking either the total magnetization $(i = 1)$ or the magnetization of one single plane $(i = 2)$ as the order parameter. The choice of the appropriate order parameter depended on the interlayer coupling strength: for low values of J_r, $J_r \leqslant 0.3$, it was found that different ordering of the layers might take place, leading to an unreasonably low value of the total magnetization, thus making the single-plane magnetization the proper choice of the order parameter. For the higher values of J_r, we could obtain better statistics by choosing the total magnetization as the order parameter.

5.1. Phase Diagram

In order to determine the phase diagram, series of simulations were performed for fixed values of J_r in the interval $J_r \in [0, 15]$. The value of $J_r = 15$ corresponds to the largest value of J_r which permitted a reasonably accurate determination of the critical point with the applied method. For each value of J_r an appropriate K interval of length $\Delta_1 K = 0.05$ was

Table I. K_c as a Function of J_r, Estimated from Monte Carlo Data by Binder's Cumulant Method

J_r	0	0.01	0.015	0.02	0.03	0.04	0.06	0.08	0.1	0.15
K_c	0.442	0.435	0.432	0.428	0.420	0.415	0.408	0.401	0.395	0.384
J_r	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.3
K_c	0.376	0.362	0.352	0.343	0.336	0.329	0.323	0.316	0.310	0.299
J_r	1.5	2	2.3	3	4	5	7	10	15	
K_c	0.290	0.277	0.269	0.256	0.244	0.237	0.229	0.223	0.218	

investigated by simulations performed in steps of $\Delta_2 K = 0.005$. This was done for various lattice sizes ranging from $l = 4$ to $l = 32$.

The data thus obtained were used to determine the critical points $K_c(J_r)$ by Binder's cumulant method.[28,29] For fixed J_r, the method was implemented by displaying three different realizations of the ratio $r_{1,2}(K) = U_{l_1,i}(K)/U_{l_2,i}(K)$: $r_{4,32}(K)$, $r_{8,20}(K)$, and $r_{24,12}(K)$, in the investigated K intervals. The existence and location of a common fixed point $r_{1,2}(K_c) = 1$ were tested. Generally, it was found that a fixed point could be found, leading to a determination of K_c with an accuracy of $\delta K_c = 0.001$ (considering only the uncertainty associated with the use of the cumulant method). For $J_r = 15$, however, the determination was less certain, as mentioned above. For this particular value the cumulant ratios were rather fluctuating.

The phase diagram obtained by using the cumulant method is shown in Fig. 1 and the pairs of (J_r, K_c) values are given in Table 1. It is seen from the table that $K_c(J_r)$ decays from a value very close to the transition point of the two-dimensional Ising model at $J_r = 0$ to about half of this value at strong couplings. The value at $J_r = 15$ is a little smaller than expected. For comparison between the theoretically predicted phase diagrams and the phase diagram obtained from Monte Carlo simulations we refer to the discussion.

5.2. Scaling Relations

The Monte Carlo simulations performed in order to test scaling relations put forward in Section 2 were designed to facilitate an investigation of the relation for the shift in critical temperature, Eq. (12), and of the finite-size scaling forms, Eq. (19). To investigate Eq. (12), the data points obtained for the phase diagram could be applied directly. To test Eq. (19), a series of simulations were performed at $K = 0.4407 \approx K_c^{2D}$ for 21 values of J_r in the interval $J_r \in [0{,}01, 1]$.

