SEPARABLE MANY-PARTICLE INTERACTIONS AND STABILITY OF CRITICAL BEHAVIOUR

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STELLINGEN

I

Laat $P(\underline{m})$ een analytische, concave functie zijn van n variabelen, en $\underline{V}_N \equiv (V_N^{(1)},\ldots,V_N^{(n)})$ een verzameling operatoren met de eigenschappen:

$\| V_N^{(i)} \| \leqslant M_i < \infty$, als m_i niet-lineair voorkomt in $P(\underline{m})$;

$\| [V_N^{(i)}, V_N^{(j)}] \| \leqslant \sigma(N)$, met $\sigma(N) \to 0$ voor $N \to \infty$.

Dan geldt:

$$\lim_{N\to\infty} \Phi_N(\beta P(\underline{V}_N)) = \inf_{\underline{m}} [\, \beta P(\underline{m}) + \sup_{\underline{h}} \lim_{N\to\infty} \Phi_N(\underline{h}\cdot(\underline{m}-\underline{V}_N)) \,],$$

waarbij $\Phi_N(..) \equiv -N^{-1} \ln \mathrm{Tr} \exp [-N(..)]$,

op voorwaarde dat de limiet in het rechterlid bestaat.

Hoofdstuk II van dit proefschrift.

II

De Van der Waals-Maxwell theorie kan zowel met interacties van het Kac type als met separabele interacties exact gerechtvaardigd worden. De resultaten verkregen met deze laatste wisselwerkingen zijn van toepassing op een grotere klasse van modelsystemen.

Hoofdstuk II van dit proefschrift.
P.C. Hemmer en J.L. Lebowitz in:
"Phase Transitions and Critical Phenomena",
C. Domb and M.S. Green, (eds.), Vol. 5B,
(Academic Press, London, 1976).

III

Het demagnetiserende effect leidt in het speciale geval van een superexchangeantiferromagneet tot kritische-exponentrenormalisatie in de zin van Fisher. In normale magnetische systemen daarentegen geeft dit effect in het algemeen aanleiding tot andere renormalisaties van kritische exponenten.

M.E. Fisher, Phys.Rev. 176 (1968) 257.
Hoofdstuk III en IV van dit proefschrift.

IV

De resultaten van Rajagopal en Ramana voor een ééndimensionaal XY-model met Dzyaloshinsky-Moriya interacties kunnen direct gevonden worden met behulp van een kanonieke transformatie.

A.K. Rajagopal en M.V. Ramana,
J.Phys. C12 (1979) L355.
J.H.H. Perk en H.W. Capel,
Phys.Lett. 58A (1976) 115.

V

De Landau ontwikkeling $g(x,y) = ux^2 + vy^2 + x^4 + px^2y^2 + y^4$ van de vrije energie in de twee ordeparameters x en y kan gebruikt worden bij de analyse van het tetrakritische en bikritische gedrag van een antiferromagneet. Een gedetailleerd onderzoek van deze ontwikkeling in de buurt van p=2 kan ook inzicht geven in meer ingewikkeld kritisch gedrag.

Kao-Chien Liu en M.E. Fisher,
J.Low Temp.Phys. 10 (1973) 655.
L. Bevaart, Proefschrift, (Leiden, 1978).

VI

Het is gewenst de opgegeven temperaturen van de vijf supergeleidende overgangspunten tussen 0,015 K en 0,210 K die sinds kort als vaste punten voor de thermometrie beschikbaar zijn door onafhankelijke metingen te verifiëren.

R.J. Soulen en R.B. Dove,
NBS Spec.Publ. 260-62 (1979).

VII

De combinatie van de transformaties die Jullien en Fields toepassen op de spin $\frac{1}{2}$ XY-keten met alternerende interacties is equivalent met een lineaire transformatie van fermionoperatoren.

R. Jullien en J.N. Fields,
Phys.Lett. 69A (1978) 214.
H.W. Capel en J.H.H. Perk,
Physica 87A (1977) 211.

VIII

Het feit dat de gebruikelijke schaalwetten niet van toepassing zijn voor de kritische exponenten van het sferisch model in vier en meer dimensies kan verklaard worden uit de competitie tussen een singuliere een een reguliere bijdrage tot de (Legendre getransformeerde van de) vrije energie.

C.K. Hall, J.Stat.Phys. 13 (1975) 157.

IX

Om het ijktheoriekarakter van de gecombineerde zwakke en elektromagnetische wisselwerkingen te testen, verdient het bestuderen van de reactie $e^+ + e^- \rightarrow W^+ + W^-$ de voorkeur boven bijvoorbeeld $e^+ + e^- \rightarrow W^+ + e^- + \bar{\nu}$.

X

Het eigenwaardeprobleem van Konno en Wadati, met als speciale keuze voor de potentialen de N-solitonoplossing ten tijde nul, gegeven door

$$-\sigma \frac{d\psi_\sigma}{dx} + \frac{2N}{\cosh 2x} \psi_{-\sigma} = \lambda\psi_\sigma , \quad \sigma = \pm 1,$$

heeft als oplossing de gebonden toestanden

$$\psi_{n,\sigma} = \frac{\text{const.}}{\cosh 2x} \left\{\sigma e^{-\sigma x} P^{n}_{N-1}(\tanh 2x) + (N+n-1)e^{\sigma x} P^{n-1}_{N-1}(\tanh 2x)\right\} ,$$

bij de eigenwaarden $\lambda_n = 2n-1$, $(n=1,\ldots,N)$.

K. Konno en M. Wadati,
Progr.Theor.Phys. 53 (1975) 1652.

XI

Tegen de bewering van Fox dat lange tijdstaarten niets anders zijn dan normeringsconstanten van Gaussische correlaties, zijn bezwaren aan te voeren.

R.F. Fox, Phys.Rep.48 (1978) 179-283, p. 222.

L.W.J. den Ouden, 20 juni 1979.

SEPARABLE MANY-PARTICLE INTERACTIONS
AND
STABILITY OF CRITICAL BEHAVIOUR

Proefschrift

ter verkrijging van de graad van doctor in de wiskunde en natuurwetenschappen aan de Rijksuniversiteit te Leiden, op gezag van de Rector Magnificus Dr. D.J. Kuenen, hoogleraar in de faculteit der wiskunde en natuurwetenschappen, volgens besluit van het college van dekanen te verdedigen op woensdag 20 juni 1979 te klokke 14.15 uur

door

Leendert Willem Jan den Ouden

geboren te Vlaardingen in 1951

Krips Repro - Meppel

Promotor: Dr. H.W. Capel

Aan mijn ouders

CONTENTS

Chapters I and III have appeared before in Physica as
L.W.J. den Ouden, H.W. Capel, J.H.H. Perk and P.A.J. Tindemans, Physica 85A (1976) 51.
H.W. Capel, L.W.J. den Ouden and J.H.H. Perk, Physica 95A (1979) 371.
Parts of chapter II have appeared in
L.W.J. den Ouden, H.W. Capel and J.H.H. Perk, Physica 85A (1976) 425.
(Physica is published by The North-Holland Publishing Co., Amsterdam).

Het in dit proefschrift beschreven werk werd gedaan als deel van het onderzoekprogramma van de Stichting voor Fundamenteel Onderzoek der Materie (F.O.M.) met financiële steun van de Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek (Z.W.O.).

INTRODUCTION AND SUMMARY.

An important problem in statistical mechanics is the evaluation of thermodynamic properties of a many-body system containing a large number (N) of particles on the basis of microscopic interactions between the particles. These properties may depend in a rather sensitive way on the range of interaction between the particles. Extreme examples are interactions of finite range which are zero when the distance between the particles becomes too large, and interactions of the so-called equivalent-neighbour type which do not depend on the distance at all. In many cases it is sufficient to evaluate the free energy per particle in the thermodynamic limit $(N \to \infty)$ from which other thermodynamic quantities can be derived.

A special class of many-particle systems is described by the hamiltonian

$$\mathcal{H}_0 = -\underline{h}^* \cdot \underline{W} = -\sum_{i=1}^{n} h_i^* W_i \ , \qquad (1)$$

in which $\underline{W} = (W_1, \ldots, W_n)$ denotes a finite set of short-range operators, acting on the Hilbert space of the N-particle system, and $\underline{h}^* = (h_1^*, \ldots, h_n^*)$ the set of coupling constants or external fields coupled to the operators $\underline{W}$. For these systems the free energy per particle in the thermodynamic limit exists [1),2)] and is given by

$$f_0(\underline{h}^*) = \lim_{N\to\infty} -(\beta N)^{-1} \ln \mathrm{Tr} \exp[-\beta\mathcal{H}_0] \ , \quad (\beta = 1/kT) \ , \qquad (2)$$

where the trace is taken over the Hilbert space of the N-particle system. A precise definition of short-range operators involves a more detailed description of the process of taking the thermodynamic limit, but all interactions with finite range belong to this category.

An example of eq. (1), with n=2, is given by the hamiltonian

$$\mathcal{H}_0 = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \ , \quad \sigma_i = \pm 1 \ , \qquad (3)$$

which describes an Ising model with interaction $J = h_1^*$ between pairs $\langle ij \rangle$ of neighbouring spins in the presence of an external magnetic field $h = h_2^*$. In this example the operators $W_1 = \sum \sigma_i \sigma_j$ and $W_2 = \sum \sigma_i$ commute, but in general $(W_1, \ldots, W_n)$ in eq. (1) can be quantummechanical operators with nontrivial commutation properties.

An interesting feature of the thermodynamic limit in eq. (2) is that for specific values of the parameters $h_1^*, \ldots, h_n^*$ the function $f_0(\underline{h}^*)$ will exhibit a nonanalytic behaviour corresponding to a phase transition in the system described by $\mathcal{H}_0$. For instance, the Ising ferromagnet described by (3) with J>0 in two and more dimensions shows a discontinuity in the magnetization [1], $m_2 = -\partial f_0/\partial h_2^*$, for sufficiently low temperatures $T<T_c$. At $T=T_c$ there is a critical point at which the second derivatives of f_0 diverge.

An equivalent description of the thermodynamic properties can be given in terms of the Legendre transform $g_0(\underline{m})$ of $f_0(\underline{h}^*)$, which is defined by

$$g_0(\underline{m}) = \sup_{\underline{h}^*} [\,\underline{h}^*\cdot\underline{m} + f_0(\underline{h}^*)\,]\,,\quad \underline{m} = (m_1,\ldots,m_n)\,. \tag{4}$$

Here the supremum exists, since $f_0(\underline{h}^*)$ is a concave function. The more conventional definition of a Legendre transform,

$$g_0(\underline{m}) = \underline{h}^*(\underline{m})\cdot\underline{m} + f_0(\underline{h}^*(\underline{m}))\quad,\quad \underline{m} = -\frac{\partial f_0}{\partial \underline{h}^*}(\underline{h}^*(\underline{m}))\,,$$

leads to some complications in the presence of first-order phase transitions, i.e. if one of the first derivatives of f_0 has a discontinuity. Between the second derivatives of f_0 and g_0 one has the relation $\underline{\underline{\chi}}_0 \equiv -\partial^2 f_0/\partial\underline{h}^*\partial\underline{h}^* = (\partial^2 g_0/\partial\underline{m}\partial\underline{m})^{-1}$, provided that the second derivatives and the inverse matrix exist. One can also obtain $f_0(\underline{h}^*)$ from $g_0(\underline{m})$ using the inverse Legendre transformation [3]

$$f_0(\underline{h}^*) = \inf_{\underline{m}} [\,-\underline{h}\cdot\underline{m} + g_0(\underline{m})\,]\,, \tag{5}$$

where the infimum must exist, since $g_0(\underline{m})$ is convex.

For most systems in two and more dimensions an exact evaluation of $f_0(\underline{h}^*)$ has not been found. An exception is the two-dimensional Ising model in zero field [4]. In other cases approximate methods have been used such as e.g. series expansions [5]. In recent years much know how has been obtained on the behaviour of $f_0(\underline{h}^*)$ in the neighbourhood of a critical point. In the case that $f_0(\underline{h}^*)$ has divergent second derivatives (at $\underline{h}^*=0$), it is appropriate to assume the homogeneity property [6]

$$f_0(b^{a_1} h_1^*,\ldots,b^{a_n} h_n^*) = b f_0(h_1^*,\ldots,h_n^*),\quad \tfrac{1}{2} < a_i < 1\quad, \tag{6}$$

where b is a parameter which tends to zero if we approach the critical point. For a number of cases, explicit values of the critical exponents a_i have been obtained using a renormalization group approach [7].

In this thesis we investigate the more general class of systems described by the hamiltonian

$$\mathcal{H} = -\underline{h}\cdot\underline{W} + NP(\underline{W}/N) \ , \tag{7}$$

in which $\underline{W} = (W_1,\ldots,W_n)$ are short-range operators acting on the Hilbert space of an N-particle system and $P(\underline{W}/N)$ is an analytic function of n variables. The different terms contributing to $NP(\underline{W}/N)$ can be expressed as products of W_i/N and may therefore be called (generalized) separable many-particle interactions.

The type of systems described by the hamiltonian in eq. (7) may be used to study the competition between a short-range operator $-\underline{h}\cdot\underline{W}$ and an additional term $NP(\underline{W}/N)$ of a quite different nature. For example, to the Ising model in eq. (3) we may add the term

$$NP(\underline{W}/N) = \lambda_1 W_1^2/N + \lambda_2 W_2^2/N = \frac{\lambda_1}{N}\sum_{\langle ij\rangle}\sum_{\langle k\ell\rangle}\sigma_i\sigma_j\sigma_k\sigma_\ell + \frac{\lambda_2}{N}\sum_{i,j}\sigma_i\sigma_j \ . \tag{8}$$

The first term in the right-hand side of eq. (8) represents a four-particle interaction of hybrid nature, which is short-range with respect to intra-pair interactions between i and j, and k and ℓ, but long-range between the pairs $\langle ij\rangle$ and $\langle k\ell\rangle$. Such a four-particle interaction can arise as a consequence of spin-phonon couplings in compressible ferromagnets [8),9)]. The second term with λ_2 corresponds to a long-range interaction of the equivalent-neighbour type. Such operators with $\lambda_2>0$ have been used in a classical description of demagnetizing effects [10)]. Exact results have been obtained by Oitmaa and Barber [9)] for the two-dimensional Ising model with $\lambda_2=0$, $\lambda_1<0$, and by Hall and Stell [11)] for the two-dimensional superexchange antiferromagnet [12)] with $\lambda_1=0$, $\lambda_2<0$.

In this thesis we derive a general result for the free energy per particle

$$f(\underline{h}) = \lim_{N\to\infty} -(\beta N)^{-1} \ln \mathrm{Tr} \exp[-\beta\mathcal{H}] \ , \tag{9}$$

corresponding to the hamiltonian (7), viz.

$$f(\underline{h}) = \inf_{\underline{m}} [-\underline{h}\cdot\underline{m} + g_0(\underline{m}) + P(\underline{m})] \ . \tag{10}$$

Here $g_0(\underline{m})$ is the Legendre transform of the free energy $f_0(\underline{h}^*)$, cf. (2) and (4), for a reference system described by the hamiltonian (1), which is a linear combination of (quantummechanical) short-range operators. Note that the reference system itself may exhibit phase transitions.

For the special case that all operators $\underline{W}$ in the hamiltonian (7) are sums of one-particle operators, such as e.g. $W_2 = \sum \sigma_i$ in the Ising model (3), eq. (10) provides a general description of the free energy in systems with long-range interactions of the equivalent-neighbour type. This problem has been treated in a fairly general way in ref. 13. Special examples include e.g. the Husimi-Temperley model, see ref. 14, the Ising chain with equivalent-neighbour interactions [15] and the exact evaluation [16),17] of the free energy starting from the reduced hamiltonian in the BCS-theory of superconductivity [18]. Also, relations which are similar to special cases of eq. (10) have been derived in models with interactions of the Kac type, (i.e. in d dimensions the interaction between two particles at distance r behaves roughly like $\gamma^d \exp(-\gamma r)$), in the limit $\gamma \downarrow 0$, see e.g. refs. 19,20.

As an application of eq. (10) we investigate in this thesis the free energy $f(\underline{h})$ in a neighbourhood of a critical point of the short-range reference system. Starting from a reference free energy with divergent second derivatives $\underline{\underline{\chi}}_0$ it is easy to see that the critical properties of the free energy (10) will be affected in a nontrivial way by a perturbation of the type $P(\underline{m})$. In fact, the second derivatives of g_0 will then tend to zero if we approach the critical point, (since $\partial^2 g_0/\partial\underline{m}\partial\underline{m} = \underline{\underline{\chi}}_0^{-1}$). If the function $P(\underline{m})$ contains a nonvanishing quadratic part, then this quadratic part will be dominant in a neighbourhood of the critical point.

In particular, if $P(\underline{m})$ is strongly convex, the value $\underline{m}$ at which the infimum in (10) occurs, is uniquely determined for each value of the coupling constants or external fields $\underline{h}$. As a consequence there can be no first-order transitions, and the susceptibility matrix $\underline{\underline{\chi}} \equiv -\partial^2 f/\partial\underline{h}\partial\underline{h}$ is finite, also at the original critical point of $g_0(\underline{m})$, (since $\underline{\underline{\chi}}^{-1} = \partial^2 g_0/\partial\underline{m}\partial\underline{m} + \partial^2 P/\partial\underline{m}\partial\underline{m}$). Also, a more detailed analysis, using the homogeneity property (6) for the reference system, leads to various regimes of critical-exponent renormalization. A special example is the Fisher critical-exponent renormalization [21], but many other renormalizations are possible.

On the other hand, if $P(\underline{m})$ is strongly concave in one direction, i.e. $\underline{e} \cdot (\partial^2 P/\partial\underline{m}\partial\underline{m}) \cdot \underline{e}$ is negative for a certain unit vector $\underline{e} = (e_1, \ldots, e_n)$, then the function between brackets in eq. (10) cannot be convex in a neighbourhood of the original critical point ($\underline{m}$=0) and the infimum cannot occur in this neighbourhood. This implies that there will be first-order transitions which may terminate in a classical critical point.

These two cases may serve as an illustration that the critical properties of a short-range system with divergent susceptibilities are unstable under small perturbations of the type $NP(\underline{W}/N)$ as in eq. (7). The actual treatment of the problem, however, is more complicated. First of all the assumption (6) for the free energy f_0 is much too restrictive. In fact, starting from n variables $h_1^*,\ldots,h_n^*$ one may introduce r variables $\varepsilon_1^*,\ldots,\varepsilon_r^*$ which affect the critical properties of the reference system and which are therefore called relevant variables, and n-r variables $\zeta_1^*,\ldots,\zeta_{n-r}^*$ which do not and may be called irrelevant. In connection with the free energy (10) one might then raise the question to which extent the "irrelevant" variables may be eliminated. This is not a trivial problem and will be taken into account in this thesis. Secondly, the free energy f_0 may have finite second derivatives with a cusp-like behaviour, i.e. an infinite derivative at the critical point. Finally, expressions like (10), but with a more general function $P(\underline{m},\underline{h})$ depending on the fields $\underline{h}$ as well, can be derived in systems with constraints on first derivatives of the free energy, and will also be taken into account. Systems with one constraint on a hidden variable have been treated from a general point of view by Fisher [21] and later on by Imry et.al. [22]. Important physical examples are e.g. the Baker-Essam model for compressible Ising ferromagnets [23], and the Syozi-models with bond-annealed [24] and site-annealed [25] impurities.

In chapters I and II we present a rigorous derivation of eq. (10) for the class of systems described by the hamiltonian (7). The proof is based on the decomposition of the function $P(\underline{m})$ into a concave part $Q(\underline{m})$ and a convex part $R(\underline{m})$. For concave $P(\underline{m}) = Q(\underline{m})$ eq. (10) can be proved using a generalization of a fundamental theorem due to Bogoliubov Jr. [17]. A simplified proof of this theorem in the case of a quadratic function $P(\underline{m}) = -\Lambda\underline{m}^2$, $\Lambda > 0$, is given in chapter I together with an evaluation of f in a special case with operators $\underline{W}$ which are sums of one-particle operators. The proof of eq. (10) for general short-range operators involves some subtle considerations on the process of taking the thermodynamic limit and is presented in chapter II.

In chapter III we give a rather general treatment on the critical properties of the free energy (10) in the neighbourhood of a critical point of the short-range reference system. The conclusions are made more explicit in chapter IV for the special case $P(\underline{m}) = P(m_1,m_2) = \frac{1}{2}\Pi_1 m_1^2 + \frac{1}{2}\Pi_2 m_2^2$, using the linear model introduced by Schofield [26] to describe the reference free energy in the neighbourhood of a simple critical point with two relevant variables and divergent second derivatives such as e.g. the critical point of the three-dimensional Ising model.

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CHAPTER I

SYSTEMS WITH SEPARABLE MANY-PARTICLE INTERACTIONS. I

1. Introduction

In recent years systems described by hamiltonians in which the interaction terms are essentially of a long-range nature have received a great deal of interest. In many cases the free energy per particle in the thermodynamic limit can be evaluated exactly and the result is usually of the molecular-field type. In connection with this two classes of long-range interactions have been investigated in detail.

For a number of models the free energy per particle has been evaluated in the presence of interactions of the so-called Kac type[1]), for which the coupling between particles located at $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ decreases roughly like $-\gamma^d \exp(-\gamma\,|\boldsymbol{r}_i - \boldsymbol{r}_j|)$, d being the dimensionality, for sufficiently large values of $|\boldsymbol{r}_i - \boldsymbol{r}_j|$. An exact result for the free energy per particle can be obtained in the so-called Van der Waals limit, *i.e.* the limit $\gamma \downarrow 0$ after taking the thermodynamic limit. The one-dimensional classical version has been treated by Kac, Uhlenbeck and Hemmer[2]). Extensions to more dimensions and quantum-mechanical situations have been dealt with by Van Kampen[3]), Lebowitz and Penrose[4]) and Lieb[5]). Ising systems with this type of interactions have been investigated by Baker[6]), Siegert and Vezzetti[7]). Recently Thompson and Silver[8]) and Pearce and Thompson[9]) treated the

n-vector spin model and the anisotropic Heisenberg model with this type of interactions.

A second class of models with long-range interactions are those with interactions of the separable type, by which we mean that the interaction $V(k, l)$ between particles k and l can be written as a product of an operator $V(k)$ acting on the Hilbert space of particle k and an operator $V(l)$, *i.e.* $V(k, l) = V(k)\,V(l)$. This class includes models with so-called equivalent-neighbour interactions, in which the coupling between two particles does not depend on the distance between the particles. A lattice-gas model with this type of interactions has been introduced and investigated by Husimi[10]), Temperley[11]) and Katsura[12]). An Ising version equivalent to this lattice-gas model has been studied in detail by Mühlschlegel and Zittartz[13]). The evaluation of the free energy in these cases is straightforward since the operators in the hamiltonian commute. In the presence of noncommuting operators, however, the situation is more difficult. Starting from the so-called reduced hamiltonian in the BCS theory of superconductivity[14]) Mühlschlegel[15]) proved, on the basis of the Laplace method, that the free energy derived by BCS[14]) is exact in the thermodynamic limit. (A different approach to this problem had been discussed earlier by Bogoliubov, Zubarev and Tserkovnikov[16]).)

Recently two of us investigated a rather general class of systems with separable interactions[17-19]). In refs. 18 and 19 we considered a hamiltonian including a one-particle operator $\sum_{k=1}^{N} T(k)$, N being the number of particles, and a finite number p of interactions of the separable type, *i.e.* $\sum_{i=1}^{p} \sum_{k,l=1}^{N} \Lambda_i V^{(i)}(k)\, V^{(i)}(l)$. Here the interaction parameters Λ_i can be positive as well as negative. For negative Λ_i, the interaction term is negative definite and may be called a separable interaction of the "ferromagnetic" type. For positive Λ_i we have an "antiferromagnetic" separable interaction. The free energy could be evaluated in terms of a "trial" hamiltonian which is a linear combination of the sums $\sum T(k)$, $\sum V^{(i)}(k)$ mentioned above.

In ref. 19 a rather simple proof was given based on a fundamental theorem due to Bogoliubov Jr.[20,21]) in the presence of only ferromagnetic interactions. This theorem applies to hamiltonians of the form $\mathscr{H}_N = N\{T - (V^{(1)^2} + \cdots + V^{(p)^2})\}$, where the operators $T, V^{(1)}, \ldots, V^{(p)}$ and the commutators $N[T, V^{(k)}]$, $N[V^{(k)}, V^{(l)}]$ $(k, l = 1, \ldots, p)$ have norms which are uniformly bounded in N.

According to this theorem the free energy per particle in the thermodynamic limit can be expressed in terms of the free energy of a trial hamiltonian which is linear in the operators T and V. The generalization of this theorem to antiferromagnetic operators is not correct, *cf.* refs. 19 and 21. An application to spin systems has been discussed by Brankov *et al.*[22]). Very recently, Bogoliubov Jr. and Plechko[23]) and also Brankov *et al.*[24]) proved that the solution of the Dicke-maser model by Hepp and Lieb[25]) can be understood in terms of a generalization of this theorem.

The fundamental theorem can be proved by deriving an upper and a lower bound for the free energy per particle, which turn out to be equal in the thermodynamic limit. The upper bound is a straightforward application of the Bogoliubov–Peierls inequality[26]). Two different approaches have been developed for the lower bound. Using some subtle inequalities and an ingenious integration over complex variables Bogoliubov Jr.[20,21]) proved that the difference between the free energy per particle of the hamiltonian and the trial hamiltonian is bounded from below by a term which is of the order $N^{-2/5}$. In ref. 19 the lower bound was derived using an integral representation for the partition function $Z = \int e^{-NG}$ and Laplace's method. The correction due to the second derivatives of G at the absolute minimum was shown to be proportional to N^{-1} except at those points where a second-order transition occurs. In ref. 19 use has been made of the assumption that the Hilbert space of particle k is finite-dimensional. This assumption is not essential in the approach of refs. 20 and 21.

Finally it may be mentioned that several systems with equivalent-neighbour interactions have been treated from a C*-algebra point of view, *cf. e.g.* ref. 27.

So far we have restricted ourselves to systems with two-body interactions. Recently models with four-body interactions and also more general interactions have been investigated in the literature. Four-particle interactions can be of importance in situations, in which the exchange coupling depends on the distance between the atoms[28]). Systems with such interactions have been treated *e.g.* in the molecular-field approximation, see Lee and Bolton[28]), Matsudaira[29]) or on the basis of an exactly soluble model with separable interactions, Bowers/McKerrell[30,31]), Thompson[32]), Oitmaa and Barber[33]), Lapushkin *et al.*[34]). In refs. 28–34, the operators in the hamiltonian commute.

In the present paper we consider the class of systems described by the hamiltonian

$$\mathscr{H}_N = N\{T_N + P(V_N)\}, \tag{1.1}$$

where T_N and V_N are "weighted" sums of bounded hermitean one-particle operators, *i.e.*

$$T_N = N^{-1}\sum_{k=1}^{N} T(k), \qquad V_N = N^{-1}\sum_{k=1}^{N} V(k) \tag{1.2}$$

and where P is a polynomial in the operator V_N of the type

$$P(V_N) = \sum_{q\geq 2}^{M} p_q V_N^q. \tag{1.3}$$

Note that in eq. (1.3) we can restrict ourselves to terms with $q \geq 2$. Also in general the operators T_N and V_N do not commute. We shall prove that the free energy per particle in the thermodynamic limit‡

$$f[\mathscr{H}] \equiv \lim_{N\to\infty} f_N[\mathscr{H}_N] \equiv \lim_{N\to\infty} -(\beta N)^{-1} \ln \operatorname{Tr} e^{-\beta \mathscr{H}_N} \tag{1.4}$$

is given by

$$f[\mathscr{H}] = \min_{\xi \in \mathscr{M}} \lim_{N\to\infty} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)] \tag{1.5}$$

where the trial hamiltonian $\mathscr{H}_{\mathrm{tr},N}(\xi)$ is defined by

$$\mathscr{H}_{\mathrm{tr},N}(\xi) = N\{T_N + P(\xi) + P'(\xi)(V_N - \xi)\}. \tag{1.6}$$

The minimum in the right-hand side of (1.5) must be taken over the set of values $\xi \in \mathscr{M}$ satisfying the molecular-field equation

$$\xi = \lim_{N\to\infty} \langle V_N \rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)}, \tag{1.7}$$

where $\langle B \rangle_A$, for arbitrary hermitean operators A and B, is the average of B with respect to A, *i.e.*

$$\langle B \rangle_A \equiv \operatorname{Tr} B\, e^{-\beta A} (\operatorname{Tr} e^{-\beta A})^{-1}. \tag{1.8}$$

Note that in general the minimum over the set $\xi \in \mathscr{M}$ does not correspond to the absolute minimum of $f[\mathscr{H}_{\mathrm{tr}}(\xi)]$. An example will be given in section 4.

In the proof of (1.5) use will be made of the general theorem of Bogoliubov Jr.[20,21]) mentioned above for ferromagnetic quadratic interactions. A simplified proof of this theorem will be given in section 2. Furthermore, we shall use a weaker assumption on $[T_N, V_N]$ than refs. 20 and 21. In section 3 we prove eq. (1.5) using the mean value theorem and general properties like the concavity of the free energy. In section 4 we deal with a model treated in ref. 32. Although this model is of a rather trivial nature, since the operators commute, it may be of interest within the context of the present treatment.

Finally it may be mentioned that the present treatment may be generalized to include a much larger class of hamiltonians. In particular the polynomial $P(V_N)$ may be replaced by an analytic function of a finite number of operators $V^{(1)}$, $V^{(2)}, \ldots, V^{(n)}$ and the operators in eq. (1.2) may be replaced by arbitrary short-range interactions. In the present paper we restrict ourselves to the hamiltonian (1.1), since the proof contains the essential features of the proof in the more general case. The generalizations mentioned above lead to some complications of a more technical nature and will be treated in a separate paper[35]).

‡ The symbol $f[\mathscr{H}]$ in eq. (1.4) has been introduced as a short-hand notation for the thermodynamic limit of $f_N[\mathscr{H}_N]$.

2. Fundamental theorem for ferromagnetic interactions

In this section we give a simplified proof of the theorem due to Bogoliubov Jr.[20,21].

Theorem: Consider a system described by the hamiltonian

$$\mathscr{H}_N = N(T_N - \Lambda V_N^2), \tag{2.1}$$

where $\Lambda > 0$ and T_N and V_N are bounded hermitean operators with a commutator which tends to zero in the thermodynamic limit, *i.e.*

$$\begin{aligned} &\|T_N\| \le M_T, \qquad \|V_N\| \le M_V, \\ &\|[T_N, V_N]\| = \varepsilon(N) \to 0, \qquad \text{if} \qquad N \to \infty. \end{aligned} \tag{2.2}$$

Then the free energy per particle in the thermodynamic limit is given by

$$f \equiv \lim_{N\to\infty} f_N[\mathscr{H}_N] = \min_{\xi} \lim_{N\to\infty} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)], \tag{2.3}$$

where the trial hamiltonian $\mathscr{H}_{\mathrm{tr},N}(\xi)$ is defined by

$$\mathscr{H}_{\mathrm{tr},N}(\xi) = N(T_N + \Lambda\xi^2 - 2\Lambda\xi V_N) \tag{2.4}$$

and where it is understood that the right-hand side of (2.3) converges in the thermodynamic limit uniformly on the interval $|\xi| \le M_V$ on which (2.3) assumes its absolute minimum.

Remark: At first sight, the theorem in refs. 20 and 21 seems to be a generalization of the present formulation, including a finite number of non-hermitean operators V. However, this generalization can be proved directly applying the present theorem successively. Note that we use a weaker condition on the commutators of the operators T_N and V_N than refs. 20 and 21.

Proof: We prove eq. (2.3) by deriving an upper and a lower bound.

Upper bound: The upper bound is almost trivial using the Bogoliubov–Peierls inequality[26])

$$F[A + B] \le F[A] + \langle B \rangle_A, \tag{2.5}$$

valid for arbitrary hermitean operators A and B, where $F[C] = -\beta^{-1} \ln \mathrm{Tr}\, e^{-\beta C}$ is the free energy corresponding to the hamiltonian C. For the free energy per particle we have

$$f_N[\mathscr{H}_N] - f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)]$$
$$\leq N^{-1}\langle \mathscr{H}_N - \mathscr{H}_{\mathrm{tr},N}(\xi)\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)} = -\Lambda\,\langle (V_N - \xi)^2\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)}$$
$$= -\Lambda\,\langle (V_N - \langle V_N\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)})^2\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)} - \Lambda\,(\langle V_N\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)} - \xi)^2 \leq 0. \qquad (2.6)$$

Note that the difference in eq. (2.6) can only be zero, if

$$\xi = \langle V_N\rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)}. \qquad (2.7)$$

Lower bound: In the derivation of the lower bound we follow essentially the procedure used by Bogoliubov Jr.[20,21]. In order to derive an upper bound for the quantity

$$a_N \equiv a_N(0) = \min_{\xi} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)] - f_N[\mathscr{H}_N], \qquad (2.8)$$

we define the function

$$a_N(\nu) \equiv \min_{\xi} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi,\nu)] - f_N[\mathscr{H}_N(\nu)], \qquad (2.9)$$

where

$$\mathscr{H}_N(\nu) \equiv \mathscr{H}_N - N\nu V_N, \qquad (2.10a)$$

$$\mathscr{H}_{\mathrm{tr},N}(\xi,\nu) \equiv \mathscr{H}_{\mathrm{tr},N}(\xi) - N\nu V_N \qquad (2.10b)$$

for real values of ν⁺.

From the mean value theorem, we have

$$l^{-1}\int_0^l \mathrm{d}\nu\, a_N(\nu) = a_N(\nu_0) \qquad (2.11)$$

for arbitrary values $l > 0$ and some value ν_0 satisfying $0 \leq \nu_0 \leq l$. Since for both hamiltonians $\mathscr{H}_{\mathrm{tr},N}(\xi,\nu)$ and $\mathscr{H}_N(\nu)$

$$\left|\frac{\partial f_N}{\partial \nu}\right| = |\langle V_N\rangle| \leq \|V_N\| \leq M_V, \qquad (2.12)$$

it follows that

$$|a_N(\nu_0) - a_N(0)| \leq 2M_V\nu_0 \qquad (2.13)$$

⁺ In refs. 20 and 21 also complex values of ν are taken into consideration. This is not necessary in the context of the present treatment, since V_N is hermitian.

and

$$a_N(0) \leq 2M_V l + l^{-1} \int_0^l \mathrm{d}\nu \, a_N(\nu). \tag{2.14}$$

Using again eq. (2.5), we have

$$\begin{aligned} a_N(\nu) &\leq \min_\xi N^{-1} \langle \mathscr{H}_{\mathrm{tr},N}(\xi,\nu) - \mathscr{H}_N(\nu)\rangle_{\mathscr{H}_N(\nu)} \\ &= \Lambda \, \langle (V_N - \langle V_N\rangle_{\mathscr{H}_N(\nu)})^2\rangle_{\mathscr{H}_N(\nu)} + \min_\xi \Lambda \, (\langle V_N\rangle_{\mathscr{H}_N(\nu)} - \xi)^2 \\ &= \Lambda \, \langle (V_N - \langle V_N\rangle_{\mathscr{H}_N(\nu)})^2\rangle_{\mathscr{H}_N(\nu)}. \end{aligned} \tag{2.15}$$

The right-hand side of (2.15) can be expressed in terms of the second derivative of the free energy f_N per particle corresponding to the hamiltonian $\mathscr{H}_N(\nu)$, *i.e.*

$$\begin{aligned} -N^{-1} \frac{\partial^2 f_N}{\partial \nu^2} &\equiv -N^{-1} \frac{\partial^2}{\partial \nu^2} f_N[\mathscr{H}_N(\nu)] \\ &= \int_0^\beta \mathrm{d}\tau \, \langle (V_N(\tau) - \langle V_N\rangle_{\mathscr{H}_N(\nu)}) (V_N - \langle V_N\rangle_{\mathscr{H}_N(\nu)})\rangle_{\mathscr{H}_N(\nu)}, \end{aligned} \tag{2.16}$$

where use has been made of the notation

$$A(\tau) = \mathrm{e}^{\tau \mathscr{H}_N(\nu)} A \, \mathrm{e}^{-\tau \mathscr{H}_N(\nu)}. \tag{2.17}$$

In order to estimate the right-hand side of eq. (2.15) we use the inequality[*]

$$\begin{aligned} \beta^{-1} \int_0^\beta \mathrm{d}\tau \, \langle A(\tau) A\rangle_{\mathscr{H}} \leq \langle A^2\rangle_{\mathscr{H}} &\leq \beta^{-1} \int_0^\beta \mathrm{d}\tau \, \langle A(\tau) A\rangle_{\mathscr{H}} \\ &+ \tfrac{1}{2} \{\langle [A, [\mathscr{H}, A]]\rangle_{\mathscr{H}}\}^{\frac{1}{2}} \left\{\int_0^\beta \mathrm{d}\tau \, \langle A(\tau) A\rangle_{\mathscr{H}}\right\}^{\frac{1}{2}}, \end{aligned} \tag{2.18}$$

where $A(\tau) = \mathrm{e}^{\tau\mathscr{H}} A \, \mathrm{e}^{-\tau\mathscr{H}}$, for arbitrary hermitean operators A and $\mathscr{H}$, *cf.* eq. (2.10) of ref. 36. Note that in eq. (2.18) the integrals over τ and the average value of $[A, [\mathscr{H}, A]]$ are positive. The inequality can be proved using a representation, in which $\mathscr{H}$ is diagonal. For details we refer to ref. 36.

Applying (2.18) to the right-hand side of (2.15), we have in view of (2.2)

$$a_N(\nu) \leq \Lambda \left\{ -(\beta N)^{-1} \frac{\partial^2 f_N}{\partial \nu^2} + (\tfrac{1}{2} M_V \varepsilon(N))^{\frac{1}{2}} \left(-\frac{\partial^2 f_N}{\partial \nu^2} \right)^{\frac{1}{2}} \right\}. \tag{2.19}$$

[*] In refs. 20 and 21 Bogoliubov Jr. uses a slightly different inequality with exponents $\frac{1}{3}$ and $\frac{2}{3}$ rather than $\frac{1}{2}$, *cf.* also ref. 22.

Using (2.14), (2.19) and the Schwarz-inequality for integrals, we have

$$a_N(0) \leq 2M_V l + \Lambda(\beta N l)^{-1} \int_0^l \mathrm{d}\nu \left(-\frac{\partial^2 f_N}{\partial \nu^2}\right)$$

$$+ \Lambda l^{-\frac{1}{2}} (\tfrac{1}{2} M_V \varepsilon(N))^{\frac{1}{2}} \left\{\int_0^l \mathrm{d}\nu \left(-\frac{\partial^2 f_N}{\partial \nu^2}\right)\right\}^{\frac{1}{2}}. \tag{2.20}$$

From (2.12) and (2.20) it follows that

$$a_N(0) \leq 2M_V \{l + \Lambda(\beta N l)^{-1} + \tfrac{1}{2}\Lambda l^{-\frac{1}{2}} \varepsilon(N)^{\frac{1}{2}}\}. \tag{2.21}$$

Eq. (2.21) holds for arbitrary positive values of l. We may now choose l so that*

$$l = \max\{(\varepsilon(N))^{1/3}, N^{-\frac{1}{2}}\} \equiv l(N) \to 0, \qquad \text{for} \quad N \to \infty. \tag{2.22}$$

Then

$$\min_{\xi} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)] - f_N[\mathscr{H}_N] \leq 2M_V(1 + \Lambda\beta^{-1} + \tfrac{1}{2}\Lambda)\, l(N), \tag{2.23}$$

which provides the desired lower bound.

Eq. (2.3) is now obvious from (2.6) and (2.23) assuming that $\lim_{N\to\infty} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)]$ exists uniformly for all values of ξ with $|\xi| \leq M_V$. Note in connection with this that the minimum of $\lim_{N\to\infty} f_N[\mathscr{H}_{\mathrm{tr},N}(\xi)]$, which is a continuous function of ξ, should occur under the condition, *cf.* (2.7),

$$\xi = \lim_{N\to\infty} \langle V_N \rangle_{\mathscr{H}_{\mathrm{tr},N}(\xi)}, \tag{2.24}$$

so that $|\xi| \leq M_V$ at the minimum. Hence, the fundamental theorem has been proved.

3. Evaluation of the free energy

In this section we shall prove eq. (1.4) in six subsequent steps.

(i) *Application of the fundamental theorem:* First we note that the hamiltonian (1.1) may be treated using the theorem of the preceding section. For this purpose we subtract a ferromagnetic operator $-\Lambda V_N^2$ ($\Lambda > 0$) from the operator $P(V_N)$, *i.e.*

$$\mathscr{H}_N = N(T_N' - \Lambda V_N^2), \tag{3.1}$$

* The treatment in refs. 20 and 21 would lead to an exponent $\frac{2}{7}$ rather than $\frac{1}{3}$ in eq. (2.22).

where

$$T'_N \equiv T_N + P(V_N) + \Lambda V_N^2. \tag{3.2}$$

In eqs. (3.1) and (3.2) we have a parameter Λ at our disposal, so that by choosing it in an appropriate way we may arrive at a lower bound for the free energy per particle.

Obviously, the operators T'_N and V_N satisfy the conditions (2.2), since in view of (1.2) the commutator $[T'_N, V_N]$ is an operator of the order N^{-1}. Applying (2.3) we have*

$$f[\mathscr{H}] = \min_{\xi} \lim_{N\to\infty} f_N[\mathscr{H}_1(\xi)], \tag{3.3}$$

where

$$\mathscr{H}_1(\xi) = N\{(T + P(V) + \Lambda V^2) + \Lambda\xi^2 - 2\Lambda\xi V\}. \tag{3.4}$$

In eq. (3.4) and also in most of the following formulae the subscripts N labeling the operators have been omitted for convenience.

We shall compare $\mathscr{H}_1(\xi)$ with a trial hamiltonian $\mathscr{H}_2(\xi \mid \eta)$ which is linear in the operator V, *i.e.*

$$\mathscr{H}_2(\xi \mid \eta) = N\{T + P(\eta) + P'(\eta)(V - \eta) + \Lambda(\xi^2 - \eta^2) - 2\Lambda(\xi - \eta)V\}. \tag{3.5}$$

In the derivation of upper and lower bounds for $f[\mathscr{H}_1(\xi)]$ use will be made of a simple lemma.

(ii) *Lemma:* Let $P(V)$ be a polynomial in the bounded hermitean operator V and let M be a constant such that $M > \|V\|$, then for all values η satisfying $|\eta| \leq M$, we have the relation

$$|\langle P(V) - P(\eta) - P'(\eta)(V - \eta)\rangle_A| \leq p_2 \langle (V - \eta)^2\rangle_A, \tag{3.6}$$

where

$$p_2 \equiv \max_{|\eta| \leq M} |P''(\eta)| \tag{3.7}$$

and $\langle\ \rangle_A$ denotes the average with respect to an arbitrary hermitean operator A#.

* The existence of the thermodynamic limit in eq. (3.3) will be shown later on in this section.

Eq. (3.6) implies that the operator $p_2(V - \eta)^2 - \{P(V) - P(\eta) - P'(\eta)(V - \eta)\}$ is positive (semi) definite.

