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Ground-state correlations and finite temperature properties of the transverse Ising model

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Abstract. We present a semi-analytic study of Ising spins on a simple square or cubic lattice coupled to a transverse magnetic field of variable strength. The formal analysis employs correlated basis functions (CBF) theory to investigate the properties of the corresponding N-body ground and excited states. For these states we discuss two different ansaetze of correlated trial wave functions and associated longitudinal and transverse excitation modes. The formalism is then generalized to describe the spin system at nonzero temperatures with the help of a suitable functional approximating the Helmholtz free energy. To test the quality of the functional in a first step we perform numerical calculations within the extended formalism but ignore spatial correlations. Numerical results are reported on the energies of the longitudinal and the transverse excitation modes at zero temperature, on critical data at finite temperatures, and on the optimized spontaneous magnetization as a function of temperature and external field strength.

PACS. 75.10.Jm Quantized spin models – 67.40.Db Quantum statistical theory; ground state, elementary excitations – 05.30.Jp Boson systems – 05.50.+q Lattice theory and statistics (Ising, Potts, etc.)

1 Introduction

Spin-lattice models have traditionally provided insights into magnetic or ferroelectric properties and structural phase transitions of crystalline materials [1–3]. Recent ab-initio studies of the transverse Ising model at zero temperature employing correlated basis functions (CBF) theory [4–6] offer valuable new perspectives on the equilibrium behaviour in a whole range of order-disorder problems [7–10]. Focusing on the transverse Ising model as a prototypical case, reference [7] presents the elements of the CBF approach for lattice systems and reports formal and numerical results on the ground-state energy, the spatial distribution function, the order parameter, and the magnon excitation energies at zero temperature. A special feature of this system is its duality to the vacuum sector of the $Z(2)$ lattice gauge model in two spatial dimensions [8].

The present contribution extends these previous investigations of the properties of the transverse Ising spin lattice in two directions, (i) we modify the variational ground-state of Hartree-Jastrow type adopted in references [7,8] and propose to explore a different kind of spatial correlations with associated spin excitations being transverse to the spontaneous magnetization, (ii) we prepare the ground for a generalization of CBF theory to investigate the spin behaviour of the system at nonzero temperatures, ignoring correlation effects at present.

Section 2 describes the basic relations of a CBF analysis of the correlated ground state of the Ising model and of its transverse and longitudinal spin excitation modes. An extended version of CBF theory applicable at nonzero temperatures is described in Section 3. In a first step of application we present numerical results on critical data of the two-dimensional transverse Ising system at finite temperatures ignoring spatial correlations (Sect. 4). We also discuss possible future studies and improvements.

2 CBF analysis

We consider a system of N Ising spins on N lattice sites in the thermodynamic limit ($N \to \infty$) on a simple square or cubic lattice subject to a transverse external magnetic field. The properties of the ground and excited states are stored in the Hamiltonian [7]

$$\mathcal{H} = \frac{1}{2}\sum_{i,j}^{N} \Delta_{ij}\sigma_i^x\sigma_j^x + \lambda\sum_{i}^{N}(1-\sigma_i^z). \qquad (1)$$

The ith spin, located at the lattice point $\mathbf{r}_i$, is represented by the Pauli vector operator σ_i with spin components σ_i^x, σ_i^y, and σ_i^z in the x, y, and z directions

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having eigenvalues ± 1. The spins interact through their x-components with $\Delta_{ij} \equiv \Delta(\mathbf{r}_i - \mathbf{r}_j) \equiv \Delta(\mathbf{n})$ taking the value -1 for nearest neighbors, $\Delta_{ij} = 2D$ for $i = j$ and $\Delta_{ij} = 0$ otherwise, where D is the spatial dimension ($D = 2$ or 3). The coupling parameter λ measures the strength of the transverse external magnetic field. The system exhibits a homogeneous ferromagnetic phase in the thermodynamic limit ($N \to \infty$, unit lattice constant) at sufficiently small coupling parameters, $0 \leq \lambda \leq \lambda_c$. The ordering is characterized by the spontaneous magnetization M_x in x-direction. At coupling parameters in the range $\lambda_c \leq \lambda \leq \infty$, the spin system is disordered ($M_x \equiv 0$) and paramagnetic.