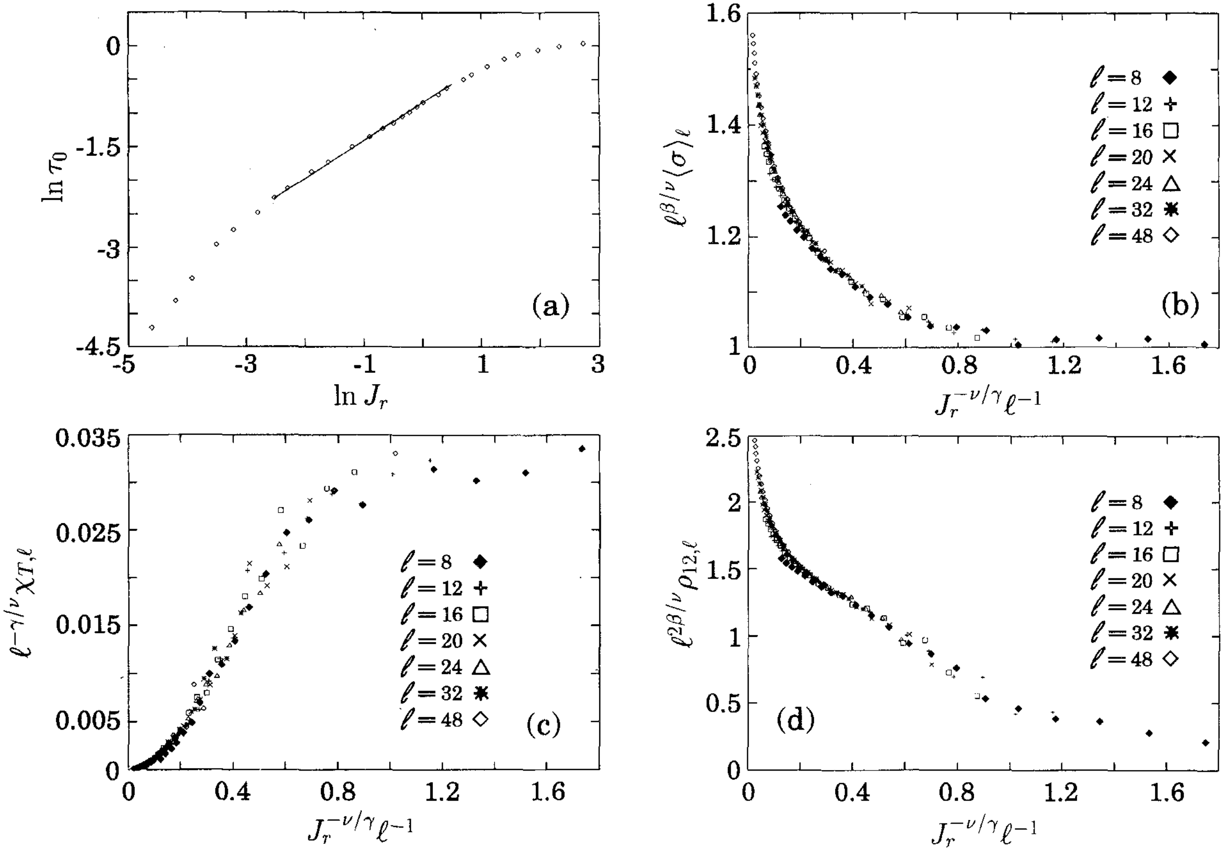

Fig. 4. (a) Test of the scaling relation for the shift in critical temperature, $\ln \tau_0$ vs. $\ln(J_r)$, using MC data obtained for the phase diagram. The proposed linear regime comprises 14 points in the region $\ln J_r \in [-2.5, 0.4]$ or $J_r \in [0.08, 1.5]$. (b–d) Test of the existence of the scaling relations at K_c^{2D} [Eq. (19)] in the form of Eq. (63) (data collapse) using MC data. Relations involving (b) the order parameter, (c) the isothermal susceptibility, and (d) the interlayer correlation function as functions of J_r are tested.

To test the relation Eq. (12), we refer to Fig. 4a, which displays τ_0 vs. J_r in a log–log plot. We have indicated the existence of three different regimes by displaying a particular linear region for $\ln(J_r) \in [-2.5, 0.4]$. In this region the slope is $\alpha = 0.5587$ ($\rho = 0.9997$), where ρ is the correlation coefficient obtained from the linear regression analysis. This result agrees within a few percent with the predicted slope. It seems reasonable to talk about two crossovers, one at high values of J_r leading to a nonscaling region, and one at low values of J_r, to a region with another type of scaling behavior, or possibly nonscaling behavior, as discussed below.