Proof: In order to prove the lemma we consider the function

$$\Phi(t) \equiv \langle P(V_t) + (1 - t) \frac{\mathrm{d}}{\mathrm{d}t} P(V_t) \rangle_A, \tag{3.8}$$

where the operator V_t is defined by

$$V_t \equiv (1 - t)\eta + tV. \tag{3.9}$$

Clearly,

$$V_0 = \eta, \qquad V_1 = V, \qquad \frac{\mathrm{d}}{\mathrm{d}t} P(V_t)\bigg|_{t=0} = P'(\eta)(V - \eta). \tag{3.10}$$

The left-hand side of (3.6) is given by $|\Phi(1) - \Phi(0)|$ and according to the mean-value theorem we have

$$\begin{aligned}\Phi(1) - \Phi(0) &= \frac{\mathrm{d}}{\mathrm{d}t} \Phi(t)\bigg|_{t=\tau} = (1 - \tau) \left\langle \frac{\mathrm{d}^2}{\mathrm{d}t^2} P(V_t)\bigg|_{t=\tau} \right\rangle_A \\ &= (1 - \tau) \langle P''(V_\tau)(V - \eta)^2 \rangle_A \end{aligned} \tag{3.11}$$

for some value τ with $0 \leq \tau \leq 1$. Hence,

$$|\Phi(1) - \Phi(0)| \leq \|P''(V_\tau)\| \langle (V - \eta)^2 \rangle_A \leq p_2 \langle (V - \eta)^2 \rangle_A. \tag{3.12}$$

Here $\|P''(V_\tau)\|$ is finite, since

$$\|V_\tau\| \leq (1 - \tau)|\eta| + \tau\|V\| \leq M. \tag{3.13}$$

(iii) *Derivation of a lower bound:* From (3.4) and (3.5) we have

$$\mathscr{H}_1(\xi) - \mathscr{H}_2(\xi \mid \eta) = N\{P(V) - P(\eta) - P'(\eta)(V - \eta) + \Lambda(V - \eta)^2\}. \tag{3.14}$$

Using the Bogoliubov–Peierls inequality, *cf.* (2.5),

$$F[A + B] \geq F[A] + \langle B \rangle_{A+B} \tag{3.15}$$

for arbitrary hermitean operators A and B, and also the lemma (3.6), it follows that

$$\begin{aligned} f_N[\mathscr{H}_1(\xi)] &\geq f_N[\mathscr{H}_2(\xi \mid \eta)] + N^{-1} \langle \mathscr{H}_1(\xi) - \mathscr{H}_2(\xi \mid \eta) \rangle_{\mathscr{H}_1(\xi)} \\ &\geq f_N[\mathscr{H}_2(\xi \mid \eta)] + (\Lambda - p_2) \langle (V - \eta)^2 \rangle_{\mathscr{H}_1(\xi)}. \end{aligned} \tag{3.16}$$

For sufficiently large values of Λ, *i.e.*

$$\Lambda \geq p_2, \tag{3.17}$$

we have

$$f_N[\mathscr{H}_1(\xi)] \geq \max_{|\eta| \leq M} f_N[\mathscr{H}_2(\xi \mid \eta)]. \tag{3.18}$$

(iv) *Derivation of an upper bound:* Using (3.14), the Bogoliubov–Peierls inequality (2.5) and the lemma (3.6), we have

$$\begin{aligned} f_N[\mathscr{H}_1(\xi)] &\leq f_N[\mathscr{H}_2(\xi \mid \eta)] + N^{-1} \langle \mathscr{H}_1(\xi) - \mathscr{H}_2(\xi \mid \eta) \rangle_{\mathscr{H}_2(\xi \mid \eta)} \\ &\leq f_N[\mathscr{H}_2(\xi \mid \eta)] + (\Lambda + p_2)(\langle V \rangle_{\mathscr{H}_2(\xi \mid \eta)} - \eta)^2 \\ &\quad + (\Lambda + p_2) \langle (V - \langle V \rangle_{\mathscr{H}_2(\xi \mid \eta)})^2 \rangle_{\mathscr{H}_2(\xi \mid \eta)}. \end{aligned} \tag{3.19}$$

Now the third term of the right-hand side of (3.19) vanishes in the thermodynamic limit, since in view of (1.2), the trial hamiltonian $\mathscr{H}_2(\xi \mid \eta)$, given by (3.5), is a sum of one-particle operators. This implies that

$$\langle V(k)\, V(l) \rangle_{\mathscr{H}_2(\xi \mid \eta)} = \langle V(k) \rangle_{\mathscr{H}_2(\xi \mid \eta)} \langle V(l) \rangle_{\mathscr{H}_2(\xi \mid \eta)}, \qquad \text{for} \quad k \neq l, \tag{3.20}$$

and therefore, using (1.2),

$$\begin{aligned} &\langle (V - \langle V \rangle_{\mathscr{H}_2(\xi \mid \eta)})^2 \rangle_{\mathscr{H}_2(\xi \mid \eta)} \\ &\quad = N^{-2} \sum_{k=1}^{N} (\langle V(k)^2 \rangle_{\mathscr{H}_2(\xi \mid \eta)} - \langle V(k) \rangle^2_{\mathscr{H}_2(\xi / \eta)}) \leq M^2 N^{-1}, \end{aligned} \tag{3.21}$$

so that the right-hand side of (3.21) vanishes in the thermodynamic limit.

We now consider the second term in (3.19). For each ξ and N we choose a parameter η_N so that

$$\eta_N - \langle V_N \rangle_{\mathscr{H}_2(\xi \mid \eta_N)} = 0. \tag{3.22}$$

Obviously, eq. (3.22) has a solution in η_N for some value η_N with $-M < \eta_N < M$, since for $\eta = -M$ the left-hand side of (3.22) is negative, whereas for $\eta = M$ it must be positive. Hence,

$$f_N[\mathscr{H}_1(\xi)] \leq f_N[\mathscr{H}_2(\xi \mid \eta_N)] + (\Lambda + p_2) M^2 N^{-1}. \tag{3.23}$$

(v) *Minimax formulation for the free energy:* Since the trial hamiltonian $\mathscr{H}_2(\xi \mid \eta)$ is a sum of one-particle operators, the associated free energy per particle and its derivatives in general exist in the thermodynamic limit $N \to \infty$ ‡. From (3.18) and (3.23), we then have

$$f[\mathscr{H}_1(\xi)] = \lim_{N\to\infty} f_N[\mathscr{H}_1(\xi)] = \max_{|\eta|\le M} f[\mathscr{H}_2(\xi\,|\,\eta)]. \tag{3.24}$$

Noting that the thermodynamic limit in eq. (3.24) exists uniformly for $|\xi| \le M$, it follows from (3.3) that

$$f[\mathscr{H}] = \min_{|\xi|\le M} \max_{|\eta|\le M} f[\mathscr{H}_2(\xi\,|\,\eta)]. \tag{3.25}$$

In eq. (3.25) the free energy per particle has been expressed in terms of the free energy of a trial hamiltonian which is linear in the operator V. Eq. (3.25), however, contains an arbitrary parameter Λ which arises from (3.2).

(vi) *Molecular-field equation:* Rather than eq. (3.25), it would be convenient to have a formulation of the free energy per particle in terms of a trial hamiltonian involving only the polynomial P. The following reasoning will lead us to such a formulation.

Let η_0 be such that

$$f[\mathscr{H}_2(\xi\,|\,\eta_0)] = \max_{|\eta|\le M} f[\mathscr{H}_2(\xi\,|\,\eta)]. \tag{3.26}$$

Then, in view of (3.16), after taking the thermodynamic limit, *cf.* (3.17),

$$\langle (V-\eta_0)^2\rangle_{\mathscr{H}_1(\xi)} = 0. \tag{3.27}$$

Hence η_0 is a unique function of ξ satisfying

$$\eta_0 \equiv \eta(\xi) = \langle V\rangle_{\mathscr{H}_1(\xi)}. \tag{3.28}$$

Moreover, at the absolute minimum, we have from (2.24)

$$\xi = \langle V\rangle_{\mathscr{H}_1(\xi)}. \tag{3.29}$$

On the other hand, taking the thermodynamic limit in eq. (3.22), *cf.* (3.28), it follows that

$$\eta(\xi) = \langle V\rangle_{\mathscr{H}_2(\xi\,|\,\eta(\xi))}. \tag{3.30}$$

Since from (3.5) and (1.6)

$$\mathscr{H}_2(\xi\,|\,\xi) = \mathscr{H}_{\mathrm{tr},N}(\xi) = N\{T_N + P(\xi) + P'(\xi)(V_N - \xi)\}, \tag{3.31}$$

‡ Of course we exclude a pathological dependence of $V(k)$ on k.

the free energy per particle is given by, *cf.* (3.25),

$$f[\mathscr{H}] = \min_{\xi \in \mathscr{M}} f[\mathscr{H}_{tr}(\xi)], \tag{3.32}$$

where $\mathscr{M}$ is the set of values ξ satisfying

$$\xi = \langle V \rangle_{\mathscr{H}_{tr}(\xi)}, \tag{3.33}$$

which is equivalent to eq. (1.7). Hence eq. (1.4) has been proved in the simple case (1.1), (1.2).

The generalizations mentioned at the end of section 1 will be treated in a following paper. This will introduce some nontrivial complications in the lemma (ii), the derivation of the upper bound (iv) and the derivation of an appropriate generalization of the definition of the set $\mathscr{M}$.

4. Example

In this section we discuss an example which has been investigated previously by Thompson[32]). The hamiltonian is defined by

$$\mathscr{H}_N = -N\{BS + P(S)\}. \tag{4.1}$$

Here B is an applied magnetic field and

$$S \equiv N^{-1} \sum_{k=1}^{N} S_k^z, \tag{4.2}$$

where $S_k^z = \pm 1$ refers to the spin of particle k. The polynomial $P(S)$ is given by

$$P(S) = J_2 S^2 + J_4 S^4. \tag{4.3}$$

In ref. 32 some features of the phase diagram of this model were treated in the ferromagnetic case $J_2 > 0$, $J_4 > 0$. A more general polynomial including higher powers of S^2 has been discussed in refs. 30, 31 in connection with higher-order critical points.

Although this model is a rather trivial example of eq. (1.1), it may be of interest to consider its phase diagram in some more detail. Moreover, the example will be used to illustrate two underlying features of the treatment in section 3, namely the restriction $\xi \in \mathscr{M}$ on taking the minimum in eq. (3.32) and the fact that minmax in eq. (3.25) cannot be replaced by maxmin.

The trial hamiltonian corresponding to (4.1) is given by, *cf.* (1.6),

$$\mathscr{H}_{\mathrm{tr},N}(\xi) = -N\{(B + P'(\xi))\,S + P(\xi) - \xi P'(\xi)\} \tag{4.4}$$

and the free energy per particle is

$$\begin{aligned} f[\mathscr{H}] &= \min_{\xi \in \mathscr{M}} f[\mathscr{H}_{\mathrm{tr}}(\xi)] \\ &= \min_{\xi \in \mathscr{M}} \{-P(\xi) + \xi P'(\xi) - \beta^{-1} \ln 2 \cosh \beta\,(B + P'(\xi))\}, \end{aligned} \tag{4.5}$$

where $\mathscr{M}$ is the set of values ξ satisfying the molecular-field equation

$$\xi = \langle S \rangle_{\mathscr{H}_{\mathrm{tr}}(\xi)} = \tanh \beta\,(B + P'(\xi)). \tag{4.6}$$

Here the "minimizing" $\xi \in \mathscr{M}$ is the magnetization per particle. Note that we do not restrict ourselves to the case $J_2 > 0$, $J_4 > 0$.

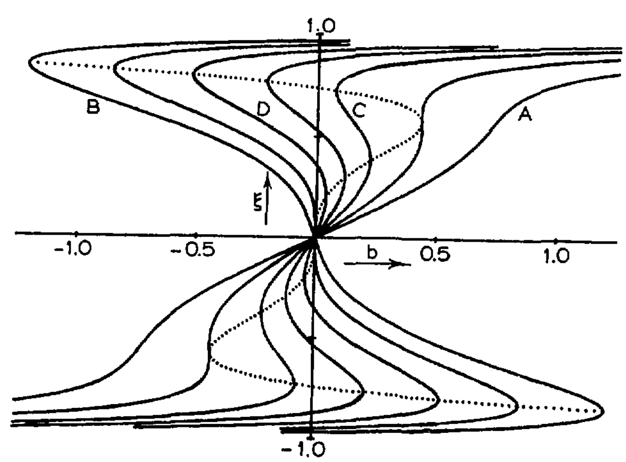

Fig. 1. $b(\xi)$ *vs.* ξ for $\varepsilon = 2$. For the curves labeled by A, B, C and D we have chosen: $\tau_{\mathrm{B}} = 3.7$, $\tau_{\mathrm{D}} = 4.3$, $\tau_{\mathrm{C}} = 4.9$ and $\tau_{\mathrm{A}} = 5.8$. The values for the intermediate curves are: $\tau_{\mathrm{BD}} = 4$, $\tau_{\mathrm{DC}} = 4.6$ and $\tau_{\mathrm{CA}} = 5\frac{1}{3}$. The dots form the spinodal curve.

In order to investigate the molecular-field solutions $\xi \in \mathscr{M}$ we first consider B/J_4 as a function of ξ. With the notations*

$$\begin{aligned} &b \equiv J_4^{-1} B, \qquad \tau \equiv J_4^{-1} \beta^{-1}, \qquad \varepsilon \equiv J_4^{-1} J_2, \\ &p(\xi) \equiv J_4^{-1} P(\xi) = \varepsilon \xi^2 + \xi^4 \end{aligned} \tag{4.7}$$

* Here we assume that $J_4 \neq 0$.

we find, *cf.* (4.6),

$$b = b(\xi) \equiv \tau \operatorname{artanh} \xi - p'(\xi) = \tau \operatorname{artanh} \xi - 2\xi (\varepsilon + 2\xi^2). \tag{4.8}$$

For different values of τ and ε, $b(\xi)$ as a function of ξ can behave in four different ways, indicated by A, B, C, D in fig. 1. Also the intermediate curves which separate one type of behaviour from another have been given. Moreover, we have indicated the spinodal curve which is the locus of points $b'(\xi) = 0$.

A partial distinction between A, B, C and D can be made by considering the zeros of the slope of $b(\xi)$, *i.e.*

$$b'(\xi) = \tau (1 - \xi^2)^{-1} - p''(\xi) = \tau (1 - \xi^2)^{-1} - 2 (\varepsilon + 6\xi^2). \tag{4.9}$$

The zeros of $b'(\xi)$ can be found from the relation

$$\tau = r(\xi^2), \qquad 0 \le \xi^2 \le 1, \tag{4.10}$$

where

$$r(\xi^2) \equiv p''(\xi) (1 - \xi^2) = \tfrac{1}{12} \{(\varepsilon + 6)^2 - (12\xi^2 + \varepsilon - 6)^2\}. \tag{4.11}$$

The function $r(\xi^2)$ assumes its maximum for $\xi_0^2 \equiv (6 - \varepsilon)/12$, which belongs to the interval $[0, 1]$ if $|\varepsilon| \le 6$. In that case eq. (4.10) has two solutions in ξ^2, provided that

$$\max \{r(0), r(1)\} = \max \{0, 2\varepsilon\} < \tau < r(\xi_0^2) = \tfrac{1}{12} (\varepsilon + 6)^2. \tag{4.12}$$

For all values of ε, eq. (4.10) has one solution, if

$$\min \{r(0), r(1)\} = \min \{0, 2\varepsilon\} < \tau < \max \{0, 2\varepsilon\}. \tag{4.13}$$

In other cases eq. (4.10) has no solution.

In fig. 2 we give the phase diagram of the system under consideration for different values of ε and τ. It consists of four regions labeled by A, B, C and D. The behaviour of $b(\xi)$ *vs.* ξ for each of these regions has been given in fig. 1.

The regions C and D in fig. 2 correspond to (4.12), so that $b(\xi)$ as a function of ξ has two maxima and two minima, *cf.* fig. 1. In region B, eq. (4.13) holds and $b(\xi)$ has only one maximum and one minimum. In the remaining part A of the phase diagram $b(\xi)$ is a monotonic function of ξ. The dotted curve in fig. 1 is the so-called spinodal curve, which can be obtained by substituting (4.10) into (4.8).

So far we have discussed the set $\mathscr{M}$ of solutions of the molecular-field equation. In the case that this equation has more than one solution we must select the solution which leads to the lowest value of the free energy. For this purpose we consider the branches of the free energy $f[\mathscr{H}_{\mathrm{tr}}(\xi)]$ corresponding to all solutions

$\xi \in \mathcal{M}$ as a function of the magnetic field b. In fig. 3 we give these branches for the four different cases labeled by A, B, C and D respectively in fig. 1. These four cases are characteristic for the regions A, B, C, D in the phase diagram in fig. 2, since the slopes of the branches of the free energy are proportional to the corresponding values of $\xi \in \mathcal{M}$, *cf.* fig. 1 and fig. 3.

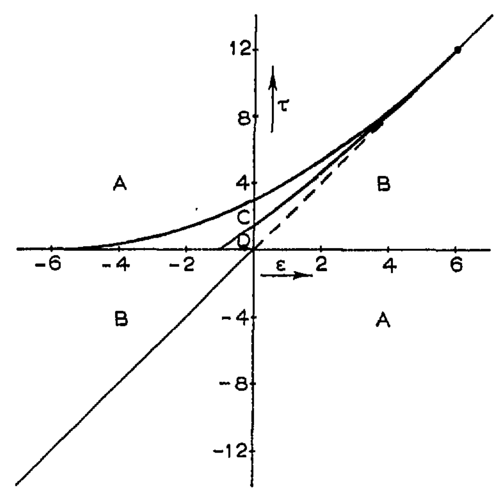

Fig. 2. The phase diagram in the ε–τ plane, showing the regions A, B, C and D. The dashed line is the unphysical phase boundary between regions B and D.

In fig. 2 the regions A and B have been defined by eqs. (4.12) and (4.13). In the remaining part of the phase diagram eq. (4.10) has two solutions in ξ^2. Two different possibilities must now be considered. In region C there are two first-order transitions in an applied magnetic field $\pm b_0$, *cf.* the kinks of the lowest branch in fig. 3c. On the other hand, in case D we have one first-order transition for $b = 0$.

From a physical point of view, *i.e.* if we restrict ourselves to the lowest branch of $f[\mathcal{H}_{tr}(\xi)]$, there is no difference between the cases B and D. This has been indicated by the dashed curve in fig. 2. The curve separating the regions C and D in fig. 2 is determined by the limiting case that both critical fields $\pm b_0$ tend to zero. This implies in particular that

$$f[\mathcal{H}_{tr}(\xi_0)] = f[\mathcal{H}_{tr}(0)], \qquad b(\xi_0) = 0, \qquad \text{with} \qquad 0 \neq \xi_0 \in \mathcal{M}. \tag{4.14}$$

Equation (4.14) can be rewritten as

$$\begin{aligned} \tau &= -2\xi_0^4 \{\xi_0 \operatorname{artanh} \xi_0 + \ln(1 - \xi_0^2)\}^{-1}, \\ \varepsilon &= \tau (2\xi_0)^{-1} \operatorname{artanh} \xi_0 - 2\xi_0^2. \end{aligned} \tag{4.15}$$

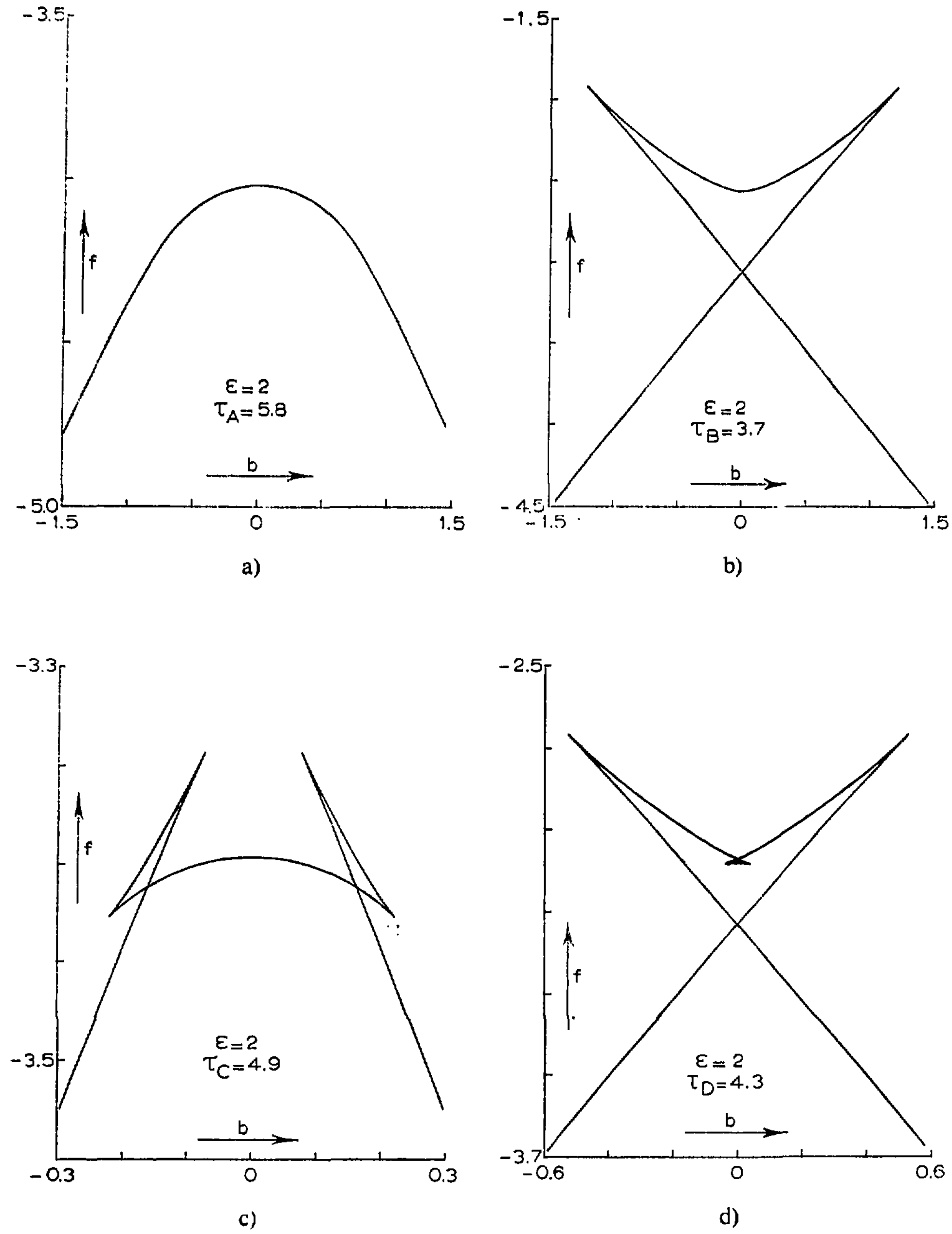

Fig. 3. The branches of the free energy $f \equiv f[\mathscr{H}_{tr}(\xi)]$, $\xi \in \mathscr{M}$, *vs.* b, *cf.* (4.5)-(4.7), for $J_4 = 1$ and the same values of ε, τ_A, τ_B, τ_C and τ_D as in fig. 1.

This curve has been evaluated numerically. In the two limiting cases $\xi_0 \to 0$, $\xi_0 \to 1$ we have $\tau \simeq 2\varepsilon \uparrow 12$ and $\tau \simeq (1 + \varepsilon)(\ln 2)^{-1} \downarrow 0$.

Finally we discuss the magnetization as a function of the magnetic field. In fig. 4 we give the isotherms for the values of the parameters used in figs. 1 and 3, *i.e.* for $\varepsilon = 2$ ($J_2 = 2J_4$) and various values of τ. The curves A, B, C and D are again characteristic for the corresponding regions in the phase diagram. The dots in fig. 4 indicate the coexistence curve which is determined by the condition that for g ven τ and b the molecular-field equation (4.8) gives two solutions $\xi \in \mathcal{M}$ leading to the absolute minimum in (4.5). This curve has been obtained numerically, solving the equations $b(\xi_1) = b(\xi_2)$, $f[\mathscr{H}_{tr}(\xi_1)] = f[\mathscr{H}_{tr}(\xi_2)]$, $\xi_1 \neq \xi_2$. Note that the coexistence curve can also be found from fig. 1 by Maxwell's equal-area construction.

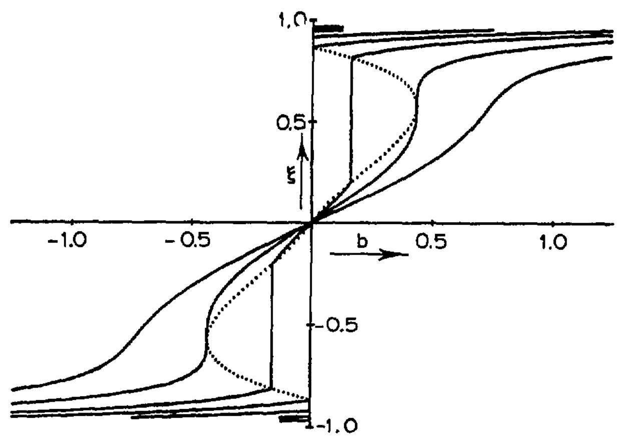

Fig. 4. The isotherms of the magnetization ξ *vs.* b fo- the same values of ε and τ as in fig. 1.

Remarks: The model described above may be useful to illustrate a few technical features of the derivation given in section 3.

i) First it may be noted that the free energy cannot be obtained by minimizing the free energy of a trial hamiltonian $f[\mathscr{H}_{tr}(\xi)]$ without taking into account the restriction $\xi \in \mathcal{M}$. In order to see this from an explicit example we consider $f[\mathscr{H}_{tr}(\xi)]$ as a function of ξ for $B = 0$, where $\mathscr{H}_{tr,N}(\xi)$ is given by (4.3) and (4.4) in the case that the four-body 'nteraction is ferromagnetic, *i.e.* $J_4 > 0$.

The extrema of $f[\mathscr{H}_{tr}(\xi)]$ are given by the equation

$$f'[\mathscr{H}_{tr}(\xi)] = P''(\xi)\{\xi - \tanh \beta P'(\xi)\} = 0. \tag{4.16}$$

For $-6 \leq \varepsilon \leq 0$ and a sufficiently large value τ, so that the point (ε, τ) belongs to region A of the phase diagram fig. 2, eq. (4.16) has two solutions

$$\xi = \pm(-\varepsilon/6)^{\frac{1}{2}}, \tag{4.17a}$$

corresponding to $P''(\xi) = 0$ for $\xi^2 \leq 1$, and a solution

$$\xi = 0, \tag{4.17b}$$

corresponding to the unique solution of the molecular-field equation $\xi = 0$, for $B = 0$, in region A. Since $f[\mathscr{H}_{\mathrm{tr}}(\xi)] \to \infty$, for $\xi \to \pm\infty$, the solutions (4.17a) determine the absolute minima of $f[\mathscr{H}_{\mathrm{tr}}(\xi)]$ and (4.17b) corresponds to the maximum of $f[\mathscr{H}_{\mathrm{tr}}(\xi)]$. Since the set $\mathscr{M}$ consists only of one point $\xi = 0$, the solution $\xi = 0$ is also the absolute minimum of $f[\mathscr{H}_{\mathrm{tr}}(\xi)]$ under the condition $\xi \in \mathscr{M}$. This feature may appear under the combined effect of ferromagnetic and antiferromagnetic interactions. If J_2 and J_4 have the same sign, $P''(\xi) \neq 0$ and all solutions of (4.16) belong to the set $\mathscr{M}$.

ii) A second remark can be made on the minimax formulation in section 3(v). It should be noted that the two procedures $\min_\xi$ and $\max_\eta$ in eq. (3.25) cannot be interchanged in general. Consider *e.g.* the special case

$$J_2 > 0, \qquad J_4 < 0, \qquad \beta^{-1} < \beta_c^{-1} \equiv 2J_2, \tag{4.18}$$

corresponding to a point (ε, τ) with $2\varepsilon < \tau < 0$ in region B of the phase diagram in fig. 2.

In this case the treatment with minmax in the correct order gives us a solution $\eta(\xi) = \xi$ with $\xi = \pm\xi_0$ for $B = 0$, where $\xi_0 > 0$ is the positive solution of the equation

$$\beta^{-1} \operatorname{artanh} \xi_0 = 2J_2\xi_0 + 4J_4\xi_0^3. \tag{4.19}$$

However, if we take the minimum first and the maximum afterwards we would have obtained [for sufficiently large Λ, *cf.* (3.17)]

$$\begin{aligned} g \equiv \max_\eta \min_\xi f[\mathscr{H}_2(\xi \mid \eta)] &= \max_\eta \min_\xi [\Lambda\xi^2 - (\Lambda - J_2 - 3J_4\eta^2)\eta^2 \\ &\quad - \beta^{-1} \ln 2\cosh\beta\{2\Lambda\xi - 2(\Lambda - J_2 - 2J_4\eta^2)\eta\}], \end{aligned} \tag{4.20}$$

rather than the correct expression (3.25) for the free energy. Clearly for fixed η, the absolute minimum with respect to ξ in (4.20) is assumed at a point $\xi(\eta)$ with

$$\operatorname{sgn}\eta = -\operatorname{sgn}\xi(\eta). \tag{4.21}$$

This can be seen by considering the difference $f[\mathscr{H}_2(\xi \mid \eta)] - f[\mathscr{H}_2(-\xi \mid \eta)]$ using (4.18). Obviously (4.21) is incompatible with the condition $\eta(\xi_0) = \xi_0 > 0$, *cf.* (3.28), (3.29), for the set $\xi \in \mathscr{M}$, arising from the minimax-procedure.

A different example of this situation has been given in ref. 18. Such examples can be used to demonstrate that the fundamental theorem (2.1) for ferromagnetic operators cannot be extended to the case of antiferromagnetic operators with the same amount of generality, *cf.* the discussion in section 8 of ref. 19.

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CHAPTER II

SYSTEMS WITH SEPARABLE MANY-PARTICLE INTERACTIONS. II

1. Introduction

In a previous paper[1]) we have considered a class of systems containing many-particle interactions of the separable type. A separable m-body interaction is defined by the property that the interaction $V(k_1, \dots, k_m)$ between particles $k_1, \dots, k_m$ can be written as a product $V(k_1) \dots V(k_m)$, where $V(k)$ is an operator acting on the Hilbert-space of particle k. Separable interactions include in particular so-called equivalent-neighbour interactions, for which the interactions between particles do not depend on the distances between the particles.

For many models with equivalent-neighbour interactions, the free energy per particle has been evaluated and the result is usually of the molecular-field type. Examples are, for instance, the Husimi–Temperley model for a lattice gas[2]), the Ising model with equivalent-neighbour interactions[3]) and other spin models[4]), the reduced hamiltonian in the BCS-theory of superconductivity[5,6]) and the Dicke maser model[7,8]). Two-body separable interactions have been treated from a more general point of view in refs. 9, 10. Many-body interactions of this type have also been investigated[11–13]). A more extensive discussion of the literature has been given in ref. 1.

Before we describe the generalizations which will be dealt with in the present treatment, we first give a brief review of the main results of our previous paper. In ref. 1 we restricted ourselves to the class of systems described by the hamiltonian

$$\mathcal{H}_N = N\{T_N + P(V_N)\}, \tag{1.1}$$

where T_N and V_N are normalized* sums of bounded hermitean one-particle operators, *i.e.*

$$T_N = N^{-1}\sum_{k=1}^{N} T(k), \quad V_N = N^{-1}\sum_{k=1}^{N} V(k) \tag{1.2}$$

and $P(V_N)$ is a polynomial in the operator V_N.

In ref. 1 the free energy per particle in the thermodynamic limit, defined by

$$f[\mathscr{H}] \equiv \lim_{N\to\infty} f_N[\mathscr{H}_N] \equiv \lim_{N\to\infty} -(\beta N)^{-1} \ln \mathrm{Tr}\, e^{-\beta\mathscr{H}_N}, \tag{1.3}$$

has been expressed in terms of a trial hamiltonian $\mathscr{H}_{tr,N}(\xi)$, which can be obtained by linearizing $\mathscr{H}_N$ with respect to V_N, *i.e.*

$$f[\mathscr{H}] = \min_{\xi\in\mathscr{M}} f[\mathscr{H}_{tr}(\xi)], \tag{1.4}$$

where

$$\mathscr{H}_{tr,N}(\xi) = N\{T_N + P(\xi) + P'(\xi)(V_N - \xi)\}. \tag{1.5}$$

The minimum in the right-hand side of (1.4) is taken over the set of values $\xi \in \mathscr{M}$ satisfying the molecular-field equation

$$\xi = \lim_{N\to\infty} \langle V_N \rangle_{\mathscr{H}_{tr,N}(\xi)}, \tag{1.6}$$

where

$$\langle B \rangle_A \equiv \mathrm{Tr}\, B\, e^{-\beta A}(\mathrm{Tr}\, e^{-\beta A})^{-1} \tag{1.7}$$

is the canonical average of B with respect to A.

As a first step in the derivation of eqs. (1.4)–(1.6) we expressed the free energy per particle in terms of a hamiltonian $\mathscr{H}_{1,N}(\xi) = \mathscr{H}_N + N\Lambda(V_N - \xi)^2$, using a fundamental theorem due to Bogoliubov Jr.[9,14]) for a hamiltonian with "ferromagnetic" quadratic operators. Applying the Bogoliubov–Peierls inequality, (see *e.g.* ref. 15), and also a lemma for the average value of $P(V_N)$ we have shown that the free energy per particle in the thermodynamic limit is given by

$$f[\mathscr{H}] = \min_{\xi} \max_{\eta} f[\mathscr{H}_2(\xi|\eta)]. \tag{1.8}$$

Here $\mathscr{H}_{2,N}(\xi|\eta)$ can be obtained by linearizing the operator $\mathscr{H}_{1,N}(\xi)$ with respect to V_N, *cf.* eqs. (3.4) and (3.5) of ref. 1. Eq. (1.8) has been proved by deriving a lower and an upper bound for $f[\mathscr{H}]$ which turn out to be equal in the thermodynamic limit; the lower bound is obvious for sufficiently large $\Lambda > 0$; in the derivation of the upper bound use has been made of a factorization property for the autocorrelation function of V_N. The final result (1.4)–(1.6) has been obtained from (1.8) using again the Bogoliubov–Peierls inequality.

* Here and from now on a normalized operator is an operator acting on the Hilbert-space of an N particle system, divided by N.

In the present paper the treatment of ref. 1 will be generalized in two ways. First the polynomial $P(V_N)$ is replaced by an arbitrary analytic function of operators $V_N^{(1)}, \ldots, V_N^{(n)}$. Moreover, these operators $V_N^{(i)}$ need not be normalized sums of one-particle operators, but can be of a much more general type, including also short-range operators. In connection with this we can mention the Ising model with two-spin and (long-range) four-spin interactions treated by Oitmaa and Barber[16]).

With regard to this more general type of operators we mention the three specific properties for the operators which have been used in the proof of ref. 1.

a) The commutator between two normalized operators V_N and V'_N (or T_N) tends to zero in the thermodynamic limit, *i.e.*

$$\|[V_N, V'_N]\| \to 0, \quad \text{if } N \to \infty. \tag{1.9}$$

b) The free energy per particle of a trial hamiltonian which is linear in the operators V_N, *i.e.*

$$\mathcal{H}_{\mathrm{tr},N} = N \sum_i h_i V_N^{(i)} \tag{1.10}$$

converges in the limit $N \to \infty$ uniformly on a bounded region in the space of the variables h_i.

c) The autocorrelation function of the normalized operator V_N with respect to the trial hamiltonian tends to zero in the thermodynamic limit, *i.e.*

$$\lim_{N\to\infty} \langle (V_N - \langle V_N \rangle_{\mathcal{H}_{\mathrm{tr},N}})^2 \rangle_{\mathcal{H}_{\mathrm{tr},N}} = 0. \tag{1.11}$$

Eq. (1.11) is essential for the derivation of an upper bound for the free energy per particle.

In the case of normalized sums of one-particle operators (1.2) the proof of eqs. (1.9)–(1.11) is trivial, assuming that the dependence of $V(k)$ on k is not of a pathological nature. Eq. (1.11) is a direct consequence of the factorization

$$\langle V(k) V(k') \rangle_{\mathcal{H}_{\mathrm{tr},N}} = \langle V(k) \rangle_{\mathcal{H}_{\mathrm{tr},N}} \langle V(k') \rangle_{\mathcal{H}_{\mathrm{tr},N}}, \quad \text{for } k \neq k'. \tag{1.12}$$

Also, in the general case under consideration here, it turns out that the free energy per particle can be obtained by minimizing the free energy of a linear trial hamiltonian over a set $\mathcal{M}$ analogous to the one in eq. (1.6). Note in connection with the definition of $\mathcal{M}$ that the average values of the operators $V^{(i)}$ may show discontinuities because of the presence of short-range interactions in the trial hamiltonian.

In section 2 we give a more precise description of the generalizations mentioned above. The theorems for the free energy will be formulated in section 3 and proved in sections 4-7. An application is given in section 8.

2. General formulation

Before we formulate the main theorems of this treatment, we discuss the extensions to more general operators V_N and functions P.

2.1. *Generalization of the operators*

In the introduction we mentioned the three properties a), b) and c) of the operators V_N, which have been used in the proof of ref. 1. These properties suggest a close relationship between the generalization of the operators V_N and the process of taking the thermodynamic limit. In order to discuss this process, we consider a sequence of (ν-dimensional) lattice systems with N particles* located on a subset Ω_N of an infinite lattice.

We shall say that the sequence of systems Ω_N tends to infinity in the sense of Van Hove, *cf.* refs. 17, 18, if for each Ω_N there exists a collection of disjoint equivalent cubes

$$C_M(K), \quad K = 1, 2, 3, \ldots, \tag{2.1}$$

with $M(N)$ sites, $L(N)$ cubes being contained in Ω_N, satisfying the conditions

$$1) \lim_{N\to\infty} M(N) = \infty, \tag{2.2}$$

$$2) \lim_{N\to\infty} L(N) = \infty, \tag{2.3}$$

$$3) \lim_{N\to\infty} \frac{L(N)M(N)}{N} = 1. \tag{2.4}$$

Furthermore, to be specific, we assume that for $N' > N$ each cube $C_{M'}$ can be constructed from cubes C_M corresponding to N, *i.e.*

$$4) \; C_{M'}(K') = \sum_K{}^{(K')} C_M(K), \tag{2.5}$$

$$M' \equiv M(N'), \quad M \equiv M(N), \quad N' > N.$$

The symbol $\Sigma^{(K')}$ is used to express that the cubes do not overlap and that the M'/M values of K which contribute to $C_{M'}(K')$ are determined by K'.

The process of taking the thermodynamic limit has been illustrated in fig. 1.

From now on each operator which has a subscript N denotes an operator acting on the direct-product Hilbert space of particles belonging to one of the systems Ω_N given above. In order to describe the generalization of the operators we decompose an arbitrary hermitean operator NV_N into an operator NV_N^0 and an operator NR_N. The operator NV_N^0 contains only the interaction between particles lying inside the same cube $C_M(K)$ of the set (2.1)

* If Ω_N is not well defined for each value of N, one can consider a sequence $\Omega_{N(n)}$ with $N(n)\to\infty$, if $n\to\infty$.

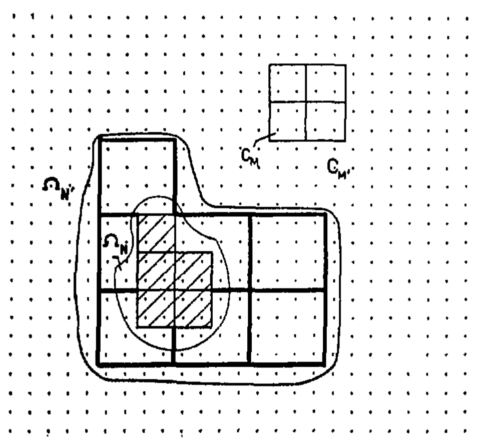

Fig. 1. Two systems with N and N' ($N' > N$) particles located on the subsets Ω_N and $\Omega_{N'}$ of the infinite lattice Ω. Ω_N contains cubes $C_M(K)$, ($M = 4$, $K = 1, \ldots, L(N) = 5$, $N = 37$), and $\Omega_{N'}$ contains cubes $C_{M'}(K')$, ($M' = 16$, $K' = 1, \ldots, L(N') = 7$, $N' = 147$).

corresponding to Ω_N and the operator R_N contains the remaining interactions. (The interaction terms in R_N involve particles belonging to different cubes and also particles which belong to the part of Ω_N outside the cubes.) The normalized operator V_N^0 can be expressed by

$$NV_N^0 = \sum_{K=1}^{L(N)} M(N) V_M^c(K), \tag{2.6}$$

where $V_M^c(K)$ is an operator acting on the Hilbert space of the particles belonging to cube $C_M(K)$. The decomposition of the normalized operator V_N can be written as

$$V_N = V_N^0 + R_N. \tag{2.7}$$

We now require that the residual operator R_N tends to zero in the thermodynamic limit, *i.e.*

$$\lim_{N\to\infty} \|R_N\| = 0. \tag{2.8}$$

Also, to be specific, we assume that for a subdivision of a large cube into smaller ones, as given by eq. (2.5), the interaction between different subcubes, *i.e.*

$$M'R_{M'|M} \equiv M'V_{M'}^c - \sum_K^{(K')} MV_M^c(K), \tag{2.9}$$

is negligible in the thermodynamic limit, *i.e.*

$$\lim_{N\to\infty} \sup_{N'>N} \|R_{M(N')|M(N)}\| = 0. \tag{2.10}$$

Furthermore it is assumed that, for sufficiently large values of N, there is a translational invariance, *i.e.*

$$TV_M^c(K)T^{-1} - V_M^c(K_T) = 0, \tag{2.11}$$

for a translation T transforming the cube K into one of the other cubes K_T*.

Eqs. (2.8), (2.10) and (2.11) will turn out to be sufficient for our purpose. From now on operators satisfying these conditions will be referred to as short-range operators. Note that this concept of short-range operator is of a rather general nature, *cf.* the discussion later on in this section. These conditions ensure that properties similar to eqs. (1.9)–(1.11) are satisfied.

In particular, for short-range hamiltonians NV_N the free energy per particle has a well-defined thermodynamic limit in the sense of Van Hove, *cf.* conditions (2.2)–(2.5), *i.e.*

$$f = \lim_{N\to\infty} f_N = \lim_{N\to\infty} f_{M(N)}^c, \tag{2.12}$$

where

$$f_N \equiv -(\beta N)^{-1} \ln \mathrm{Tr}_N\, e^{-\beta N V_N} \tag{2.13}$$

and

$$f_M^c \equiv -(\beta M)^{-1} \ln \mathrm{Tr}_M\, e^{-\beta M V_M^c} \tag{2.14}$$

are the free energies per particle of the system Ω_N and the cube $C_M(K)$ resp. Using eqs. (2.8), (2.10), (2.11) and the Bogoliubov–Peierls inequality[15]), we have

$$|f_{M'}^c - f_M^c| \leq \|R_{M'|M}\| \to 0, \quad (M, M' \to \infty) \tag{2.15}$$

and

$$|f_N - f_{M(N)}^c| \leq \|R_N\| + (1 - LMN^{-1})|f_M^c| \to 0, \quad (N \to \infty), \tag{2.16}$$

from which eq. (2.12) follows.