The energy-expectation value for the exact or approximate N-body state $|\Psi\rangle$ can be expressed by the functional [7,8]

$$E_0 = \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = V + V_M \tag{2}$$

with

$$V = ND(1 - M_x^2)\left[1 + \frac{1}{2D}\sum_{\mathbf{n}} \Delta(\mathbf{n}) G_x(\mathbf{n})\right], \tag{3}$$

$$V_M = N\lambda\Big[1 - (1 - M_x^2)^{\frac{1}{2}}\; n_{12}\Big]. \tag{4}$$

The components V and V_M represent, respectively, the internal interaction energy and the magnetic energy. The quantities appearing in (3) and (4) are the spontaneous magnetization M_x (the order parameter of the ferromagnetic phase) the spin-exchange strength n_{12} and the modified spatial distribution function $G_x(\mathbf{n})$, defined, respectively, by

$$M_x = \frac{\langle\Psi|\sigma_i^x|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \quad n_{12} = \left[(1 - M_x^2)^{-\frac{1}{2}}\right] \frac{\langle\Psi|\sigma_i^z|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{5}$$

and

$$G_x(\mathbf{n}) = (1 - M_x^2)^{-1}\left[g_x(\mathbf{n}) - \delta_{\mathbf{n0}} - (1 - \delta_{\mathbf{n0}})M_x^2\right]. \tag{6}$$

Here, function $G_x(\mathbf{n})$ is the short-ranged part of the spin distribution function

$$g_x(\mathbf{n}) = \frac{\langle\Psi|\sigma_i^x\sigma_j^x|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{7}$$

We may generate excited states with definite momentum $\hbar\mathbf{k}$ by applying an appropriate excitation operator $\rho(\mathbf{k})$ on the trial ground state of the spin system. The associated excitation energy is given by the Feynman formula [11], $\omega(\mathbf{k}) = \epsilon_0(\mathbf{k})/S_0(\mathbf{k})$. The single-particle energy at zero temperature is

$$\varepsilon_0(\mathbf{k}) = \frac{\langle\Psi|[\rho(\mathbf{k}), [\mathcal{H}, \rho(-\mathbf{k})]]|\Psi\rangle}{2N\langle\Psi|\Psi\rangle} \tag{8}$$

and quantity $S_0(\mathbf{k})$ is the corresponding structure function

$$S_0(\mathbf{k}) = \frac{\langle\Psi|\rho(\mathbf{k})\rho(-\mathbf{k})|\Psi\rangle}{N\langle\Psi|\Psi\rangle}. \tag{9}$$

To construct the correlated ground states and excitation operators of interest for an interacting many-body system one has to resort to approximation procedures. The simplest technique is provided by a mean-field assumption that completely ignores correlation effects. In this case the ground states are assumed to be represented by a product of single-particle (single-site) states, i.e., by N-body trial states of Hartree type. In a next step we may employ CBF theory on a variational level to account for correlations induced by the spin-spin interactions. Usually, one begins with an ansatz of Hartree-Jastrow form for the ground state and adopts Feynman's single-particle (single-site) approximation for the excitation operator. The variational principle for the energy is then employed to determine the optimal Hartree-Jastrow wave function. CBF theory may be systematically continued by incorporating triplet correlations in the ground-state trial function and two-body components in the excitation operator. Such calculations have been extensively performed in theoretical and numerical studies of quantum fluids [12] yielding valuable analytic insights and quantitative results of high numerical accuracy.