To test the scaling relations in Eq. (19), we have analyzed the data obtained from a simulation at $K = K_c^{2D}$ in terms of the quantities

$$x = \frac{J^{-\nu/\gamma}}{l}, \qquad \Omega_1 = l^{\beta/\nu} \langle \sigma \rangle_{l,2}, \qquad \Omega_2 = l^{-\gamma/\nu} \chi_{T,l,2}, \qquad \Omega_3 = l^{2\beta/\nu} g_{12,l} \qquad (60)$$

which derive from a reformulation of Eq. (19), with x as the basic scaling variable. If the scaling relations are valid, we expect a data collapse in the form of $\Omega_i = f_i(x)$. The individual Ω_i are displayed vs. x in Figs. 4b–4d. Each individual curve was generated for $l = 8$ to $l = 48$ and $J_r \in [0{,}01, 1]$. A cutoff of larger values of J_r was chosen since, for these values, no scaling behavior was expected. One sees from the figures that the data are approximately collapsing in all three cases, that is, universal scaling functions do seem to exist, at least for low values of the scaling variable. The opposite limit corresponds to small lattice sizes and/or weak interlayer coupling strengths. In this limit, more scattering in the data is observed, which may reflect a breakdown of the numerical method applied and/or that the scaling theory does not apply in this limit. If the latter is true, we recover two crossovers.

5.3. Behavior of the Interlayer Correlation Function

The behavior of the interlayer correlation function (or the force) in the (J_r, K) plane was investigated by the following method. From the simulations performed at K_c^{2D} it was concluded that the interlayer correlation function shows weak scaling in the sense that the finite-size correction to the scaling form for the interlayer correlation function [cf. Eq. (19)], which is a function of x, converged quite rapidly, implying that for $J_r > 0.1$ the behavior for different lattices with $l > 24$ was independent of the lattice size. Clearly, this type of behavior cannot be expected in any part of the (K, J_r) plane, especially not in the vicinity of the critical points. However, intuitively it may be expected that for any smaller value of K the finite-size corrections are indeed of reduced importance sufficiently far from the critical point at this particular K value and for sufficiently large l values. We have here decided to extract the qualitative behavior of the interlayer correlation function for the $l=32$ lattice, assuming that the approach to the critical points is well represented on lattices of this size.

A series of simulations was performed on an $l=32$ lattice for four different K values, $K=0.244$, $K=0.310$, $K=0.343$, and $K=0.395$, corresponding to the estimated values of K_c at $J_r=4$, 1, 0.5, and 0.1. For each K value, J_r was allowed to vary in an interval that made the system pass from the disordered state across the critical region into the ordered region. Representative data for the behavior in the vicinity of a critical region are shown in Fig. 2. The critical region is indicated by an asterisk on the curves, corresponding to the respective values of the interlayer correlation function calculated at the estimated transition points. From Fig. 2 we conclude that ρ_{12} is increasing quite rapidly before the critical region is approached, $\rho_{12,c} \approx 0.35$ for $K=0.395$ and $\rho_{12,c} \approx 0.88$ for $K=0.244$. In the log–log plot the variation appears to take place linearly with a slope close to $\alpha=1$. This is independent of the K value. In the critical region we see no abnormal behavior. This may be the result of finite-size effects. On passing the critical line there is a crossover to a region with a marked flattening of the curves which seems to reflect a "saturation effect." No linear behavior resembling the scaling behavior for $t=0$ is apparent, but again this picture may be modified by finite-size effects.

6. DISCUSSION

In the previous sections we have been concerned with various theoretical and numerical approaches to the thermodynamics of two coupled Ising planes. We shall now make some comparisons between the various results obtained.

Approximations to the phase diagram of the system were obtained from five different types of calculation, namely by two types of applications of mean-field theory (MFI and MFII), by two different approximative implementations of the Migdal–Kadanoff scheme (MKI and MKII), and by Monte Carlo (MC) simulations (Fig. 1). We will take the MC result as our reference, since the least problematic approximations were involved in the implementation of this method. Quite generally we find good agreement between MC results and the results from MKII and MFII, although MFII is not valid in the vicinity of K_c^{2D}. The results agree well with data obtained by series expansions for weak couplings.[7] Both MKII and MFII and the MC results verify that $K_c(J_r \to \infty) = \frac{1}{2} K_c(J_r = 0)$. On the other hand, MFI and MKI represent the phase diagram in a less precise way, although MKI predicts the behavior in the weak-coupling limit reasonably well and MFI predicts the doubling of the transition temperature in the strong-coupling limit. All this reflects the expected level of precision of the methods. However, perhaps unexpectedly, the methods do not systematically overestimate the critical temperatures when we disregard MFI.