2.2. *Discussion*

It should be mentioned that eqs. (2.8) and (2.10) are satisfied for "(not too) long-range" interactions, *cf.* eq. (2B.24) of ref. 19 or eq. (2.2.8) of ref. 18. To see this, note that the action of an arbitrary operator V on the system Ω_N can be written as **,†

$$NV_N = \sum_{\substack{k \\ k\in\Omega_N}} \sum_{\substack{\omega_k \\ \omega_k\subset\Omega_N}} V(\omega_k), \tag{2.17}$$

* Equation (2.11) can be relaxed assuming that the left-hand side tends to zero for $N \to \infty$.

** Equation (2.17) is equivalent to the definition by Ruelle and Griffiths. For comparison, note that NV_N can be written as $\Sigma_{\omega\subset\Omega_N} \Phi(\omega)$, where $\Phi(\omega) \equiv N(\omega)V(\omega)$, $N(\omega)$ being the number of particles in ω.

†In eq. (2.17) we restrict ourselves to open boundary conditions. The effect of other boundary conditions can be included in the operator R_N in eq. (2.7), without affecting the line of reasoning.

where k labels the sites in Ω_N and where the summation over ω_k involves the different subsets of Ω_N containing particles which interact with particle k. In eq. (2.17) an m-body interaction $V(\omega)$ between m particles $k_1, \ldots, k_m$ occurs m times, namely as one of the terms $V(\omega_{k_i})$, for $i = 1, \ldots, m$ resp. (A set ω containing *e.g.* two neighbouring particles 1 and 2 corresponds to a nearest neighbour interaction between 1 and 2 and the corresponding $V(\omega)$ occurs twice, namely as a term $V(\omega_k)$ for $k = 1, 2$ resp.).

As in refs. 18 and 19, we assume that for sufficiently large values of N the interaction is invariant under translations from one cube to another and also that the sum of the interactions $V(\omega_k)$ over an infinite lattice is finite for fixed k, *i.e.*

$$\text{A)}\quad TV(\omega_k)T^{-1} = V(\omega_{kT}), \tag{2.18}$$

where T is the operator associated with the translation from one cube $C_M(K)$ into another cube $C_M(K_T)$ and where ω_{kT} is the subset obtained from ω_k after application of the translation T.

$$\text{B)}\quad \sum_{\omega_k} \|V(\omega_k)\| \leq v_1 < \infty, \tag{2.19}$$

where the summation in the left-hand side is over all finite subsets ω_k, containing particle k, of the infinite lattice.

In view of (2.7), the operator R_N does not contain the interaction terms $V(\omega)$ for which ω is included in one single cube. From this we have the inequality

$$\|R_N\| \leq \frac{N - LM}{N} v_1 + \frac{LM}{N} v_M. \tag{2.20}$$

Here the first term is an upper bound for the interactions involving particles which do not belong to one of the cubes, and Mv_M is an upper bound for the interaction of the particles belonging to a cube C_M with particles outside that cube, *i.e.*.

$$Mv_M = \sum_{\substack{k \\ k \in C_M}} \sum_{\substack{\omega_k \\ \omega_k \not\subset C_M}} \|V(\omega_k)\|. \tag{2.21}$$

In order to estimate (2.21) we consider the restricted sum of interactions with a particle k such that the "diameter" $D(\omega_k)$ of the subset ω_k is larger than some fixed distance d. From (2.19) it follows that

$$\sum_{\substack{\omega_k \\ D(\omega_k) \geq d}} \|V(\omega_k)\| \leq v_{1d} \to 0, \quad \text{for } d \to \infty. \tag{2.22}$$

Using (2.22) we can give separate estimates for the contributions to Mv_M from particles $k \in C_M$ lying at a distance larger than d from one of the sides of the cube and for the contributions from the other particles in C_M. We then have, for each value of d,

$$v_M \leq v_{1d} + 2\nu d\, M^{-1/\nu} v_1. \tag{2.23}$$

In eq. (2.23) it has been used that the number of sites in C_M at a distance less than d from one of the sides of the cube is bounded by $2\nu d\,M^{(\nu-1)/\nu}$, where ν is the dimensionality of the lattice. Since eq. (2.23) is valid for all d, we can take as an upper bound for v_M the infimum of the right-hand side with respect to d, which is a function of the variable M. As a result we have

$$v_M \to 0, \quad \text{for } M \to \infty. \tag{2.24}$$

Hence, in view of (2.20), R_N tends to zero if we take the thermodynamic limit in the sense of Van Hove, so that eq. (2.8) and also eq. (2.10) are satisfied. This shows that operators satisfying eqs. (2.18) and (2.19) are included in our treatment.

As an example one may consider a spin model for a ν-dimensional lattice with anisotropic Heisenberg interactions, described by the hamiltonian

$$NV_N = \sum_{k,k'} \boldsymbol{S}_k \cdot \mathbf{J}_{kk'} \cdot \boldsymbol{S}_{k'}. \tag{2.25}$$

The decomposition (2.7) is then determined by

$$NV_N^0 = \sum_{K=1}^{L(N)} \sum_{k,k'} \boldsymbol{S}_k \cdot \mathbf{J}_{kk'} \cdot \boldsymbol{S}_{k'} \delta_k(K)\delta_{k'}(K), \tag{2.26a}$$

$$NR_N = \sum_{k,k'} \boldsymbol{S}_k \cdot \mathbf{J}_{kk'} \cdot \boldsymbol{S}_{k'} \left\{ 1 - \sum_{K=1}^{L(N)} \delta_k(K)\delta_{k'}(K) \right\}, \tag{2.26b}$$

where

$$\delta_k(K) = \begin{cases} 1, & \text{if } k \in C_M(K), \\ 0, & \text{otherwise.} \end{cases} \tag{2.27}$$

The factor between brackets in the right-hand side of (2.26b) expresses that R_N contains only contributions from particles k and k' which do not belong to the same cube.

Now R_N in (2.26b) tends to zero in the thermodynamic limit under rather general conditions. If the interactions $\mathbf{J}_{kk'}$ in eq. (2.25) are of finite range D, *i.e.*

$$\mathbf{J}_{kk'} = 0, \quad \text{if } |\boldsymbol{R}_k - \boldsymbol{R}_{k'}| > D, \tag{2.28a}$$

where $\boldsymbol{R}_k$ and $\boldsymbol{R}_{k'}$ are the lattice sites corresponding to particles k and k', then $v_{1d} = 0$ in (2.22) for $d > D$, and $R_N \to 0$ because of (2.19), (2.20) and (2.23). Also for interactions with a Kac-type dependence on the distance , *i.e.*

$$\mathbf{J}_{kk'} = \mathbf{J}\gamma^{\nu}\, e^{-\gamma|\boldsymbol{R}_k - \boldsymbol{R}_{k'}|}, \quad \gamma > 0, \tag{2.28b}$$

R_N tends to zero.

2.3. *Generalization of the polynomial*

In ref. 1 we dealt with the simple case of a polynomial $P(V_N)$ of one normalized sum of one-particle operators. In order to discuss the generalization to an "analytic" function of more operators we consider a finite number of normalized hermitean short-range operators $V_N^{(i)}$, $i = 1, 2, \ldots, n$, which we may assume to be uniformly bounded, *i.e.*

$$\|V_N^{(i)}\| \leqslant M_i < \infty, \quad i = 1, 2, \ldots, n, \tag{2.29}$$

independent of N*'**. An arbitrary analytic function P of these operators is determined by its series expansion, *i.e.*

$$P(\boldsymbol{V}_N) \equiv \sum_{m=1}^{\infty} \sum_{i_1, \ldots, i_m = 1}^{n} p(i_1, \ldots, i_m) V_N^{(i_1)} \ldots V_N^{(i_m)}. \tag{2.30}$$

In eq. (2.30) use has been made of a vector notation

$$\boldsymbol{V}_N \equiv (V_N^{(1)}, \ldots, V_N^{(n)}). \tag{2.31}$$

Furthermore, it is assumed that

$$p(i_m, \ldots, i_1) = p(i_1, \ldots, i_m)^*, \tag{2.32}$$

so that the operator $P(\boldsymbol{V}_N)$ is hermitean.

For the coefficients $p(i_1, \ldots, i_m)$ it is sufficient to impose the "analyticity" condition:

$$\mathscr{P}(\boldsymbol{M}^+) = p_0 < \infty, \tag{2.33}$$

where

$$\mathscr{P}(\boldsymbol{\eta}) \equiv \sum_{m=1}^{\infty} \sum_{i_1, \ldots, i_m = 1}^{n} |p(i_1, \ldots, i_m)| \eta_{i_1} \ldots \eta_{i_m}, \tag{2.34}$$

for some values of $M_i^+ > M_i$, $i = 1, \ldots, n$.

* Note that for the operator given by (2.17) $\|V_N\| \leqslant v_1$, independent of N, *cf.* (2.19).

** Non-hermitean operators J_N, as have been used in refs. 9, 14, can also be treated using the decomposition $J = \{\frac{1}{2}(J^\dagger + J)\} + \mathrm{i}\{\frac{1}{2}\mathrm{i}(J^\dagger - J)\}$.

3. Theorems.

In section 2 we have given the definition of an analytic function of short-range operators. With this definition a number of theorems can be formulated for the free energy per particle of a system described by the hamiltonian

$$\mathcal{H}_N(\underline{h}) = N(P(\underline{V}_N) - \underline{h}\cdot\underline{V}_N) . \tag{3.1}$$

Here $P(\underline{V}_N)$ is defined by (2.30) and the coefficients $p(i_1,\dots,i_m)$ satisfy eqs. (2.32) and (2.33). The vector $\underline{V}_N$, cf. (2.31), denotes a finite set of normalized operators $V_N^{(i)}$, $i = 1,\dots,N$, which are uniformly bounded, cf. (2.29), and which satisfy the short-range conditions (2.8), (2.10) and (2.11). The vector $\underline{h} = (h_1,\dots,h_n)$ denotes the fields or coupling constants conjugate to the operators $N\underline{V}_N$.

In this chapter it will be shown that the free energy per particle in the thermodynamic limit, i.e.

$$f(\underline{h}) = -\lim_{N\to\infty} (\beta N)^{-1} \ln \mathrm{Tr} \exp[-\beta\mathcal{H}_N(\underline{h})] , \tag{3.2}$$

exists and can be expressed in terms of the free energy per particle of a reference system described by a hamiltonian which is a short-range operator.

Note that the hamiltonian (3.1) is not a short-range operator, if P contains nonlinear terms. For example, if $NV_N^{(1)}$ describes an anisotropic Heisenberg interaction, cf. (2.25), and $NV_N^{(2)}$ the magnetization operator in the direction of the vector $\vec{H}$, i.e.

$$NV_N^{(1)} = \sum_{k,k'} \vec{S}_k\cdot\vec{\vec{J}}_{kk'}\cdot\vec{S}_{k'} , \qquad NV_N^{(2)} = \vec{H}\cdot\sum_k \vec{S}_k , \tag{3.3}$$

and if P is a quadratic function

$$P(\underline{V}_N) = \lambda_1 V_N^{(1)2} + \lambda_2 V_N^{(2)2} , \tag{3.4}$$

then the hamiltonian (3.1) is given by

$$\mathcal{H}_N(\underline{h}) = -h_1 \sum_{k,k'} \vec{S}_k\cdot\vec{\vec{J}}_{kk'}\cdot\vec{S}_{k'} - h_2\vec{H}\cdot\sum_k \vec{S}_k + \frac{\lambda_1}{N}\sum_{k,k'}\sum_{\ell,\ell'} \vec{S}_k\cdot\vec{\vec{J}}_{kk'}\cdot\vec{S}_{k'}\, \vec{S}_\ell\cdot\vec{\vec{J}}_{\ell\ell'}\cdot\vec{S}_{\ell'} + \frac{\lambda_2}{N}\sum_{k,\ell} \vec{H}\cdot\vec{S}_k\, \vec{H}\cdot\vec{S}_\ell . \tag{3.5}$$

Apart from the usual (short-range) bilinear exchange between spins located at k and k' and the Zeeman term, eq. (3.5) contains a four-spin interaction of hybrid type, (i.e. long-range between the pairs with indices (k,k') and (ℓ,ℓ'), and short-range between the spins k,k' and the spins ℓ,ℓ'), and a pair interaction of the equivalent-neighbour type. Four-spin interactions can arise in compressible spin systems, in which there is a coupling between the spins and the lattice [20]. An exactly solvable Ising model with four-spin interactions has been treated in ref. 16. Also four-spin interactions are important in the framework of renormalization group theory [21]. Equivalent-neighbour interactions can be used e.g. in the classical description of demagnetizing effects [22]. An exactly solvable model which can be obtained from the two-dimensional super-exchange antiferromagnet [23] adding an equivalent-neighbour interaction has been investigated in ref. 24, see also refs. 25-27 for one-dimensional short-range systems with equivalent-neighbour interactions.

In this chapter we shall prove a number of theorems relating the free energy per particle (3.2) to the free energy per particle

$$f_0(\underline{h}) = -\lim_{N\to\infty} (\beta N)^{-1} \ln \mathrm{Tr} \exp [\beta N \underline{h}\cdot\underline{V}_N] \tag{3.6}$$

of a reference system described by the hamiltonian

$$\mathcal{H}_{0,N}(\underline{h}) = -N\underline{h}\cdot\underline{V}_N \ . \tag{3.7}$$

First of all we have a minimax-theorem, which can be considered as a generalization of eq. (1.8), derived in chapter I. This theorem is formulated in terms of the decomposition of the function P in (3.1) into a strongly concave and a strongly convex part, i.e.

$$P(\underline{\xi}) = Q(\underline{\xi}) + R(\underline{\xi}) \ , \tag{3.8}$$

with

$$\underline{e}\cdot\frac{\partial^2 Q}{\partial\underline{\xi}\partial\underline{\xi}}\cdot\underline{e} < 0, \quad \underline{e}\cdot\frac{\partial^2 R}{\partial\underline{\xi}\partial\underline{\xi}}\cdot\underline{e} > 0 \ , \tag{3.9}$$

for every (n-dimensional) vector $\underline{e}$. A decomposition like (3.8) is always possible, at least for the values $\underline{\xi}$ satisfying $|\xi_i| \leq M_i$, $i = 1,\ldots,n$, cf. (2.29), which is sufficient for our purpose. Note that the decomposition is not unique, one may choose e.g. $Q(\underline{\xi}) = -\Lambda\underline{\xi}\cdot\underline{\xi}$ with Λ positive and sufficiently large, similar to ref. 1, but many other choices are possible.

Using (3.8) it can be shown that

$$f(\underline{h}) = \min_{\underline{\xi}} \max_{\underline{\eta}} [\, Q(\underline{\xi}) - \underline{\xi}\cdot\underline{Q}'(\underline{\xi}) + R(\underline{\eta}) - \underline{\eta}\cdot\underline{R}'(\underline{\eta}) + f_0(\underline{h} - \underline{Q}'(\underline{\xi}) - \underline{R}'(\underline{\eta}))\,], \qquad (3.10)$$

with $\underline{Q}'(\underline{\xi}) = \partial Q/\partial\underline{\xi}$, $\underline{R}'(\underline{\eta}) = \partial R/\partial\underline{\eta}$. The minimax-theorem can be proved using a generalization of a fundamental theorem due to Bogoliubov Jr., see refs. 9, 14 and chapter I. In contrast with the situation in chapter I, the special case of convex P, (i.e. Q=0, P=R), is far from trivial and requires some subtle considerations on short-range operators in the thermodynamic limit. Eq. (3.10) for the special case P=R will be proved in section 4, the derivation for general P is given in section 5.

From the minimax result (3.10) we shall derive in section 6 a different result,

$$f(\underline{h}) = \inf_{\underline{m}} [\, - \underline{h}\cdot\underline{m} + g_0(\underline{m}) + P(\underline{m})\,], \qquad (3.11)$$

involving the Legendre transform

$$g_0(\underline{m}) = \sup_{\underline{h}} [\, \underline{h}\cdot\underline{m} + f_0(\underline{h})\,] \qquad (3.12)$$

of the reference free energy (3.6). Eq. (3.11) shows that the minimax result (3.10) does not depend on the details of the decomposition (3.8).

Eq. (3.11) can be used for various purposes. For instance, when all operators $\underline{V}_N$ are sums of one-particle operators, it can be used as a starting point for Landau expansions providing an explicit realization of various types of classical critical behaviour, see e.g. refs. 1, 11, 12 for examples, ref. 28 for a systematic classification and ref. 29 for the relation with the theory of catastrophes [30),31)]. On the other hand, the reference system can contain short-range interactions, which give rise to phase transitions, also in the absence of $P(\underline{m})$ in (3.11), so that eq. (3.11) can be used to study the stability of critical behaviour of a system with short-range interactions under the influence of a perturbation P describing interactions of a different nature. This problem will be treated extensively in chapter III. Note that in the absence of $P(\underline{m})$, eq. (3.11) amounts to the inverse Legendre transform of (3.12), as is well-known from the theory of convex functions, see refs. 32-38 and in particular refs. 33, 34, 38 for Legendre transformations in more than one variable. Expressions like (3.11) have also been derived e.g. for the Ising model with quadratic equivalent-neighbour interactions using the Laplace method or a rigorous version of the Bragg-Williams approximation, see e.g. refs. 2, 3, 11, 39.

Introducing the Legendre transform

$$g(\underline{m}) = \sup_{\underline{h}} [\, \underline{h}\cdot\underline{m} + f(\underline{h}) \,] \tag{3.13}$$

of the free energy per particle (3.2), eq. (3.11) can be rewritten in the form

$$g(\underline{m}) = \sup_{\underline{h}} \inf_{\underline{m}'} [\, \underline{h}\cdot(\underline{m}-\underline{m}') + g_0(\underline{m}') + P(\underline{m}') \,] = \mathrm{CE}\{g_0(\underline{m}) + P(\underline{m})\} \quad , \tag{3.14}$$

where CE denotes the convex envelope, i.e. CE $\phi(\underline{x})$ is the maximum over all functions $\psi(\underline{x})$ satisfying

$$\begin{aligned} &\psi(\underline{x}) \leq \phi(\underline{x}) \ , \\ &\psi(\lambda\underline{x} + (1-\lambda)\underline{y}) \leq \lambda\psi(\underline{x}) + (1-\lambda)\psi(\underline{y}) \ , \qquad 0 < \lambda < 1 \end{aligned} \tag{3.15}$$

Relations like eq. (3.14) have been derived [40)-42)] for the free energy per particle in a classical Van der Waals gas with interactions of the Kac type [43)], see also refs. 44 and 45 for an analogous treatment of the Ising model. For a more extensive discussion of related literature, see e.g. refs. 39, 46, 47. It may be noted that most treatments including Kac potentials are restricted to models of classical gases [40)-43)], Ising models [44),45),48)] and classical Heisenberg models [49),50)]; as far as quantummechanical systems are considered, only a few specific models have been treated [51),52)]. In the present chapter, eq. (3.14) will be proved for general hamiltonians of the type (3.1) containing analytic functions of a finite number of quantummechanical short-range operators.

From eq. (3.14) we derive in section 7 a generalization of eqs. (1.4) and (1.6). In the case of short-range operators, which can give rise to first-order transitions, the molecular-field equation is more complicated, since the average values of the operators $V_N^{(i)}$ may show discontinuities in the thermodynamic limit.

4. Convex functions.

In this section we prove the minimax-theorem (3.10) in the special case that P is a strongly convex function of n variables. The theorem can then be formulated as follows:

Let Ω_N be a sequence of systems described by the hamiltonian

$$\mathcal{H}_N = NR(\underline{V}_N), \tag{4.1}$$

where R is a strongly convex function of n variables satisfying the second inequality of (3.9) and the properties (2.30)-(2.34) with R, r and $\mathcal{R}$ instead of P, p and $\mathcal{P}$. The operators $V_N^{(i)}$, i=1,...,N, are uniformly bounded, cf. (2.29), and satisfy the short-range conditions (2.8), (2.10) and (2.11).

Then the free energy per particle f in the thermodynamic limit is given by

$$f = \max_{\underline{\eta}} f_t(\underline{\eta}), \tag{4.2}$$

where

$$f \equiv \lim_{N\to\infty} f_N[\mathcal{H}_N] \quad , \quad f_t(\underline{\eta}) \equiv \lim_{N\to\infty} f_N[\mathcal{H}_{t,N}(\underline{\eta})] \quad , \tag{4.3}$$

cf. (1.3) for the notation. The hamiltonian $\mathcal{H}_{t,N}(\underline{\eta})$ can be obtained linearizing $\mathcal{H}_N$ with respect to $\underline{V}_N$, i.e.

$$\mathcal{H}_{t,N}(\underline{\eta}) = N\{R(\underline{\eta}) + \underline{R}'(\underline{\eta})\cdot(\underline{V}_N-\underline{\eta})\} \quad . \tag{4.4}$$

In the proof of eq. (4.2) use will be made of two lemma's.

Lemma 1: Let $V^{(1)},\dots,V^{(n)}$ be a finite set of bounded hermitean operators. Let $P(\underline{V})$ be an analytic function of these operators, as defined in subsection 2.3. Let ρ be a density operator acting on the same Hilbert space as the operators V. Then, for all parameters $\underline{\eta}$ with $|\eta_i| \le M_i$, where $\underline{M}$ satisfies $M_i \ge \|V^{(i)}\|$, we have the inequality

$$|\mathrm{Tr}\ \rho\{P(\underline{V}) - P(\underline{\eta}) - P'(\underline{\eta})\cdot(\underline{V}-\underline{\eta})\}| \le p_2\ \mathrm{Tr}\ \rho(\underline{V}-\underline{\eta})^2 + p_3 \quad , \tag{4.5}$$

$$p_2 \equiv \tfrac{1}{2} \max_{\underline{e}} \left[\underline{e}\cdot\frac{\partial^2\mathcal{P}}{\partial\underline{\eta}\partial\underline{\eta}}\bigg|_{\underline{\eta}=\underline{M}}\cdot\underline{e}\right] \quad , \tag{4.6}$$

$$p_3 \equiv \frac{\partial^3\mathcal{P}}{\partial\underline{\eta}\partial\underline{\eta}\partial\underline{\eta}}\bigg|_{\underline{\eta}=\underline{M}} \vdots\ \underline{M}\ \|[\underline{V},\underline{V}]\| \quad , \tag{4.7}$$

where $\underline{e}$ is a real unit vector and $\mathcal{P}$ is defined as in eq. (2.34). For the details of the proof we refer to appendix A.

Lemma 2: Let $V_N^{(1)},\dots,V_N^{(n)}$ be a finite set of operators acting on an N-particle system, described by a hamiltonian $\mathcal{H}_N$, such that, for i.j=1,...,n,

$$\|V_N^{(i)}\| \le M_i \quad , \tag{4.8}$$

$$\|[V_N^{(i)}, V_N^{(j)}]\| = \varepsilon_{ij}(N) \quad , \tag{4.9}$$

$$\| [\mathcal{H}_N, V_N^{(i)}] \| = N\varepsilon_i(N) \ , \tag{4.10}$$

$$\varepsilon_{ij}(N) \to 0, \quad \varepsilon_i(N) \to 0, \quad \text{if} \quad N \to \infty \ . \tag{4.11}$$

Let $F(\underline{\nu})$ be an integrable function of n variables satisfying the continuity condition

$$|F(\underline{\nu}) - F(\underline{0})| \leq \sum_{i=1}^{n} F_i |\nu_i| \quad , \tag{4.12}$$

for some $F_i \geq 0$, $i=1,\dots,n$, and also the inequality

$$F(\underline{\nu}) \leq \langle P(\underline{V}_N)\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N} - P(\langle \underline{V}_N\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N}) \quad , \tag{4.13}$$

cf. (1.7) for the notation, for every value of $\underline{\nu}$, where P is an analytic function, as defined in subsection 2.3.

Then we have the inequality

$$F(\underline{0}) \leq c_N \ , \tag{4.14}$$

where

$$c_N \to 0, \quad \text{if } N \to \infty \ . \tag{4.15}$$

Eq. (4.14), which may be considered to be a generalization of the inequalities used in the derivation of the fundamental theorem in section 2 of chapter I, will be proved in appendix B.

We will now prove eq. (4.2) by deriving a lower and an upper bound to f, which will be equal to $f_t(\underline{\eta})$ in the thermodynamic limit.

<u>Lowerbound</u>: From the Bogoliubov-Peierls inequality, see eq. (2.5) of chapter I, it follows that

$$\begin{aligned} F(\underline{\nu}) &\equiv f_N[\mathcal{H}_{t,N}(\underline{\eta}) - N\underline{\nu}\cdot\underline{V}_N] - f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N] \\ &\leq - \langle R(\underline{V}_N) - R(\underline{\eta}) - \underline{R}'(\underline{\eta})\cdot(\underline{V}_N - \underline{\eta})\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N} \quad . \end{aligned} \tag{4.16}$$

Since R is a convex function,

$$R(\underline{\eta}) + \underline{R}'(\underline{\eta})\cdot(\langle \underline{V}_N\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N} - \underline{\eta}) \leq R(\langle \underline{V}_N\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N}) \quad , \tag{4.17}$$

so that

$$F(\underline{\nu}) \leq -\langle R(\underline{V}_N)\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N} + R(\langle \underline{V}_N\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N}) \quad , \tag{4.18}$$

for every value of $\underline{\nu}$.

For short-range operators $\underline{V}_N$ and the hamiltonian (4.1) the commutation relations (4.9)-(4.11) are satisfied, cf. appendix C. The lemma (4.14) applied to $F(\underline{\nu})$ in (4.16) then provides the lower bound

$$f_N[\mathcal{H}_N] - f_N[\mathcal{H}_{t,N}(\underline{\eta})] \geq c_N \quad , \tag{4.19}$$

where $c_N \to 0$, if $N \to \infty$, cf. (4.15).

Upper bound: In section 3(iv) of chapter I an upper bound was derived using the Bogoliubov-Peierls inequality, lemma 1 and the factorization property (1.12). This property could be proved easily in chapter I noting that the operator NV_N and the hamiltonian are sums of one-particle operators $V(k)$. Here, however, $N\underline{V}_N$ are short-range operators and the validity of an equation like (1.11) is not obvious. Yet, a factorization property seems to be a basic ingredient for the derivation of an upper bound. For that reason averages will be taken with respect to the hamiltonian $\mathcal{H}^0_{t,N}(\underline{\eta})$, which can be obtained from (4.4) replacing the $V_N^{(i)}$ by the corresponding operators $V_N^{0(i)}$, cf. (2.6), so that $\mathcal{H}^0_{t,N}(\underline{\eta})$ is a sum of operators acting on the Hilbert-spaces associated with the cubes $C_M(K)$ originating from the sub-division of the system Ω_N, cf. (2.1)-(2.5). Since the operators $NV_N^{(i)}$ occurring in $\mathcal{H}_{t,N}(\underline{\eta})$ are short-range operators, use can be made of the decomposition properties (2,7), (2.8) for each i, so that

$$\underline{V}_N = \underline{V}_N^0 + \underline{R}_N \ , \tag{4.20}$$

with

$$\| R_N^{(i)} \| \to 0, \quad \text{if } N \to \infty, \quad i=1,\dots,n, \tag{4.21}$$

and

$$\mathcal{H}_{t,N}(\underline{\eta}) = \mathcal{H}^0_{t,N}(\underline{\eta}) + N\underline{R}'(\underline{\eta})\cdot\underline{R}_N \ , \tag{4.22}$$

with

$$\mathcal{H}^0_{t,N}(\underline{\eta}) = N(R(\underline{\eta}) - \underline{\eta}\cdot\underline{R}'(\underline{\eta}) + \underline{R}'(\underline{\eta})\cdot\underline{V}_N^0) \ . \tag{4.23}$$

From the Bogoliubov-Peierls inequality it follows that

$$\begin{aligned} f_N[\mathcal{H}_N] &\leq f_N[\mathcal{H}^0_{t,N}(\underline{\eta})] + N^{-1}\langle\mathcal{H}_N - \mathcal{H}^0_{t,N}(\underline{\eta})\rangle_{\mathcal{H}^0_{t,N}(\underline{\eta})} \\ &\leq f_N[\mathcal{H}_{t,N}(\underline{\eta})] + N^{-1}\langle\mathcal{H}^0_N - \mathcal{H}^0_{t,N}(\underline{\eta})\rangle_{\mathcal{H}^0_{t,N}(\underline{\eta})} \\ &\quad + N^{-1}\|\mathcal{H}^0_{t,N}(\underline{\eta}) - \mathcal{H}_{t,N}(\underline{\eta})\| + N^{-1}\|\mathcal{H}_N - \mathcal{H}^0_N\| \ , \end{aligned} \tag{4.24}$$

where $\mathcal{H}_N^0 \equiv N h(\underline{V}_N^0)$, cf. (4.1). In view of the norm-estimates

$$N^{-1}\|\mathcal{H}_{t,N}^0(\underline{n}) - \mathcal{H}_{t,N}(\underline{n})\| \leq \underline{r}_1 \cdot \|\underline{R}_N\| \ , \quad N^{-1}\|\mathcal{H}_N - \mathcal{H}_N^0\| < \underline{r}_1 \cdot \|\underline{R}_N\| \quad , \tag{4.25}$$

with

$$\underline{r}_1 \equiv \frac{\partial \mathcal{R}}{\partial \underline{n}}\bigg|_{\underline{n}=\underline{M}} \quad , \tag{4.26}$$

cf. appendix C, and the lemma (4.5), with $\underline{V}_N^0$, R, r_2, $r_{3,N}$ instead of $\underline{V}$, P, p_2, p_3, we have

$$f_N[\mathcal{H}_N] \leq f_N[\mathcal{H}_{t,N}(\underline{n})] + r_2(\langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} - \underline{n})^2$$

$$+ r_2 \langle (\underline{V}_N^0 - \langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})})^2 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} + r_{3,N} + 2\underline{r}_1 \cdot \|\underline{R}_N\| \quad , \tag{4.27}$$

with $r_{3,N} \to 0$, $\underline{r}_1 \cdot \|\underline{R}_N\| \to 0$, if $N \to \infty$, cf. (4.7), (4.21). Since $N\underline{V}_N^0$ and $\mathcal{H}_{t,N}^0(\underline{n})$ are linear combinations of $M(N)\underline{V}_M^c(K)$, cf. (2.6), acting on the cubes $C_M(K)$, K=1,...,L(N), we have the factorization property

$$\langle \underline{V}_M^c(K)\underline{V}_M^c(K') \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} = \langle \underline{V}_M^c(K) \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} \langle \underline{V}_M^c(K') \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} \quad , \tag{4.28}$$

for different cubes K'≠K, and therefore

$$\langle (\underline{V}_N^0 - \langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})})^2 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} \leq \underline{M}^2/L(N) \to 0, \quad \text{if } N \to \infty. \tag{4.29}$$

From (4.27) and (4.29) we have the upper bound

$$f_N[\mathcal{H}_N] - f_N[\mathcal{H}_{t,N}(\underline{n})] \leq q_N + r_2(\langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} - \underline{n})^2 \quad , \tag{4.30}$$

with $q_N \to 0$, if $N \to \infty$.

From (4.30) and the lower bound (4.19) it follows that

$$c_N \leq f_N[\mathcal{H}_N] - \max_{\underline{n}} f_N[\mathcal{H}_{t,N}(\underline{n})] \leq q_N \ . \tag{4.31}$$

Here it has been used that, for each finite value of N, $\underline{n}$ may be chosen such that

$$\underline{n} = \langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})} \quad , \tag{4.32}$$

which is a consequence of a fixed-point theorem due to Brouwer [53], since the vector field $\phi(\underline{n}) = \langle \underline{V}_N^0 \rangle_{\mathcal{H}_{t,N}^0(\underline{n})}$ gives a continuous mapping of the region $|n_i| \leq M_i$, i=1,...,n, onto itself. In the thermodynamic limit (4.31) reduces to

$$f = \lim_{N\to\infty} \max_{\underline{\eta}} f_N[\mathcal{H}_{t,N}(\underline{\eta})] = \max_{\underline{\eta}} f_t(\underline{\eta}) \ , \tag{4.33}$$

which completes the proof of theorem (4.2).

Remark: The free energy per particle f is also given by

$$f = f_t(\underline{\eta}_m) \ , \tag{4.34}$$

$$\underline{\eta}_m = \lim_{N\to\infty} \langle \underline{V}_N \rangle_{\mathcal{H}_N} \ . \tag{4.35}$$

Proof: The function $f_t(\underline{\eta})$ is concave in $\underline{\eta}$, so that $f = \max f_t(\underline{\eta}) = f_t(\underline{\eta}_m)$ for some value $\underline{\eta}_m$. Since R is strongly convex, cf. (3.9), we can write

$$R(\underline{\eta}) = \varepsilon\underline{\eta}^2 + \tilde{R}(\underline{\eta}) \ , \tag{4.36}$$

in which $\varepsilon>0$ and $\tilde{R}(\underline{\eta})$ is convex for $|\eta_i| \leq M_i$. Following the line of reasoning leading to (4.19), (with $F(\underline{\nu}) - \varepsilon\langle(\underline{V}_N-\underline{\eta})^2\rangle$ and $\tilde{R}$ instead of $F(\underline{\nu})$ and R in (4.16)-(4.18)), we obtain

$$f_N[\mathcal{H}_N] - f_N[\mathcal{H}_{t,N}(\underline{\eta})] \geq c_N + \varepsilon\langle(\underline{V}_N-\underline{\eta})^2\rangle_{\mathcal{H}_N} \ , \tag{4.37}$$

which implies that $\underline{\eta}_m$ in (4.34) must satisfy (4.35).

5. Minimax theorem.

In this section the minimax theorem (3.10) will be proved using an extension of the fundamental theorem due to Bogoliubov Jr. This extension can be formulated as follows.

Let Ω_N be a sequence of systems described by the hamiltonian

$$\mathcal{H}_N = N\{T_N + Q(\underline{V}_N)\} \ , \tag{5.1}$$

where $Q(\underline{V}_N)$ is a strongly concave function of n variables satisfying the first inequality of (3.9) and the properties (2.30)-(2.34) with Q, q and $\mathcal{Q}$ instead of P, p and $\mathcal{P}$. The operators T_N and $\underline{V}_N$ satisfy the (commutation) properties, for i,j=1,...,n,

$$\| V_N^{(i)} \| \leq M_i \tag{5.2}$$

$$\| [V_N^{(i)}, V_N^{(j)}] \| = \varepsilon_{ij}(N) \ , \tag{5.3}$$

$$\| [T_N, V_N^{(i)}] \| = \varepsilon_i(N) \ , \tag{5.4}$$

$$\varepsilon_{ij}(N) \to 0, \quad \varepsilon_i(N) \to 0, \quad \text{if } N \to \infty. \tag{5.5}$$

Then the free energy per particle f in the thermodynamic limit is given by

$$f = \min_{\underline{\xi}} f_t(\underline{\xi}) \tag{5.6}$$

where

$$f = \lim_{N\to\infty} f_N[\mathcal{H}_N] \ , \quad f_t(\underline{\xi}) = \lim_{N\to\infty} f_N[\mathcal{H}_{t,N}(\underline{\xi})] \ , \tag{5.7}$$

$$\mathcal{H}_{t,N}(\underline{\xi}) = N\{T_N + Q(\underline{\xi}) + Q'(\underline{\xi}) \cdot (\underline{V}_N - \underline{\xi})\} \ . \tag{5.8}$$

The thermodynamic limit of $f_N[\mathcal{H}_{t,N}(\underline{\xi})]$ is assumed to exist for $|\xi_i| \leq M_i$.

Note that eq. (5.6) can be considered to be equivalent to eq. (3.10) for the special case of concave P=Q. For the validity of (5.6), however, only the commutation relations (5.3)-(5.5) are required and no short-range conditions are imposed on the operators $\underline{V}_N$. This will turn out to be an essential feature for the proof of eq. (3.10) for general P = Q+R.

Eq. (5.6) will be proved by deriving an upper and a lower bound for $f_N[\mathcal{H}_N]$ which turn out to be equal in the thermodynamic limit. (The special case of one variable has also been treated in ref. 54).

Upper bound: Using the Bogoliubov-Peierls inequality and the concavity of the function Q, we have

$$\begin{aligned} F(\underline{\nu}) &\equiv f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N] - f_N[\mathcal{H}_{t,N}(\underline{\xi}) - N\underline{\nu}\cdot\underline{V}_N] \\ &\leq \langle Q(\underline{V}_N) - Q(\underline{\xi}) - \underline{Q}'(\underline{\xi}) \cdot (\underline{V}_N - \underline{\xi})\rangle_{\mathcal{H}_{t,N}(\underline{\xi}) - N\underline{\nu}\cdot\underline{V}_N} \\ &\leq \langle Q(\underline{V}_N)\rangle_{\mathcal{H}_{t,N}(\underline{\xi}) - N\underline{\nu}\cdot\underline{V}_N} - Q(\langle \underline{V}_N\rangle_{\mathcal{H}_{t,N}(\underline{\xi}) - N\underline{\nu}\cdot\underline{V}_N}) \ . \end{aligned} \tag{5.9}$$

The lemma (4.14), applied to $F(\underline{\nu})$ in (5.9), gives

$$f_N[\mathcal{H}_N] - f_N[\mathcal{H}_{t,N}(\underline{\xi})] \leq c_N \ , \tag{5.10}$$

where $c_N \to 0$, if $N \to \infty$, cf. (4.15).

Lower bound: Using the Bogoliubov-Peierls inequality and the concavity of

Q, we have

$$F(\underline{\nu}) \equiv \min_{\underline{\xi}} f_N[\mathcal{H}_{t,N}(\underline{\xi}) - N\underline{\nu}\cdot\underline{V}_N] - f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N]$$
$$\leq \min_{\underline{\xi}} \langle Q(\underline{\xi}) + Q'(\underline{\xi})\cdot(\underline{V}_N-\underline{\xi}) - Q(\underline{V}_N)\rangle_{\mathcal{H}_N-N\underline{\nu}\cdot\underline{V}_N}$$
$$= -\langle Q(\underline{V}_N)\rangle_{\mathcal{H}_N-N\underline{\nu}\cdot\underline{V}_N} + Q(\langle\underline{V}_N\rangle_{\mathcal{H}_N-N\underline{\nu}\cdot\underline{V}_N}) , \tag{5.11}$$

and from the lemma (4.14) it follows that

$$f_N[\mathcal{H}_N] - \min_{\xi} f_N[\mathcal{H}_{t,N}(\underline{\xi})] \geq c'_N , \tag{5.12}$$

where $c'_N \to 0$, if $N\to\infty$.
Eq. (5.6) is now a direct consequence of (5.10) and (5.12).

<u>Remark</u>: Suppose that the minimum in (5.6) occurs at $\underline{\xi}=\underline{\xi}_m$, then

$$f = f_t(\underline{\xi}_m) , \tag{5.13}$$

and $\underline{\xi}_m$ must satisfy the implicit equation

$$\underline{\xi}_m = \lim_{N\to\infty} \langle\underline{V}_N\rangle_{\mathcal{H}_{t,N}(\underline{\xi}_m)} . \tag{5.14}$$

<u>Proof</u>: Since Q is strongly concave we can write

$$Q(\underline{\xi}) = -\varepsilon\underline{\xi}^2 + \tilde{Q}(\underline{\xi}) , \tag{5.15}$$

in which $\varepsilon>0$ and $\tilde{Q}$ is concave. Using (5.15) to derive an upper bound, we find (5.14).

We now proceed to prove the minimax theorem (3.10) for a sequence of systems described by the hamiltonian (3.1) with a general function P sarisfying eqs. (2.30)-(2.34), in which the operators $V_N^{(i)}$ are uniformly bounded and satisfy the short-range conditions (2.8), (2.10) and (2.11). Here we can take $\underline{h}=\underline{0}$ without loss of generality, since the operator $\underline{h}\cdot\underline{V}_N$ can be included in $P(\underline{V}_N)$.

Using the decomposition (3.8) the hamiltonian (3.1), with $\underline{h}=\underline{0}$, can be written

$$\mathcal{H}_N = N\{T_N + Q(\underline{V}_N)\} , \tag{5.16}$$

where

$$T_N = R(\underline{V}_N) , \tag{5.17}$$

and where the strongly concave function $Q(\underline{V}_N)$ and the strongly convex function $R(\underline{V}_N)$ satisfy the properties (2.30)-(2.34), (with Q, q, $\mathcal{Q}$ and R, r, $\mathcal{R}$ instead of P, p, $\mathcal{P}$).

For the set of operators T_N and $\underline{V}_N$ under consideration the (commutation) relations (5.2)-(5.5) are satisfied, cf. appendix C. From theorem (5.6) it then follows that the free energy per particle f in the thermodynamic limit is given by

$$f = \lim_{N\to\infty} f_N[\mathcal{H}_N] = \min_{\underline{\xi}} \lim_{N\to\infty} f_N[\mathcal{H}_{t,N}(\underline{\xi})] \ , \tag{5.18}$$

with

$$\mathcal{H}_{t,N}(\underline{\xi}) = N\left[Q(\underline{\xi}) - \underline{\xi}\cdot\underline{Q}'(\underline{\xi}) + R(\underline{V}_N) + \underline{Q}'(\underline{\xi})\cdot\underline{V}_N\right] \ . \tag{5.19}$$

From theorem (4.2) for convex functions of short-range operators we conclude that the free energy per particle f in the thermodynamic limit exists and is given by

$$f = \min_{\underline{\xi}} \max_{\underline{\eta}} \lim_{N\to\infty} f_N[\mathcal{H}_{t,N}(\underline{\xi},\underline{\eta})] \ , \tag{5.20}$$

with

$$\mathcal{H}_{t,N}(\underline{\xi},\underline{\eta}) = N\left[Q(\underline{\xi}) - \underline{\xi}\cdot\underline{Q}'(\underline{\xi}) + R(\underline{\eta}) - \underline{\eta}\cdot\underline{R}'(\underline{\eta}) + \{\underline{Q}'(\underline{\xi}) + \underline{R}'(\underline{\eta})\}\cdot\underline{V}_N\right] \ . \tag{5.21}$$

Eqs. (5.20), (5.21) are equivalent with (3.10), noting that a term $-N\underline{h}\cdot\underline{V}_N$ in the hamiltonian (3.1) can be present in $Q(\underline{V}_N)$ or $R(\underline{V}_N)$.

In the derivation use has been made of the validity of eq. (5.6) for a larger class of operators involving also nonlinear terms occurring in $R(\underline{V}_N)$ which do not satisfy the short-range conditions. However, these conditions have been used in an essential way in the derivation of the upper bound in theorem (4.2) for convex functions. In appendix D it is shown by an explicit example that eq. (5.20) cannot be valid with the same amount of generality as eq. (5.6), see also refs. 1 and 55.

6. Legendre transform.

In this section we derive eq. (3.11) which relates the free energy per particle of the hamiltonian (3.1) to the Legendre transform (3.12) of the reference free energy.