In a mean-field approximation of CBF theory correlations are neglected, hence function (6) is set zero and the strength factor n_{12} is unity [7,8]. In this case the optimal order parameter is of the analytic form $M_x = \sqrt{1 - (\lambda/2D)^2}$ in the ordered phase, $0 \leq \lambda \leq \lambda_c = 2D$. Further, the associated excitation operator is restricted to a sum of N single-spin operators. To find the best operator of this kind, we choose (i) $\rho(\mathbf{k}) = \rho^x(\mathbf{k})$ or, (ii) $\rho(\mathbf{k}) = \rho^y(\mathbf{k})$ with

$$\rho_{\mathbf{k}}^x = \sum_i^N e^{i\mathbf{k}\cdot\mathbf{r}_i}\sigma_i^x, \tag{10}$$

$$\rho_{\mathbf{k}}^y = \sum_i^N e^{i\mathbf{k}\cdot\mathbf{r}_i}\sigma_i^y, \tag{11}$$

respectively. The excitation operator (10) generates a longitudinal mode with spin component in direction of the spontaneous magnetization M_x, case (ii) describes a spin mode transverse to the external field and to the spontaneous magnetization. Due to the neglect of correlations the structure function $S_0(\mathbf{k})$ is independent of wave number k in both cases (10) and (11). However, the corresponding excitation energies to branch (10) differ from those of case (11). For the longitudinal ansatz (10) we find $\omega(\mathbf{k}) = 2\lambda$ in the paramagnetic phase and $\omega(\mathbf{k}) = 8$ in the ferromagnetic phase ($D = 2$). In contrast, the results for case (ii) are:

$$\omega(\mathbf{k}) = 2(\lambda - \lambda_c) + 2\sum_{\mathbf{n}} \Delta(\mathbf{n})\left(e^{i\mathbf{k}\cdot\mathbf{n}} - 1\right) \tag{12}$$

($D = 2$) for the excitations in the paramagnetic phase, $\lambda > \lambda_c = 4$, and

$$\omega(\mathbf{k}) \;=\; 8\left[1 - \left(\frac{\lambda}{4}\right)^2\right] \;+\; 2\left(\frac{\lambda}{4}\right)^2 \sum_{\mathbf{n}} \Delta(\mathbf{n})\left(e^{i\mathbf{k}\cdot\mathbf{n}} - 1\right), \tag{13}$$

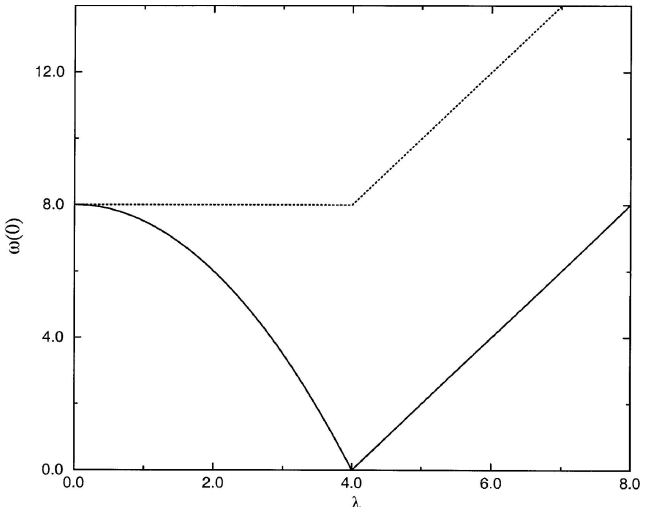

Fig. 1. The energy gap at $\mathbf{k} = 0$ of the longitudinal and the transverse excitation modes of the Ising model on a simple square lattice. The solid line indicates the energy of the transverse excitations given by (12) and (13). The dotted line gives the excitation energy of the longitudinal branch.

for the ordered phase, i.e., for $\lambda < \lambda_c = 4$. Figure 1 displays the energy gap (at $\mathbf{k} = 0$) of both excitation branches. The energy gap of the transverse excitations vanishes at the critical coupling strength.