From the point of view of further refinement of the theoretical methods used in the general description of critical phenomena, our results seem to indicate that it is still worthwhile to try to improve approximate theoretical descriptions of lattice critical phenomena. As we have seen, it is in fact possible to improve traditional mean-field descriptions as well as the original Migdal–Kadanoff RG scheme for the present model system. However, in the case of MFII the improvement was based on the close relation between our model and the two-dimensional Ising model, and MKII suffered from a somewhat *ad hoc* treatment of the new types of bonds appearing in the problem after the decimation. Thus, the proposed types of solutions may be limited to the present model.

From the MC data the scaling relations between J_r and different variables were tested, including the shift in critical temperature τ_0, the order parameter, the isothermal susceptibility, as well as the interlayer correlation function evaluated at the transition point of the two-dimensional Ising model. The common result of the test is that, in an intermediate range of J_r values, the relations do indeed seem to be obeyed. At large J_r values, there seems to be a crossover to a nonscaling region. At small J_r values a rather interesting crossover to a new type of behavior is observed. This is common to all the scaling plots and does not agree with the estimated Ginzburg critical region.[18] Assuming that this shift is not connected with a reduction in numerical precision, this signals a breakdown of the mean-field-based scaling theory and it may be proposed that this is a new scaling regime, where an independent scaling behavior, governed by strong fluctuations near the transition point of the two-dimensional Ising model, is present. We have no theory to support this or even to guide us in the proper way to construct relevant scaling functions, and we have not tried to build up trail scaling functions, but from the individual simulations we found that, e.g., a linear variation of ρ_{12} with J_r seems to be a reasonable assumption. It is interesting to note that this is also the qualitative behavior observed in the disordered phase at higher temperatures.

Another interesting feature of this proposition is that it may imply that critical fluctuations have a quite special influence on two interacting surfaces in the ordered state and close to a critical point. Assuming J_r to be a decreasing function of the distance r, keeping the system at K_c^{2D} and decreasing the distance will be equivalent to passing a "fluctuating region" where the force increases strongly with r, into a "mean-field region" where the force increases less strongly with r. From our MC investigations, it seems that the equivalent of this behavior for $K < K_c^{2D}$ is the increase before and after the passage of the critical line. However, here there is apparently not a crossover from one scaling regime to another, but rather a change from a linear regime, which is predicted by mean-field calculations, to a nonscaling region.

It is clear that further investigation of these phenomena might be of some interest in the further study of forces influenced or governed by fluctuations. However, it is felt that the present model underestimates the potential importance of fluctuations for the effective interactions between surfaces containing many degrees of freedom. Here, we think not only of the sign of the force, but generally of the extent to which the force is affected by the fluctuations in the order parameter distribution, that is, how strongly it couples to the order–disorder transition. It is likely that more complex interlayer couplings, for instance, four-spin couplings known from the Ashkin–Teller model, and the associated richer phase diagram, could add some more interesting features to the study of forces. Clearly, addition of various types of more complex degrees of freedom to the problem would be of particular interest in relation to biological systems. Likewise, addition of a fluctuating medium between the surfaces would mimic the situation in a real bilayer system. A study of this sort could be performed by investigating the effect of a critical wetting layer associated with tricritical behavior.

7. CONCLUSION

In the present paper we have investigated the problem of two ferromagnetically coupled Ising planes with local two-spin interactions by using various numerical and theoretical methods to determine the phase diagram, to investigate the scaling behavior of the model as a function of the interlayer coupling strength, and to make a qualitative study of the interlayer correlation function in the critical regions. The phase diagrams predicted by special implementations of mean-field theory and the Migdal–Kadanoff RG scheme are in good agreement with the phase diagram obtained by MC simulations. All these methods confirm the prediction that the transition temperature in the strong-coupling limit is twice the value obtained for the ordinary Ising model. Mean-field arguments suggest scaling relations involving the shift in critical temperature, the order parameter, the susceptibility, as well as the interlayer correlation function, as functions of the interlayer coupling strength at $K = K_c^{2D}$. The scaling relations are obeyed in an intermediate range of coupling strengths. This opens up the possibility of a crossover to another type of scaling behavior with a more rapid increase in the various variables for very small values of the interlayer coupling strength. Since the interlayer correlation function measures the force between the layers and since the coupling strength is expected to decrease with distance, this situation implies a more rapid increase of the force in the long-distance regime than in the short-distance regime. From the qualitative study at higher temperatures, we observe that an equivalent type of behavior is associated with the disorder–order transition.

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