Substituting the inverse Legendre transformation of (3.12), i.e.

$$f_0(\underline{h}) = \inf_{\underline{m}} [- \underline{h}\cdot\underline{m} + g_0(\underline{m})] , \tag{6.1}$$

into the minimax theorem (3.10), we have

$$f(\underline{h}) = \min_{\underline{\xi}} \max_{\underline{\eta}} \inf_{\underline{m}} [- \underline{h}\cdot\underline{m} + g_0(\underline{m}) + \tilde{Q}(\underline{\xi},\underline{m}) + \tilde{R}(\underline{\eta},\underline{m})] , \tag{6.2}$$

with

$$\tilde{Q}(\underline{\xi},\underline{m}) = Q(\underline{\xi}) + \underline{Q}'(\underline{\xi})\cdot(\underline{m}-\underline{\xi}) , \tag{6.3}$$

$$\tilde{R}(\underline{\eta},\underline{m}) = R(\underline{\eta}) + R'(\underline{\eta})\cdot(\underline{m}-\underline{\eta}) . \tag{6.4}$$

The expression between brackets in the right-hand side of (6.2) is a convex function of $\underline{m}$, and has a unique maximum over $\underline{\eta}$. This follows from the strong convexity of $R(\underline{\eta})$, which implies that, for each $\underline{m}$, $\tilde{R}(\underline{\eta},\underline{m})$ has a uniquely determined maximum.

Under these conditions the maximum over $\underline{\eta}$ and the infimum over $\underline{m}$ in (6.2) can be interchanged [56], see also appendix E. Interchanging also the infimum over $\underline{m}$ and the minimum over $\underline{\xi}$, we find

$$f(\underline{h}) = \inf_{\underline{m}} [-\underline{h}\cdot\underline{m} + g_0(\underline{m}) + \tilde{P}(\underline{m})] , \tag{6.5}$$

with

$$\tilde{P}(\underline{m}) = \min_{\underline{\xi}} \max_{\underline{\eta}} [\tilde{Q}(\underline{\xi},\underline{m}) + \tilde{R}(\underline{\eta},\underline{m})] . \tag{6.6}$$

The minimum of $\tilde{Q}(\underline{\xi},\underline{m})$ occurs at $\underline{\xi}=\underline{m}$, (since $Q(\underline{\xi})$ is concave), and the maximum of $\tilde{R}(\underline{\eta},\underline{m})$ at $\underline{\eta}=\underline{m}$, so that

$$\tilde{P}(\underline{m}) = Q(\underline{m}) + R(\underline{m}) = P(\underline{m}) , \tag{6.7}$$

which completes the proof of (3.11).

7. Generalized molecular-field equation.

In this section we derive the generalization of the molecular-field equation (1.6), taking into account that here the reference hamiltonian (3.7) can be a short-range operator which can give rise to first-order phase transitions in the thermodynamic limit. Inserting the expression (3.12) for the Legendre transform g_0 in eq. (3.11), we have

$$f(\underline{h}) = \inf_{\underline{m}} \sup_{\underline{h}'} [(\underline{h}'-\underline{h})\cdot\underline{m} + f_0(\underline{h}') + P(\underline{m})] . \tag{7.1}$$

At fixed $\underline{m}$, the supremum in (7.1) occurs at $\underline{h}'=\underline{h}'(\underline{m})$ for which

$$\underline{h}'\cdot\underline{m} + f_0(\underline{h}') \geq \underline{h}''\cdot\underline{m} + f_0(\underline{h}'') , \tag{7.2}$$

for all values of $\underline{h}''$. With the notation $\underline{h}''=\underline{h}'+\nu\underline{e}$, with $\underline{e}$ any unit vector, (7.2) can be written

$$- [f_0(\underline{h}'+\nu\underline{e}) - f_0(\underline{h}')] \geq \nu\underline{e}\cdot\underline{m} . \tag{7.3}$$

Since f_0 is a concave function, its left and right derivatives with respect to ν exist and from (7.3) it follows that $\underline{h}'$ satisfies

$$\lim_{\nu\uparrow 0} - \frac{d}{d\nu} f_0(\underline{h}'+\nu\underline{e}) \leq \underline{e}\cdot\underline{m} \leq \lim_{\nu\downarrow 0} - \frac{d}{d\nu} f_0(\underline{h}'+\nu\underline{e}) , \tag{7.4}$$

for any unit vector $\underline{e}$.

The infimum in (7.1) occurs at those values of $\underline{m}$ for which

$$(\underline{h}'(\underline{m}) - \underline{h})\cdot\underline{m} + f_0(\underline{h}'(\underline{m})) + P(\underline{m}) \leq (\underline{h}'(\underline{m}') - \underline{h})\cdot\underline{m}' + f_0(\underline{h}'(\underline{m}')) + P(\underline{m}'), \tag{7.5}$$

for all values of $\underline{m}'$. Using (7.2), (with $\underline{h}'=\underline{h}'(\underline{m})$ and $\underline{h}''=\underline{h}'(\underline{m}')$), and the notation $\underline{m}'=\underline{m}+\nu\underline{e}$, with $\underline{e}$ any unit vector, (7.5) can be written

$$\nu\underline{e}\cdot\underline{h}'(\underline{m}+\nu\underline{e}) \geq \nu\underline{e}\cdot\underline{h} - P(\underline{m}+\nu\underline{e}) + P(\underline{m}) , \tag{7.6}$$

so that $\underline{m}$ satisfies

$$\lim_{\nu\uparrow 0} \underline{e}\cdot\underline{h}'(\underline{m}+\nu\underline{e}) \leq \underline{e}\cdot(\underline{h}-\underline{P}'(\underline{m})) \leq \lim_{\nu\downarrow 0} \underline{e}\cdot\underline{h}'(\underline{m}+\nu\underline{e}) , \tag{7.7}$$

for any unit vector $\underline{e}$. Eq. (7.7) implies that, for the values of $\underline{m}$ for which the infimum in (7.1) occurs, we may use for $\underline{h}'$ the value

$$\underline{h}' = \underline{h} - \underline{P}'(\underline{m}) . \tag{7.8}$$

In connection with this relation it may be noted that for systems with short-range interactions the function $\underline{h}'(\underline{m})$ defined by (7.4) is in general continuous [57),58)], in which case (7.8) is identical with (7.7).

Inserting (7.8) in the condition (7.4) for the supremum we obtain a necessary, but in general not sufficient, condition to determine the infimum. This condition which we call the generalized molecular-field equation reads

$$\lim_{\nu\uparrow 0} - \frac{d}{d\nu} f_0(\underline{h} - \underline{P}'(\underline{m}) + \nu\underline{e}) \leq \underline{e}\cdot\underline{m} \leq \lim_{\nu\downarrow 0} - \frac{d}{d\nu} f_0(\underline{h} - \underline{P}'(\underline{m}) + \nu\underline{e}) , \tag{7.9}$$

for any unit vector $\underline{e}$.

As a result the free energy $f(\underline{h})$ can be written

$$f(\underline{h}) = \min_{\underline{m}\in\mathcal{M}} [\, f_0(\underline{h} - \underline{P}'(\underline{m})) + P(\underline{m}) - \underline{m}\cdot\underline{P}'(\underline{m}) \,] , \tag{7.10}$$

where $\mathcal{M}$ is defined as the set of solutions $\underline{m}$ of eq. (7.9). Note that in eq. (7.10) the restriction $\underline{m}\in\mathcal{M}$ is necessary, since at the infimum over $\underline{m}$ in (7.1), eq. (7.8) gives a correct solution to the problem of taking the supremum over $\underline{h}'$, cf. e.g. remark i) of section 4 of chapter I for example. Furthermore, we need the minimalization procedure over the solutions $\underline{m}\in\mathcal{M}$, in order to exclude unphysical solutions of (7.9) which do not correspond to the infimum.

Eqs. (7.9) and (7.10) are identical to eqs. (2.41) and (2.42) derived in ref. 59, apart from some minor changes in notation. In this chapter, (7.9) and (7.10) have been derived starting from (3.11), or (3.14), so that these equations must also be valid in systems described by Kac-like long-range interactions, provided that the Legendre transform $g(\underline{m})$ of the free energy is given by a convex-envelope expression as in (3.14).

In the absence of first-order transitions (7.9) reduces to the implicit equation

$$\underline{m} = -\frac{\partial}{\partial \underline{h}} \; f_0(\underline{h} - \underline{P}'(\underline{m})) \;, \tag{7.11}$$

which can be considered as a molecular-field type of equation.

Remark: Eqs. (7.10) and (7.11) have some direct applications for time-independent correlation functions of normalized short-range operators. For this purpose we consider a system described by the hamiltonian

$$\mathcal{H}_N = N\{P(\underline{V}_N) + \lambda\Pi(\underline{V}_N)\} \;, \tag{7.12}$$

where $P(\underline{V}_N)$ and $\Pi(\underline{V}_N)$ are analytic functions of a finite number of normalized short-range operators and λ is a real parameter. The free energy per particle corresponding to $\mathcal{H}_N$ in the thermodynamic limit is given by, cf. (7.10),

$$\begin{aligned} f(\lambda) &\equiv \lim_{N\to\infty} f_N[N\{P(\underline{V}_N) + \lambda\Pi(\underline{V}_N)\}] \\ &= \min_{\underline{m}\in\mathcal{M}} \lim_{N\to\infty} f_N[N\{P(\underline{m}) + \underline{P}'(\underline{m})\cdot(\underline{V}_N-\underline{m}) + \lambda\Pi(\underline{m}) + \lambda\underline{\Pi}'(\underline{m})\cdot(\underline{V}_N-\underline{m})\}] . \end{aligned} \tag{7.13}$$

In the absence of first-order transitions $\underline{m}=\underline{m}(\lambda)\in\mathcal{M}$ satisfies the molecular-field equation (7.11). Taking the derivative with respect to λ, it follows that

$$\lim_{N\to\infty} \langle \Pi(\underline{V}_N)\rangle_{NP(\underline{V}_N)} = \left.\frac{df(\lambda)}{d\lambda}\right|_{\lambda=0} = \Pi(\underline{m}(0))$$

$$= \Pi(\lim_{N\to\infty} \langle \underline{V}_N\rangle_{NP'(\underline{m})\cdot\underline{V}_N}) = \Pi(\lim_{N\to\infty} \langle \underline{V}_N\rangle_{NP(\underline{V}_N)}) \quad , \tag{7.14}$$

cf. also (4.35), (5.14). Relations like (7.14) have also been established in an algebraic approach [0),61].

8. Dicke maser type of models.

In this section we consider the class of systems described by the hamiltonian

$$\mathcal{H}_N = \sum_k \omega_k a_k^\dagger a_k + \sqrt{N} \sum_k (\lambda_k^* a_k V_N^{(k)^\dagger} + \lambda_k a_k^\dagger V_N^{(k)}) + NT_N. \tag{8.1}$$

In (8.1) a_k and $a_k^\dagger$ are boson construction operators, i.e.

$$[a_k, a_\ell] = [a_k^\dagger, a_\ell^\dagger] = 0, \qquad [a_k, a_\ell^\dagger] = \delta_{k\ell}, \tag{8.2}$$

acting on the Hilbert space h_B. The normalized operators $T_N = T_N^\dagger$ and $V_N^{(k)}$ act on the Hilbert space h_N of an N particle system, and satisfy the (commutation) relations

$$\|V_N^{(k)}\| \leq M \ , \tag{8.3}$$

$$\|[V_N^{(k)}, V_N^{(\ell)}]\| \leq \varepsilon_a(N), \quad \|[V_N^{(k)^\dagger}, V_N^{(\ell)}]\| \leq \varepsilon_a(N) \ , \tag{8.4}$$

$$\|[T_N, V_N^{(k)}]\| \leq \varepsilon_b(N) \ , \tag{8.5}$$

$$\varepsilon_a(N),\ \varepsilon_b(N) \to 0, \quad \text{if } N\to\infty. \tag{8.6}$$

The hamiltonian $\mathcal{H}_N$ acts on the direct product Hilbert space $h_B \otimes h_N$, the constants ω_k and λ_k satisfy

$$\omega_k > 0, \quad \sum_k |\lambda_k| / \sqrt{\omega_k} < \infty . \tag{8.7}$$

The second condition in (8.7) is trivially satisfied if the number of modes k which are coupled to the N particle system is finite.

A special case of (8.1) is the Dicke maser model, in which

$$NT_N = \sum_{i=1}^{N} S_i^z \ , \quad NV_N^{(1)} = \sum_{i=1}^{N} S_i^- \ , \quad NV_N^{(1)^\dagger} = \sum_{i=1}^{N} S_i^+ \quad , \tag{8.8}$$

for one mode k=1, where $\vec{S}_i$ is the spin of particle i. This model has first been solved by Hepp and Lieb [7], see also ref. 62 for polynomial extensions.

For the general hamiltonian (8.1) Bogoliubov Jr. and Plechko [8], cf. also ref. 63, have proved a theorem which can be formulated as follows.

<u>Theorem</u>: The free energy per particle in the thermodynamic limit of the class of systems described by (8.1)-(8.7) is given by

$$\lim_{N\to\infty} f_N[\mathcal{H}_N] = \lim_{N\to\infty} f_N[\tilde{\mathcal{H}}_N] \ , \tag{8.9}$$

where

$$\tilde{\mathcal{H}}_N = \sum_k \omega_k a_k^\dagger a_k + N\{T_N - \sum_k \frac{|\lambda_k|^2}{\omega_k} V_N^{(k)^\dagger} V_N^{(k)}\} \ . \tag{8.10}$$

In (8.9) the traces are taken over the Hilbert space $h_B \otimes h_N$.

The free energy in the right-hand side of eq. (8.9) can be further evaluated applying the theorem (5.6), (using the decomposition $\underline{V}_N = \underline{V}_N' + i\underline{V}_N''$, with $\underline{V}_N'$ and $\underline{V}_N''$ hermitean). We first give a direct proof of eq. (8.9), deriving an upper and a lower bound for $f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N]$.

<u>Upper bound</u>: Consider the hamiltonian

$$\tilde{\mathcal{H}}_{N,\alpha} = \sum_k \omega_k (a_k^\dagger - \sqrt{N}\alpha_k^*)(a_k - \sqrt{N}\alpha_k) + N\{T_N - \sum_k \frac{|\lambda_k|^2}{\omega_k} V_N^{(k)^\dagger} V_N^{(k)}\} \ . \tag{8.11}$$

Since the (Bogoliubov) transformation

$$a_k \to a_k - \sqrt{N}\alpha_k, \qquad a_k^\dagger \to a_k^\dagger - \sqrt{N}\alpha_k^* \ , \tag{8.12}$$

is a canonical transformation, cf. e.g. refs. 64, 65, we have

$$f_N[\tilde{\mathcal{H}}_{N,\alpha}] = f_N[\tilde{\mathcal{H}}_N] \quad , \tag{8.13}$$

for any set of complex numbers $\{\alpha_k\}$. Applying the Bogoliubov-Peierls inequality it follows that

$$f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N] \leq N^{-1}\langle \mathcal{H}_N - \tilde{\mathcal{H}}_{N,\alpha}\rangle_{\tilde{\mathcal{H}}_{N,\alpha}}$$

$$= \sum_k \omega_k \langle (\frac{a_k^\dagger}{\sqrt{N}} - \alpha_k^*)(\frac{\lambda_k}{\omega_k} V_N^{(k)} + \alpha_k) + (\frac{\lambda_k^*}{\omega_k} V_N^{(k)^\dagger} + \alpha_k^*)(\frac{a_k}{\sqrt{N}} - \alpha_k)$$

$$+ (\frac{\lambda_k^*}{\omega_k} V_N^{(k)^\dagger} + \alpha_k^*)(\frac{\lambda_k}{\omega_k} V_N^{(k)} + \alpha_k)\rangle_{\tilde{\mathcal{H}}_{N,\alpha}}$$

$$= \sum_k \frac{|\lambda_k|^2}{\omega_k} \left\{\langle V_N^{(k)^\dagger} V_N^{(k)}\rangle_{\tilde{\mathcal{H}}_N} - \langle V_N^{(k)^\dagger}\rangle_{\tilde{\mathcal{H}}_N}\langle V_N^{(k)}\rangle_{\tilde{\mathcal{H}}_N}\right\} \quad . \tag{8.14}$$

In (8.14) we have used that

$$\langle \frac{a_k}{\sqrt{N}}\rangle_{\tilde{\mathcal{H}}_{N,\alpha}} = \langle \frac{a_k}{\sqrt{N}}\rangle_{\omega_k(a_k^\dagger - \sqrt{N}\alpha_k^*)(a_k - \sqrt{N}\alpha_k)} = \alpha_k \ , \tag{8.15}$$

and we have substituted for $\{\alpha_k\}$ the values

$$\alpha_k \equiv -\frac{\lambda_k}{\omega_k} \langle V_N^{(k)}\rangle_{\tilde{\mathcal{H}}_N} = -\frac{\lambda_k}{\omega_k}\langle V_N^{(k)}\rangle_{\tilde{\mathcal{H}}_{N,\alpha}} \quad . \tag{8.16}$$

Using a line of reasoning similar to the derivation of (4.14), see appendix F for further details, it follows from (8.14) that

$$f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N] \leq c_N \ , \tag{8.17}$$

with $c_N \to 0$, if $N \to \infty$.

<u>Lower bound</u>: Consider now the hamiltonian

$$\mathcal{H}_{N,x} = \sum_k x_k \omega_k a_k^\dagger a_k + N\{T_N - \sum_k \frac{|\lambda_k|^2}{(1-x_k)\omega_k} V_N^{(k)^\dagger} V_N^{(k)}\} \quad , \tag{8.18}$$

with $0 < x_k < 1$. Using the Bogoliubov-Peierls inequality we have

$$f_N[\mathcal{H}_N] - f_N[\mathcal{H}_{N,x}] \geq N^{-1}\langle \mathcal{H}_N - \mathcal{H}_{N,x}\rangle_{\mathcal{H}_N}$$

$$= \sum_k (1-x_k)\omega_k \langle (\frac{a_k^\dagger}{\sqrt{N}} + \frac{\lambda_k^*}{(1-x_k)\omega_k} V_N^{(k)^\dagger})(\frac{a_k}{\sqrt{N}} + \frac{\lambda_k}{(1-x_k)\omega_k} V_N^{(k)})\rangle_{\mathcal{H}_N} \geq 0 \ , \tag{8.19}$$

and therefore

$$f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N] \geq f_N[\mathcal{H}_{N,x}] - f_N[\tilde{\mathcal{H}}_N]$$

$$\geq - \sum_k \langle \frac{(1-x_k)\omega_k}{N} a_k^\dagger a_k + \frac{x_k |\lambda_k|^2}{(1-x_k)\omega_k} v_N^{(k)\dagger} v_N^{(k)} \rangle_{\mathcal{H}_{N,x}} \quad . \tag{8.20}$$

Inserting

$$\langle a_k^\dagger a_k \rangle_{\mathcal{H}_{N,x}} = (e^{\beta x_k \omega_k} - 1)^{-1} \leq \frac{1}{\beta x_k \omega_k} , \tag{8.21}$$

gives, cf. also (8.3) ,

$$f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N] \geq - \sum_k \left(\frac{1-x_k}{\beta x_k N} + \frac{x_k |\lambda_k|^2 M^2}{(1-x_k)\omega_k} \right). \tag{8.22}$$

Choosing for the set $\{x_k\}$ the values

$$\frac{x_k}{1-x_k} = \left(\frac{\omega_k}{\beta N |\lambda_k|^2 M^2} \right)^{\frac{1}{2}} , \tag{8.23}$$

we get the lower bound

$$f_N[\mathcal{H}_N] - f_N[\tilde{\mathcal{H}}_N] \geq - \sum_k \frac{2|\lambda_k| M}{\sqrt{\beta \omega_k N}} \equiv b_N , \tag{8.24}$$

with $b_N \to 0$, if $N \to \infty$, cf. (8.7).

The theorem (8.9) is now a direct consequence of eqs. (8.17) and (8.24).

Remark: Theorem (3.11) can be used to obtain various further evaluations of the free energy of Dicke maser type of models.

Consider e.g. the hamiltonian

$$\mathcal{H}_N = \sum_k \omega_k a_k^\dagger a_k + \sqrt{N} \left\{ a_0 Q^\dagger(\underline{V}_N) + a_0^\dagger Q(\underline{V}_N) \right\} + N \left\{ P(\underline{V}_N) - \underline{h} \cdot \underline{V}_N \right\} , \tag{8.25}$$

where $N\underline{V}_N \equiv (NV_N^{(1)}, \ldots, NV_N^{(n)})$ are hermitean short-range operators satisfying (2.8),(2.10), (2.11) and P and Q are analytic functions, cf. (2.30)-(2.34), Q not necessarily being a real function.

Then the free energy per particle in the thermodynamic limit can be written

$$f(\underline{h}) = \inf_{\underline{m}} [-\underline{h} \cdot \underline{m} + g_0(\underline{m}) + P(\underline{m}) - |Q(\underline{m})|^2/\omega_0] + f_b \quad , \tag{8.26}$$

where f_b is the free energy per particle corresponding to $\sum_k \omega_k a_k^\dagger a_k$ and $g_0(\underline{m})$ is the Legendre transform (3.12) of the free energy per particle $f_0(\underline{h})$

corresponding to the short-range hamiltonian $-N\underline{h}\cdot\underline{V}_N$.

Eq. (8.26) can be derived from (8.9), with $\lambda_k=0$ if $k\neq 0$, noting that the operators $P(\underline{V}_N)$ and $Q(\underline{V}_N)$ for short-range interactions $(NV_N^{(1)},\ldots,NV_N^{(n)})$ satisfy the requirements (8.3)-(8.6) imposed on the operators in (8.1). Then

$$f(\underline{h}) = \lim_{N\to\infty} f_N[\tilde{\mathcal{H}}_N] \,, \tag{8.27}$$

where

$$\tilde{\mathcal{H}}_N = \sum_k \omega_k a_k^\dagger a_k + N\{P(\underline{V}_N) - Q^\dagger(\underline{V}_N)Q(\underline{V}_N)/\omega_0 - \underline{h}\cdot\underline{V}_N\} \tag{8.28}$$

and eq. (8.26) follows as a direct consequence of (8.27), (8.28) and (3.11).

Eq. (8.26) also holds when the operators $\underline{V}_N$ in (8.25) are not short-range, but satisfy the (commutation) relations (5.2)-(5.5), in the case that $P(\underline{m}) - |Q(\underline{m})|^2/\omega_0$ is strongly concave, cf. (5.6).

Appendix A.

In this appendix the proof of the lemma (4.5)-(4.7) will be given. We start with an analytic function $P(\underline{V})$, as defined in section 2.3, and an arbitrary density operator ρ. Then we apply Taylor's theorem with Lagrange's form for the remainder, i.e.

$$\phi(t) = \phi(0) + t\phi'(0) + \tfrac{1}{2}t^2\phi''(\tau) \,, \tag{A.1}$$

for some value τ with $0 < \tau < t$, to the function

$$\phi(t) \equiv \mathrm{Tr}\ \rho P(\underline{V}_t) \,, \tag{A.2}$$

where

$$\underline{V}_t \equiv \underline{n} + t(\underline{V}-\underline{n}) \,. \tag{A.3}$$

Choosing $t=1$, we have

$$X \equiv \mathrm{Tr}\ \rho\{P(\underline{V}) - P(\underline{n}) - \underline{P}'(\underline{n})\cdot(\underline{V}-\underline{n})\} = \tfrac{1}{2}\,\mathrm{Tr}\left\{\rho\,\frac{d^2}{dt^2}P(\underline{V}_t)\Big|_{t=\tau}\right\} \,, \tag{A.4}$$

for some τ with $0 < \tau < 1$.

According to (2.30) we write

$$P(\underline{V}_t) = \sum_{m=1}^{\infty} \sum_{i_1,\ldots,i_m=1}^{n} p(i_1,\ldots,i_m)\, V_t^{(i_1)}\ldots V_t^{(i_m)} \,, \tag{A.5}$$

so that in view of eq. (A.3)

$$\tfrac{1}{2}\frac{d^2}{dt^2}P(\underline{V}_t) = \sum_{m=2}^{\infty}\sum_{i_1,\ldots,i_m=1}^{n} p(i_1,\ldots,i_m)\sum_{a=1}^{m-1}\sum_{b=a+1}^{m}\left(\prod_{\ell=1}^{a-1} V_t^{(i_\ell)}\right)$$

$$\times\,(V^{(i_a)}-\eta_{i_a})\left(\prod_{\ell=a+1}^{b-1} V_t^{(i_\ell)}\right)(V^{(i_b)}-\eta_{i_b})\left(\prod_{\ell=b+1}^{m} V_t^{(i_\ell)}\right) \quad . \tag{A.6}$$

We now shift the factor $(V^{(i_a)}-\eta_{i_a})$ to the left and the factor $(V^{(i_b)}-\eta_{i_b})$ to the right. This leads to

$$\tfrac{1}{2}\frac{d^2}{dt^2}P(\underline{V}_t)\bigg|_{t=\tau} = (\underline{V}-\underline{\eta})\cdot\underline{\underline{P}}^{(2)}\cdot(\underline{V}-\underline{\eta}) + P^{(3)} \ , \tag{A.7}$$

where

$$P^{(2)}_{ij} = \sum_{m=2}^{\infty}\sum_{i_1,\ldots,i_m=1}^{n} p(i_1,\ldots,i_m)\sum_{a=1}^{m-1}\sum_{b=a+1}^{m}\delta_{i,i_a}\delta_{j,i_b}\left(\prod_{\substack{\ell=1\\ \ell\neq a,b}}^{m} V_\tau^{(i_\ell)}\right). \tag{A.8}$$

The contribution arising from $P^{(3)}$ can be estimated as follows:

$$|\mathrm{Tr}\,\rho P^{(3)}| \leqslant \|P^{(3)}\| \leqslant \sum_{m=3}^{\infty}\sum_{i_1,\ldots,i_m=1}^{n} |p(i_1,\ldots,i_m)|$$

$$\times\left\{\sum_{a=2}^{m-1}\sum_{b=a+1}^{m}\sum_{c=1}^{a-1}\|[V^{(i_c)},V^{(i_a)}]\|\,\|V^{(i_b)}-\eta_{i_b}\|\left(\prod_{\substack{\ell=1\\ \ell\neq a,b,c}}^{m}\|V_\tau^{(i_\ell)}\|\right)\right.$$

$$\left.+\sum_{a=1}^{m-2}\sum_{b=a+1}^{m-1}\sum_{c=b+1}^{m}\|V^{(i_a)}-\eta_{i_a}\|\,\|[V^{(i_b)},V^{(i_c)}]\|\left(\prod_{\substack{\ell=1\\ \ell\neq a,b,c}}^{m}\|V_\tau^{(i_\ell)}\|\right)\right\}$$

$$\leqslant \sum_{m=3}^{\infty}\sum_{i_1,\ldots,i_m=1}^{n} |p(i_1,\ldots,i_m)|$$

$$\times\ \tfrac{1}{2}\sum_{a\neq b\neq c\neq a}\left(\prod_{\ell\neq a,b,c}\|V_\tau^{(i_\ell)}\|\right)\|V^{(i_a)}-\eta_{i_a}\|\,\|[V^{(i_b)},V^{(i_c)}]\|$$

$$\leqslant \frac{\partial^3\mathcal{P}}{\partial\underline{\eta}\partial\underline{\eta}\partial\underline{\eta}}\bigg|_{\underline{\eta}=\underline{M}} \vdots\ \underline{M}\ \|[\underline{V},\underline{V}]\| \equiv p_3, \tag{A.9}$$

cf. (2.29), (2.33), (2.34). Note that the last line of eq. (A.9) is identical to (4.7).

We now proceed to derive an inequality for the quantity X defined by

(A.4). From (A.7) and (A.9) we have

$$|X| \leq \text{Tr}\ \rho(\underline{V}-\underline{\eta})\cdot\underline{\underline{P}}^{(2)}\cdot(\underline{V}-\underline{\eta})| + p_3$$

$$\leq \sum_{i,j=1}^{n} |\text{Tr}\ \rho(V^{(i)}-\eta_i)\ P_{ij}^{(2)}\ (V^{(j)}-\eta_j)| + p_3\ . \qquad \text{(A.10)}$$

The first term in the right-hand side of (A.10) can be estimated using the Schwarz inequality

$$|\text{Tr ABC}| \leq (\text{Tr}\ A^\dagger A)^{\frac{1}{2}}\{\text{Tr}\ C^\dagger(B^\dagger B)C\}^{\frac{1}{2}} \leq (\text{Tr}\ A^\dagger A)^{\frac{1}{2}}\ \|B\|\ (\text{Tr}\ C^\dagger C)^{\frac{1}{2}}, \qquad \text{(A.11)}$$

with

$$A = \rho^{\frac{1}{2}}(V^{(i)}-\eta_i), \quad B = P_{ij}^{(2)}, \quad C = (V^{(j)}-\eta_j)\rho^{\frac{1}{2}}\ . \qquad \text{(A.12)}$$

We then have

$$|X| \leq \sum_{i,j=1}^{n} \left[\{\text{Tr}\ \rho(V^{(i)}-\eta_i)^2\}^{\frac{1}{2}}\ \|P_{ij}^{(2)}\|\ \{\text{Tr}\ \rho(V^{(j)}-\eta_j)^2\}^{\frac{1}{2}}\right] + p_3\ , \qquad \text{(A.13)}$$

where

$$P_{ij}^{(2)} \leq \frac{1}{2}\ \frac{\partial^2 \mathcal{P}}{\partial\eta_i\partial\eta_j}\bigg|_{\underline{\eta}=\underline{M}} \equiv p_{ij}^{(2)}\ , \qquad \text{(A.14)}$$

cf. (2.29), (2.33), (2.34) and (A.8). From (A.13) and (A.14) we conclude

$$|X| \leq p_2\ \{\sum_{i=1}^{n} \text{Tr}\ \rho(V^{(i)}-\eta_i)^2\} + p_3\ , \qquad \text{(A.15)}$$

where p_2 is the largest eigenvalue of the matrix $p_2^{(2)}$. Hence, the lemma (4.5)-(4.7) has been proved.

Appendix B.

In this appendix we prove eq. (4.14), using the (commutation) relations (4.8)-(4.11), which can be written as

$$\|V_N^{(i)}\| \leq M, \quad \|[V_N^{(i)},V_N^{(j)}]\| \leq \varepsilon_a(N), \quad \|[\mathcal{H}_N,V_N^{(i)}]\| \leq N\varepsilon_b(N)\ ,$$
$$\varepsilon_a(N), \quad \varepsilon_b(N) \to 0, \quad \text{if } N\to\infty, \qquad \text{(B.1)}$$

and also the inequalities (4.12) and (4.13).
From (4.13) and the lemma (4.5) we have

$$F(\underline{\nu}) \leq p_{3,N} + \sum_{i=1}^{n} p_2\langle (V_N^{(i)} - \langle V_N^{(i)}\rangle_{\mathcal{H}_N-N\underline{\nu}\cdot\underline{V}_N})^2\rangle_{\mathcal{H}_N-N\underline{\nu}\cdot\underline{V}_N}, \qquad \text{(B.2)}$$

where p_2 and $p_{3,N}$ are independent of $\underline{\nu}$, and $p_{3,N} \to 0$, if $N \to \infty$, cf. (4.6), (4.7), (B.1). Applying eqs. (2.16) and (2.18) of chapter I to the auto-correlation function in (B.2), we have

$$F(\underline{\nu}) \leq p_{3,N} + \sum_{i=1}^{n} p_2 \left[\frac{1}{\beta N} \{- \frac{\partial^2}{\partial \nu_i^2} f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N]\} + \right.$$

$$\left. + \sqrt{\tfrac{1}{2}N\tilde{\varepsilon}(N)}\, \{- \frac{\partial^2}{\partial \nu_i^2} f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N]\}^{\frac{1}{2}}\right], \tag{B.3}$$

where we have also used the estimate, cf. (B.1).

$$\langle [V_N^{(i)}, [\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N, V_N^{(i)}]]\rangle_{\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N}$$

$$\leq 2NM \left\{\varepsilon_b(N) + \sum_{j=1}^{n} \ell_j \varepsilon_a(N)\right\} = 2NM\tilde{\varepsilon}(N) , \tag{B.4}$$

restricting $\underline{\nu}$ to the interval $0 \leq \nu_i \leq \ell_i$, for $i=1,\ldots,n$, where $\ell_1,\ldots,\ell_n$ are arbitrary positive constants. Note that $\tilde{\varepsilon}(N) \to 0$, if $N \to \infty$, independent of $\underline{\nu}$.

As a consequence of the mean value theorem we have

$$\left(\prod_{i=1}^{n} \ell_i\right)^{-1} \int_0^{\ell_1} d\nu_1 \ldots \int_0^{\ell_n} d\nu_n\, F(\underline{\nu}) = F(\underline{\nu}_0), \tag{B.5}$$

for some vector $\underline{\nu}_0$ with $0 \leq \nu_{0,i} \leq \ell_i$. From (B.5) and (4.12) we have the inequality

$$F(\underline{0}) \leq \sum_{i=1}^{n} F_i \ell_i + \left(\prod_{i=1}^{n} \ell_i\right)^{-1} \int_0^{\ell_1} d\nu_1 \ldots \int_0^{\ell_n} d\nu_n\, F(\underline{\nu}) . \tag{B.6}$$

Applying (B.3) to the $F(\underline{\nu})$ in (B.6), and using the Schwarz inequality for integrals and (B.1), i.e.

$$\int_0^{\ell_i} d\nu_i \{- \frac{\partial^2}{\partial \nu_i^2} f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N]\}^{\frac{1}{2}} \leq \sqrt{\ell_i} \left[\int_0^{\ell_i} d\nu_i \{- \frac{\partial^2}{\partial \nu_i^2} f_N[\mathcal{H}_N - N\underline{\nu}\cdot\underline{V}_N]\}\right]^{\frac{1}{2}}$$

$$\leq \sqrt{2M\ell_i} , \tag{B.7}$$

we obtain

$$F(\underline{0}) \leq p_{3,N} + \sum_{i=1}^{n} \left[F_i \ell_i + p_2 M \left\{\frac{2}{\beta N \ell_i} + \left(\frac{\tilde{\varepsilon}(N)}{\ell_i}\right)^{\frac{1}{2}}\right\}\right]. \tag{B.8}$$

So far $\ell_1,\ldots,\ell_n$ are arbitrary positive constants. Choosing the ℓ_i such that

$$\ell_i \equiv \ell(N) = \max\left\{\left(\frac{2p_2}{\beta N}\right)^{\frac{1}{2}},\ (p_2^2\ \tilde{\varepsilon}(N))^{\frac{1}{3}}\right\}, \tag{B.9}$$

we have

$$F(\underline{0}) \leq p_{3,N} + \sum_{i=1}^{n} (F_i+2M)\ell(N) \equiv c_N, \tag{B.10}$$

and eqs. (4.14) and (4.15) have been proved.

Appendix C.

In this appendix we treat some properties of the normalized short-range operators $V_N^{(i)}$, $i=1,\ldots,n$, defined in section 2.1. We first derive the commutation relations

$$\| [V_N^{(i)}, V_N^{(j)}] \| = \varepsilon_{ij}(N) \to 0, \quad \text{if } N\to\infty. \tag{C.1}$$

Using the decomposition (2.6)-(2.8) of the operators $\underline{V}_N$, i.e.

$$\underline{V}_N = \underline{V}_N^0 + \underline{R}_N, \quad \underline{V}_N^0 = N^{-1}\sum_{K=1}^{L(N)} M(N)\underline{V}_M^c(K),$$
$$\|\underline{R}_N\| \to 0, \quad \text{if } N\to\infty, \tag{C.2}$$

and the norm estimates

$$\|V_N^{(i)}\| \leq M_i, \quad \|V_N^{0(i)}\| \leq M_i, \quad (i=1,\ldots,n), \tag{C.3}$$

which hold for sufficiently large M_i, we have

$$\begin{aligned}\|[V_N^{(i)}, V_N^{(j)}]\| = \Big\| \Big\{ & L(N)^{-2}\sum_{K=1}^{L(N)} [V_M^{c(i)}(K), V_M^{c(j)}(K)] \\ & + [V_N^{0(i)}, R_N^{(j)}] + [R_N^{(i)}, V_N^{0(j)}] + [R_N^{(i)}, R_N^{(j)}]\Big\}\Big\| \\ & \leq 2\Big\{L(N)^{-1}M_iM_j + M_i\|R_N^{(j)}\| + M_j\|R_N^{(i)}\| + \|R_N^{(i)}R_N^{(j)}\|\Big\},\end{aligned} \tag{C.4}$$

which proves (C.1), cf. (2.3) and (C.2).

As a corollary we have the commutation relations

$$\|[R(\underline{V}_N), V_N^{(i)}]\| = \varepsilon_i(N) \to 0, \quad \text{if } N\to\infty, \tag{C.5}$$

where $R(\underline{V}_N)$ is an analytic function of n variables, defined in section 2.3. Equation (C.5) follows from (2.30), (2.33) and (2.34), (with R, r, $\mathcal{R}$

instead of P, p, $\mathcal{P}$), which lead to

$$\|[R(\underline{V}_N),\, V_N^{(i)}]\| \leq \sum_{m=1}^{\infty} \sum_{\ell=1}^{m} \sum_{i_1,\ldots,i_m=1}^{n} |r(i_1,\ldots,i_m)|$$

$$\times \left(\prod_{a=1}^{\ell-1} M_{i_a}\right) \|[V_N^{(i_\ell)},\, V_N^{(i)}]\| \left(\prod_{b=\ell+1}^{m} M_{i_b}\right)$$

$$= \sum_{j=1}^{n} r_{1,j} \|[V_N^{(j)},\, V_N^{(i)}]\| \;, \tag{C.6}$$

with

$$\underline{r}_1 \equiv \frac{\partial \mathcal{R}}{\partial \underline{\eta}}\bigg|_{\underline{\eta}=\underline{M}} \tag{C.7}$$

Finally, a second inequality involving $\underline{r}_1$ has been used in eq. (4.25), i.e.

$$\|R(\underline{V}_N) - R(\underline{V}_N^0)\| \leq \sum_{m=1}^{\infty} \sum_{\ell=1}^{m} \sum_{i_1,\ldots,i_m=1}^{n} |r(i_1,\ldots,i_m)|$$

$$\times \left(\prod_{a=1}^{\ell-1} M_{i_a}\right) \|R_N^{(i_\ell)}\| \left(\prod_{b=\ell+1}^{m} M_{i_b}\right) = \underline{r}_1 \cdot \|\underline{R}_N\| \;. \tag{C.8}$$

Appendix D.

In order to see that (5.20) or (3.10) does not hold under the same general conditions for operators as (5.6), we consider the hamiltonian

$$\mathcal{H}_N = N(T_N + wW_N^2), \quad (w > 0) \;, \tag{D.1}$$

where T_N and W_N are general operators satisfying eqs. (5.2)-(5.5). From the Bogoliubov-Peierls inequality it follows that

$$f = \lim_{N\to\infty} f_N[\mathcal{H}_N] \geq g \;, \tag{D.2}$$

with

$$g = \max_{\eta} \lim_{N\to\infty} f_N[N(T_N + 2\eta w W_N - w\eta^2)] \;, \tag{D.3}$$

assuming that the thermodynamic limits in (D.2) and (D.3) exist. If T_N and W_N are short-range operators we can apply (5.20), (or (4.2)). As a result we would have f=g.

In general, however, f can be larger than g, even if the thermodynamic limits in (D.2) and (D.3) exist, i.e.

$$f > g \, , \tag{D.4}$$

which implies that the theorem (3.10) cannot be extended to more general operators satisfying (5.2)-(5.5).

As an example of (D.1) we consider the hamiltonian

$$\mathcal{H}_N = N(-vV_N^2 + wW_N^2), \quad (v,w > 0; \quad T_N = -vV_N^2) \, , \tag{D.5}$$

where V_N and W_N are normalized short-range operators. From (D.3) and (5.6) it follows that

$$g = \max_{\eta} \min_{\xi} \phi(\xi,\eta) \, , \tag{D.6}$$

with

$$\phi(\xi,\eta) = \lim_{N\to\infty} f_N[N(-2\xi vV_N + v\xi^2 + 2\eta wW_N - w\eta^2)] \quad . \tag{D.7}$$

On the other hand, from (3.10) it follows that

$$f = \min_{\xi} \max_{\eta} \phi(\xi,\eta) \, . \tag{D.8}$$

The operators V_N and W_N can be chosen in such a way that (D.6) and (D.8) lead to the inequality (D.4), which implies that (3.10) is not valid for the hamiltonian (D.1) with the operator $T_N = -vV_N^2$.

Explicit examples have been given in refs. 1, 55. A very simple example can be obtained choosing

$$V_N = W_N = N^{-1} \sum_{k=1}^{N} \sigma_k, \quad w > v > 0 \, , \tag{D.9}$$

where $\sigma_k = \pm 1$ refers to the spin of particle k. In this case we have

$$\phi(\xi,\eta) = v\xi^2 - w\eta^2 - \beta^{-1} \ln 2 \cosh 2\beta(v\xi - w\eta) \, . \tag{D.10}$$

For sufficiently low temperatures, (i.e. $2\beta v > 1$), the absolute minimum over ξ of $\phi(\xi,\eta)$ occurs for (ξ,η)-values such that

$$|\xi| > \xi_1 \, , \quad 2\beta w\eta = 2\beta v\xi - \operatorname{artanh} \xi, \tag{D.11}$$

where ξ_1 is the positive solution of $2\beta v\xi_1 = \operatorname{artanh} \xi_1$. The absolute maximum over η occurs for (ξ,η) such that

$$2\beta v\xi = 2\beta w\eta + \operatorname{artanh} \eta \, . \tag{D.12}$$

Since the curves in eqs. (D.11) and (D.12) do not intersect, the function ϕ

does not have a saddle-point and therefore $f>g$. (The equality $f=g$ would imply the existence of a saddle-point, see e.g. lemma (36.2) of ref. 38). Explicitly we have

$$f = -\beta^{-1} \ln 2 > g = v\xi_1^2 - \beta^{-1} \ln 2 \cosh 2\beta v \xi_1 \ . \tag{D.13}$$

In eq. (D.13) it has been used that the min-max of ϕ occurs at $\xi=\eta=0$ and the max-min at $\xi=\xi_1$, $\eta=0$.

Appendix E.

In this appendix we give a proof of the following theorem [56].

Theorem: Let $K(x,y)$ be a continuous function of the variables $x \equiv (x_1,\ldots,x_p)$, $y \equiv (y_1,\ldots,y_q)$, for each $x \in X$, $y \in Y$, with X and Y bounded regions in the x and y space. Let K have a unique maximum at $x = u(y) \in X$, for each $y \in Y$, and a unique minimum at $y = v(x) \in Y$, for each $x \in X$. Then

$$\max_x \min_y K(x,y) = \min_y \max_x K(x,y) \ , \tag{E.1}$$

with the maximum and minimum taken over $x \in X$, $y \in Y$.