To include the effects of spatial spin correlations on the ground state of the spin system in cases (i) and (ii), we take, respectively, account of the longitudinal excitations generated by the operator $\rho^x(\mathbf{k})$ or the transverse excitations described by the operator $\rho^y(\mathbf{k})$. This is done by virtually exciting and de-exciting the uncorrelated ground state in analogy to the paired-phonon analysis familiar from CBF theory of liquid helium [13]. In the first case, we therefore begin the CBF analysis with a Hartree-Jastrow ansatz of form [7,8]

$$|\Psi_x\rangle = \exp(M_x U_M + U)|0\rangle, \tag{14}$$

for the correlated ground states. The trial ansatz holds for the ordered phase ($0 \leq M_x \leq 1$) and for the disordered phase ($M_x \equiv 0$). The vacuum reference state $|0\rangle$ is taken as a symmetric product of single-spin eigenstates of the spin components σ_i^z, with eigenvalues $+1$. The pseudopotentials defining the exponent appearing in (14) are

$$U = \frac{1}{2}\sum_{i<j}^{N} u(\mathbf{r}_{ij})\sigma_i^x\sigma_j^x, \tag{15}$$

$$U_M = \sum_{i}^{N} u_1(\mathbf{r}_i)\sigma_i^x + \frac{1}{4}\sum_{i<j}^{N} u_M(\mathbf{r}_{ij})(\sigma_i^x + \sigma_j^x). \tag{16}$$

The trial functions $u_1(\mathbf{r}_i)$, $u(\mathbf{r}_{ij})$, and $u_M(\mathbf{r}_{ij})$ are to be determined by minimizing the associated energy functional of the ground states. For an infinitely extended lattice ($N \to \infty$), function $u_1(\mathbf{r}_i)$ is constant and independent of the lattice site, while $u(\mathbf{r}_{ij})$ and $u_M(\mathbf{r}_{ij})$ depend only on the relative distance $|\mathbf{n}| = |\mathbf{r}_i - \mathbf{r}_j|$. The ansatz, of course, recovers the mean-field approximation by setting the two-body pseudopotentials zero. The real magnon excitations corresponding to ansatz (14−16) are described in Feynman approximation by the excited states $\rho^x(\mathbf{k})|\Psi_x\rangle$. In this case the energy (8) can be cast into the explicit form

$$\varepsilon_0(\mathbf{k}) = 2\lambda n_{12}(1 - M_x^2)^{\frac{1}{2}}. \tag{17}$$

The associated approximate structure function $S_0(\mathbf{k}) = (1 - M_x^2)^{\frac{1}{2}} S(\mathbf{k})$ needed for the evaluation of the energy $\omega(\mathbf{k})$ is given by the Fourier transform

$$S(\mathbf{k}) = 1 + \sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}}\, G_x(\mathbf{n}). \tag{18}$$

References [7,8] provide explicit expressions for the energy functional $E[G_x(\mathbf{n}), M_x; \lambda]$ and for the set of Euler-Lagrange equations which determine the optimal physical quantities of interest. These references also report numerical results on the energy of the correlated ground state represented by the optimal state of type (14) and on the corresponding optimized excitation energies of the longitudinal mode. The numerical results show that the spatial correlations strongly influence the excitation energies of the longitudinal mode. Compared with the mean-field result $\omega(0) = 4D = 8$ at the critical coupling parameter (see Fig. 1) the correlation effects drastically reduce the energy gap by about a factor 3/8. However, we learn from Figure 1 that the energies of the transverse mode in mean-field approximation are still lower than the energies of the longitudinal mode even if spatial correlations in x-direction are taken into account.

It is therefore of interest to investigate also case (ii) where the correlated trial ground states are generated by the pairing of virtual transverse spin excitations and de-excitations with total momentum zero. The associated excited states have then to be constructed with the help of operator (11). The corresponding Hartree-Jastrow ansatz for the correlated trial ground states differs, of course, from ansatz (14−16) and is of form

$$|\Psi\rangle = \exp(M_x U'_M + U')|0\rangle \tag{19}$$

with pseudopotentials of the following form:

$$U' = \frac{1}{2}\sum_{i<j}^{N} u'(\mathbf{r}_{ij})\sigma_i^y\sigma_j^y, \tag{20}$$

$$U'_M = \mathrm{i}\sum_{\mathrm{i}}^{\mathrm{N}} \mathrm{u}'_1(\mathbf{r}_\mathrm{i})\sigma_\mathrm{i}^\mathrm{y}. \tag{21}$$

Note that the pseudopotential U'_M generates a unitary transformation of the reference state $|0\rangle$ in contrast to the operator U_M, equation (16). The optimization of the associated energy functional may be performed in close analogy to the explicit construction of Euler-Lagrange equations for ansatz (14−16) described in detail in references [7,8]. These references also report numerical results on the energies of the optimized ground and excited states

and other physical quantities of interest corresponding to ansatz (14−16). In case (ii) we have derived explicit formal expressions for the energy functional, the Euler-Lagrange equations, and the excitation energies corresponding to ansatz (19−21). However, at present, numerical calculations within CBF theory based on ansatz (19−21) are not yet available.