Proof : From Brouwer's fixed point theorem [53] it follows that the set of equations

$$\begin{aligned} x &= u(y) \\ y &= v(x) \end{aligned} \tag{E.2}$$

has a solution $(\bar{x},\bar{y})$ which is a saddle-point of K, i.e.

$$K(x,\bar{y}) \leq K(\bar{x},\bar{y}) \leq K(\bar{x},y) \ , \tag{E.3}$$

for each $x \in X$, $y \in Y$, cf. e.g. ref. 38. Using the notation

$$f(x) \equiv \min_y K(x,y) \ , \quad g(y) \equiv \max_x K(x,y) \ , \tag{E.4}$$

it follows from (E.3) that

$$\max_x f(x) \geq f(\bar{x}) = K(\bar{x},\bar{y}) = g(\bar{y}) \geq \min_y g(y) \ . \tag{E.5}$$

Since $f(x) \leq K(x,y) \leq g(y)$ for each $x \in X$, $y \in Y$, we also have

$$\max_x f(x) \leq \min_y g(y) \ , \tag{E.6}$$

and therefore

$$\max_x \min_y K(x,y) = \max_x f(x) = K(\bar{x},\bar{y}) = \min_y g(y) = \min_y \max_x K(x,y) \ . \tag{E.7}$$

Remark: Eq. (E.1) also holds when the maximum of $K(x,y)$ over x occurs at a convex set $U(y) \subset X$, for each $y \in Y$, (and the minimum over y at a convex set $V(x) \subset Y$, for each $x \in X$) , instead of a unique point $u(y)$, (and $v(x)$), see ref. 56.

Appendix F.

In this appendix we prove eq. (8.17). From eq. (8.14), using the replacement, $(\alpha=1,2)$,

$$T_N \to T_N - \sum_{\alpha,k} \nu_{\alpha,k} V_N^{(\alpha,k)} , \tag{F.1}$$

with

$$V_N^{(1,k)} = \tfrac{1}{2}(V_N^{(k)\dagger} + V_N^{(k)}), \quad V_N^{(2,k)} = \tfrac{1}{2}i(V_N^{(k)\dagger} - V_N^{(k)}) \quad , \tag{F.2}$$

we have the inequality

$$F[\{\nu_{\alpha,k}\}] \equiv f_N[\mathcal{H}_{N,\nu}] - f_N[\tilde{\mathcal{H}}_{N,\nu}]$$
$$\leq p_{3,N} + \sum_{\alpha,k} \frac{|\lambda_k|^2}{\omega_k} \langle (V_N^{(\alpha,k)} - \langle V_N^{(\alpha,k)}\rangle_{\tilde{\mathcal{H}}_{N,\nu}})^2 \rangle_{\tilde{\mathcal{H}}_{N,\nu}} , \tag{F.3}$$

with

$$\mathcal{H}_{N,\nu} = \mathcal{H}_N - N \sum_{\alpha,k} \nu_{\alpha,k} V_N^{(\alpha,k)} , \tag{F.4}$$

$$\tilde{\mathcal{H}}_{N,\nu} = \tilde{\mathcal{H}}_N - N \sum_{\alpha,k} \nu_{\alpha,k} V_N^{(\alpha,k)} , \tag{F.5}$$

$$p_{3,N} = \sum_k \frac{|\lambda_k|^2}{\omega_k} \langle i[V_N^{(1,k)}, V_N^{(2,k)}] \rangle_{\tilde{\mathcal{H}}_{N,\nu}} . \tag{F.6}$$

Using also the inequality

$$|F(\{\nu_{\alpha,k}\}) - F(\{0\})| \leq \sum_{\alpha,k} F_{\alpha,k} |\nu_{\alpha,k}| , \tag{F.7}$$

(with $F_{\alpha,k} \leq 2M$, cf. (8.3)), we have, following the same line of reasoning as in the derivation leading from eq. (B.2) to (B.10) in appendix B,

$$F(\{0\}) \leq \sum_{\alpha,k} (F_{\alpha,k} + 2M)\ell_k(N) \equiv c_N \; , \tag{F.8}$$

with

$$\ell_k(N) = \max \left\{ \left(\frac{2|\lambda_k|^2}{\beta\omega_k N}\right)^{\frac{1}{2}} , \left(\frac{|\lambda_k|^4}{\omega_k^2} \tilde{\varepsilon}(N)\right)^{\frac{1}{3}} \right\} \; , \tag{F.9}$$

$$\tilde{\varepsilon}(N) = \tilde{\varepsilon}_b(N) + \sum_{\alpha,k} \ell_k(N)\varepsilon_a(N) \; , \tag{F.10}$$

$$\tilde{\varepsilon}_b(N) = \varepsilon_b(N) + \sum_k \frac{|\lambda_k|^2}{\omega_k} 2M\varepsilon_a(N) \; , \tag{F.11}$$

cf. (8.3)-(8.5), (8.7).

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CHAPTER III

STABILITY OF CRITICAL BEHAVIOUR, CRITICAL-EXPONENT RENORMALIZATION AND FIRST-ORDER TRANSITIONS

1. Introduction

When one considers a compressible (Ising) ferromagnet, the critical behaviour will be unstable. Two types of instabilities have been discussed extensively in the literature; there can be first-order transitions or a continuous transition with renormalized critical exponents.

The first-order transitions have been discussed first by Rice[1]) and Domb[2]) on the basis of an instability (i.e. a negative value) of the compressibility, see also ref. 3, and by Larkin and Pikin[4]) on the basis of a microscopic hamiltonian containing magnetoelastic couplings with acoustic phonons. More recently Oitmaa and Barber[5]) have derived first-order transitions in the context of an exactly solvable Ising model with an attractive four-spin interaction originating from spin–phonon coupling[6]).

Another exactly solvable model is the Baker–Essam model[7]) in which the partition function can be obtained by an integration over the distances between neighbouring spins. In the constant-volume ensemble this model leads to renormalized critical exponents[8–10]). In the constant-pressure ensemble there may be first-order transitions or critical-exponent renormalization[11,12]) and also tricritical behaviour[13–16]). The Baker–Essam model is a typical example of a constrained system. More detailed treatments of compressible Ising ferromagnets have been given on the basis of ϵ-expansions in renormalization group theory[17-22]).

Another type of constrained system is the Syozi model[23,24]) for Ising ferromagnets with (bond) annealed impurities. The constraint is here the condition that the impurity concentration is constant[25-29]). This model leads also to the Fisher critical-exponent renormalization[8,9]), as can be understood from a Legendre transformation. A different renormalization has been found by Essam and Place[30]) for Ising magnets with site-annealed impurities.

From a more general point of view systems with a constrained hidden variable have been treated by Fisher[9]) who also discussed several examples and showed that the constraint would lead to critical-exponent renormalization. Later on Imry et al.[31]) pointed out that constraints can also lead to first-order transitions[31]) and to tricritical behaviour[32,33]), see also refs. 15, 16.

Instabilities will also occur as a consequence of long-range pair interactions. An exactly solvable model in terms of the two-dimensional superexchange antiferromagnet of Fisher[34]) has been treated by Esipov[35]) and Hall and Stell[36]). Furthermore, the classical description of demagnetizing effects[37]) can be obtained from a hamiltonian containing long-range repulsive pair interactions, see e.g. ref. 38, p.65. As a consequence one has no first-order transitions, a finite susceptibility, but also more subtle effects such as a renormalization of the critical exponent δ[30]). More detailed results have been found using an ϵ-expansion on the basis of a Landau–Ginzburg hamiltonian with dipolar couplings[39,40]). For Ising systems with an attractive long-range interaction there is a classical critical point[41]). Emery[42]) has treated an n-component classical spin model which can be solved exactly in the limit $n \to \infty$ and which leads to critical-exponent renormalization and tricritical phenomena, see also refs. 43, 44 for related models.

In view of this one may conjecture that also under more general conditions the critical behaviour of an Ising system, or a more general reference system with short-range interactions and with a divergent second derivative of the free energy, will be unstable under small perturbations of a different nature. The perturbation can arise from additional terms in the hamiltonian such as e.g. long-range interactions[35,36,41]) or four-particle interactions of hybrid nature[5,6]), but also from one or more constrained hidden variables[9]).

It is the purpose of the present paper to present a more general formulation and a systematic analysis of instabilities in critical behaviour. The results are of a rather general nature and independent of a number of specific details such as e.g. the number and (commutation) properties of the operators in the hamiltonian, or the number and nature of hidden variables. For a brief and partial account, see ref. 45.

In order to give an outline of the problem we consider an N-particle reference system described by the hamiltonian

$$\mathcal{H}_{0,N} = -N\boldsymbol{h}^* \cdot \boldsymbol{V}_N, \tag{1.1}$$

where $N\boldsymbol{V}_N = \{NV_N^{(1)}, \ldots, NV_N^{(n)}\}$, ($n$ finite), is a set of short-range operators[46,47]) and $\boldsymbol{h}^* = \{h_1^*, \ldots, h_n^*\}$ denotes the coupling constants or fields appearing in the hamiltonian (1.1). The free energy per particle in the thermodynamic limit is given by

$$f_0(\boldsymbol{h}^*) = -\lim_{N\to\infty} N^{-1} \ln \operatorname{Tr} \exp[-\mathcal{H}_{0,N}], \tag{1.2}$$

where the inverse temperature $\beta = 1/kT$ has been absorbed in $\boldsymbol{h}^*$. Starting from (1.2) we can define the Legendre transform, see refs. 47–51,

$$g_0(\boldsymbol{m}) = \sup_{\boldsymbol{h}^*}[\boldsymbol{h}^* \cdot \boldsymbol{m} + f_0(\boldsymbol{h}^*)], \tag{1.3}$$

where the $m_1, m_2, \ldots, m_n$ are thermodynamic variables conjugate to $h_1^*, h_2^*, \ldots, h_n^*$.

Consider now the class of systems for which the free energy per particle $f(\boldsymbol{h})$ as a function of n external-field or coupling parameters $h_1, \ldots, h_n$ is given by

$$f(\boldsymbol{h}) = \inf_{\boldsymbol{m}}[-\boldsymbol{h} \cdot \boldsymbol{m} + g_0(\boldsymbol{m}) + P(\boldsymbol{m})]. \tag{1.4}$$

Here $g_0(\boldsymbol{m})$ has been defined by (1.3) and $P(\boldsymbol{m})$ is an analytic function of $m_1, m_2, \ldots, m_n$.

Let us assume that the reference free energy $f_0(\boldsymbol{h}^*)$ has a critical point at $\boldsymbol{m}_c$. Then, if $f_0(\boldsymbol{h}^*)$ has a divergent second derivative at the critical point, we have

$$\boldsymbol{e} \cdot \frac{\partial^2 g_0}{\partial \boldsymbol{m} \partial \boldsymbol{m}} \cdot \boldsymbol{e} \to 0, \qquad \text{if } \boldsymbol{m} \to \boldsymbol{m}_c, \tag{1.5}$$

for a certain unit vector $\boldsymbol{e}$. If now the matrix of second derivatives of $P(\boldsymbol{m})$ at $\boldsymbol{m}_c$ has eigenvalues different from zero, then $P(\boldsymbol{m})$ dominates $g_0(\boldsymbol{m})$ in the direction $\boldsymbol{e}$ in a neighbourhood of $\boldsymbol{m}_c$ and the critical behaviour of the reference system will be unstable. This will apply no matter how small the perturbation $P(\boldsymbol{m})$ actually is.

Eq. (1.4) has been derived rigorously[52]) from the hamiltonian which can be obtained by adding a term $NP(\boldsymbol{V}_N)$ to $-N\boldsymbol{h} \cdot \boldsymbol{V}_N$ where $P(\boldsymbol{V}_N)$ is an analytic function of n variables. In this hamiltonian we have a competition between a short-range hamiltonian and an operator of a different nature. In the proof of (1.4) which has been given in ref. 52, see also[53,54]), use has been made of a fundamental theorem by Bogoliubov Jr.[55,56]).

An expression similar to (1.4) but with a more general function $P(\boldsymbol{m},\boldsymbol{h})$ which may also depend on the field variables $h_1,\dots,h_n$ can be derived starting from a general expression for the free energy in constrained systems, i.e.

$$f(\boldsymbol{h})=\inf_{\{\xi_1,\dots,\xi_q\}}\sup_{\{\eta_1,\dots,\eta_p\}}[f_0(\boldsymbol{h}^*(\boldsymbol{h},\{\xi_j\},\{\eta_i\}))+K(\boldsymbol{h},\{\xi_j\},\{\eta_i\})], \tag{1.6}$$

where $\xi_1,\dots,\xi_q$ and $\eta_1,\dots,\eta_p$ are hidden variables and $\boldsymbol{h}^*$ and K are regular functions of $h_1,\dots,h_n$, $\xi_1,\dots,\xi_q$ and $\eta_1,\dots,\eta_p$. (In ref. 9 one variable η has been taken into account.)

In section 2 we review some details concerning the derivation of eq. (1.4) and give a discussion on the instabilities in critical behaviour arising from (1.4). In section 3 we derive eq. (1.4) with the more general function $P(\boldsymbol{m},\boldsymbol{h})$ starting from the constraint (1.6). We also discuss some examples of constraints and instabilities in critical behaviour.

In many cases it will be necessary to consider the free energy of the reference hamiltonian in more detail. More specifically we shall assume in section 4 that the singular part of the free energy is a homogeneous function[57,58]) of the relevant fields $\epsilon_1^*,\dots,\epsilon_r^*$, i.e.

$$f_s(b^{a_1}\epsilon_1^*,\dots,b^{a_r}\epsilon_r^*)=bf_s(\epsilon_1^*,\dots,\epsilon_r^*), \tag{1.7}$$

$\frac{1}{2}<a_k<1$. We also evaluate the Legendre transform $g_0(\boldsymbol{m})=\hat{g}_0(\boldsymbol{E},\boldsymbol{Z})$, where $\boldsymbol{E}=\{E_1,\dots,E_r\}$ and $\boldsymbol{Z}=\{Z_1,\dots,Z_{n-r}\}$ denote relevant and irrelevant thermodynamic variables conjugate to $\epsilon_1^*,\dots,\epsilon_r^*$ and the irrelevant field variables $\zeta_1^*,\dots,\zeta_{n-r}^*$ resp.

In section 5 we eliminate the irrelevant variables $\boldsymbol{Z}$ from the problem and derive for the free energy $f(\boldsymbol{h})=\hat{f}(\boldsymbol{\epsilon},\boldsymbol{\zeta})$ as a function of relevant and irrelevant external fields an expression like eq. (1.4) containing a function Π of the relevant variables $\boldsymbol{E}$, which will be defined uniquely in terms of $P(\boldsymbol{m},\boldsymbol{h})$.

In section 6 the convexity properties of the function Π will be used for the classification of instabilities in the critical behaviour of the reference system. If all the eigenvalues of the $r\times r$ matrix $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ at $\boldsymbol{E}=\boldsymbol{0}$ are positive, then the function Π is locally strongly convex, the system will not undergo a first-order transition in a neighbourhood of $\boldsymbol{E}=\boldsymbol{0}$ and all second derivatives of the free energy are finite. If one of the eigenvalues is negative, there will be first-order transitions, so that the infimum, cf. (1.4), cannot be reached in a neighbourhood of $\boldsymbol{E}=\boldsymbol{0}$. Finally, if the lowest eigenvalue is zero, there will be multicritical features.

The critical-exponent renormalization in the case of convex Π will be treated in section 7. The results include the renormalizations of refs. 9, 30, but also a combination of both effects and various other renormalizations. The critical-exponent renormalization is derived on the basis of the homogeneity property (1.7) of $f_s(\boldsymbol{\epsilon}^*)$ and properties of the Legendre transformation.

2. Separable interactions

In this section we review some details concerning eq. (1.4) and equivalent results which have been obtained rigorously for a class of systems described by the hamiltonian[52,54])

$$\mathcal{H}_N(\boldsymbol{h}) = \mathcal{H}_{0,N}(\boldsymbol{h}) + NP(\boldsymbol{V}_N), \tag{2.1}$$

$$\mathcal{H}_{0,N}(\boldsymbol{h}) = N(T_N - \boldsymbol{h} \cdot \boldsymbol{V}_N). \tag{2.2}$$

Here NT_N and $N\boldsymbol{V}_N \equiv \{NV_N^{(1)}, \ldots, NV_N^{(n)}\}$, ($n$ finite), are short-range operators acting on an N-particle system. Short-range operators NV_N are defined by

$$NV_N = \sum_{\omega \subset \Omega_N} N(\omega) V(\omega), \tag{2.3}$$

and

$$\sum_{\omega \ni k} \|V(\omega)\| \equiv v < \infty, \tag{2.4}$$

for any given particle k. Here Ω_N is a sequence of subsets of an infinite lattice which tends to infinity in the thermodynamic limit $N \to \infty$ in the sense of Van Hove[46,47]). The summation over ω in (2.4) contains all subsets $\omega \subset \Omega_N$, $N(\omega)$ is the number of particles and $V(\omega)$ the interaction between the particles in subset ω. Equation (2.4) implies that the total interaction per particle in the infinite lattice is finite. More specifically one may consider sums of one-particle operators for which $V(\omega) = 0$, if $N(\omega) \neq 1$, i.e.

$$NV_N = \sum_{k=1}^{N} V(k), \tag{2.5}$$

where $V(k)$ is an operator acting on particle k, or short-range pair interactions, with $V(\omega) = 0$ for $N(\omega) \neq 2$, i.e.

$$NV_N = \sum_{\langle k,l \rangle} V(k, l) \tag{2.6}$$

in which $V(k, l)$ denotes the interaction between the particles k and l.

The function $P(\boldsymbol{V}_N)$ in (2.1) is an analytic function of n variables, i.e. $P(\xi_1, \ldots, \xi_n)$ is analytic for $|\xi_i| \leq M_i$, $(i = 1, \ldots, n)$, where $M_i > \|V_N^{(i)}\|$ for all N. The operator $P(\boldsymbol{V}_N)$ will contain terms (quadratic and higher order in the $V_N^{(i)}$)

which are different from short-range interactions. For example, if $NV_N^{(1)}$ is a pair-interaction of the type (2.6) and $NV_N^{(2)}$ is a sum of one-particle operators, then

$$N\lambda_1 V_N^{(1)2} + N\lambda_2 V_N^{(2)2} = \lambda_1 N^{-1} \sum_{\langle i,j\rangle} \sum_{\langle k,l\rangle} V(i,j)V(k,l) + \lambda_2 N^{-1} \sum_{k,l} V(k)V(l). \tag{2.7}$$

The first term with λ_1 in (2.7) corresponds to a four-particle interaction of hybrid nature, which is short-range with respect to intra-pair interactions between i and j and between k and l, but long-range between the pairs $\langle i,j\rangle$ and $\langle k,l\rangle$. Such operators can be used in the description of compressible Ising ferromagnets[6]). Exact results have been obtained in ref. 5 by taking for $NV_N^{(1)}$ the hamiltonian of the (two-dimensional) Ising model. The second term with λ_2 in eq. (2.7) corresponds to a long-range interaction of the equivalent-neighbour type. Such operators with $\lambda_2 > 0$ have been used in a classical description of demagnetizing effects[38]). An exactly solvable model in which $\mathscr{H}_{0,N}(\boldsymbol{h})$ is the hamiltonian of the two-dimensional superexchange Ising antiferromagnet of Fisher[34]) and $NP(V_N) = N^{-1}J' \sum_{i,j} \sigma_i\sigma_j$, $(\sigma = \pm 1)$, has been treated in refs. 35, 36. Furthermore, the terms with λ_2 can serve as a simplified model for interactions of the Kac type, i.e., in d dimensions the interaction between two particles at distance r behaves roughly like $-J\gamma^d \exp(-\gamma r)$. Rigorous results for the free energy per particle have been obtained in the Van der Waals limit $\gamma \downarrow 0$, see e.g. refs. 41, 59–62; the results are in general equal to those for an equivalent-neighbour coupling.

For the class of hamiltonians (2.1), the free energy per particle in the thermodynamic limit

$$f(\boldsymbol{h}) \equiv -\lim_{N\to\infty} N^{-1} \ln \operatorname{Tr} \exp[-\mathscr{H}_N(\boldsymbol{h})], \tag{2.8}$$

where $\beta = 1/kT$ has been absorbed in $\boldsymbol{h}$, is given by eq. (1.4). In eq. (1.4) $g_0(\boldsymbol{m})$ is the Legendre transform of the free energy per particle $f_0(\boldsymbol{h}^*)$ of the reference hamiltonian (2.2) which is linear in the short-range operators.

The proof of eq. (1.4) in ref. 52 is based on the decomposition of

$$P(\boldsymbol{V}_N) = Q(\boldsymbol{V}_N) + R(\boldsymbol{V}_N) \tag{2.9}$$

into a concave part $Q(\boldsymbol{V}_N)$ and a convex part $R(\boldsymbol{V}_N)$, and on the minimax result[52,54])

$$f(\boldsymbol{h}) = \min_{\boldsymbol{\xi}} \max_{\boldsymbol{\eta}} [f_0(\boldsymbol{h} - \boldsymbol{Q}'(\boldsymbol{\xi}) - \boldsymbol{R}'(\boldsymbol{\eta})) + Q(\boldsymbol{\xi}) - \boldsymbol{\xi}\cdot\boldsymbol{Q}'(\boldsymbol{\xi}) + R(\boldsymbol{\eta}) - \boldsymbol{\eta}\cdot\boldsymbol{R}'(\boldsymbol{\eta})], \tag{2.10}$$

where $\boldsymbol{Q}' \equiv \partial Q/\partial\boldsymbol{\xi}$ and $\boldsymbol{R}' \equiv \partial R/\partial\boldsymbol{\eta}$. For concave $P(\boldsymbol{V}_N) = Q(\boldsymbol{V}_N)$, eq. (2.10) reduces to the theorem by Bogoliubov Jr.[55,56]). The validity of this theorem for a larger class of operators V_N, including also long-range interactions, is an essential feature of the proof of (2.10) for short-range operators. In ref. 52 also alternative expressions for $f(\boldsymbol{h})$ have been given. Moreover, for the Legendre transform of $f(\boldsymbol{h})$ we have from (1.4) the result

$$g(\boldsymbol{m}) \equiv \sup_{\boldsymbol{h}}[\boldsymbol{h} \cdot \boldsymbol{m} + f(\boldsymbol{h})] = \underset{\boldsymbol{m}}{\mathrm{CE}}[g_0(\boldsymbol{m}) + P(\boldsymbol{m})], \tag{2.11}$$

where CE denotes the convex envelope, i.e. the maximum of all convex functions which lie below $g_0(\boldsymbol{m}) + P(\boldsymbol{m})$.

Starting from (1.4) or (2.11) we can discuss the instabilities in the critical behaviour of the reference system described by $g_0(\boldsymbol{m})$ or $f_0(\boldsymbol{h}^*)$ due to a small perturbation. Here we consider the two special cases that the eigenvalues of $\partial^2 P/\partial\boldsymbol{m}\partial\boldsymbol{m}$ are positive, ($P(\boldsymbol{m})$ strongly convex), or negative ($P(\boldsymbol{m})$ strongly concave), resp.

2.1. P(m) strongly convex

In eq. (2.11) we can then omit the convex envelope, since $g_0(\boldsymbol{m})$ itself is also convex, so that

$$g(\boldsymbol{m}) = g_0(\boldsymbol{m}) + P(\boldsymbol{m}). \tag{2.12}$$

From (2.12) we conclude:

i) If the reference hamiltonian has a critical point, i.e. a non-analytic behaviour of $g_0(\boldsymbol{m})$, at $\boldsymbol{m} = \boldsymbol{m}_c$, then the hamiltonian (2.1) has also a critical point (non-analytic behaviour of $g(\boldsymbol{m})$) at $\boldsymbol{m} = \boldsymbol{m}_c$.
ii) There will not be any first-order transitions. In fact, the function $g_0(\boldsymbol{m}) + P(\boldsymbol{m})$ cannot contain straight parts on which the external fields $\boldsymbol{h} = \partial g/\partial \boldsymbol{m}$ would be constant. (This is also true if the reference hamiltonian has a first-order transition, i.e. $g_0(\boldsymbol{m})$ has a straight part on which the internal fields $\boldsymbol{h}^* = \partial g_0/\partial \boldsymbol{m}$ are constant.) The absence of first-order transitions may be considered as a generalization of the well-known demagnetizing effect, see also section 3 for a more detailed discussion.
iii) For the matrix of second derivatives of the free energy we have

$$\chi \equiv -\frac{\partial^2 f}{\partial \boldsymbol{h}\partial \boldsymbol{h}} = \left(\frac{\partial^2 g}{\partial \boldsymbol{m}\partial \boldsymbol{m}}\right)^{-1} = \left(\frac{\partial^2 g_0}{\partial \boldsymbol{m}\partial \boldsymbol{m}} + \frac{\partial^2 P}{\partial \boldsymbol{m}\partial \boldsymbol{m}}\right)^{-1} < \infty, \tag{2.13}$$

which implies that the second derivatives at any critical point remain finite. For the effects of critical-exponent renormalization, see section 7.

2.2. $P(\boldsymbol{m})$ strongly concave

Assume that the free energy $f_0(\boldsymbol{h}^*)$ of the reference hamiltonian has a divergent second derivative at all critical points $\boldsymbol{m}_c$, i.e. at $\boldsymbol{m}_c$ eq. (1.5) holds for a unit vector $\boldsymbol{e}$. Then for all values of $\boldsymbol{m}$ in a sufficiently small neighbourhood U_m of any $\boldsymbol{m}_c$ we must have

$$\boldsymbol{e}\cdot\left(\frac{\partial^2 g_0}{\partial\boldsymbol{m}\partial\boldsymbol{m}}+\frac{\partial^2 P}{\partial\boldsymbol{m}\partial\boldsymbol{m}}\right)\cdot\boldsymbol{e}<0,\qquad \boldsymbol{m}\in U_m. \tag{2.14}$$

On the other hand, the infimum over $\boldsymbol{m}$ in eq. (1.4) must occur at a point where $g_0(\boldsymbol{m})+P(\boldsymbol{m})$ is convex. This implies that, for the values $\boldsymbol{m}\in U_m$, $g(\boldsymbol{m})$ belongs to the straight portions of the convex envelope in (2.11). Hence:

i) Any critical point $\boldsymbol{m}_c$ of the reference hamiltonian is unstable.
ii) There will be first-order transitions and new critical points $\boldsymbol{m}_0$. These critical points are of a classical nature, as can be seen from a Landau expansion of $g_0(\boldsymbol{m})+P(\boldsymbol{m})$, which is an analytic function in the neighbourhood of $\boldsymbol{m}_0$. A systematic classification of classical critical behaviour can be given following the treatment of ref. 63, or the theory of catastrophes[64,65]).

3. Constrained systems

In this section we consider the free energy per particle in systems with constraints from a more general point of view. We shall deal successively with sup-constraints, inf-constraints and inf-sup-constraints.

3.1. Sup-constraints

Assume that the free energy per particle $f(\boldsymbol{h})$ is given by

$$f(\boldsymbol{h})=\sup_{\{\eta_i\}} f(\boldsymbol{h},\{\eta_i\}),\qquad i=1,\ldots,p, \tag{3.1}$$

where

$$f(\boldsymbol{h},\{\eta_i\})=f_0(\boldsymbol{h}^*(\boldsymbol{h},\{\eta_i\}))+K(\boldsymbol{h},\{\eta_i\}). \tag{3.2}$$

In eq. (3.2) $f_0(\boldsymbol{h}^*)$ is the free energy per particle (1.2) of a reference hamiltonian (1.1) and $\boldsymbol{h}^*$ and K are regular functions of the fields $h_1,\ldots,h_n$ and the hidden variables $\eta_1,\ldots,\eta_p$. Eqs. (3.1) and (3.2) are a generalization of the relations for $p=1$ introduced by Fisher[9]). If $f(\boldsymbol{h},\{\eta_i\})$ for fixed $\boldsymbol{h}$ is a concave function of the variables $\eta_1,\ldots,\eta_p$, then the supremum in (3.1) defines unique functions $\eta_1(\boldsymbol{h}),\ldots,\eta_p(\boldsymbol{h})$.

3.1.1. Legendre transform

From (3.1), (3.2) and the definition, cf. (2.11), of the Legendre transform $g(\boldsymbol{m})$, we have

$$g(\boldsymbol{m}) = \sup_{\boldsymbol{h}} \sup_{\{\eta_i\}} [\boldsymbol{h} \cdot \boldsymbol{m} + f_0(\boldsymbol{h}^*(\boldsymbol{h}, \{\eta_i\})) + K(\boldsymbol{h}, \{\eta_i\})]. \tag{3.3}$$

Using the inverse transformation

$$\boldsymbol{h} = \boldsymbol{h}(\boldsymbol{h}^*, \{\eta_i\}) \tag{3.4}$$

and interchanging both suprema in (3.3), we find

$$\begin{aligned} g(\boldsymbol{m}) &= \sup_{\{\eta_i\}} \sup_{\boldsymbol{h}^*} [\boldsymbol{h}(\boldsymbol{h}^*, \{\eta_i\}) \cdot \boldsymbol{m} + f_0(\boldsymbol{h}^*) + K(\boldsymbol{h}(\boldsymbol{h}^*, \{\eta_i\}), \{\eta_i\})] \\ &= \sup_{\boldsymbol{h}^*} [\boldsymbol{h}^* \cdot \boldsymbol{m} + f_0(\boldsymbol{h}^*) + R(\boldsymbol{m}, \boldsymbol{h}^*)], \end{aligned} \tag{3.5}$$

with

$$R(\boldsymbol{m}, \boldsymbol{h}^*) = \sup_{\{\eta_i\}} [(\boldsymbol{h}(\boldsymbol{h}^*, \{\eta_i\}) - \boldsymbol{h}^*) \cdot \boldsymbol{m} + K(\boldsymbol{h}(\boldsymbol{h}^*, \{\eta_i\}), \{\eta_i\})]. \tag{3.6}$$

The function $R(\boldsymbol{m}, \boldsymbol{h}^*)$ is a convex function of $\boldsymbol{m}$, i.e.

$$R(\lambda \boldsymbol{m}_1 + (1-\lambda)\boldsymbol{m}_2, \boldsymbol{h}^*) \leq \lambda R(\boldsymbol{m}_1, \boldsymbol{h}^*) + (1-\lambda) R(\boldsymbol{m}_2, \boldsymbol{h}^*), \quad 0 < \lambda < 1, \tag{3.7}$$

which is trivial because of the sup and the linear dependence on $\boldsymbol{m}$ in eq. (3.6). From (3.5) it follows that the function $g(\boldsymbol{m})$ is also convex,

$$g(\lambda \boldsymbol{m}_1 + (1-\lambda)\boldsymbol{m}_2) \leq \lambda g(\boldsymbol{m}_1) + (1-\lambda) g(\boldsymbol{m}_2), \qquad 0 < \lambda < 1. \tag{3.8}$$

3.1.2. Examples

i) Consider the hamiltonian (2.1) in which $P(\boldsymbol{V}_N) = R(\boldsymbol{V}_N)$ is convex. Then (2.10) is equivalent to (3.1) and (3.2) with $p = n$ and $\boldsymbol{h}^* = \boldsymbol{h} - \boldsymbol{R}'(\boldsymbol{\eta})$, $K = R(\boldsymbol{\eta}) - \boldsymbol{\eta} \cdot \boldsymbol{R}'(\boldsymbol{\eta})$. Using the Legendre transformation (1.3), eq. (2.12) is equivalent to (3.5), since $R(\boldsymbol{m}, \boldsymbol{h}^*) = R(\boldsymbol{m})$†. A special case is the classical description[37,38]) of demagnetizing effects which can be obtained taking $R(\boldsymbol{m}) = \frac{1}{2}\boldsymbol{m} \cdot \boldsymbol{D} \cdot \boldsymbol{m}$, in which $\boldsymbol{m} = (m_x, m_y, m_z)$ is the magnetization per particle and $\boldsymbol{D}$ is the tensor of the demagnetizing field.

ii) Consider an Ising system with the free energy per particle

$$f(\eta, \eta') = -\lim_{N\to\infty} N^{-1} \ln \sum_{\{\sigma_i\}} \left(\prod_{\langle i,j \rangle} \int dx_{ij}\, e^{-\mathscr{H}_{ij}}\right)\left(\prod_i \int dx_i\, e^{-\mathscr{H}_i}\right), \tag{3.9}$$

$$\begin{aligned} \mathscr{H}_{ij} &= -\phi_1(x_{ij}) - \eta x_{ij} - J(x_{ij})\sigma_i\sigma_j - H(x_{ij})(\sigma_i + \sigma_j), \\ \mathscr{H}_i &= -\phi_2(x_i) - \eta' x_i - h(x_i)\sigma_i, \end{aligned} \tag{3.10}$$

† This can also be seen from (3.6), since in view of the convexity of $R(\boldsymbol{\eta})$ the supremum occurs at $\boldsymbol{\eta} = \boldsymbol{m}$.

where $\langle i, j\rangle$ denotes pairs of nearest neighbours and $i = 1, \ldots, N$ the lattice sites, $\sigma_i = \pm 1$. (The inverse temperature $\beta = 1/kT$ has been included in $\mathcal{H}_{ij}$ and $\mathcal{H}_i$).

Special cases of (3.10), with $H(x_{ij}) = 0$, are:

a) $e^{\phi_1(x)}$ regular, $\quad e^{\phi_2(x)} = \delta(x)$. (3.11)

Eq. (3.9) reduces to the Baker–Essam model[7]) in the constant-stress ($\eta = \lambda$) ensemble[12]). The function $J(x)$ describes the dependence of the exchange coupling on the interatomic distance.

b) $e^{\phi_1(x)} = \delta(x) + \delta(x-1), \quad e^{\phi_2(x)} = \delta(x)$. (3.12)

Eq. (3.12) gives the double-bond Syozi model[27]) with two different interaction strengths $J(0)$, $J(1)$; η is the chemical potential for bonds $J(1)$. The n-bond Syozi model with n different exchange couplings[28,29]) can be included by an obvious generalization of (3.12).

c) $e^{\phi_1(x)} = \delta(x), \quad e^{\phi_2(x)} = \delta(x) + \delta(x-1)$. (3.13)

Eq. (3.13) leads to a two-component model[30]) in which the magnetic field can have two different values, $h(0) = h + h_{loc}$, $h(1) = h - h_{loc}$, where h is the applied magnetic field and h_{loc} a local field[30]); η' is the chemical potential for fields $h(1)$.

The free energy $f(\eta, \eta')$ for $H(x_{ij}) = 0$ can be written†

$$f(\eta, \eta') = f_0(J^*(\eta, \beta), h^*(\eta', \beta, h)) - A_1(\eta, \beta) - A_2(\eta', \beta, h), \tag{3.14}$$

where $f_0(J^*, h^*)$ is the free energy of a rigid Ising model, i.e.

$$f_0(J^*, h^*) = -\lim_{N\to\infty} N^{-1} \ln \sum_{\{\sigma_i\}} \exp\Big(J^* \sum_{\langle i,j\rangle} \sigma_i\sigma_j + h^* \sum_i \sigma_i\Big), \tag{3.15}$$

with

$$J^*(\eta, \beta) = \tfrac{1}{2} \ln\Big[\int dx\, e^{\phi_1(x)+\eta x+J(x)} \Big/ \int dx\, e^{\phi_1(x)+\eta x-J(x)}\Big],$$

$$h^*(\eta', \beta, h) = \tfrac{1}{2} \ln\Big[\int dx\, e^{\phi_2(x)+\eta' x+h(x)} \Big/ \int dx\, e^{\phi_2(x)+\eta' x-h(x)}\Big]. \tag{3.16}$$

The functions $A_1(\eta, \beta)$ and $A_2(\eta', \beta, h)$ are given by

$$A_1(\eta, \beta) = \tfrac{1}{4} z \ln\Big[\int dx\, e^{\phi_1(x)+\eta x+J(x)} \int dx\, e^{\phi_1(x)+\eta x-J(x)}\Big],$$

$$A_2(\eta', \beta, h) = \tfrac{1}{2} \ln\Big[\int dx\, e^{\phi_2(x)+\eta' x+h(x)} \int dx\, e^{\phi_2(x)+\eta' x-h(x)}\Big]. \tag{3.17}$$

† The more complicated expressions for the case $H(x_{ij}) \neq 0$ will not be given here, see e.g. ref. 26.

Here z is the coordination number of the lattice. The inverse temperature $\beta = 1/kT$ has been added to indicate that in (3.9), as well as in (3.15), β has been included in the coupling constants, so that (3.16) and (3.17) depend in a non-trivial way on β. Furthermore $h(x)$ depends on the external field $\boldsymbol{h}$, so that $\boldsymbol{h}^*$ and A_2 depend also on h. (An h-dependence of J^* and A_1 e.g. through ϕ_1 may also be taken into account.)

From (3.14) it follows that the critical behaviour in the constant η, η'-ensemble (i.e. constant stress in the case of (3.11) and constant chemical potential for (3.12) and (3.13)) is given by the critical behaviour of the rigid Ising system.

From a physical point of view it is often more appealing to pass to the ensemble in which the quantities

$$a = \lim_{N\to\infty}(\tfrac{1}{2}zN)^{-1}\sum_{\langle i,j\rangle}\langle x_{ij}\rangle = -(\tfrac{1}{2}z)^{-1}\frac{\partial f}{\partial \eta},$$
$$a' = \lim_{N\to\infty} N^{-1}\sum_{i}\langle x_i\rangle = -\frac{\partial f}{\partial \eta'} \qquad (3.18)$$

are constant[12,27,30]). This can be done using the L gendre transformation

$$\psi(a, a') = \sup_{\eta,\eta'}[\tfrac{1}{2}za\eta + a'\eta' + f_0(J^*, h^*) - A_1(\eta, \beta) - A_2(\eta', \beta, h)]. \qquad (3.19)$$

In (3.19) we should have sup, since according to its definition $f(\eta, \eta')$ is concave in η and η'. The function ψ describes the free energy of the Baker–Essam model in the constant-volume (constant-interatomic distance a) ensemble[12]), cf. (3.11), or the free energy for Ising systems with bond-annealed impurities[27]), (3.12), or site-annealed impurities[30]), (3.13), in which the concentration of bonds $J(1)$, or fields $h(1)$ resp., are kept constant. Therefore the free energy in these cases can be obtained by a sup-constraint of the form (3.1) which leads to (3.5) with a function $R(\boldsymbol{m}, \boldsymbol{h}^*)$ depending on $\boldsymbol{h}^*$ via (3.15)–(3.17) and (3.4), (3.6). Note that in all three cases (3.11)–(3.13), eq. (3.19) reduces to a non-trivial constraint in one variable ($p = 1$).

3.1.3. Remarks

i) If $R(\boldsymbol{m}, \boldsymbol{h}^*)$ is strongly convex in $\boldsymbol{m}$, i.e. $\partial^2 R/\partial \boldsymbol{m}\partial \boldsymbol{m}$ is positive definite, then, cf. the discussion below eq. (2.12):

a) A critical point of the reference hamiltonian at $\boldsymbol{h}^* = \boldsymbol{h}_c^*$ will lead to a critical point of the constrained system (3.1) at $\boldsymbol{h} = \boldsymbol{h}_c^* + (\partial R/\partial \boldsymbol{m})(\boldsymbol{m}, \boldsymbol{h}_c^*)$, where $\boldsymbol{m}$ is the solution of $\boldsymbol{m} = -(\partial f_0/\partial \boldsymbol{h}^*)(\boldsymbol{h}_c^*) - (\partial R/\partial \boldsymbol{h}^*)(\boldsymbol{m}, \boldsymbol{h}_c^*)$.

b) There are no first-order transitions, i.e. no straight line segments on which $\boldsymbol{h} = \partial g/\partial \boldsymbol{m}$ is constant.

c) The second derivatives of the free energy are finite.

ii) Not always will the function $R(\boldsymbol{m}, \boldsymbol{h}^*)$ be strongly convex. Especially, when the number of constraints is smaller than the number of variables $\boldsymbol{h}$, i.e. $p < n$ in eq. (3.1), one can expect that $\boldsymbol{e}' \cdot (\partial^2 R/\partial \boldsymbol{m} \partial \boldsymbol{m}) \cdot \boldsymbol{e}' = 0$ for certain directions $\boldsymbol{e}'$. If the reference free energy has divergent second derivatives, i.e. (1.5) holds for an arbitrary direction $\boldsymbol{e}$, then the constrained system (3.1) has a critical point at which some of the second derivatives $-\partial^2 f/\partial \boldsymbol{h} \partial \boldsymbol{h}$ become finite and others remain infinite. This situation occurs in the three examples (3.11)–(3.13) in which we have only one non-trivial constraint ($p = 1$) for the free energy $\psi(a, a')$ and two variables β and h.

iii) From (3.5) it follows that the value $\boldsymbol{h}^*$ at the supremum is uniquely determined by, cf. refs. 52, 54,

$$\mu_0^-(\boldsymbol{h}^*, \boldsymbol{e}) \equiv \lim_{\nu \uparrow 0} -\frac{\mathrm{d}}{\mathrm{d}\nu} f_0(\boldsymbol{h}^* + \nu \boldsymbol{e}) \leq \boldsymbol{e} \cdot \left(\boldsymbol{m} + \frac{\partial R}{\partial \boldsymbol{m}}(\boldsymbol{m}, \boldsymbol{h}^*) \right)$$
$$\leq \lim_{\nu \downarrow 0} -\frac{\mathrm{d}}{\mathrm{d}\nu} f_0(\boldsymbol{h}^* + \nu \boldsymbol{e}) \equiv \mu_0^+(\boldsymbol{h}^*, \boldsymbol{e}), \tag{3.20}$$

for all unit vectors $\boldsymbol{e}$.

If the reference system has a first-order transition at $\boldsymbol{h}^* = \boldsymbol{c}$, i.e. $\mu_0^-(\boldsymbol{c}, \boldsymbol{e}') < \mu_0^+(\boldsymbol{c}, \boldsymbol{e}')$ for a certain direction $\boldsymbol{e}'$, then for all $\boldsymbol{m}$-values satisfying (3.20) with $\boldsymbol{h}^* = \boldsymbol{c}$, we have

$$\boldsymbol{h} = \frac{\partial g}{\partial \boldsymbol{m}} = \boldsymbol{c} + \frac{\partial R}{\partial \boldsymbol{m}}(\boldsymbol{m}, \boldsymbol{c}). \tag{3.21}$$

For the special case $R(\boldsymbol{m}) = \frac{1}{2}\boldsymbol{m} \cdot \boldsymbol{D} \cdot \boldsymbol{m}$ we obtain $\boldsymbol{h}^* = \boldsymbol{h} - \boldsymbol{D} \cdot \boldsymbol{m}$, which is the wellknown relation[37,38]) between the internal field $\boldsymbol{h}^*$ and the applied field $\boldsymbol{h}$ in the classical description of demagnetizing effects.

3.2. Inf-constraints

Assume that the free energy per particle $f(\boldsymbol{h})$ is given by

$$f(\boldsymbol{h}) = \inf_{\{\xi_j\}} f(\boldsymbol{h}, \{\xi_j\}), \qquad j = 1, \ldots, q, \tag{3.22}$$

where

$$f(\boldsymbol{h}, \{\xi_j\}) = f_0(\boldsymbol{h}^*(\boldsymbol{h}, \{\xi_j\})) + K(\boldsymbol{h}, \{\xi_j\}). \tag{3.23}$$

In eq. (3.23) $f_0(\boldsymbol{h}^*)$ is the free energy of a reference hamiltonian and $\boldsymbol{h}^*$ and K are regular functions.

3.2.1. Legendre transform

Using the inverse Legendre transformation of (1.3), i.e.

$$f_0(\boldsymbol{h}^*) = \inf_{\boldsymbol{m}}[-\boldsymbol{h}^* \cdot \boldsymbol{m} + g_0(\boldsymbol{m})] \tag{3.24}$$

and interchanging the infima over m and $\{\xi_j\}$, we have

$$f(\boldsymbol{h}) = \inf_{\{\xi_j\}} \inf_{\boldsymbol{m}} [-\boldsymbol{h}^*(\boldsymbol{h}, \{\xi_j\}) \cdot \boldsymbol{m} + g_0(\boldsymbol{m}) + K(\boldsymbol{h}, \{\xi_j\})]$$

$$= \inf_{\boldsymbol{m}} [-\boldsymbol{h} \cdot \boldsymbol{m} + g_0(\boldsymbol{m}) + Q(\boldsymbol{m}, \boldsymbol{h})] \tag{3.25}$$

with

$$Q(\boldsymbol{m}, \boldsymbol{h}) = \inf_{\{\xi_j\}} [(\boldsymbol{h} - \boldsymbol{h}^*(\boldsymbol{h}, \{\xi_j\})) \cdot \boldsymbol{m} + K(\boldsymbol{h}, \{\xi_j\})]. \tag{3.26}$$

The function $Q(\boldsymbol{m}, \boldsymbol{h})$ is a concave function of $\boldsymbol{m}$, i.e.

$$Q(\lambda \boldsymbol{m}_1 + (1-\lambda)\boldsymbol{m}_2, \boldsymbol{h}) \geqslant \lambda Q(\boldsymbol{m}_1, \boldsymbol{h}) + (1-\lambda) Q(\boldsymbol{m}_2, \boldsymbol{h}), \qquad 0 < \lambda < 1, \tag{3.27}$$

as follows from the infimum and the linear dependence on $\boldsymbol{m}$ in (3.26).

3.2.2. Remarks

i) If $Q(\boldsymbol{m}, \boldsymbol{h})$ is strongly concave in one direction, i.e. $\boldsymbol{e}' \cdot (\partial^2 Q / \partial \boldsymbol{m} \partial \boldsymbol{m}) \cdot \boldsymbol{e}' < 0$ for a certain unit vector $\boldsymbol{e}'$, and the free energy of the reference system has only divergent second derivatives at any critical point, i.e. eq. (1.5) holds for any direction $\boldsymbol{e}$, then

a) any critical point of the reference system is unstable,

b) there will be first-order transitions and classical critical points.

ii) The same conclusions a) and b) can be reached, if $Q(\boldsymbol{m}, \boldsymbol{h})$ is a strongly concave function, i.e. $\boldsymbol{e} \cdot (\partial^2 Q / \partial \boldsymbol{m} \partial \boldsymbol{m}) \cdot \boldsymbol{e} < 0$ for all unit vectors $\boldsymbol{e}$, and the free energy of the reference system has at least one divergent second derivative at any critical point, i.e. eq. (1.5) holds for a certain direction $\boldsymbol{e}'$.

3.2.3. Examples

i) Consider the hamiltonian (2.1) in which $P(\boldsymbol{V}_N) = Q(\boldsymbol{V}_N)$ is concave. Then (2.10) is equivalent to (3.22) and (3.23) with $q = n$ and $\boldsymbol{h}^* = \boldsymbol{h} - \boldsymbol{Q}'(\boldsymbol{\xi})$, $K = Q(\boldsymbol{\xi}) - \boldsymbol{\xi} \cdot \boldsymbol{Q}'(\boldsymbol{\xi})$. Eq. (1.4) has the form (3.25) with $Q(\boldsymbol{m}, \boldsymbol{h}) = Q(\boldsymbol{m}) = P(\boldsymbol{m})$.

ii) Consider now the Dicke maser type of model[66–69,54])

$$\mathcal{H} = N[T_N + P(\boldsymbol{V}_N) - \boldsymbol{h} \cdot \boldsymbol{V}_N] + \sum_k \omega_k a_k^\dagger a_k - \sqrt{N}(\alpha a_0^\dagger + \alpha^* a_0)$$

$$+ \sqrt{N}(a_0^\dagger Q(\boldsymbol{V}_N) + a_0 Q^\dagger(\boldsymbol{V}_N)), \tag{3.28}$$

where NT_N and $N\boldsymbol{V}_N$ are short-range operators, cf. (2.3), (2.4), $a_k^\dagger, a_k$ are boson operators and P and Q are analytic functions, $Q(\boldsymbol{V}_N)$ not necessarily being hermitean. The case in which $N[T_N + P(\boldsymbol{V}_N) - \boldsymbol{h} \cdot \boldsymbol{V}_N]$ and $Q(\boldsymbol{V}_N)$ are linear in the components of the total spin has first been solved exactly by Hepp and Lieb[66]), cf. also ref. 67 for polynomial extensions. Eq. (3.28) with short-range operators is more general, since a (reference) hamiltonian linear in short-range operators can give rise to phase transitions.

For the reference hamiltonian

$$\mathcal{H}_0 = N[T_N - \boldsymbol{h} \cdot \boldsymbol{V}_N] + \sum_k \omega_k a_k^\dagger a_k - \sqrt{N}(\alpha a_0^\dagger + \alpha^* a_0) \tag{3.29}$$

the free energy per particle (1.2) in the thermodynamic limit is given by

$$f_0(\boldsymbol{h}, \alpha) = f_{sr}(\boldsymbol{h}) + f_b - |\alpha|^2/\omega_0, \tag{3.30}$$

where $f_{sr}(\boldsymbol{h})$ and f_b are the free energies per particle corresponding to $N[T_N - \boldsymbol{h} \cdot \boldsymbol{V}_N]$ and $\Sigma_k \omega_k a_k^\dagger a_k$ resp. The Legendre transform is given by

$$g_0(\boldsymbol{m}, d) = \sup_{\boldsymbol{h},\alpha,\alpha^*}[\boldsymbol{h} \cdot \boldsymbol{m} + \alpha d^* + \alpha^* d + f_0(\boldsymbol{h}, \alpha)] = g_{sr}(\boldsymbol{m}) + f_b + \omega_0|d|^2, \tag{3.31}$$

where $g_{sr}(\boldsymbol{m})$ is the Legendre transform of $f_{sr}(\boldsymbol{h})$.

The free energy per particle for the total hamiltonian (3.28) can be shown to be[68,69,52,54]), taking $\alpha = 0$,

$$\begin{aligned} f(\boldsymbol{h}, 0) &= \inf_{\boldsymbol{m},d,d^*}[-\boldsymbol{h} \cdot \boldsymbol{m} + g_0(\boldsymbol{m}, d) + P(\boldsymbol{m}) + d^*Q(\boldsymbol{m}) + dQ^*(\boldsymbol{m})] \\ &= \inf_{\boldsymbol{m}}[-\boldsymbol{h} \cdot \boldsymbol{m} + g_{sr}(\boldsymbol{m}) + f_b + P(\boldsymbol{m}) - |Q(\boldsymbol{m})|^2/\omega_0] \\ &= \inf_{d,d^*}[\psi(\boldsymbol{h}, d) + f_b + \omega_0|d|^2] \end{aligned} \tag{3.32}$$

with the function

$$\begin{aligned} \psi(\boldsymbol{h}, d) = -\lim_{N\to\infty} N^{-1} \ln \operatorname{Tr} \exp[-N\{T_N + P(\boldsymbol{V}_N) - \boldsymbol{h} \cdot \boldsymbol{V}_N \\ + d^*Q(\boldsymbol{V}_N) + dQ^\dagger(\boldsymbol{V}_N)\}]. \end{aligned} \tag{3.33}$$

Equation (3.32) gives three inf-constraints; the third type with $P = 0$ and linear Q has been used in magnetothermomechanics[1-3]), where the effect of lattice compressibility on the magnetic phase transition in the rigid lattice system leads to a mechanical instability, (ψ is a concave function which dominates $\omega_0|d|^2$ for small d), and a first-order transition.

3.3. *Inf-sup-constraints*

Assume that the free energy per particle is given by (1.6), i.e. eq. (3.22) in which

$$f(\boldsymbol{h}, \{\xi_j\}) = \sup_{\{\eta_i\}}[f_0(\boldsymbol{h}^*(\boldsymbol{h}, \{\xi_j\}, \{\eta_i\})) + K(\boldsymbol{h}, \{\xi_j\}, \{\eta_i\})] \tag{3.34}$$

is assumed to be a concave function of $\boldsymbol{h}$ and where $\boldsymbol{h}^*(\boldsymbol{h},\{\xi_j\},\{\eta_i\})$ and $K(\boldsymbol{h},\{\xi_j\},\{\eta_i\})$ are regular functions.

3.3.1. Legendre transform

Inserting the identity

$$\inf_{\boldsymbol{m}'} \sup_{\boldsymbol{h}'}[(\boldsymbol{h}'-\boldsymbol{h})\cdot \boldsymbol{m}' + \Phi(\boldsymbol{h}')] = \Phi(\boldsymbol{h}) \tag{3.35}$$

for an arbitrary concave function Φ, cf. e.g. appendix A of ref. 52, we have, cf. eqs. (3.22) and (3.34),

$$f(\boldsymbol{h}) = \inf_{\{\xi_j\}} \inf_{\boldsymbol{m}'} \sup_{\boldsymbol{h}'} \sup_{\{\eta_i\}}[(\boldsymbol{h}'-\boldsymbol{h})\cdot \boldsymbol{m}' + f_0(\boldsymbol{h}^*(\boldsymbol{h}',\{\xi_j\},\{\eta_i\})) + K(\boldsymbol{h}',\{\xi_j\},\{\eta_i\})]. \tag{3.36}$$

Using the inverse transformation of $\boldsymbol{h}^*(\boldsymbol{h}',\{\xi_j\},\{\eta_i\})$, i.e.

$$\boldsymbol{h}' = \boldsymbol{h}'(\boldsymbol{h}^*,\{\xi_j\},\{\eta_i\}) \tag{3.37}$$

and following the treatment of section 3.1.1 we find

$$f(\boldsymbol{h}) = \inf_{\{\xi_j\}} \inf_{\boldsymbol{m}'} \sup_{\boldsymbol{h}^*}[(\boldsymbol{h}^*-\boldsymbol{h})\cdot \boldsymbol{m}' + f_0(\boldsymbol{h}^*) + R(\boldsymbol{m}',\boldsymbol{h}^*,\{\xi_j\})] \tag{3.38}$$

with

$$R(\boldsymbol{m}',\boldsymbol{h}^*,\{\xi_j\}) = \sup_{\{\eta_i\}}[(\boldsymbol{h}'(\boldsymbol{h}^*,\{\xi_j\},\{\eta_i\}) - \boldsymbol{h}^*)\cdot \boldsymbol{m}' + K(\boldsymbol{h}'(\boldsymbol{h}^*,\{\xi_j\},\{\eta_i\}),\{\xi_j\},\{\eta_i\})]. \tag{3.39}$$

We want to investigate the stability (under very small constraints) of a reference system with a critical point which may be chosen at $\boldsymbol{h}^* = \boldsymbol{0}$. If we expand the function R in terms of $\boldsymbol{h}^*$, then

$$R(\boldsymbol{m}',\boldsymbol{h}^*,\{\xi_i\}) = R_0(\boldsymbol{m}',\{\xi_j\}) + \boldsymbol{R}_1(\boldsymbol{m}',\{\xi_j\})\cdot \boldsymbol{h}^* + R^q(\boldsymbol{m}',\boldsymbol{h}^*,\{\xi_j\}), \tag{3.40}$$

where R^q contains quadratic and higher order terms in $\boldsymbol{h}^*$. The term R^q may be ignored close to the critical point assuming for the moment that the reference free energy has divergent second derivatives. This assumption, however, should not be taken too literally, in view of the description of the reference free energy in section 4, section 7.4 and appendix G. Omitting the term R^q in (3.40) and using the Legendre transform (1.3), we have

$$f(\boldsymbol{h}) = \inf_{\{\xi_j\}} \inf_{\boldsymbol{m}'}[-\boldsymbol{h}\cdot \boldsymbol{m}' + g_0(\boldsymbol{m}' + \boldsymbol{R}_1(\boldsymbol{m}',\{\xi_j\})) + R_0(\boldsymbol{m}',\{\xi_j\})]. \tag{3.41}$$

Finally, introducing the variable $\boldsymbol{m} = \boldsymbol{m}' + R_1(\boldsymbol{m}',\{\xi_j\})$ with the inverse transformation $m' = m'(m, \{\xi_j\})$ we obtain

$$f(h) = \inf_m [-h \cdot m + g_0(m) + P(m, h)], \tag{3.42}$$

with

$$P(m, h) = \inf_{\{\xi_j\}} [h \cdot (m - m'(m, \{\xi_j\})) + R_0(m'(m, \{\xi_j\}), \{\xi_j\})]. \tag{3.43}$$

Eq. (3.42) is a more general expression than (1.4), since the function $P(m, h)$ depends also on the variables h. In principle not much can be said on the convexity (or concavity) properties of the function $P(m, h)$ given by (3.43), (3.39) and (3.40). Therefore a more detailed treatment, taking into account the homogeneity properties of the reference free energy, is needed to investigate the critical behaviour arising from (3.42), see sections 4–7.

3.3.2. Remarks and examples

i) The restriction to linear terms in h^* in (3.40) is not necessary in the case that the function $\mathcal{H}(\{\eta_i\}) = [K(h, \{\xi_j\}, \{\eta_i\}) - h^*(h, \{\xi_j\}, \{\eta_i\}) \cdot m]$ has a uniquely determined maximum over $\{\eta_i\}$ for all values of $\{\xi_j\}$ and h. (This condition is satisfied e.g., if the function $\mathcal{H}(\{\eta_i\})$ is (quasi)concave.) In that case we may interchange[49]) the infimum over m and the supremum over $\{\eta_i\}$ in the expression

$$f(h) = \inf_{\{\xi_j\}} \sup_{\{\eta_i\}} \inf_m [-h^*(h, \{\xi_j\}, \{\eta_i\}) \cdot m + g_0(m) + K(h, \{\xi_j\}, \{\eta_i\})] \tag{3.44}$$

which follows from (3.34) and (3.24).

As a result $f(h)$ can be expressed in the form (3.42) with

$$P(m, h) = \inf_{\{\xi_j\}} \sup_{\{\eta_i\}} [(h - h^*(h, \{\xi_j\}, \{\eta_i\})) \cdot m + K(h, \{\xi_j\}, \{\eta_i\})]. \tag{3.45}$$

ii) Consider the hamiltonian (2.1) in which $P(V_N) = Q(V_N) + R(V_N)$, cf. (2.9). Then (2.10) is equivalent to eq. (1.6) with $p = q = n$ and $h^* = h - Q'(\xi) - R'(\eta)$, $K = Q(\xi) - \xi \cdot Q'(\xi) + R(\eta) - \eta \cdot R'(\eta)$. Equation (1.4) has then the form (3.42) with $P(m, h) = P(m)$, cf. (3.45).

iii) Consider the anisotropic Baker–Essam model on a d-dimensional (hyper-) cubic lattice in which the exchange interaction $J_\delta(x_\delta)$ between neighbouring atoms as well as the function $\phi_\delta(x_\delta)$ depends on the direction $\delta = 1, \ldots, d$. Then, by an obvious generalization of the considerations in subsection 3.1.2 the free energy $\psi(a_1, \ldots, a_d)$ as a function of the average distances a_δ between neighbouring atoms in the directions $\delta = 1, \ldots, d$, can be evaluated to be

$$\psi(a_1, \ldots, a_d) = \sup_{\eta_1, \ldots, \eta_d} \left[\sum_{\delta=1}^{d} a_\delta \eta_\delta + f_0(J_1^*, \ldots, J_d^*) - \sum_{\delta=1}^{d} A_\delta(\eta_\delta, \beta) \right] \tag{3.46}$$

in which $J_\delta^*(\eta_\delta, \beta)$ is given by the first equation of (3.16) with $\phi_\delta(x_\delta)$, η_δ, $J_\delta(x_\delta)$ instead of $\phi_1(x)$, η, $J(x)$ and

$$A_\delta(\eta_\delta, \beta) = \tfrac{1}{2}\ln\left[\int \mathrm{d}x_\delta\ \mathrm{e}^{\phi_\delta(x_\delta)+\eta_\delta x_\delta + J_\delta(x_\delta)} \int \mathrm{d}x_\delta\ \mathrm{e}^{\phi_\delta(x_\delta)+\eta_\delta x_\delta - J_\delta(x_\delta)}\right]. \tag{3.47}$$

By taking the (Legendre) transform

$$\phi(p) = \inf_{a_1,\ldots,a_d} [pa_1 \ldots a_d + \psi(a_1, \ldots, a_d)], \tag{3.48}$$

one obtains the Gibbs free energy in the constant-pressure ensemble. (The existence of the infimum in (3.48) with positive values of p, $a_1, \ldots, a_d$ is not entirely trivial, but will be ensured under (physical) conditions on the functions ϕ_δ and J_δ.) From (3.48) and (3.46) the Gibbs free energy can be expressed in terms of an inf-sup constraint of the type (1.6). Furthermore using the inequalities $|m_\delta| \leq 1$ for the correlations between nearest neighbours and the concavity of the functions $-J_\delta^*(\eta_\delta, \beta)m_\delta - A_\delta(\eta_\delta, \beta)$, $\phi(p)$ can be expressed in the form (3.42), (3.45) with

$$P(\boldsymbol{m}, \boldsymbol{h}) - \boldsymbol{h} \cdot \boldsymbol{m} = \inf_{a_1,\ldots,a_d} \sup_{\eta_1,\ldots,\eta_d} \left[p \prod_{\delta=1}^{d} a_\delta + \sum_{\delta=1}^{d} \{a_\delta \eta_\delta - J_\delta^*(\eta_\delta, \beta)m_\delta - A_\delta(\eta_\delta, \beta)\}\right]. \tag{3.49}$$

Equations (3.42) and (3.49) may lead to renormalized critical exponents if $P(\boldsymbol{m}, \boldsymbol{h})$ is convex as a function of $\boldsymbol{m}$, to first-order transitions, if $P(\boldsymbol{m}, \boldsymbol{h})$ is concave in at least one direction, and to multicritical behaviour, see also sections 6.3 and 6.4, if the matrix $\partial^2 P/\partial \boldsymbol{m}\partial \boldsymbol{m}$ has a lowest eigenvalue zero at $\boldsymbol{m}_c$ for suitable β and p. (The tricritical point in the Baker–Essam model and compressible ferromagnets has first been discussed in refs. 13–16 from a slightly different point of view).

iv) Finally, there might be some relation with recent results obtained using a variational approach *in renormalization group* theory[70–72]). A variational principle for the free energy involving a finite number of variables may lead to constraints as treated in this section.

4. Critical properties of the reference hamiltonian

4.1. Reference free energy

In this section we give a description of the free energy per particle $f_0(\boldsymbol{h}^*)$ of the reference hamiltonian defined by (1.1) and (1.2) in the neighbourhood of a (multi)critical point C. After an appropriate choice of origin, C may be assumed to occur at $\boldsymbol{h}^* = \mathbf{0}$ with zero values $\boldsymbol{m} = \mathbf{0}$ of the first derivatives of f_0 at C.

Using a local (linear) transformation, the free energy can be expressed in terms of relevant fields $\epsilon_1^*, \ldots, \epsilon_r^*$ and irrelevant fields $\zeta_1^*, \ldots, \zeta_{n-r}^*$, i.e.

$$\hat{\boldsymbol{h}}^* = \{\epsilon_1^*, \ldots, \epsilon_r^*, \zeta_1^*, \ldots, \zeta_{n-r}^*\} = \boldsymbol{S} \cdot \boldsymbol{h}^*, \tag{4.1}$$

and

$$f_0(\boldsymbol{h}^*) = f_0(\boldsymbol{S}^{-1} \cdot \hat{\boldsymbol{h}}^*) = \hat{f}_0(\hat{\boldsymbol{h}}^*) = \hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*), \tag{4.2}$$

where $\boldsymbol{\epsilon}^* = \{\epsilon_1^*, \ldots, \epsilon_r^*\}$ and $\boldsymbol{\zeta}^* = \{\zeta_1^*, \ldots, \zeta_{n-r}^*\}$ are r and $n-r$ dimensional vectors resp.

The variables $\boldsymbol{\epsilon}^*$ and $\boldsymbol{\zeta}^*$ in (4.1) are chosen such that

i) critical points C′ of the same nature as C occur at $\boldsymbol{\epsilon}^* = 0$, also for $\boldsymbol{\zeta}^* \neq \mathbf{0}$,
ii) in a neighbourhood of $(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) = (\mathbf{0}, \mathbf{0})$ there are no critical points of higher order, (i.e. with a larger number of relevant variables),
iii) the second derivatives $-\partial^2 \hat{f}_0 / \partial \boldsymbol{\zeta}^* \partial \boldsymbol{\zeta}^*$ and $-\partial^2 \hat{f}_0 / \partial \boldsymbol{\zeta}^* \partial \boldsymbol{\epsilon}^*$ exist at the critical points C, C′ and are finite,
iv) the second derivatives $-\partial^2 \hat{f}_0 / \partial \boldsymbol{\epsilon}^* \partial \boldsymbol{\epsilon}^*$ with respect to the relevant variables at the critical points C, C′ are infinite.

More specifically we shall assume that the reference free energy can be expressed as, choosing the standard representation for the quadratic terms,

$$\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) = f_s(\boldsymbol{\epsilon}^*) - \tfrac{1}{2}\boldsymbol{\zeta}^* \cdot \boldsymbol{\zeta}^* + F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*). \tag{4.3}$$

Here $f_s(\boldsymbol{\epsilon}^*)$ is a non-analytic function with divergent second derivatives at $\boldsymbol{\epsilon}^* = \mathbf{0}$ satisfying the homogeneity property (1.7) with $\frac{1}{2} < a_k < 1$. (We shall not take into account terms for which $a_k = \frac{1}{2}$; usually divergent second derivatives with $a_k = \frac{1}{2}$ involve logarithmic corrections which require a more detailed analysis, cf. e.g. refs. 9, 73, 74.) Eq. (1.7) implies that the first and second derivatives of $f_s(\boldsymbol{\epsilon}^*)$,

$$\mu_k(\boldsymbol{\epsilon}^*) \equiv -\frac{\partial f_s}{\partial \epsilon_k^*}, \qquad \chi_{kl}(\boldsymbol{\epsilon}^*) \equiv -\frac{\partial^2 f_s}{\partial \epsilon_k^* \partial \epsilon_l^*}, \tag{4.4}$$

satisfy the homogeneity relations[57,58])

$$\begin{aligned} \mu_k(b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*) &= b^{1-a_k}\mu_k(\epsilon_1^*, \ldots, \epsilon_r^*), \\ \chi_{kl}(b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*) &= b^{1-a_k-a_l}\chi_{kl}(\epsilon_1^*, \ldots, \epsilon_r^*). \end{aligned} \tag{4.5}$$

As an example we may mention a simple ferromagnet for which $r = 2$, $\epsilon_1^* = 1 - T/T_c$, $\epsilon_2^* = H$ and

$$a_1 = 1/(2-\alpha), \qquad a_2 = \Delta/(2-\alpha), \tag{4.6}$$

where α is the exponent of the specific heat and $\Delta = \beta\delta$ the gap exponent, i.e. $\beta = 2-\alpha-\Delta$, $-\gamma = 2-\alpha-2\Delta$.

The second term in (4.3) originates from a contribution to the regular part which is quadratic in the irrelevant field variables. The function $F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ is a small correction containing regular parts, e.g. quadratic terms in $\boldsymbol{\epsilon}^*$ (or cross-terms $\epsilon_i^*\zeta_j^*$) and higher-order terms, but also next-leading singularities which may be neglected close to the critical point. The precise meaning of the function $F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ being small is specified in eq. (4.10).

At first sight the simple choice (4.3) may seem a restriction of generality. Our purpose, however, is to analyze the critical behaviour of the free energy (3.42), in which $g_0(\boldsymbol{m})$ is the Legendre transform of the reference free energy $f_0(\boldsymbol{h}^*)$ and $P(\boldsymbol{m}, \boldsymbol{h})$ an analytic function arising from a constraint of the type (1.6). In doing so we shall obtain by choosing an appropriate function $P_0(\boldsymbol{m}, \boldsymbol{h})$ a more general expression for the free energy $\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ with also finite second derivatives, i.e. $0 < a_k < 1$ in eq. (1.7). From (3.42) with general $P(\boldsymbol{m}, \boldsymbol{h})$ one can then investigate the stability of the critical properties of the more general $\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ under the influence of a perturbation $P(\boldsymbol{m}, \boldsymbol{h}) - P_0(\boldsymbol{m}, \boldsymbol{h})$, see section 7.4.

We shall now take into account the leading terms of the order b in the free energy, where b is the parameter, cf. (1.7), that tends to zero if we approach the critical point. Equation (4.3) can be rewritten as

$$\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) = f_h(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) + F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*), \tag{4.7}$$

where

$$f_h(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) = f_s(\boldsymbol{\epsilon}^*) - \tfrac{1}{2}\boldsymbol{\zeta}^* \cdot \boldsymbol{\zeta}^* \tag{4.8}$$

satisfies the homogeneity relation, cf. (1.7),

$$f_h(b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*, b^{1/2}\zeta_1^*, \ldots, b^{1/2}\zeta_{n-r}^*) = bf_h(\epsilon_1^*, \ldots, \epsilon_r^*, \zeta_1^*, \ldots, \zeta_{n-r}^*). \tag{4.9}$$

The assumption that $F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ is small may be formulated by the property

$$F(b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*, b^{1/2}\zeta_1^*, \ldots, b^{1/2}\zeta_{n-r}^*) = o(b^{1+\eta}), \tag{4.10}$$

for some $\eta > 0$, where $o(b^{1+\eta})$ is a shorthand notation for a function satisfying

$$\lim_{b \downarrow 0} o(b^{1+\eta})b^{-(1+\eta)} = 0. \tag{4.11}$$

4.2. Legendre transform

We now consider the Legendre transform $\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z})$ of $\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$, i.e.

$$\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z}) = \sup_{\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*}[\boldsymbol{\epsilon}^* \cdot \boldsymbol{E} + \boldsymbol{\zeta}^* \cdot \boldsymbol{Z} + \hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)], \tag{4.12}$$

where

$$\boldsymbol{E} = \{E_1, \ldots, E_r\}, \qquad \boldsymbol{Z} = \{Z_1, \ldots, Z_{n-r}\} \tag{4.13}$$

are the relevant and irrelevant thermodynamic variables conjugate to the (internal) fields $\epsilon_1^*, \ldots, \epsilon_r^*$ and $\zeta_1^*, \ldots, \zeta_{n-r}^*$ resp.

When we ignore the term $F(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ in (4.7) we obtain the Legendre transform

$$g_h(\boldsymbol{E}, \boldsymbol{Z}) = \sup_{\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*}[\boldsymbol{\epsilon}^* \cdot \boldsymbol{E} + \boldsymbol{\zeta}^* \cdot \boldsymbol{Z} + f_h(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)], \tag{4.14}$$

so that, cf. (4.8),

$$g_h(\boldsymbol{E}, \boldsymbol{Z}) = g_s(\boldsymbol{E}) + \tfrac{1}{2}\boldsymbol{Z} \cdot \boldsymbol{Z}, \tag{4.15}$$

where

$$g_s(\boldsymbol{E}) = \sup_{\boldsymbol{\epsilon}^*}[\boldsymbol{\epsilon}^* \cdot \boldsymbol{E} + f_s(\boldsymbol{\epsilon}^*)] \tag{4.16}$$

is the Legendre transform of $f_s(\boldsymbol{\epsilon}^*)$. From (4.16) and (1.7) it follows that $g_s(\boldsymbol{E})$ is a homogeneous function of the variables $E_1, \ldots, E_r$, i.e.

$$g_s(b^{1-a_1}E_1, \ldots, b^{1-a_r}E_r) = b g_s(E_1, \ldots, E_r). \tag{4.17}$$

In fact

$$\begin{aligned} g_s(b^{1-a_1}E_1, \ldots, b^{1-a_r}E_r) &= \sup_{\epsilon_1^*, \ldots, \epsilon_r^*}\left[\sum_{k=1}^{r} \epsilon_k^* b^{1-a_k}E_k + f_s(\epsilon_1^*, \ldots, \epsilon_r^*)\right] \\ &= \sup_{b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*}\left[\sum_{k=1}^{r} b^{a_k}\epsilon_k^* b^{1-a_k}E_k + f_s(b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*)\right] \\ &= b\left\{\sup_{b^{a_1}\epsilon_1^*, \ldots, b^{a_r}\epsilon_r^*}\left[\sum_{k=1}^{r} \epsilon_k^* E_k + f_s(\epsilon_1^*, \ldots, \epsilon_r^*)\right]\right\} = b g_s(E_1, \ldots, E_r). \end{aligned}$$

Eq. (4.17) implies that the first and second derivatives,

$$\epsilon_k^* = \frac{\partial g_s}{\partial E_k}, \qquad (\chi^{-1})_{kl} = \frac{\partial^2 g_s}{\partial E_k \partial E_l}, \tag{4.18}$$

satisfy the homogeneity relations

$$\begin{aligned} \epsilon_k^*(b^{1-a_1}E_1, \ldots, b^{1-a_r}E_r) &= b^{a_k}\epsilon_k^*(E_1, \ldots, E_r), \\ \chi^{-1}{}_{kl}(b^{1-a_1}E_1, \ldots, b^{1-a_r}E_r) &= b^{a_k+a_l-1}\chi^{-1}{}_{kl}(E_1, \ldots, E_r). \end{aligned} \tag{4.19}$$

For the Legendre transform $\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z})$ it can be shown that

$$\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z}) = g_h(\boldsymbol{E}, \boldsymbol{Z}) + G(\boldsymbol{E}, \boldsymbol{Z}), \tag{4.20}$$

where $G(\boldsymbol{E}, \boldsymbol{Z})$ is a small correction satisfying

$$G(b^{1-a_1}E_1, \ldots, b^{1-a_r}E_r, b^{1/2}Z_1, \ldots, b^{1/2}Z_{n-r}) = o(b^{1+\eta}), \tag{4.21}$$

with the same $\eta > 0$ as in (4.10). For a derivation, see appendix A. If we ignore terms of order higher than b we may take

$$\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z}) \simeq g_h(\boldsymbol{E}, \boldsymbol{Z}), \tag{4.22}$$

where $g_h(\boldsymbol{E}, \boldsymbol{Z})$ has been given by (4.15). Eq. (4.22) will be the starting point of further considerations.

5. Elimination of irrelevant variables

In this section we eliminate the irrelevant variables $\boldsymbol{Z}$, replacing the function $P(\boldsymbol{m}, \boldsymbol{h})$ by a new function Π depending on the relevant variables $\boldsymbol{E}$. We also give a discussion on the origin of possible terms appearing in Π.

5.1. Elimination of Z

Consider the free energy per particle (3.42) in which $g_0(\boldsymbol{m})$ is defined by (1.3). Instead of $\boldsymbol{h}^*$ we introduced in (4.1) relevant and irrelevant (internal) parameters $\hat{\boldsymbol{h}}^* = (\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*) = \boldsymbol{S} \cdot \boldsymbol{h}^*$. Furthermore, in eq. (4.13) we introduced relevant and irrelevant variables

$$\hat{\boldsymbol{m}} = \{E_1, \ldots, E_r, Z_1, \ldots, Z_{n-r}\} = \tilde{\boldsymbol{S}}^{-1} \cdot \boldsymbol{m}, \tag{5.1}$$

where $\boldsymbol{E}$ and $\boldsymbol{Z}$ are conjugate to $\boldsymbol{\epsilon}^*$ and $\boldsymbol{\zeta}^*$ resp. and $\boldsymbol{m}$ denotes the variables conjugate to $\boldsymbol{h}^*$, i.e. $\boldsymbol{m} \cdot \boldsymbol{h}^* = \hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{h}}^*$. The tilde in (5.1) denotes the transposed matrix. The Legendre transform defined by (4.12) is related to $g_0(\boldsymbol{m})$, defined by (1.3), by

$$\begin{aligned} \hat{g}_0(\boldsymbol{E}, \boldsymbol{Z}) = \hat{g}_0(\hat{\boldsymbol{m}}) &= \sup_{\hat{\boldsymbol{h}}^*}[\hat{\boldsymbol{h}}^* \cdot \hat{\boldsymbol{m}} + \hat{f}_0(\hat{\boldsymbol{h}}^*)] \\ &= \sup_{\boldsymbol{h}^*}[\boldsymbol{h}^* \cdot \tilde{\boldsymbol{S}} \cdot \hat{\boldsymbol{m}} + f_0(\boldsymbol{h}^*)] = g_0(\tilde{\boldsymbol{S}} \cdot \hat{\boldsymbol{m}}) = g_0(\boldsymbol{m}). \end{aligned} \tag{5.2}$$

We now express the free energy per particle $f(\boldsymbol{h})$ in (3.42) as a function of external parameters

$$\hat{\boldsymbol{h}} = \{\epsilon_1, \ldots, \epsilon_r, \zeta_1, \ldots, \zeta_{n-r}\} = \boldsymbol{S} \cdot \boldsymbol{h}, \tag{5.3}$$

$$\hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = \hat{f}(\hat{\boldsymbol{h}}) = f(\boldsymbol{S}^{-1} \cdot \hat{\boldsymbol{h}}) = f(\boldsymbol{h}), \tag{5.4}$$

where $\epsilon_1, \ldots, \epsilon_r$ and $\zeta_1, \ldots, \zeta_{n-r}$ are conjugate to $E_1, \ldots, E_r$ and $Z_1, \ldots, Z_{n-r}$ resp. Using (3.42) and (5.2)–(5.4) we obtain

$$\begin{aligned} \hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) &= \inf_{\boldsymbol{m}}[-\hat{\boldsymbol{h}} \cdot \tilde{\boldsymbol{S}}^{-1} \cdot \boldsymbol{m} + g_0(\boldsymbol{m}) + P(\boldsymbol{m}, \boldsymbol{S}^{-1} \cdot \hat{\boldsymbol{h}})] \\ &= \inf_{\hat{\boldsymbol{m}}}[-\hat{\boldsymbol{h}} \cdot \hat{\boldsymbol{m}} + \hat{g}_0(\hat{\boldsymbol{m}}) + P(\tilde{\boldsymbol{S}} \cdot \hat{\boldsymbol{m}}, \boldsymbol{S}^{-1} \cdot \hat{\boldsymbol{h}})], \end{aligned} \tag{5.5}$$

which can be written in the form

$$\hat{f}(\epsilon, \zeta) = \inf_{E,Z}[-\epsilon \cdot E - \zeta \cdot Z + \hat{g}_0(E, Z) + \hat{P}(E, Z, \epsilon, \zeta)], \tag{5.6}$$

with

$$\hat{P}(E, Z, \epsilon, \zeta) = P(\tilde{S} \cdot \hat{m}, S^{-1} \cdot \hat{h}) = P(m, h). \tag{5.7}$$

Using the estimate $Z_k \sim b^{1/2}$, cf. (4.21), we have the expansion

$$\hat{P}(E, Z, \epsilon, \zeta) = \hat{P}(E, 0, \epsilon, \zeta) + P_Z(E, \epsilon, \zeta) \cdot Z + \tfrac{1}{2} Z \cdot P_{ZZ} \cdot Z, \tag{5.8}$$

where terms of the order $b^{1+\eta}$ with $\eta > 0$ have been ignored. (In the last term the matrix $P_{ZZ}(E, \epsilon, \zeta)$ has been replaced by $P_{ZZ}(0, 0, 0) = P_{ZZ}$.) Inserting (5.8) into (5.6), we have

$$\begin{aligned}\hat{f}(\epsilon, \zeta) = \inf_{E,Z}[&-\epsilon \cdot E - \zeta \cdot Z + g_s(E) + \tfrac{1}{2} Z \cdot Z \\ &+ \hat{P}(E, 0, \epsilon, \zeta) + P_Z(E, \epsilon, \zeta) \cdot Z + \tfrac{1}{2} Z \cdot P_{ZZ} \cdot Z].\end{aligned} \tag{5.9}$$

From the trivial property

$$\inf_{Z}[\tfrac{1}{2} Z \cdot (1 + P_{ZZ}) \cdot Z + T \cdot Z] = -\tfrac{1}{2} T \cdot (1 + P_{ZZ})^{-1} \cdot T \tag{5.10}$$

it follows that

$$\begin{aligned}\hat{f}(\epsilon, \zeta) = \inf_{E}[&-\epsilon \cdot E + g_s(E) + \hat{P}(E, 0, \epsilon, \zeta) \\ &- \tfrac{1}{2}(P_Z(E, \epsilon, \zeta) - \zeta) \cdot (1 + P_{ZZ})^{-1} \cdot (P_Z(E, \epsilon, \zeta) - \zeta)].\end{aligned} \tag{5.11}$$

We now use the relations

$$\begin{aligned}\hat{P}(E, 0, \epsilon, \zeta) &= P_0(\epsilon, \zeta) + P_E(\epsilon, \zeta) \cdot E + P^q(E, \epsilon, \zeta), \\ P_Z(E, \epsilon, \zeta) &= P_Z(0, \epsilon, \zeta) + P_{ZE}(\epsilon, \zeta) \cdot E + P_Z^q(E, \epsilon, \zeta),\end{aligned} \tag{5.12}$$

in which P^q and P_Z^q contain only quadratic and higher order terms in the variables E. The terms P_0 and P_Z independent of E can be included in the regular part of $\hat{f}(\epsilon, \zeta)$. The linear terms in E can be taken into account by introducing new relevant parameters

$$\tilde{\epsilon} = \epsilon - P_E(\epsilon, \zeta) + (P_Z(0, \epsilon, \zeta) - \zeta) \cdot (1 + P_{ZZ})^{-1} \cdot P_{ZE}(\epsilon, \zeta). \tag{5.13}$$

Using the inverse transformation of (5.13), i.e.

$$\epsilon = \tilde{\epsilon} - p(\tilde{\epsilon}, \zeta), \tag{5.14}$$

eq. (5.11) can be rewritten as

$$\hat{f}(\epsilon, \zeta) = \inf_{E}[-\tilde{\epsilon} \cdot E + g_s(E) + \Pi(E, \tilde{\epsilon}, \zeta)] + \Pi_r(\tilde{\epsilon}, \zeta), \tag{5.15}$$

where

$$\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = P^q - \boldsymbol{P}^q_Z \cdot (1 + \boldsymbol{P}_{ZZ})^{-1} \cdot (\boldsymbol{P}_Z - \boldsymbol{\zeta})$$
$$- \tfrac{1}{2}(\boldsymbol{P}^q_Z + \boldsymbol{E} \cdot \tilde{\boldsymbol{P}}_{ZE}) \cdot (1 + \boldsymbol{P}_{ZZ})^{-1} \cdot (\boldsymbol{P}^q_Z + \boldsymbol{P}_{ZE} \cdot \boldsymbol{E}), \tag{5.16}$$

$$\Pi_r(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = P_0 - \tfrac{1}{2}(\boldsymbol{P}_Z - \boldsymbol{\zeta}) \cdot (1 + \boldsymbol{P}_{ZZ})^{-1} \cdot (\boldsymbol{P}_Z - \boldsymbol{\zeta}). \tag{5.17}$$

In (5.16) and (5.17) the following abbreviations have been used:

$$\begin{aligned} &P^q \equiv P^q(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}} - \boldsymbol{p}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \boldsymbol{\zeta}), \qquad \boldsymbol{P}^q_Z \equiv \boldsymbol{P}^q_Z(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}} - \boldsymbol{p}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \boldsymbol{\zeta}), \\ &\boldsymbol{P}_Z \equiv \boldsymbol{P}_Z(\boldsymbol{0}, \bar{\boldsymbol{\epsilon}} - \boldsymbol{p}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \boldsymbol{\zeta}), \qquad \boldsymbol{P}_{ZE} \equiv \boldsymbol{P}_{ZE}(\bar{\boldsymbol{\epsilon}} - \boldsymbol{p}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \boldsymbol{\zeta}), \\ &P_0 \equiv P_0(\bar{\boldsymbol{\epsilon}} - \boldsymbol{p}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \boldsymbol{\zeta}), \end{aligned} \tag{5.18}$$

all these functions being regular in $\boldsymbol{E}$, $\bar{\boldsymbol{\epsilon}}$ and $\boldsymbol{\zeta}$.

5.2. Discussion

We now discuss some features of the transformation (5.13) and the result (5.15), (5.16) for the free energy. Here we shall assume that the function P is small.

The transformation (5.13) should be considered as a nonlinear transformation; in general there are $\epsilon\epsilon$ and $\epsilon\zeta$ contributions to the second and third term of the right-hand side of (5.13) which may be more important than linear terms. First order contributions in P arise from the terms

$$\epsilon\epsilon P_{E\epsilon\epsilon}, \qquad \epsilon\zeta P_{E\epsilon\zeta}, \qquad \epsilon\zeta P_{ZE\epsilon}. \tag{5.19a}$$

Second order contributions $\sim P^2$ are provided by products like

$$\begin{aligned} &\epsilon\epsilon P_{Z\epsilon\epsilon} P_{ZE}, \quad \epsilon P_{Z\epsilon}\epsilon P_{ZE\epsilon}, \quad P_Z\epsilon\epsilon P_{ZE\epsilon\epsilon}, \quad \zeta P_{ZZ}\epsilon P_{ZE\epsilon}, \\ &\epsilon\zeta P_{Z\epsilon\zeta} P_{ZE}, \quad \epsilon P_{Z\epsilon}\zeta P_{ZE\zeta}, \quad \zeta P_{Z\zeta}\epsilon P_{ZE\epsilon}, \quad P_Z\epsilon\zeta P_{ZE\epsilon\zeta}, \end{aligned} \tag{5.19b}$$

where e.g. $P_{ZE\epsilon\zeta}$ denotes a four-fold derivative of $\hat{P}(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta})$ with respect to one variable Z, one variable E, one variable ϵ and one variable ζ. (Also, there may be quadratic terms $\sim \zeta\zeta$, which have been omitted here.)

In the free energy expression (5.15), cf. (5.16), we can have quadratic terms in E, in first order arising from EEP^q_{EE} and in second order from products $E\tilde{P}_{ZE}P_{ZE}E$ and $EEP^q_{ZEE}P_Z$. These terms will dominate close to the critical point $\boldsymbol{E} = \boldsymbol{0}$, if the eigenvalues of the matrix of second derivatives $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ at $(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$ are different from zero. If one of the eigenvalues is zero, then other terms such as EEE and higher order terms in E may be important in (5.15), but also terms like $\bar{\epsilon}EE$ and ζEE which depend on the external variables. First order contributions to $\bar{\epsilon}EE$ and ζEE can arise from

$$\bar{\epsilon}EEP^q_{\epsilon EE}, \qquad \zeta EEP^q_{\zeta EE}, \qquad \zeta EEP^q_{ZEE} \tag{5.20a}$$

and second order contributions $\sim P^2$ from products

$$\begin{array}{llll} \bar{\epsilon}EEP^q_{Z\epsilon EE}P_Z, & EEP^q_{ZEE}\bar{\epsilon}P_{Z\epsilon}, & E\bar{\epsilon}P_{ZE\epsilon}P_{ZE}E, & \\ \zeta EEP^q_{Z\zeta EE}P_Z, & EEP^q_{ZEE}\zeta P_{Z\zeta}, & E\zeta P_{ZE\zeta}P_{ZE}E, & EEP^q_{ZEE}P_{ZZ}\zeta, \end{array} \tag{5.20b}$$

but there are also terms

$$\bar{\epsilon}EEP^q_{EE\epsilon}(\partial p/\partial\bar{\epsilon}), \qquad \zeta EEP^q_{EE\epsilon}(\partial p/\partial\zeta), \tag{5.20c}$$

which arise from the linear part of the transformation (5.13), cf. also the expression for P^q in (5.18).