3 Extension to nonzero temperatures

For quantum fluids such as liquid helium or para-hydrogen CBF theory has been adequately generalized to describe such systems at nonzero temperatures [14,15]. This so-called correlated density matrix (CDM) theory [16–18] begins with a suitable trial ansatz for the correlated N-body density matrix from which one constructs an appropriate approximation for the Helmholtz free energy. Thereupon a minimum principle for the free energy functional is employed. Functional variation then leads to associated Euler-Lagrange equations which determine the optimal density-matrix elements and excitation energies of the correlated Bose fluid.

This CDM theory may be properly adapted for an ab-initio study of spin-lattice systems at finite temperatures. To derive an explicit expression for the free energy one must construct the functionals which represent the internal energy at nonzero temperatures and the entropy. To do so we start from the CBF ground-state functional $E[G_x(\mathbf{n}), M_x; \lambda]$ and proceed – as in the case of quantum fluids – to the more general functional of the internal energy that includes the energy component of real excitations. At present we have explicitly constructed an extension of ansatz (14−16) involving only real and virtual spin excitations of longitudinal type to nonzero temperatures.

For a first and quick numerical test of this approach we specialize the adapted CDM formalism by ignoring the spatial correlations of the Ising model, i.e., we set $G_x(\mathbf{n})$ zero, evaluate the associated Euler-Lagrange equations, and calculate their optimal solutions, in particular, the order parameter M_x as a function of temperature and coupling strength. Under this assumption the internal energy per spin reads

$$E/N = E_0/N + \frac{1}{N}\sum_{\mathbf{k}} \varepsilon(\mathbf{k}) n_1(\mathbf{k}) \tag{22}$$

with functional E_0 being of the same form as for the uncorrelated groundstate and an additional term that represents the energy contributions of the excitations. The single-magnon distribution function $n_1(\mathbf{k})$ of the real excitations is a Bose function of the explicit form

$$n_1(\mathbf{k}) = \frac{1}{(e^{\beta\omega(\mathbf{k})} - 1)} \tag{23}$$

at temperature $T = 1/(\beta k_B)$ and excitation energy $\omega(\mathbf{k})$. The single-particle energy appearing in the sum of (22) is given by

$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k})(1 - M_x^2)^{-1} \exp \frac{2}{N}\sum_{\mathbf{k}} \frac{n_1(\mathbf{k})[1 - n_1(\mathbf{k})]}{S(\mathbf{k})(1 - M_x^2)}. \tag{24}$$

The entropy is represented by the familiar expression for independent bosons,

$$TS_e = \frac{1}{\beta}\sum_{\mathbf{k}} \{[1 + n_1(\mathbf{k})] \ln[1 + n_1(\mathbf{k})] - n_1(\mathbf{k}) \ln n_1(\mathbf{k})\}. \tag{25}$$

The free energy functional is then the difference of the components (22) and (25). It depends on the distribution $n_1(\mathbf{k})$, the spontaneous magnetization M_x, and the external parameter T and λ. Upon variation with respect to the first two variables we obtain the associated Euler-Lagrange equations

$$\frac{1}{N}\frac{\partial F}{\partial n_1(\mathbf{k})} = 0 \tag{26}$$

and

$$\frac{1}{N}\frac{\partial F}{\partial M_x^2} = 0. \tag{27}$$

Equation (27) is only needed for the ordered phase and can be discarded in the paramagnetic regime. The Euler-Lagrange equation (26) yields the optimal spectrum $\omega(\mathbf{k})$ via

$$\varepsilon_0(\mathbf{k}) = S_0(\mathbf{k})\omega(\mathbf{k}) \tanh \frac{1}{2}\beta\omega(\mathbf{k}). \tag{28}$$

Evaluation of the derivative in equation (27) leads to an explicit expression for the optimal spontaneous magnetization,

$$M_x^2 = 1 - \left(\frac{\lambda}{\Lambda}\right)^2, \tag{29}$$

with the Hartree-field

$$\Lambda = \frac{2D}{n_{12}(T)(1 + H_1)}. \tag{30}$$

The component H_1 is defined by

$$H_1 = -2(1 - M_x^2)\frac{\partial}{\partial M_x^2} \ln n_{12}(T). \tag{31}$$

The spin exchange strength $n_{12}(T)$ at a finite temperature T is given by

$$n_{12}(T) = n_{12} \exp\left(-\frac{2}{N}\sum_{\mathbf{k}} \frac{n_1(\mathbf{k})[1 - n_1(\mathbf{k})]}{S(\mathbf{k})(1 - M_x^2)}\right). \tag{32}$$

We may interpret equation (29) as a Hartree equation for the order parameter M_x that characterizes the ferromagnetic phase in the range of coupling parameters

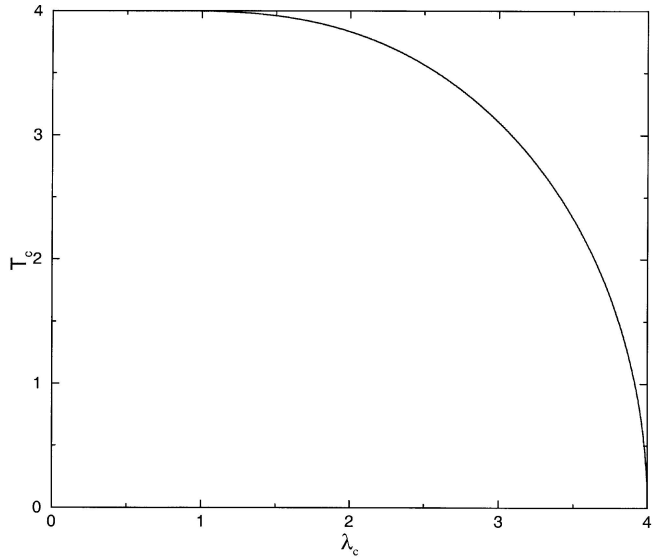

Fig. 2. Mean-field results on the temperature dependence of the critical coupling parameter of the transverse Ising model in the (T_c, λ_c) phase diagram, in two spatial dimensions $(D = 2)$. The phase-boundary curve separates the ferromagnetic region from the paramagnetic phase regime.

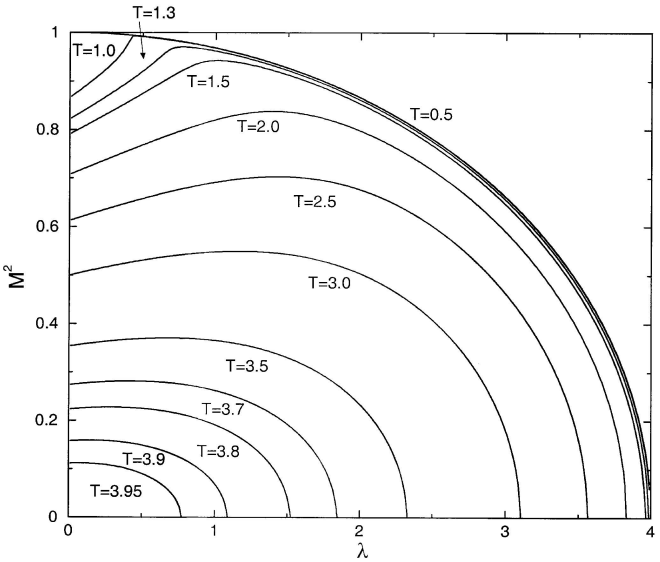

Fig. 3. Mean-field results for the squared optimal order parameter (magnetization M_x) of the ferromagnetic phase of the two dimensional transverse Ising model as function of the coupling strength λ, at various temperatures.