Note that a function $P(\boldsymbol{m})$, independent of $\boldsymbol{h}$, as in eq. (1.4), which can be derived from the hamiltonian (2.1), cannot give rise to $\bar{\epsilon}EE$ and ζEE terms apart from the term ζEEP^q_{ZEE} in (5.20a). Also, in that case the transformation (5.13) is a linear transformation, i.e.

$$\bar{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon} - \boldsymbol{P}_E - \boldsymbol{\zeta}\cdot(1+\boldsymbol{P}_{ZZ})^{-1}\cdot\boldsymbol{P}_{ZE}. \tag{5.21}$$

Furthermore, if $\hat{P}(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta})$ is a quadratic function of the variables $\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta}$, the transformation is linear and no terms $\bar{\epsilon}EE$ and ζEE can arise.

Finally, if the function $P(\boldsymbol{m}, \boldsymbol{h})$ is an even function, i.e. $P(\boldsymbol{m}, \boldsymbol{h}) = P(-\boldsymbol{m}, -\boldsymbol{h})$, then all contributions (5.19) and (5.20) vanish. First order contributions to terms $\epsilon\epsilon\epsilon$ and $\epsilon\epsilon\zeta$ in the transformation (5.13) are then provided by

$$\epsilon\epsilon\epsilon P_{E\epsilon\epsilon\epsilon}, \qquad \zeta\epsilon\epsilon P_{E\zeta\epsilon\epsilon}, \qquad \zeta\epsilon\epsilon P_{ZE\epsilon\epsilon}. \tag{5.22}$$

First order contributions to terms $\bar{\epsilon}\bar{\epsilon}EE$ and $\bar{\epsilon}\zeta EE$ can arise from

$$\bar{\epsilon}\bar{\epsilon}EEP^q_{\epsilon\epsilon EE}, \qquad \bar{\epsilon}\zeta EEP^q_{\epsilon\zeta EE}, \qquad \zeta\bar{\epsilon}EEP^q_{Z\epsilon EE}. \tag{5.23}$$

6. Stability of critical behaviour

In order to discuss the stability of critical phenomena we distinguish between the following three cases:

i) The matrix of second derivatives $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ of the function $\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (5.15) at $(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$ has positive eigenvalues.
ii) The matrix $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ at $(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$ has a negative eigenvalue.
iii) The matrix $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ at $(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$ has a lowest eigenvalue 0.

The cases i), ii) and iii) will be treated in subsections 6.1, 6.2 and 6.3 resp. The different types of critical behaviour may be described in terms of a multicritical scaling law as given in subsection 6.4.

6.1. Positive eigenvalues

In this case the function $\Pi(\boldsymbol{E}, \mathbf{0}, \mathbf{0})$ is strongly convex at $\boldsymbol{E} = \mathbf{0}$, i.e.

$$\boldsymbol{e} \cdot \frac{\partial^2 \Pi}{\partial \boldsymbol{E} \partial \boldsymbol{E}}(\mathbf{0}, \mathbf{0}, \mathbf{0}) \cdot \boldsymbol{e} > 0, \tag{6.1}$$

for an arbitrary unit vector $\boldsymbol{e}$. Since the singular part $f_s(\boldsymbol{\epsilon}^*)$ of the reference free energy has divergent second derivatives, cf. (4.5), we also have

$$\boldsymbol{e} \cdot \frac{\partial^2 g_s}{\partial \boldsymbol{E} \partial \boldsymbol{E}}(\boldsymbol{E}, \mathbf{0}, \mathbf{0}) \cdot \boldsymbol{e} \to 0, \qquad \text{for } \boldsymbol{E} \to \mathbf{0}, \tag{6.2}$$

for an arbitrary direction $\boldsymbol{e}$. From (6.1) and (6.2) it follows that the function

$$\psi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = g_s(\boldsymbol{E}) + \Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) \tag{6.3}$$

is strongly convex for sufficiently small $\boldsymbol{E}$, $\bar{\boldsymbol{\epsilon}}$ and $\boldsymbol{\zeta}$, i.e. $\boldsymbol{E} \in U_E$, $\bar{\boldsymbol{\epsilon}} \in U_\epsilon$, $\boldsymbol{\zeta} \in U_\zeta$, where U_E, U_ϵ and U_ζ are neighbourhoods of the origin. For $\boldsymbol{E}$ outside U_E the function $g_s(\boldsymbol{E})$ may be assumed to be larger than a positive constant. Therefore, the function $\psi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ will assume its absolute minimum as a function of $\boldsymbol{E}$ for fixed $\bar{\boldsymbol{\epsilon}} \in U_\epsilon$, $\boldsymbol{\zeta} \in U_\zeta$, in the neighbourhood U_E, provided that $\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ is sufficiently small.

Then, for $\bar{\boldsymbol{\epsilon}} \in U_\epsilon$, $\boldsymbol{\zeta} \in U_\zeta$, the infimum over $\boldsymbol{E}$ defines a unique function $\boldsymbol{E}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ with the property $\boldsymbol{E}(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) \to 0$, if $\bar{\boldsymbol{\epsilon}} \to \mathbf{0}$, cf. (5.15), (5.16). From this the following conclusions can be drawn:

i) The free energy $\hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta})$ has a critical point with $\boldsymbol{E} = \mathbf{0}$ for $\bar{\boldsymbol{\epsilon}} = \mathbf{0}$, just as the reference free energy $\hat{f}_0(\boldsymbol{\epsilon}^*, \boldsymbol{\zeta}^*)$ has a critical point with $\boldsymbol{E} = \mathbf{0}$ at $\boldsymbol{\epsilon}^* = \mathbf{0}$. (In terms of the variables $\boldsymbol{\epsilon}$ and $\boldsymbol{\zeta}$ the critical point has been shifted, i.e. $\boldsymbol{\epsilon} \neq \mathbf{0}$, cf. (5.13).)
ii) There cannot be first-order transitions for $\bar{\boldsymbol{\epsilon}} \in U_\epsilon$, $\boldsymbol{\zeta} \in U_\zeta$, and the second derivatives $-\partial^2 \hat{f}/\partial \bar{\boldsymbol{\epsilon}} \partial \bar{\boldsymbol{\epsilon}}$ (and also $-\partial^2 \hat{f}/\partial \boldsymbol{\epsilon} \partial \boldsymbol{\epsilon}$) remain finite. In fact, from (5.15) it can be shown that

$$-\frac{\partial^2 \hat{f}}{\partial \bar{\boldsymbol{\epsilon}} \partial \bar{\boldsymbol{\epsilon}}} = \left(1 - \frac{\partial^2 \Pi}{\partial \bar{\boldsymbol{\epsilon}} \partial \boldsymbol{E}}\right) \cdot \left(\frac{\partial^2 g_s}{\partial \boldsymbol{E} \partial \boldsymbol{E}} + \frac{\partial^2 \Pi}{\partial \boldsymbol{E} \partial \boldsymbol{E}}\right)^{-1} \cdot \left(1 - \frac{\partial^2 \Pi}{\partial \boldsymbol{E} \partial \bar{\boldsymbol{\epsilon}}}\right) - \frac{\partial^2 \Pi}{\partial \bar{\boldsymbol{\epsilon}} \partial \bar{\boldsymbol{\epsilon}}} - \frac{\partial^2 \Pi_r}{\partial \bar{\boldsymbol{\epsilon}} \partial \bar{\boldsymbol{\epsilon}}}. \tag{6.4}$$

iii) There will be effects analogous to the demagnetizing effect, if the reference free energy $f_s(\boldsymbol{\epsilon}^*)$ has a first-order transition at $\boldsymbol{\epsilon}^* = \boldsymbol{c}$. In fact, the Legendre transform $g_s(\boldsymbol{E})$ of $f_s(\boldsymbol{\epsilon}^*)$ has then a straight portion,

$$g_s(\boldsymbol{E}) - g_s(\boldsymbol{E}_0) = \boldsymbol{c} \cdot (\boldsymbol{E} - \boldsymbol{E}_0), \tag{6.5}$$

for a set of $\boldsymbol{E}$-values satisfying

$$\mu_s^-(\boldsymbol{c}, \boldsymbol{e}) \equiv \lim_{\nu \uparrow 0} -\frac{\mathrm{d}}{\mathrm{d}\nu} f_s(\boldsymbol{c} + \nu \boldsymbol{e}) \leq \boldsymbol{e} \cdot \boldsymbol{E} \leq \lim_{\nu \downarrow 0} -\frac{\mathrm{d}}{\mathrm{d}\nu} f_s(\boldsymbol{c} + \nu \boldsymbol{e}) \equiv \mu_s^+(\boldsymbol{c}, \boldsymbol{e}), \tag{6.6}$$

for all unit vectors $\boldsymbol{e}$, and

$$\mu_s^-(\boldsymbol{c}, \boldsymbol{e}') < \mu_s^+(\boldsymbol{c}, \boldsymbol{e}'), \tag{6.7}$$

for at least one unit vector $\boldsymbol{e}'$. Taking into account the condition for the infimum in (5.15), i.e.

$$\frac{\partial}{\partial \boldsymbol{E}} g_s(\boldsymbol{E}) = \boldsymbol{c} = \tilde{\boldsymbol{\epsilon}} - \frac{\partial}{\partial \boldsymbol{E}} \Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \tag{6.8}$$

one can determine the external parameters $\tilde{\boldsymbol{\epsilon}}$ as a function of the variables $\boldsymbol{E}$, for fixed internal parameters $\boldsymbol{c}$. (In the special case that $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = \frac{1}{2}\boldsymbol{E} \cdot \boldsymbol{D} \cdot \boldsymbol{E}$, eq. (6.8) reduces to $\boldsymbol{c} = \tilde{\boldsymbol{\epsilon}} - \boldsymbol{D} \cdot \boldsymbol{E}$, which corresponds to the classical description of the demagnetizing effect[37,38].)

Similar results have been discussed for the special cases considered in sections 2.1 and 3.1. In section 7 a more detailed analysis of the effects of critical-exponent renormalization will be given.

6.2. *Negative eigenvalue*

If the matrix $\partial^2 \Pi / \partial \boldsymbol{E} \partial \boldsymbol{E}$ has a negative eigenvalue at $(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$ there can be found a unit vector $\boldsymbol{e}'$ and neighbourhoods U_E, U_ϵ and U_ζ of the origin so that

$$\boldsymbol{e}' \cdot \frac{\partial^2}{\partial \boldsymbol{E} \partial \boldsymbol{E}} \Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) \cdot \boldsymbol{e}' < -\delta < 0, \tag{6.9}$$

for $\boldsymbol{E} \in U_E$, $\tilde{\boldsymbol{\epsilon}} \in U_\epsilon$, $\boldsymbol{\zeta} \in U_\zeta$ and some positive number δ. On the other hand, at the infimum of (5.15), the function $\psi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (6.3) should be convex as a function of $\boldsymbol{E}$, so that

$$\delta < \boldsymbol{e}' \cdot \frac{\partial^2 g_s}{\partial \boldsymbol{E} \partial \boldsymbol{E}} \cdot \boldsymbol{e}' = \mathcal{O}(b^{\min 2a_k - 1}), \tag{6.10}$$

cf. (4.19), (6.9). This implies that a neighbourhood of the critical point of the reference free energy, i.e. the values of b where (6.10) does not hold, cannot be reached. Hence, there will be first-order transitions in such a neighbourhood.

Further away, there may be critical points of a classical nature, or other critical points arising from the reference free energy. In the neighbourhood of a classical critical point the function $\psi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ is an analytic function of the variables $\boldsymbol{E}$ and the critical properties can be derived from a Landau expansion involving only relevant variables. The first-order transition may also end on a critical point C′ of the reference system which can be described in terms of r' relevant variables $E'_1, \ldots, E'_{r'}, (r' \leq r)$. Following the treatment of sections 4 and 5 one can obtain a function Π' of the r' relevant variables of which the matrix of second derivatives has a lowest eigenvalue zero at C′, see subsection 6.3.

6.3. *Other cases*

We are left with the case that $\partial^2\Pi/\partial E\partial E$ has a lowest eigenvalue 0 at $(E, \bar{\epsilon}, \zeta) = (0, 0, 0)$. Then higher order terms $\sim EEE$, $\sim \bar{\epsilon}EE$, $\sim \zeta EE$, etc. can be essential to describe the (multi)critical behaviour. If there is for example a ζEE term of the type $\Pi_3\zeta_1 E \cdot E$, $(\Pi_3 > 0)$, then for $\zeta_1 > 0$ the function $\Pi(E, \bar{\epsilon}, \zeta) = \Pi(E, \bar{\epsilon}, 0) + \Pi_3\zeta_1 E \cdot E$ is strongly convex as a function of E in a neighbourhood of $E = 0$, for sufficiently small $\bar{\epsilon}$. On the other hand, for $\zeta_1 < 0$, we have $e' \cdot (\partial^2\Pi/\partial E\partial E) \cdot e' < 0$ for a certain unit vector e' in a neighbourhood of $E = 0$, for sufficiently small $\bar{\epsilon}$.

For $\zeta_1 > 0$, the free energy $\hat{f}(\epsilon, \zeta)$ will have a critical point at $\bar{\epsilon} = 0$ arising from a critical point of the reference hamiltonian, but with finite second derivatives and no first-order transitions in a neighbourhood of $\bar{\epsilon} = 0$, as treated under 6.1. However, for $\zeta_1 < 0$ a neighbourhood of $E = 0$ cannot be reached for small $\bar{\epsilon}$ and there will be first-order transitions, as treated under 6.2. This situation is characteristic for multicritical behaviour, see e.g. refs. 12–16, 32, 33.

If the terms $\sim \zeta EE$ vanish, then higher order terms, e.g. $\sim \zeta\zeta EE$ and $\sim \zeta\zeta\zeta EE$ can affect the multicritical properties[44,75,76]). In discussing the origin of these terms it may also become important to take into account terms of the order $b^{1+\eta}$, which have been ignored in (5.8). From (5.6), however, one can derive the formal expression

$$\hat{f}(\epsilon, \zeta) = \inf_{E}[-\epsilon \cdot E + g_s(E) + \mathcal{P}(E, \epsilon, \zeta)], \tag{6.11}$$

with

$$\mathcal{P}(E, \epsilon, \zeta) = \inf_{Z}[-\zeta \cdot Z + \tfrac{1}{2}Z \cdot Z + \hat{P}(E, Z, \epsilon, \zeta)]. \tag{6.12}$$

We can now expand the function $\mathcal{P}(E, \epsilon, \zeta)$ in the same way as the functions in (5.12). The term with $E = 0$ contributes to the regular part, the linear terms in E can be taken into account introducing new parameters $\bar{\epsilon}$ and a different function $p(\bar{\epsilon}, \zeta)$. The quadratic and higher order terms in E can be expressed by a function $\Pi(E, \bar{\epsilon}, \zeta)$ analogous to the one in (5.15). One may now have terms $\sim \zeta\zeta EE$ arising from terms $\sim EZZ$ and $\sim EEZZ$ in $\hat{P}(E, Z, \epsilon, \zeta)$, which have been ignored in (5.8). An example is given in appendix B, where we also discuss some features arising from such terms.

6.4. *Multicritical scaling*

To discuss multicritical scaling we expand the function $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (5.16), or the more general Π arising from (6.12), as a power series in $\boldsymbol{E}$,

$$\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = \sum_{k_1,\ldots,k_s}{}' \Pi_{k_1\ldots k_s}(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) E_{k_1} \ldots E_{k_s}, \tag{6.13}$$

where the prime indicates that we can restrict ourselves to terms with indices $k_1, \ldots, k_s$, $(s \geq 2)$, satisfying

$$\sum_{j=1}^{s} (1 - a_{k_j}) \leq 1. \tag{6.14}$$

The function $\psi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (6.3) may be regarded as a homogeneous function of the variables $\boldsymbol{E}$ and the coefficients $\Pi_{k_1\ldots k_s}$, i.e.

$$\psi[\{b^{1-a_k} E_k\}, \{b^{1-s+a_{k_1}+\cdots+a_{k_s}} \Pi_{k_1\ldots k_s}\}] = b\psi[\{E_k\}, \{\Pi_{k_1\ldots k_s}\}]. \tag{6.15}$$

For the function

$$f_s[\{\tilde{\epsilon}_k\}, \{\Pi_{k_1\ldots k_s}\}] = \inf_{\boldsymbol{E}}[-\tilde{\boldsymbol{\epsilon}} \cdot \boldsymbol{E} + \psi] = \hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) - \Pi_r(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \tag{6.16}$$

cf. (6.3) and (5.15), we have the homogeneity property

$$f_s[\{b^{a_k}\tilde{\epsilon}_k\}, \{b^{1-s+a_{k_1}+\cdots+a_{k_s}} \Pi_{k_1\ldots k_s}\}] = bf_s[\{\tilde{\epsilon}_k\}, \{\Pi_{k_1\ldots k_s}\}], \tag{6.17}$$

cf. the derivation of (4.17).

Using the estimate $\tilde{\epsilon}_k \sim b^{a_k}$, $(a_k > \frac{1}{2})$, cf. (6.17), we can expand the functions $\Pi_{k_1\ldots k_s}$ up to linear terms in $\tilde{\boldsymbol{\epsilon}}$,

$$\Pi_{k_1\ldots k_s}(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = \Pi^0_{k_1\ldots k_s}(\boldsymbol{\zeta}) + \sum_l{}' \Pi^1_{k_1\ldots k_s, l}(\boldsymbol{\zeta})\tilde{\epsilon}_l, \tag{6.18}$$

with $k_1, \ldots, k_s$ satisfying (6.14), taking only into account terms with a summation index l for which

$$\sum_{j=1}^{s} (1 - a_{k_j}) \leq 1 - a_l. \tag{6.19}$$

For the singular part of the free energy f_s as a function of $\tilde{\boldsymbol{\epsilon}}$ and the coefficients Π^0 and Π^1 we have the homogeneity property

$$\begin{aligned} f_s[\{b^{a_k}\tilde{\epsilon}_k\}, \{b^{1-s+a_{k_1}+\cdots+a_{k_s}} \Pi^0_{k_1\ldots k_s}(\boldsymbol{\zeta})\}, \{b^{1-s+a_{k_1}+\cdots+a_{k_s}-a_l} \Pi^1_{k_1\ldots k_s, l}(\boldsymbol{\zeta})\}] \\ = bf_s[\{\tilde{\epsilon}_k\}, \{\Pi^0_{k_1\ldots k_s}(\boldsymbol{\zeta})\}, \{\Pi^1_{k_1\ldots k_s, l}(\boldsymbol{\zeta})\}], \end{aligned} \tag{6.20}$$

which may be used in studying the multicritical behaviour.

As a special case we mention the tricritical point in compressible Ising ferromagnets, cf. refs. 13, 15, 16, 32, 33.

7. Critical-exponent renormalization.

In this section we discuss the case of a small strongly-convex Π as treated in section 6.1. We shall show that close to the critical point there is a "complete" critical-exponent renormalization in which case all second derivatives of the singular part of the free energy tend to zero with well-defined (renormalized) exponents. Sufficiently far from all critical points (or for sufficiently small Π) no difference can be seen between the singular behaviour of second derivatives of the actual free energy and the reference free energy, and there will be no renormalization of critical exponents.

For the sake of presentation we will first derive the homogeneity properties in the case of a "partial" critical-exponent renormalization in which some of the second derivatives diverge and others remain finite. This type of critical behaviour may show up in intermediate regions, i.e. not too far from and not too close to the critical point, but also in special cases in which the lowest eigenvalue of the matrix $\partial^2\Pi/\partial \boldsymbol{E}\partial \boldsymbol{E}$ is zero, see subsection 6.3. The two cases of complete renormalization and unrenormalized exponents follow as corollaries of the treatment of partial renormalization.

So far we have only taken into account a reference free energy for which the singular part has divergent second derivatives, cf. (4.3). In a final remark a more general reference free energy containing also finite (cusp-like) second derivatives, i.e. $0 < a_k < 1$ in eq. (1.7), will be taken into consideration.

7.1. *Homogeneity properties*

In order to discuss the homogeneity properties (in the case of partial critical-exponent renormalization) let us assume that the relevant variables $\boldsymbol{E}$ can be decomposed into variables

$$\boldsymbol{E}_a = \{E_1, \dots, E_q\}, \qquad \boldsymbol{E}_b = \{E_{q+1}, \dots, E_r\}, \tag{7.1}$$

so that

$$\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = \Pi^a(\boldsymbol{E}_a, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) + \Pi^b(\boldsymbol{E}_b, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}). \tag{7.2}$$

Assuming "continuity of the pressure"[47,77]) for the reference system, i.e. the free energy $f_0(\boldsymbol{h}^*)$ is strictly concave and $g_0(\boldsymbol{m})$ has continuous first derivatives ($\boldsymbol{h}^* = \partial g_0/\partial \boldsymbol{m}$), we have at the infimum in (5.15) that

$$\tilde{\boldsymbol{\epsilon}}_a = \frac{\partial g_s}{\partial \boldsymbol{E}_a}(\boldsymbol{E}_a, \boldsymbol{E}_b) + \frac{\partial \Pi^a}{\partial \boldsymbol{E}_a}(\boldsymbol{E}_a, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \quad \tilde{\boldsymbol{\epsilon}}_b = \frac{\partial g_s}{\partial \boldsymbol{E}_b}(\boldsymbol{E}_a, \boldsymbol{E}_b) + \frac{\partial \Pi^b}{\partial \boldsymbol{E}_b}(\boldsymbol{E}_b, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}), \tag{7.3}$$

which yield unique solutions $\boldsymbol{E}_a(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$, $\boldsymbol{E}_b(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ since $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ is assumed to be a strongly convex function of $\boldsymbol{E}$, cf. section 6.1.

Let us also assume that in a certain region of external parameters $\tilde{\boldsymbol{\epsilon}}$ and $\boldsymbol{\zeta}$, we have the inequalities, (which are satisfied in a trivial way with $q = r$ far from all critical points and with $q = 0$ sufficiently close to the critical point),

$$\left|\frac{\partial g_s}{\partial E_a}\right| \gg \left|\frac{\partial \Pi^a}{\partial E_a}\right|, \qquad \left|\frac{\partial g_s}{\partial E_b}\right| \ll \left|\frac{\partial \Pi^b}{\partial E_b}\right|, \tag{7.4}$$

so that in eq. (7.3) for $\bar{\epsilon}_a$, as well as in (5.15) for the free energy $\hat{f}(\epsilon, \zeta)$, we can neglect Π^a. Under these conditions we shall derive the homogeneity property for the (dominant) singular part of $\hat{f}(\epsilon, \zeta)$.

From (5.15) and (7.4) we have

$$\hat{f}(\epsilon, \zeta) = \inf_{E_a, E_b} [-\bar{\epsilon}_a \cdot E_a - \bar{\epsilon}_b \cdot E_b + g_s(E_a, E_b) + \Pi^b(E_b, \bar{\epsilon}, \zeta)] + \Pi_r(\bar{\epsilon}, \zeta). \tag{7.5}$$

Using the partial (inverse) Legendre transform

$$\phi_s(\bar{\epsilon}_a, E_b) = \inf_{E_a} [-\bar{\epsilon}_a \cdot E_a + g_s(E_a, E_b)], \tag{7.6}$$

we have

$$\hat{f}(\epsilon, \zeta) = \inf_{E_b} [-\bar{\epsilon}_b \cdot E_b + \phi_s(\bar{\epsilon}_a, E_b) + \Pi^b(E_b, \bar{\epsilon}, \zeta)] + \Pi_r(\bar{\epsilon}, \zeta). \tag{7.7}$$

Here ϕ_s satisfies the homogeneity relation, cf. the derivation of (4.17),

$$\begin{aligned} &\phi_s(b^{a_1}\bar{\epsilon}_1, \ldots, b^{a_q}\bar{\epsilon}_q, b^{1-a_{q+1}}E_{q+1}, \ldots, b^{1-a_r}E_r) \\ &\quad = b\phi_s(\bar{\epsilon}_1, \ldots, \bar{\epsilon}_q, E_{q+1}, \ldots, E_r), \qquad (a_k > \tfrac{1}{2}). \end{aligned} \tag{7.8}$$

From (7.8) we see that the variables $\bar{\epsilon}_k$ with $k \leq q$ behave like b^{a_k}. Furthermore, since $\Pi_r(\bar{\epsilon}, \zeta)$ contains a term $-\frac{1}{2}\zeta \cdot \zeta$ independent of $\hat{P}(E, Z, \epsilon, \zeta)$ and since Π^b is a strongly convex function of E_b, so that for small ζ terms like $\zeta\zeta E_b$, $\zeta\zeta E_b E_b$ cannot influence the phase diagram, we also may use the estimate $\zeta \sim b^{1/2}$. Then we can restrict ourselves to linear terms in $\bar{\epsilon}_a$ and ζ in the expansion of Π^b, i.e.

$$\Pi^b(E_b, \bar{\epsilon}_a, \bar{\epsilon}_b, \zeta) = \Pi^b_0(E_b, \bar{\epsilon}_b) + \Pi^b_a(E_b, \bar{\epsilon}_b) \cdot \bar{\epsilon}_a + \Pi^b_\zeta(E_b, \bar{\epsilon}_b) \cdot \zeta. \tag{7.9}$$

The infimum over E_b in (7.7) is determined by the equation

$$\bar{\epsilon}_b = \frac{\partial \Pi^b_0}{\partial E_b}(E_b, \bar{\epsilon}_b) + \frac{\partial}{\partial E_b}(\phi_s + \Pi^b_a \cdot \bar{\epsilon}_a + \Pi^b_\zeta \cdot \zeta). \tag{7.10}$$

Here the first term involving Π^b_0 is the dominant term, cf. (7.4), (7.9). From (7.7) and (7.10) it can be shown that†

$$\begin{aligned} \hat{f}(\epsilon, \zeta) = {} & \phi_s(\bar{\epsilon}_a, \epsilon^*_b(\bar{\epsilon}_b)) - \bar{\epsilon}_b \cdot \epsilon^*_b(\bar{\epsilon}_b) + \Pi^b_0(\epsilon^*_b(\bar{\epsilon}_b), \bar{\epsilon}_b) \\ & + \Pi^b_a(\epsilon^*_b(\bar{\epsilon}_b), \bar{\epsilon}_b) \cdot \bar{\epsilon}_a + \Pi^b_\zeta(\epsilon^*_b(\bar{\epsilon}_b), \bar{\epsilon}_b) \cdot \zeta + \Pi_r(\bar{\epsilon}, \zeta) + \Phi(\bar{\epsilon}, \zeta), \end{aligned} \tag{7.11}$$

† The notation for the scaling fields ϵ^*_a, ϵ^*_b should not be confused with the one for the relevant field variables of the reference system in section 4. In the remark at the end of this section, however, a free energy of the form (7.11) will be regarded as a new reference free energy.

where $\boldsymbol{\epsilon}_b^*(\bar{\boldsymbol{\epsilon}}_b)$ is the unique solution of the equation

$$\bar{\boldsymbol{\epsilon}}_b = \frac{\partial \Pi_0^b}{\partial \boldsymbol{E}_b}(\boldsymbol{\epsilon}_b^*(\bar{\boldsymbol{\epsilon}}_b), \bar{\boldsymbol{\epsilon}}_b) \tag{7.12}$$

and where $\Phi(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ is a small correction which can be omitted. The proof of (7.11) is not entirely trivial and is given in appendix C.

Ignoring the term $\Phi(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ and using

$$\bar{\boldsymbol{\epsilon}}_b = \bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*), \qquad \bar{\boldsymbol{\epsilon}}_a = \boldsymbol{\epsilon}_a^*, \tag{7.13}$$

where $\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*)$ is the inverse transformation of $\boldsymbol{\epsilon}_b^* = \boldsymbol{\epsilon}_b^*(\bar{\boldsymbol{\epsilon}}_b)$ in (7.12), we obtain

$$\hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = \phi_s(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_b^*) + \phi_r(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_b^*, \boldsymbol{\zeta}) \tag{7.14}$$

with

$$\begin{aligned}\phi_r(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_b^*, \boldsymbol{\zeta}) = &-\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*)\cdot\boldsymbol{\epsilon}_b^* + \Pi_0^b(\boldsymbol{\epsilon}_b^*, \bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*))\\ &+\Pi_a^b(\boldsymbol{\epsilon}_b^*, \bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*))\cdot\boldsymbol{\epsilon}_a^* + \Pi_\zeta^b(\boldsymbol{\epsilon}_b^*, \bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*))\cdot\boldsymbol{\zeta} + \Pi_r(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}).\end{aligned} \tag{7.15}$$

The function ϕ_s in (7.14) satisfies the homogeneity relation, cf. (7.8),

$$\begin{aligned}&\phi_s(b^{a_1}\epsilon_1^*, \ldots, b^{a_q}\epsilon_q^*, b^{1-a_{q+1}}\epsilon_{q+1}^*, \ldots, b^{1-a_r}\epsilon_r^*)\\ &\quad = b\phi_s(\epsilon_1^*, \ldots, \epsilon_q^*, \epsilon_{q+1}^*, \ldots, \epsilon_r^*).\end{aligned} \tag{7.16}$$

Expanding the function $p(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in the transformation (5.14) to linear terms in $\bar{\boldsymbol{\epsilon}}_a$ and $\boldsymbol{\zeta}$, i.e.

$$p(\bar{\boldsymbol{\epsilon}}_a, \bar{\boldsymbol{\epsilon}}_b, \boldsymbol{\zeta}) = p_0(\bar{\boldsymbol{\epsilon}}_b) + \mathbf{p}_a(\bar{\boldsymbol{\epsilon}}_b)\cdot\bar{\boldsymbol{\epsilon}}_a + \mathbf{p}_\zeta(\bar{\boldsymbol{\epsilon}}_b)\cdot\boldsymbol{\zeta} \tag{7.17}$$

we have to leading order

$$\begin{aligned}\boldsymbol{\epsilon}_a &= \boldsymbol{\epsilon}_a^* - p_0^a(\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*)) - \mathbf{p}_a^a(\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*))\cdot\boldsymbol{\epsilon}_a^* - \mathbf{p}_\zeta^a(\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*))\cdot\boldsymbol{\zeta},\\ \boldsymbol{\epsilon}_b &= \bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*) - p_0^b(\bar{\boldsymbol{\epsilon}}_b(\boldsymbol{\epsilon}_b^*)),\end{aligned} \tag{7.18}$$

where p_0^a and p_0^b denote the components $k \leq q$ and $k > q$ resp. of the vector p_0. In the second equation, for $\boldsymbol{\epsilon}_b$, we have ignored terms involving $\bar{\boldsymbol{\epsilon}}_a = \boldsymbol{\epsilon}_a^*$ and $\boldsymbol{\zeta}$ which go with $o(b^{1/2})$ and $b^{1/2}$ resp., whereas in view of (7.16) and the fact that Π_0^b in (7.12) and (7.9) contains only quadratic and higher order terms in $\boldsymbol{E}_b$, $\boldsymbol{\epsilon}_b^*$ and $\bar{\boldsymbol{\epsilon}}_b$ tend to zero with $o(b^{1/2-\eta})$, $(\eta > 0)$.

Equations (7.14), (7.15) and (7.18), in which all functions Π_0^b, Π_a^b, Π_ζ^b, p_0^a, $\mathbf{p}_a^a$, $\mathbf{p}_\zeta^a$ and p_0^b are regular functions of $\boldsymbol{\epsilon}_b^*$, are a general representation of the free energy $\hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta})$ given by (7.5).

7.2. Partial critical-exponent renormalization

As a consequence of (7.16) we have for the second derivatives

$$X_{kl} \equiv -\frac{\partial^2}{\partial \epsilon_k^* \partial \epsilon_l^*} \phi_s(\epsilon_a^*, \epsilon_b^*) \tag{7.19}$$

the homogeneity relations

$$\begin{aligned} &X_{kl}(b^{a'_1}\epsilon_1^*, \dots, b^{a'_q}\epsilon_q^*, b^{a'_{q+1}}\epsilon_{q+1}^*, \dots, b^{a'_r}\epsilon_r^*) \\ &\quad = b^{1-a'_k-a'_l} X_{kl}(\epsilon_1^*, \dots, \epsilon_q^*, \epsilon_{q+1}^*, \dots, \epsilon_r^*) \end{aligned} \tag{7.20}$$

with

$$\begin{aligned} a'_k &= a_k, \qquad & k &= 1, \dots, q, \\ a'_k &= 1 - a_k, \qquad & k &= q+1, \dots, r. \end{aligned} \tag{7.21}$$

Equations (7.20) and (7.21) imply that, ($b \downarrow 0$),

i) X_{kl} diverges with $b^{1-a_k-a_l}$, if $k, l \leq q$,
ii) X_{kl} tends to zero with $b^{a_k+a_l-1}$, if $k, l > q$,
iii) $X_{kl} \sim b^{a_k-a_l}$, ($k > q, l \leq q$), diverges if $a_k < a_l$ and tends to zero if $a_k > a_l$.

The results (7.16), (7.20) and (7.21) are characteristic for a partial renormalization of critical exponents. The physical interpretation of (7.20) is not trivial, since the transformation (7.18) from ϵ_a^*, ϵ_b^* to ϵ_a, ϵ_b is in general a nonlinear transformation. In special cases, however, simplifications occur, see appendix D.

7.3. Corollaries

As an application we now consider the general case of a (small) function $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ which is strongly convex at $(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\mathbf{0}, \mathbf{0}, \mathbf{0})$ as treated in section 6.1.

i) Sufficiently far from the critical points (for small $\tilde{\boldsymbol{\epsilon}}$ and $\boldsymbol{\zeta}$), we have the inequality $b^{\max(2a_k-1)} \gg \|\Pi\|$, where $\|\Pi\|$ denotes the largest eigenvalue of $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$. We may neglect the function $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$, so that we have (7.4), (7.5) with $q = r$, i.e. $\boldsymbol{E} \equiv \boldsymbol{E}_a$. Therefore, (7.20) holds with $a'_k = a_k$, for $k = 1, \dots, r$, leading to the same exponents as the second derivatives of the reference free energy. Furthermore, in view of (7.16) with $q = r$, ($a_k > \frac{1}{2}$), the regular part (7.15) reduces to $\Pi_r(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$. Finally, since there are only variables $\boldsymbol{\epsilon}_a^* = \boldsymbol{\epsilon}^*$ in this case, the first equation of (7.18) reduces to a linear transformation, in which $\boldsymbol{p}_0^a$, $\boldsymbol{p}_a^a$ and $\boldsymbol{p}_\zeta^a$ are constant. Note that the transformation coefficients originate from the linear terms in $\boldsymbol{E}$ in $\hat{P}(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta})$, cf. (5.12)–(5.14), whereas the function $\Pi(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$, which has been neglected, arises from quadratic and higher order terms in $\boldsymbol{E}$, cf. (5.16).
ii) Sufficiently close to the critical point we have the inequality $b^{\min(2a'_k-1)} \ll \delta$, where $\delta > 0$ is the lowest eigenvalue of $\partial^2\Pi/\partial\boldsymbol{E}\partial\boldsymbol{E}$ at $(\boldsymbol{E}, \tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\mathbf{0}, \mathbf{0}, \mathbf{0})$. We

then have eqs. (7.4), (7.5) with $q = 0$, i.e. $\boldsymbol{E} \equiv \boldsymbol{E}_b$, and (7.20) holds with $a_k' = 1 - a_k$ for $k = 1, \ldots, r$. As a consequence all second derivatives of the free energy remain finite, cf. the regular part (7.15), and the singular parts X_{kl} tend to zero with $b^{a_k + a_l - 1}$. This situation is characteristic for the case of complete critical-exponent renormalization. Furthermore, since we now only have variables $\boldsymbol{\epsilon}_b^* = \boldsymbol{\epsilon}^*$, the second equation of (7.18) is a nonlinear transformation $\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}}(\boldsymbol{\epsilon}^*) - p_0(\bar{\boldsymbol{\epsilon}}(\boldsymbol{\epsilon}^*))$. In the special case that $\frac{1}{2} < a_k < \frac{3}{4}$, i.e. $\frac{1}{4} < a_k' < \frac{1}{2}$, $(k = 1, \ldots, r)$, all nonlinear terms in the transformation may be neglected, cf. appendix D, but this condition will not be satisfied in practice, if the magnetic field is one of the relevant fields.

iii) In intermediate cases, i.e. not too far from and not too close to the critical point one may have eq. (7.4) with both $\boldsymbol{E}_a$ and $\boldsymbol{E}_b$, $(0 < q < r)$, under suitable assumptions for the function $\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$. In principle, one could distinguish between $2^r - 2$ of such regimes corresponding to all partial Legendre transformations (7.6), although it is by no means obvious that all these regimes would have a clear physical meaning in actual cases. From (7.20), (7.21) one finds that certain second derivatives X_{kl} diverge at the critical point, whereas others, i.e. those with $k, l > q$, or $k > q$, $l \leq q$ and $a_k > a_l$, tend to zero. This situation corresponds to partial critical-exponent renormalization. Examples are the Fisher renormalization[9]) with $\alpha' = -\alpha/(1-\alpha)$, $\delta' = \delta$, or the renormalization in ref. 30 with $\alpha' = \alpha$, $\delta' = 1/\delta$. Partial critical-exponent renormalization can also exist down to the critical point, in the special case that the lowest eigenvalue of $\partial^2 \Pi / \partial \boldsymbol{E} \partial \boldsymbol{E}$ vanishes at $(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\mathbf{0}, \mathbf{0}, \mathbf{0})$. Such a situation, however, is not stable under small perturbations which can give rise to multicritical features, cf. section 6.3.

As an example of i)–iii) we give in appendix E the four possible sets of exponents in case of a simple ferromagnet with two relevant variables $\epsilon_1 = 1 - T/T_c$, $\epsilon_2 = H$.

In the treatment presented here, the properties of critical-exponent renormalization have been derived on the basis of homogeneity relations and (partial) Legendre transformation. In the simple case of one relevant variable $(r = 1)$, it is worthwhile to use an iterative procedure for the solution of implicit equations. Such a procedure provides also higher order (confluent) singularities which contribute to terms of the order $b^{1+\eta}$, $(\eta > 0)$, in the free energy and which have been neglected in the general treatment of this paper. The case with one variable is discussed in appendix F.

7.4. Remark

So far we have considered a reference free energy with divergent second derivatives, i.e. eq. (4.3) in which the singular part satisfies the homogeneity relation (1.7) with $\frac{1}{2} < a_k < 1$. It is now straightforward to take into account a more general situation in which some second derivatives diverge, say $\frac{1}{2} < a_k < 1$, $(k = 1, \ldots, q)$, and others remain finite, $0 < a_k < \frac{1}{2}$, $(k = q + 1, \ldots, r)$. (Here we exclude values $a_k = \frac{1}{2}$ which usually would require logarithmic corrections and further analysis, cf. e.g. refs. 9, 73, 74.) To see this note that a general expression for the reference free energy is provided by eqs. (7.14), (7.15), (7.18) in section 7.1, which has been obtained from the simple expression (4.3) after adding a suitable function $\hat{P}(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta})$ in (5.6).

To be specific, if we choose a function $\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (5.15) which depends only on the variables $\boldsymbol{E}_b = \{E_{q+1}, \ldots, E_r\}$, i.e. $\Pi^a = 0$ in eq. (7.2), then in view of the analysis in section 7.1 we obtain a free energy of the form

$$\begin{aligned} \hat{f}(\boldsymbol{\epsilon}, \boldsymbol{\zeta}) = {} & \phi_s(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_b^*) + C(\boldsymbol{\epsilon}_b^*) + \boldsymbol{C}_a(\boldsymbol{\epsilon}_b^*) \cdot \boldsymbol{\epsilon}_a^* \\ & + \boldsymbol{C}_\zeta(\boldsymbol{\epsilon}_b^*) \cdot \boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\zeta} \cdot \boldsymbol{\zeta} + \text{small terms}. \end{aligned} \tag{7.22}$$

Here ϕ_s satisfies the homogeneity property (7.16) which is of a more general type than (1.7), since, in view of (7.21), $\frac{1}{2} < a'_k < 1$ for $k = 1, \ldots, q$ and $0 < a'_k < \frac{1}{2}$ for $k = q + 1, \ldots, r$. The functions C, $\boldsymbol{C}_a$, $\boldsymbol{C}_\zeta$ are regular functions of the variables $\boldsymbol{\epsilon}_b = \{\epsilon_{q+1}^*, \ldots, \epsilon_r^*\}$ which can be expressed in terms of the functions $\bar{\boldsymbol{\epsilon}}_b$, Π_0^b, Π_a^b, Π_ζ^b and $\Pi_t(\bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (7.15).

The variables $\boldsymbol{\epsilon}^*$ can be found from $\boldsymbol{\epsilon}$ by a transformation of the type

$$\begin{aligned} \boldsymbol{\epsilon}_a^* &= \boldsymbol{\epsilon}_a + \boldsymbol{A}(\boldsymbol{\epsilon}_b) + \boldsymbol{A}_a(\boldsymbol{\epsilon}_b) \cdot \boldsymbol{\epsilon}_a + \boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b) \cdot \boldsymbol{\zeta}, \\ \boldsymbol{\epsilon}_b^* &= \boldsymbol{B}(\boldsymbol{\epsilon}_b), \end{aligned} \tag{7.23}$$

in which $\boldsymbol{A}$, $\boldsymbol{A}_a$, $\boldsymbol{A}_\zeta$ and $\boldsymbol{B}$ are regular functions of $\boldsymbol{\epsilon}_b$. These functions can be obtained taking the inverse transformation of (7.18), or also from the function $\boldsymbol{\epsilon}_b^*(\bar{\boldsymbol{\epsilon}}_b)$ in (7.12) and the definition $\boldsymbol{\epsilon}_a^* = \bar{\boldsymbol{\epsilon}}_a$ in (7.13) using the explicit expression for $\bar{\boldsymbol{\epsilon}}$ in terms of $\boldsymbol{\epsilon}$ and $\boldsymbol{\zeta}$ which can be obtained linearizing the right-hand side of (5.13) with respect to the variables $\boldsymbol{\epsilon}_a$ and $\boldsymbol{\zeta}$.