$0 \leq \lambda \leq \lambda_c$. The temperature dependence of the critical coupling parameter λ_c is determined by the simple analytic expression

$$\lambda_c = 2D \tanh \beta\lambda_c. \tag{33}$$

Taking the limit $\beta \to \infty$ we correctly recover the mean-field result $\lambda_c = 4$ at zero temperature. In the limit $\lambda_c \to 0$ equation (33) specializes to $\lambda_c = 2D\beta\lambda_c$, i.e., the critical temperature is $T_c = 2D$. This agrees with Pfeuty's and Elliot's result [19]. Condition (33) recovers also the results of reference [20] derived in standard mean-field theory. Figure 2 displays results on critical data, i.e., on the solutions of equation (33), in the (T, λ) phase diagram $(D = 2)$.

4 Numerical results and conclusions

We have solved the Hartree equation (29) for the optimal spontaneous magnetization M_x of the transverse Ising model on a simple square lattice as a function of the external parameters T and λ. For a numerical comparison we have also repeated standard mean-field calculations [21] on the magnetization M_x. In Figure 3 the results on the squared magnetization M_x^2 derived from (29) and (30) are plotted as a function of the strength parameter at various fixed temperatures in the ferromagnetic domain. The dependence of the squared optimized order parameter on temperature T at various fixed parameter values λ is shown in Figure 4. The order parameter vanishes as the external field approaches the critical strength which increases with decreasing temperature. At $T = 0$ we have the exact result $\lambda_c = 4$. On the other hand, if the temperature approaches the critical value $T = 4$ K the critical

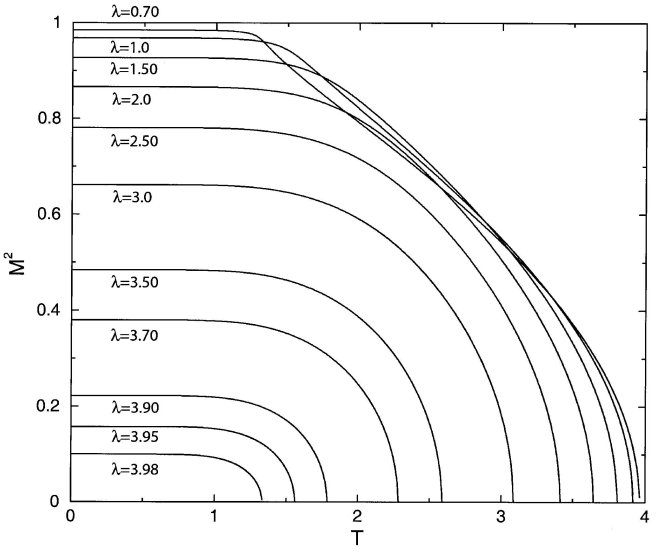

Fig. 4. Mean-field results for the squared optimal order parameter M_x of the ferromagnetic phase of the transverse Ising model on a simple square lattice, at differing strengths λ of the external field.

strength is zero, as it should be. As seen in Figure 3, the magnetization at a given strength λ decreases monotonically with increasing temperature.

By comparing the above results with those of a standard mean-field approach [21] we find, however, some unexpected features. In contrast to the monotonous decrease of the spontaneous magnetization with increasing strength parameter as familiar from standard mean-field results the solutions of (29) and (30) develop a nonmonotonous dependence on the parameter λ for temperatures $T < 3.8$ K and coupling strengths $\lambda < 2$. This feature is particularly

pronounced at relatively low temperatures. This unusual behaviour is also reflected in Figure 4 by the results on quantity M_x^2 for coupling parameters $\lambda < 2$. We interpret this numerical outcome as an artifact of the adopted approximation for the free energy functional at nonzero temperatures and of the corresponding approximate excitation generator $\rho^x(\mathbf{k})$. We believe that ansatz (19−21) in conjunction with the choice $\rho^y(\mathbf{k})$ for the excitation operator will lead to an improved energy functional for the ground state and low lying excitations and, in consequence, also to a more accurate quantitative treatment of correlation effects in the Helmholtz free energy functional of the transverse Ising model within CBF and CDM theory.

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