Equations (7.22) and (7.23) can be considered to be a general expression for the free energy of a reference system, in which some of the second derivatives of the singular part diverge and others have a cusp-like behaviour, involving a homogeneous function of nonlinear scaling fields, see e.g. refs. 78, 79, 44. (This result is of course of a formal nature and does not imply that the behaviour of such a reference system should be interpreted in terms of a simpler system as in eq. (4.3), subjected to a number of constraints leading to eq. (5.6).) The stability of such a reference system may now be discussed on the basis of a function $\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ of the form (7.2), in which $\Pi^b(\boldsymbol{E}_b, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ contributes to the reference free energy and $\Pi^a(\boldsymbol{E}_a, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ is a small perturbation which will affect the critical behaviour. (Of course one may also evaluate the Legendre transform $\hat{g}_0(\boldsymbol{E}, \boldsymbol{Z})$ of (7.22), see appendix G for further details, and discuss the stability of critical behaviour on the basis of (5.15).)

Then, following the line of reasoning of section 6, we are led to the following conclusions:

i) If $\Pi^a(\boldsymbol{E}_a, \boldsymbol{0}, \boldsymbol{0})$ is strongly convex as a function of $\boldsymbol{E}_a$ in a neighbourhood of $\boldsymbol{E}_a = \boldsymbol{0}$, then there is a critical point at $\bar{\boldsymbol{\epsilon}} = \boldsymbol{0}$, just as the reference hamiltonian has a critical point at $\boldsymbol{\epsilon}^* = \boldsymbol{0}$. There will be no first-order transitions, the second derivatives of the free energy are finite and close to the critical point there is a complete critical-exponent renormalization described by (7.20), (7.21) with $a'_k = 1 - a_k$ for $k = 1, \dots, r$.

ii) If $\partial^2\Pi^a/\partial\boldsymbol{E}_a\partial\boldsymbol{E}_a$ has a negative eigenvalue at $(\boldsymbol{E}_a, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = (\boldsymbol{0}, \boldsymbol{0}, \boldsymbol{0})$, then the critical point of the reference hamiltonian cannot be reached, there will be first-order transitions which may terminate in classical critical points or on a critical point of the reference system, cf. section 6.2.

iii) If the lowest eigenvalue of $\partial^2\Pi^a/\partial\boldsymbol{E}_a\partial\boldsymbol{E}_a$ is zero there may be multicritical behaviour, see also the discussion in section 6.3.

Finally, if the reference free energy has a critical point with only finite second derivatives, i.e. $\boldsymbol{\epsilon}^* \equiv \boldsymbol{\epsilon}^*_b$, $\boldsymbol{E} \equiv \boldsymbol{E}_b$, see (7.20), (7.21) with $a'_k = 1 - a_k$ for $k = 1, \dots, r$, then the critical behaviour will be stable under small perturbations. Only a finite perturbation can give rise to qualitatively different effects such as e.g. multicritical behaviour[14,15]), where at the multicritical point one may observe "inverse" critical-exponent renormalization ($a_k = 1 - a'_k$).

Appendix A

To give a proof of (4.21) we start from the relation

$$\hat{g}_0(\{m_j\}) = g_h(\{m_j\}) + \int_0^{\boldsymbol{m}} \mathrm{d}\boldsymbol{m}' \int_0^{\boldsymbol{m}'} \mathrm{d}\boldsymbol{m}'' \colon \boldsymbol{K}(\{m''_j\}), \tag{A.1}$$

cf. (4.12), (4.14), in which $\boldsymbol{m} = \{m_1, \dots, m_n\}$ denotes an n-dimensional vector with relevant components $m_k = E_k$, $(k = 1, \dots, r)$, and irrelevant components $m_{l+r} = Z_l$, $(l = 1, \dots, n-r)$, conjugate to the fields ϵ_k^* and ζ_l^* resp. appearing in eq. (4.1) for the vector $\hat{\boldsymbol{h}}^*$. The matrix $\boldsymbol{K}$ is given by

$$\boldsymbol{K} = (\boldsymbol{X}_h + \boldsymbol{Y})^{-1} - \boldsymbol{X}_h^{-1} = -\boldsymbol{X}_h^{-1} \cdot \boldsymbol{Y} \cdot \boldsymbol{X}_h^{-1} \cdot (1 + \boldsymbol{Y} \cdot \boldsymbol{X}_h^{-1})^{-1} \tag{A.2}$$

with

$$\boldsymbol{X}_h = -\partial^2 f_h / \partial \hat{\boldsymbol{h}}^* \partial \hat{\boldsymbol{h}}^*, \qquad \boldsymbol{Y} = -\partial^2 F / \partial \hat{\boldsymbol{h}}^* \partial \hat{\boldsymbol{h}}^*. \tag{A.3}$$

For values $\boldsymbol{m}$ satisfying $m_j = b^{1-a_j} \hat{m}_j$, in which $a_1, \dots, a_r$ are given by (1.7) and $a_j = \frac{1}{2}$ for $j = r+1, \dots, n$, use can be made of the estimates, cf. (4.9), (4.10),

$$\begin{aligned} &|(X_h^{-1})_{pq}| \leq C_{pq} b^{a_p + a_q - 1}, \\ &|Y_{pq}| \leq D_{pq} b^{1 - a_p - a_q}, \qquad \|\boldsymbol{D}\| = \mathcal{O}(b^{\eta}). \end{aligned} \tag{A.4}$$

From (A.4) we have

$$|\{\boldsymbol{X}_h^{-1} \cdot (\boldsymbol{Y} \cdot \boldsymbol{X}_h^{-1})^n\}_{pq}| \leq \{\boldsymbol{C} \cdot (\boldsymbol{D} \cdot \boldsymbol{C})^n\}_{pq} b^{a_p + a_q - 1}, \tag{A.5}$$

leading to

$$|K_{pq}| = \left| \sum_{n=1}^{\infty} (-1)^n \{\boldsymbol{X}_h^{-1} \cdot (\boldsymbol{Y} \cdot \boldsymbol{X}_h^{-1})^n\}_{pq} \right| \leq \frac{\|\boldsymbol{C}\|^2 \|\boldsymbol{D}\|}{1 - \|\boldsymbol{C}\| \|\boldsymbol{D}\|} b^{a_p + a_q - 1}. \tag{A.6}$$

Inserting (A.6) into (A.1) we arrive at the relation

$$\hat{g}_0(\{b^{1-a_j} \hat{m}_j\}) = b g_h(\{\hat{m}_j\}) + \mathcal{O}(b^{1+\eta}). \tag{A.7}$$

Equation (4.21) follows immediately from (A.7) identifying $\{\hat{m}_1, \dots, \hat{m}_n\}$ with $\{E_1, \dots, E_r, Z_1, \dots, Z_{n-r}\}$.

Appendix B

In this appendix we discuss the influence of terms like $\zeta\zeta EE$ in $\Pi(E, \tilde{\epsilon}, \zeta)$ on the basis of the example

$$\hat{f}(\epsilon, \zeta) = \inf_{E,Z} [-\epsilon E - \zeta Z + |E|^x + \tfrac{1}{2} Z^2 + A(E) Z + \tfrac{1}{2} B(E) Z^2]. \tag{B.1}$$

Equation (B.1) has the form (5.6) with one variable E, one variable Z, $\hat{g}_0(E, Z) = |E|^x + \frac{1}{2} Z^2$ and a simple function $\hat{P}(E, Z) = A(E) Z + \frac{1}{2} B(E) Z^2$ which depends only on E and Z. In eq. (5.9) the term $\frac{1}{2} B(E) Z^2$ has been ignored, apart from an E-independent contribution $\frac{1}{2} P_{ZZ} Z^2$.

The infimum over Z occurs at

$$Z_{\text{inf}} = (\zeta - A(E)) / (1 + B(E)), \tag{B.2}$$

so that

$$\hat{f}(\epsilon, \zeta) = \inf_E[-\epsilon E + |E|^x - \tfrac{1}{2}(\zeta - A(E))^2/(1 + B(E))]. \tag{B.3}$$

Assuming that $2 < x < 3$, i.e. $f_s(\epsilon^*) \sim |\epsilon^*|^{2-\alpha}$ with $0 < \alpha < \frac{1}{2}$, $x = (2 - \alpha)/(1 - \alpha)$, we may expand

$$A(E) = A_1E + \tfrac{1}{2}A_2E^2, \qquad B(E) = B_1E + \tfrac{1}{2}B_2E^2, \tag{B.4}$$

and

$$\hat{f}(\epsilon, \zeta) = \inf_E[|E|^x - \tfrac{1}{2}\zeta^2 + E\{-\epsilon + \zeta A_1 + \tfrac{1}{2}\zeta^2 B_1\}$$

$$+ \tfrac{1}{2}E^2\{\zeta A_2 + \tfrac{1}{2}\zeta^2 B_2 - (A_1 + \zeta B_1)^2\}]. \tag{B.5}$$

Note that in eq. (B.5) we have two ζ^2E^2 terms, one arising from B_1, i.e. the EZ^2 term in $\hat{P}(E, Z)$ and the other one from B_2, i.e. the E^2Z^2 term in $\hat{P}(E, Z)$.

Equation (B.5) leads to a first-order transition, if the right-hand side for fixed ϵ and ζ has two equal infima. This will occur, if the coefficient of E vanishes and the coefficient of E^2 is negative, i.e.

$$\epsilon = \zeta A_1 + \tfrac{1}{2}\zeta^2 B_1, \tag{B.6}$$

$$\zeta A_2 + \tfrac{1}{2}\zeta^2 B_2 - (A_1 + \zeta B_1)^2 < 0. \tag{B.7}$$

We now discuss different cases:

i) If $A_1 \neq 0$, i.e. $\hat{P}(E, Z)$ contains a nonvanishing EZ term, then the function $\Pi(E, \zeta)$, cf. (5.16), in the right-hand side of (B.5) is concave for small ζ and there is always a first-order transition, see section 6.2.

ii) If $A_1 = 0$, $A_2 \neq 0$, i.e. $\hat{P}(E, Z)$ contains a nonvanishing E^2Z term, then the function $\Pi(E, \zeta)$, if we neglect terms $\sim \zeta^2$, is convex for $A_2\zeta > 0$ and concave for $A_2\zeta < 0$. For $\zeta = 0$ the free energy has divergent second derivatives at $\epsilon = 0$. For $A_2\zeta > 0$, we have a critical point with $E = 0$ at $\epsilon = \frac{1}{2}\zeta^2 B_1$ with finite second derivatives of the free energy, for $A_2\zeta < 0$ there is a first-order transition at $\epsilon = \frac{1}{2}\zeta^2 B_1$, see the discussion on $E^2\zeta$ terms in section 6.3.

iii) If $A_1 = A_2 = 0$, then, as a consequence of the ζ^2E^2 terms in (B.5), we have a critical point at $E = 0$ with finite second derivatives, if $B_1^2 < \frac{1}{2}B_2$, and a first-order transition for $B_1^2 > \frac{1}{2}B_2$, provided that $\zeta \neq 0$. Here the coefficients B_1 and B_2 arise from EZ^2 and E^2Z^2 terms in the expansion of $\hat{P}(E, Z)$. For $\zeta = 0$ the critical behaviour is identical to that of the reference system.

We now consider the second derivative of $\hat{f}(\epsilon, \zeta)$ with respect to the variable ζ at $\zeta = 0$ in the cases ii) and iii) with $A_1 = 0$, where we do not have a first-order transition for $\zeta = 0$. From (B.1) and (B.2) we have

$$\chi_{\zeta\zeta}\Big|_{\zeta=0} = -\frac{\partial^2 \hat{f}}{\partial\zeta^2}\Big|_{\zeta=0} = \frac{dZ_{inf}}{d\zeta}\Big|_{\zeta=0}$$
$$= \frac{1}{1+B(E)} - \left[\frac{A'(E)}{1+B(E)} - \frac{A(E)B'(E)}{(1+B(E))^2}\right]\frac{dZ_{inf}}{d\epsilon}\Big|_{\zeta=0}$$
$$= \frac{1}{1+B(E)} + \left[\frac{A'(E)}{1+B(E)} - \frac{A(E)B'(E)}{(1+B(E))^2}\right]^2\frac{dE_{inf}}{d\epsilon}\Big|_{\zeta=0}, \tag{B.8}$$

where, ignoring the last term in the right-hand side of (B.3),

$$E_{inf} = \left|\frac{\epsilon}{x}\right|^{1/(x-1)} \operatorname{sgn}\epsilon, \qquad \frac{dE_{inf}}{d\epsilon}\Big|_{\zeta=0} = \frac{1}{x(x-1)}\left|\frac{\epsilon}{x}\right|^{(2-x)/(x-1)}. \tag{B.9}$$

Expanding the right-hand side of (B.8) with $A_1 = 0$ up to quadratic terms in E, we have

$$\chi_{\zeta\zeta}\Big|_{\zeta=0} = 1 - B_1E_{inf} - (\tfrac{1}{2}B_2 - B_1^2)E_{inf}^2 + A_2^2E_{inf}^2\frac{dE_{inf}}{d\epsilon}\Big|_{\zeta=0}, \tag{B.10}$$

in which the three terms with B_1, $\frac{1}{2}B_2 - B_1^2$, A_2^2 behave like $|\epsilon/x|^{1/(x-1)}\operatorname{sgn}\epsilon$, $|\epsilon/x|^{2/(x-1)}$, $|\epsilon/x|^{(4-x)/(x-1)}$ resp. Thus we have derived three singular contributions to the susceptibility $\chi_{\zeta\zeta}$ for $\zeta = 0$ which arise from EZ^2, E^2Z^2, E^2Z terms resp. in $\hat{P}(E, Z)$, see also refs. 75, 76 for similar results derived using a renormalization group approach starting from a Landau–Ginzburg hamiltonian.

To give an example of the effect of nonlinear transformations, let us consider the Legendre transform of (B.1) in the special case that $A(E) = 0$, i.e.

$$\hat{g}(E, Z) = \sup_{\epsilon,\zeta}[\epsilon E + \zeta Z + \hat{f}(\epsilon, \zeta)] = \underset{E,Z}{\mathrm{CE}}[|E|^x + \tfrac{1}{2}Z^2 + \tfrac{1}{2}B(E)Z^2]. \tag{B.11}$$

Using the new variable

$$\hat{Z} = Z\{1 + B(E)\}^{1/2} \tag{B.12}$$

eq. (B.11) can be rewritten

$$\hat{g}(E, Z) = \underset{E,Z}{\mathrm{CE}}[|E|^x + \tfrac{1}{2}\hat{Z}^2]. \tag{B.13}$$

Ignoring the nonlinear features of (B.12) and replacing the convex envelope over E and Z in (B.13) by the convex envelope over E and $\hat{Z}$, one may infer $\hat{g}(E, Z) = |E|^x + \frac{1}{2}\hat{Z}^2$, which is wrong, also because it does not lead to any first-order transition for $B_1^2 > \frac{1}{2}B_2$, cf. the discussion under iii).

Appendix C

To prove eq. (7.11) we note that the solution of (7.10) can be expressed as

$$E_b = \epsilon_b^*(\bar{\epsilon}_b) + \epsilon_b'(\bar{\epsilon}_a, \bar{\epsilon}_b, \zeta), \tag{C.1}$$

where $\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b)$ has been defined by (7.12) and where $\boldsymbol{\epsilon}_b'(\tilde{\boldsymbol{\epsilon}}_a, \tilde{\boldsymbol{\epsilon}}_b, \boldsymbol{\zeta})$ is a small correction. In fact, in (7.10) the first term $\partial \Pi_0^b/\partial \boldsymbol{E}_b$ will contain linear terms in E_k, $(k > q)$, which behave like b^{1-a_k}, $(a_k > \frac{1}{2})$. On the other hand, $\partial\phi_s/\partial E_k$, $(k > q)$, tends to zero with the power b^{a_k}, the coefficients $\boldsymbol{\Pi}_a^b$ and $\boldsymbol{\Pi}_\zeta^b$ tend to zero with a positive power of b, and the components $\tilde{\epsilon}_l$, $(l \leq q)$, of $\tilde{\boldsymbol{\epsilon}}_a$, and $\boldsymbol{\zeta}$ behave like b^{a_l} and $b^{1/2}$ resp.

Inserting (C.1) into (7.10) we obtain

$$\boldsymbol{\epsilon}_b'(\tilde{\boldsymbol{\epsilon}}_a, \tilde{\boldsymbol{\epsilon}}_b, \boldsymbol{\zeta}) = -\left[\frac{\partial^2 \Pi_0^b}{\partial \boldsymbol{E}_b \partial \boldsymbol{E}_b}(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b), \tilde{\boldsymbol{\epsilon}}_b)\right]^{-1} \cdot \frac{\partial}{\partial \boldsymbol{E}_b}(\phi_s + \boldsymbol{\Pi}_a^b \cdot \tilde{\boldsymbol{\epsilon}}_a + \boldsymbol{\Pi}_\zeta^b \cdot \boldsymbol{\zeta})$$
$$+ \text{ higher order terms.} \tag{C.2}$$

In eq. (C.2) it is of interest that $\boldsymbol{\epsilon}_b'(\tilde{\boldsymbol{\epsilon}}_a, \tilde{\boldsymbol{\epsilon}}_b, \boldsymbol{\zeta})$ tends to zero with $b^{(1+\eta)/2}$, where $\eta > 0$; the precise form of $\boldsymbol{\epsilon}_b'$ will not be used for the derivation of (7.11).

Inserting (C.1) and (7.9) into (7.7) we find (7.11) with

$$\begin{aligned}
\Phi(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) = &-\tilde{\boldsymbol{\epsilon}}_b \cdot \boldsymbol{\epsilon}_b' + \phi_s(\tilde{\boldsymbol{\epsilon}}_a, \boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b) + \boldsymbol{\epsilon}_b') - \phi_s(\tilde{\boldsymbol{\epsilon}}_a, \boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b))\\
&+ \Pi_0^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b) + \boldsymbol{\epsilon}_b', \tilde{\boldsymbol{\epsilon}}_b) - \Pi_0^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b), \tilde{\boldsymbol{\epsilon}}_b)\\
&+ \{\boldsymbol{\Pi}_a^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b) + \boldsymbol{\epsilon}_b', \tilde{\boldsymbol{\epsilon}}_b) - \boldsymbol{\Pi}_a^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b), \tilde{\boldsymbol{\epsilon}}_b)\} \cdot \tilde{\boldsymbol{\epsilon}}_a\\
&+ \{\boldsymbol{\Pi}_\zeta^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b) + \boldsymbol{\epsilon}_b', \tilde{\boldsymbol{\epsilon}}_b) - \boldsymbol{\Pi}_\zeta^b(\boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b), \tilde{\boldsymbol{\epsilon}}_b)\} \cdot \boldsymbol{\zeta}\\
= &\left\{-\tilde{\boldsymbol{\epsilon}}_b + \frac{\partial}{\partial \boldsymbol{E}_b}(\phi_s + \Pi_0^b + \boldsymbol{\Pi}_a^b \cdot \tilde{\boldsymbol{\epsilon}}_a + \boldsymbol{\Pi}_\zeta^b \cdot \boldsymbol{\zeta})\right\} \cdot \boldsymbol{\epsilon}_b' + \tfrac{1}{2}\boldsymbol{\epsilon}_b' \cdot \boldsymbol{L} \cdot \boldsymbol{\epsilon}_b'\\
= &\tfrac{1}{2}\boldsymbol{\epsilon}_b' \cdot \boldsymbol{L} \cdot \boldsymbol{\epsilon}_b',
\end{aligned} \tag{C.3}$$

where $\boldsymbol{L}$ is a matrix which depends on $\boldsymbol{\epsilon}_b'$. The derivative in (C.3) has been taken at the point $\boldsymbol{E}_b = \boldsymbol{\epsilon}_b^*(\tilde{\boldsymbol{\epsilon}}_b) + \boldsymbol{\epsilon}_b'$, so that the last step follows using (7.10). Since the right-hand side of (C.3) is of the order $b^{1+\eta}$, with positive η, the term $\Phi(\tilde{\boldsymbol{\epsilon}}, \boldsymbol{\zeta})$ in (7.11) can be omitted.

Appendix D

In this appendix we discuss some simplifications which may occur in the transformation (7.18) and in eq. (7.15) for the regular part $\phi_r(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_b^*, \boldsymbol{\zeta})$.

i) If for all critical exponents a_k, we have $\frac{1}{2} < a_k < \frac{3}{4}$, then, with $(\boldsymbol{\epsilon}_a^*)_k \sim b^{a_k}$, $(\boldsymbol{\epsilon}_b^*)_k \sim b^{1-a_k}$, cf. (7.16), the $\boldsymbol{\epsilon}_b^*$-dependence in $\boldsymbol{p}_a^a$ and $\boldsymbol{p}_\zeta^a$ can be neglected, as well as third order terms $\sim \boldsymbol{\epsilon}_b^*\boldsymbol{\epsilon}_b^*\boldsymbol{\epsilon}_b^*$ in p_0^a and quadratic terms $\sim \boldsymbol{\epsilon}_b^*\boldsymbol{\epsilon}_b^*$ in $\boldsymbol{p}_0^b$. Furthermore, $\boldsymbol{\Pi}_a^b$ and $\boldsymbol{\Pi}_\zeta^b$, which contain only quadratic and higher order terms in $\boldsymbol{\epsilon}_b^*$, cf. (5.16), (7.2), (7.9), can be neglected. If in addition $\frac{1}{2} < a_k < \frac{2}{3}$, the terms $\sim \boldsymbol{\epsilon}_b^*\boldsymbol{\epsilon}_b^*$ in p_0^a can be neglected, so that (7.18) becomes a linear transformation. However, if the magnetic field is one of the relevant variables, i.e.

$\epsilon_k^* = H$, $a_k = \delta/(\delta+1)$, the condition $\frac{1}{2} < a_k < \frac{3}{4}$ will not be satisfied in practice for all k.

ii) In the case of two relevant variables $\epsilon_1^*, \epsilon_2^*$, such that $\partial^2\phi_s/\partial\epsilon_1^{*2} \sim b^{1-2a_1} \to \infty$ and $\partial^2\phi_s/\partial\epsilon_2^{*2} \sim b^{2a_2-1} \to 0$, we have $\epsilon_1^* = \epsilon_a^*$, $\epsilon_2^* = \epsilon_b^*$. Then the quadratic term $\sim \epsilon_b^{*2}$ in p_0^a in (7.18) can be neglected, provided that $2(1-a_2) > a_1$. This inequality implies also that the ϵ_b^*-dependence in $\boldsymbol{p}_a^a$ and $\boldsymbol{p}_\zeta^a$, i.e. the nonlinear terms in the transformation (7.18), can be ignored. As a further consequence of this inequality the terms Π_a^b and Π_ζ^b in (7.15) which, by definition, are at least quadratic in ϵ_b^*, can be neglected. Also, when we express $\Pi_r(\bar{\epsilon}, \boldsymbol{\zeta})$ in (7.15) in terms of ϵ_a^*, ϵ_b^*, $\boldsymbol{\zeta}$, all quadratic terms involving ϵ_a^* are of the order $b^{1+\eta}$, $(\eta > 0)$, provided that $a_1 > a_2$.

As an example we consider a ferromagnet with relevant variables $1 - T/T_c, H$. If the exponent of the specific heat is renormalized[9], i.e. $a_2 = 1/(2-\alpha)$, $a_1 = \delta/(\delta+1)$, which is e.g. the case in the Baker–Essam model in the constant-volume ensemble[12] or the bond-annealed Syozi model[27], then the inequality $a_2 < a_1 < 2(1-a_2)$, or equivalently $1/(1-\alpha) < \delta < 2(1-\alpha)/\alpha$, will be satisfied in practice. As a consequence the transformation (7.18) can be considered to be a linear transformation and terms like $\epsilon_a^*\epsilon_b^*$ and $\epsilon_b^{*2}\zeta$ in the regular part ϕ_r can be ignored. In the opposite case in which the exponent of the susceptibility is renormalized[30], i.e. $a_1 = 1/(2-\alpha)$, $a_2 = \delta/(\delta+1)$, the inequality will not be satisfied and nonlinear terms in (7.18) and couplings $\epsilon_a^*\epsilon_b^*$ and $\epsilon_b^{*2}\zeta$ in (7.15) can be important.

Appendix E

As an example of critical-exponent renormalization we consider a ferromagnet with two relevant variables $\epsilon_1 = 1 - T/T_c$, $\epsilon_2 = H$ in the simple case that

$$\Pi(\boldsymbol{E}, \bar{\boldsymbol{\epsilon}}, \boldsymbol{\zeta}) \equiv \Pi(\boldsymbol{E}) = \tfrac{1}{2}\Pi_1 E_1^2 + \tfrac{1}{2}\Pi_2 E_2^2, \qquad (\Pi_1, \Pi_2 > 0). \tag{E.1}$$

We may then distinguish between four different regimes,

I $\quad b^{2a_1-1} \gg \Pi_1,\ b^{2a_2-1} \gg \Pi_2$,

II $\quad b^{2a_1-1} \ll \Pi_1,\ b^{2a_2-1} \gg \Pi_2$,

III $\quad b^{2a_1-1} \gg \Pi_1,\ b^{2a_2-1} \ll \Pi_2$,

IV $\quad b^{2a_1-1} \ll \Pi_1,\ b^{2a_2-1} \ll \Pi_2$,

leading to new critical exponents a_1', a_2' and $\alpha', \beta', \gamma', \delta', \Delta'$, which in the four regimes are given by

	a_1'	a_2'	α'	β'	γ'	δ'	Δ'	
I	a_1	a_2	α	β	γ	δ	Δ	
II	$1-a_1$	a_2	$-\alpha/(1-\alpha)$	$\beta/(1-\alpha)$	$\gamma/(1-\alpha)$	δ	$\Delta/(1-\alpha)$	(E.2)
III	a_1	$1-a_2$	α	Δ	$-\gamma$	$1/\delta$	β	
IV	$1-a_1$	$1-a_2$	$-\alpha/(1-\alpha)$	$\Delta/(1-\alpha)$	$-\gamma/(1-\alpha)$	$1/\delta$	$\beta/(1-\alpha)$.	

Regime I corresponds to the case of unrenormalized critical exponents far from the critical point; regime IV to the case of complete exponent renormalization close to the critical point. In regimes II and III there is a partial renormalization, i.e. Fisher renormalization[9]) in regime II and the renormalization found in ref. 30 in regime III. Partial renormalization can occur in an intermediate region, but also close to the critical point, if one of the constants Π_1 or Π_2 is zero. This is the case, (cf. section 3), for the constraints ($\Pi_2 = 0$) in the context of compressible Ising ferromagnets[12]) and the bond-annealed Syozi models[27]). The classical description of the demagnetizing effects[37,38]) and also the site-annealed model of ref. 30 provide a natural constraint with $\Pi_2 \neq 0$. In practice, however, it may not be easy to distinguish between the exponents in regimes II and IV.

Appendix F

In the case of one relevant variable, ($r = 1$), the critical exponent renormalization, but also higher order (confluent) singularities can be obtained from an iterative procedure. We consider the example

$$f(\epsilon) = \inf_E[-\epsilon E + \frac{1}{x}|E|^x + \tfrac{1}{2}\Pi E^2], \tag{F.1}$$

where $x = (2-\alpha)/(1-\alpha) > 2$ and $\Pi > 0$.

Introducing

$$y = \frac{\Pi}{\epsilon} E, \qquad z = \frac{1}{|\epsilon|}\left|\frac{\epsilon}{\Pi}\right|^{x-1}, \tag{F.2}$$

eq. (F.1) can be rewritten

$$f(\epsilon) = \frac{\epsilon^2}{\Pi} \inf_y\left[-y + \frac{1}{x} z|y|^x + \tfrac{1}{2}y^2\right]. \tag{F.3}$$

The function under the infimum of (F.3) is an analytic function of y and z, for $y \neq 0$, with a positive second derivative with respect to y. The infimum in (F.3) must occur for $y \neq 0$ and therefore the solution of the inf as well as $f(\epsilon)$ can be expressed as analytic functions of z. In fact,

$$f(\epsilon)=\frac{\epsilon^2}{\Pi}\left(-\frac{1}{2}+\frac{1}{x}z-\frac{1}{2}z^2+\frac{1}{2}(x-1)z^3-\frac{1}{6}(x-1)(4x-5)z^4+\cdots\right). \qquad \text{(F.4)}$$

As a result the different terms of $f(\epsilon)$ behave like ϵ^2, $\epsilon^{2+(x-2)}$, $\epsilon^{2+2(x-2)}, \ldots$, or more generally $\epsilon^{2+m(x-2)}$. The first term ($m=0$) is the regular part, the second term is the effect of critical-exponent renormalization, ($x-2=\alpha/(1-\alpha)$), and the third and higher order terms give confluent singularities. In the more general case of a convex function $\Pi(E)$ involving also terms $\sim E^3$ and higher order terms the free energy will contain singular terms of the type $\epsilon^{2+m(x-2)+n}$, where m and n are non-negative integers.

Appendix G

In this appendix we evaluate the Legendre transform

$$\hat{g}(\boldsymbol{E},\boldsymbol{Z})=\sup_{\epsilon_a,\epsilon_b,\zeta}[\boldsymbol{\epsilon}\cdot\boldsymbol{E}+\boldsymbol{\zeta}\cdot\boldsymbol{Z}+\hat{f}(\boldsymbol{\epsilon},\boldsymbol{\zeta})] \qquad \text{(G.1)}$$

of the free energy $\hat{f}(\boldsymbol{\epsilon},\boldsymbol{\zeta})$ given by (7.22), in which the relation between the coordinates $\boldsymbol{\epsilon}_a^*$, $\boldsymbol{\epsilon}_b^*$ and $\boldsymbol{\epsilon}_a$, $\boldsymbol{\epsilon}_b$, $\boldsymbol{\zeta}$ is given by (7.23). In (7.23), $\boldsymbol{A}(\boldsymbol{\epsilon}_b)$ contains quadratic and higher order terms in $\boldsymbol{\epsilon}_b$ and $\boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b)$ is at least linear in $\boldsymbol{\epsilon}_b$. (The linear terms in $\boldsymbol{A}(\boldsymbol{\epsilon}_b)$ and the constant terms in $\boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b)$ have been included in the definition of the coordinates $\boldsymbol{\epsilon}_a$.)

From (7.23) we have

$$\begin{aligned}\boldsymbol{\epsilon}_b&=\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*),\\ \boldsymbol{\epsilon}_a&=[1+\boldsymbol{A}_a(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))]^{-1}\cdot(\boldsymbol{\epsilon}_a^*-\boldsymbol{A}(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))-\boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))\cdot\boldsymbol{\zeta}).\end{aligned} \qquad \text{(G.2)}$$

Inserting (G.2) and (7.22) into (G.1) and taking the supremum over ζ, we find

$$\hat{g}(\boldsymbol{E},\boldsymbol{Z})=\sup_{\epsilon_a^*,\epsilon_b^*}[\phi_s(\boldsymbol{\epsilon}_a^*,\boldsymbol{\epsilon}_b^*)+\Gamma(\boldsymbol{E},\boldsymbol{Z},\boldsymbol{\epsilon}_b^*)+\boldsymbol{\Gamma}_a(\boldsymbol{E}_a,\boldsymbol{\epsilon}_b^*)\cdot\boldsymbol{\epsilon}_a^*], \qquad \text{(G.3)}$$

where

$$\begin{aligned}\Gamma(\boldsymbol{E},\boldsymbol{Z},\boldsymbol{\epsilon}_b^*)&=C(\boldsymbol{\epsilon}_b^*)-\boldsymbol{E}_a\cdot[1+\boldsymbol{A}_a(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))]^{-1}\cdot\boldsymbol{A}(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))+\boldsymbol{E}_b\cdot\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*)\\ &\quad+\tfrac{1}{2}\{\boldsymbol{Z}+\boldsymbol{C}_\zeta(\boldsymbol{\epsilon}_b^*)-\boldsymbol{E}_a\cdot[1+\boldsymbol{A}_a(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))]^{-1}\cdot\boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))\}^2,\\ \boldsymbol{\Gamma}_a(\boldsymbol{E}_a,\boldsymbol{\epsilon}_b^*)&=\boldsymbol{C}_a(\boldsymbol{\epsilon}_b^*)+\boldsymbol{E}_a\cdot[1+\boldsymbol{A}_a(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_b^*))]^{-1}.\end{aligned} \qquad \text{(G.4)}$$

The supremum over $\boldsymbol{\epsilon}_b^*$ can be evaluated using the considerations of appendix C. In fact, in view of the estimate $\partial\phi_s/\partial\boldsymbol{\epsilon}_b^*\sim\mathcal{O}(b^{(1+\eta)/2})$ for some $\eta>0$, cf. (7.16), the supremum over $\boldsymbol{\epsilon}_b^*$ occurs at

$$\boldsymbol{\epsilon}_b^*=\boldsymbol{\omega}(\boldsymbol{E},\boldsymbol{Z},\boldsymbol{\epsilon}_a^*)+\boldsymbol{\omega}'(\boldsymbol{E},\boldsymbol{Z},\boldsymbol{\epsilon}_a^*), \qquad \text{(G.5)}$$

where $\epsilon_b^* = \omega(E, Z, \epsilon_a^*)$ is the solution of the equation

$$\frac{\partial}{\partial \epsilon_b^*} \Gamma(E, Z, \epsilon_b^*) + \frac{\partial}{\partial \epsilon_b^*} \Gamma_a(E_a, \epsilon_b^*) \cdot \epsilon_a^* = 0, \tag{G.6}$$

and where $\omega'(E, Z, \epsilon_a^*)$ is a small correction of the order $o(b^{(1+\eta)/2})$. Inserting (G.5) into (G.3) we obtain

$$\hat{g}(E, Z) = \sup_{\epsilon_a^*}[\phi_s(\epsilon_a^*, \epsilon_b^*) + \Gamma(E, Z, \omega(E, Z, \epsilon_a^*)) + \Gamma_a(E_a, \omega(E, Z, \epsilon_a^*)) \cdot \epsilon_a^*], \tag{G.7}$$

Here we have neglected a correction quadratic in ω' which is of the order $o(b^{1+\eta})$.

Since $\epsilon_a^* \sim o(b^{(1+\eta)/2})$ we may expand $\omega(E, Z, \epsilon_a^*)$ up to linear terms in ϵ_a^*, i.e.

$$\omega(E, Z, \epsilon_a^*) = E_b^*(E, Z) + \omega_a(E, Z) \cdot \epsilon_a^*, \tag{G.8}$$

where $E_b^*(E, Z)$ is the solution of

$$\frac{\partial \Gamma}{\partial \epsilon_b^*}(E, Z, E_b^*(E, Z)) = 0. \tag{G.9}$$

Inserting (G.8) into (G.7) and noting that, in view of (G.9), the contribution of $\omega_a(E, Z)$ is of the order $o(b^{1+\eta})$, we arrive at the expression

$$\begin{aligned}\hat{g}(E, Z) &= \sup_{\epsilon_a^*}[\phi_s(\epsilon_a^*, E_b^*(E, Z)) + \Gamma(E, Z, E_b^*(E, Z)) + \Gamma_a(E_a, E_b^*(E, Z)) \cdot \epsilon_a^*] \\ &= g_s(E_a^*(E, Z), E_b^*(E, Z)) + \Gamma(E, Z, E_b^*(E, Z)),\end{aligned} \tag{G.10}$$

cf. (7.6), where

$$E_a^*(E, Z) = \Gamma_a(E_a, E_b^*(E, Z)). \tag{G.11}$$

Here E_a^*, E_b^* and Γ are regular functions.

In the presence of a constraint leading to a function $\hat{P}(E, Z, \epsilon, \zeta)$, the free energy per particle is given by, cf. (3.42), (3.45),

$$\hat{f}(\epsilon, \zeta) = \inf_{E,Z}[-\epsilon \cdot E - \zeta \cdot Z + g_s(E_a^*, E_b^*) + \Gamma(E, Z, E_b^*) + \hat{P}(E, Z, \epsilon, \zeta)]. \tag{G.12}$$

Note that in contrast with eq. (5.6), the function $g_s(E_a^*, E_b^*)$ depends on variables $E_a^*(E, Z)$, $E_b^*(E, Z)$ which can be obtained from E, Z by a nonlinear transformation (G.9), (G.11). This feature should be taken into account in deriving an equation like (5.15) with a function $\Pi(E_a^*, E_b^*, \bar{\epsilon}, \zeta)$. (Furthermore, in the case that eq. (3.45) is not valid, it can be mentioned that the supremum over h^* in (3.38) can be carried out without using the linear approximation

(3.40) for the variables ϵ_ζ^*. In fact, the supremum can be evaluated following the treatment in this appendix, using (7.22), (7.23) and a relation like

$$f_0(\boldsymbol{h}^*) + R(\boldsymbol{m}', \boldsymbol{h}^*, \{\xi_j\}) = \phi_s(\boldsymbol{\epsilon}_a^*, \boldsymbol{\epsilon}_\zeta^*) - \tfrac{1}{2}\boldsymbol{\zeta} \cdot \boldsymbol{\zeta} + D(\boldsymbol{m}', \boldsymbol{\epsilon}_\zeta^*, \{\xi_j\}) + \boldsymbol{D}_a(\boldsymbol{m}', \boldsymbol{\epsilon}_\zeta^*, \{\xi_j\}) \cdot \boldsymbol{\epsilon}_a^* + \boldsymbol{D}_\zeta(\boldsymbol{m}', \boldsymbol{\epsilon}_\zeta^*, \{\xi_j\}) \cdot \boldsymbol{\zeta}, \tag{G.13}$$

leading to eq. (3.42) with a function $P(\boldsymbol{m}, \boldsymbol{h})$ which may be different from the one given in (3.43).)

For the function $\Gamma(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{E}_\zeta^*)$ in (G.12) it can be shown that

$$\Gamma(\boldsymbol{E}, \boldsymbol{Z}, \boldsymbol{E}_\zeta^*) = \tfrac{1}{2}\boldsymbol{E}_b \cdot \boldsymbol{Y}_{bb}(\boldsymbol{E}_a, \boldsymbol{E}_b, \boldsymbol{Z}) \cdot \boldsymbol{E}_b + \tfrac{1}{2}\boldsymbol{Z} \cdot \boldsymbol{Y}_{ZZ}(\boldsymbol{E}_a, \boldsymbol{E}_b, \boldsymbol{Z}) \cdot \boldsymbol{Z} + \boldsymbol{E}_b \cdot \boldsymbol{Y}_{bZ}(\boldsymbol{E}_a, \boldsymbol{E}_b, \boldsymbol{Z}) \cdot \boldsymbol{Z}, \tag{G.14}$$

in which $\boldsymbol{Y}_{bb}$ and $\boldsymbol{Y}_{ZZ}$ are strictly positive definite for sufficiently small $\boldsymbol{E}_a, \boldsymbol{E}_b$ and $\boldsymbol{Z}$. Equation (G.14) may be derived from (G.4) and (G.9) and the relation

$$\boldsymbol{E}_\zeta^* = \boldsymbol{U}_b(\boldsymbol{E}_a, \boldsymbol{E}_b, \boldsymbol{Z}) \cdot \boldsymbol{E}_b + \boldsymbol{U}_Z(\boldsymbol{E}_a, \boldsymbol{E}_b, \boldsymbol{Z}) \cdot \boldsymbol{Z}, \tag{G.15}$$

in which the matrix $\boldsymbol{U}_b$ is nonsingular. Here it has been taken into account that $C(\boldsymbol{\epsilon}_\zeta^*)$ and $A(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_\zeta^*))$ are at least quadratic in $\boldsymbol{\epsilon}_\zeta^*$ and that $\boldsymbol{C}_\zeta(\boldsymbol{\epsilon}_\zeta^*)$ and $\boldsymbol{A}_\zeta(\boldsymbol{\epsilon}_b(\boldsymbol{\epsilon}_\zeta^*))$ do not contain terms independent of $\boldsymbol{\epsilon}_\zeta^*$.

From (G.12) and (G.14) it can be inferred that the critical behaviour of a reference free energy described by (7.22) and (7.23) will be unstable under small perturbations like e.g. $\boldsymbol{E}_a \cdot \boldsymbol{\Lambda} \cdot \boldsymbol{E}_a$, in which $\boldsymbol{\Lambda}$ is a constant matrix, independent of $\boldsymbol{E}_b, \boldsymbol{Z}, \boldsymbol{\epsilon}, \boldsymbol{\zeta}$.

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CHAPTER IV

STABILITY OF CRITICAL BEHAVIOUR IN SCHOFIELD'S LINEAR MODEL UNDER PERTURBATIONS INVOLVING TWO (RELEVANT) VARIABLES

1. Introduction.

In the previous chapter we considered the class of systems for which the free energy per particle is given by

$$f(\underline{h}) = \inf_{\underline{m}} [-\underline{h}\cdot\underline{m} + g_0(\underline{m}) + P(\underline{m},\underline{h})] \ . \tag{1.1}$$

Here $\underline{h} = (h_1,\ldots,h_n)$ denotes a finite set of coupling constants or external fields, $\underline{m} = (m_1,\ldots,m_n)$ the thermodynamic variables conjugate to $\underline{h}$, and

$$g_0(\underline{m}) \equiv \sup_{\underline{h}^*} [\underline{h}^*\cdot\underline{m} + f_0(\underline{h}^*)] \tag{1.2}$$

is the Legendre transform of the free energy per particle $f_0(\underline{h}^*)$ of a reference system with short-range interactions as a function of (internal) coupling constants or fields $\underline{h}^* = (h_1^*,\ldots,h_n^*)$. The analytic function $P(\underline{m},\underline{h})$ can depend on the variables $\underline{m}$ as well as the variables $\underline{h}$. Such a term can arise e.g. from a perturbation with a long-range nature in the hamiltonian, or from one or more constraints imposed on the system, cf. sections 2 and 3 of chapter III for examples and references to the literature.

In chapter III we studied from a general point of view the stability of the critical behaviour of the reference system under small perturbations $P(\underline{m},\underline{h})$. In case that $f_0(\underline{h}^*)$ has a critical point with one or more divergent second derivatives, a very small term $P(\underline{m},\underline{h})$ in general will lead to different critical behaviour, such as e.g. a critical point with finite second derivatives, or to first-order transitions terminating in classical critical points.

In order to be more specific we shall investigate in this chapter in some detail a special case of two (relevant) variables, (e.g. temperature and magnetic field), i.e.

$$f(h_1,h_2) = \inf_{m_1,m_2} [-h_1m_1 - h_2m_2 + g_0(m_1,m_2) + \tfrac{1}{2}\Pi_1m_1^2 + \tfrac{1}{2}\Pi_2m_2^2] , \tag{1.3}$$

$$g_0(m_1,m_2) = \sup_{h_1^*,h_2^*} [h_1^*m_1 + h_2^*m_2 + f_0(h_1^*,h_2^*)] \ , \qquad (1.4)$$

where $f_0(h_1^*,h_2^*)$ satisfies the homogeneity property

$$f_0(b^{a_1}h_1^*, b^{a_2}h_2^*) = bf_0(h_1^*,h_2^*) \quad , \qquad (1.5)$$

with $\frac{1}{2} < a_i < 1$, $(i=1,2)$. Eq. (1.5) implies that f_0 has a critical point at $h_1^* = h_2^* = 0$, with critical exponents $\alpha = (2a_1-1)/a_1$, $\beta = (1-a_2)/a_1$, $\gamma = (2a_2-1)/a_1$, $\Delta = a_2/a_1$, $\delta = a_2/(1-a_2)$.

From (1.5) it follows that $g_0(m_1,m_2)$ satisfies the homogeneity property

$$g_0(b^{1-a_1}m_1, b^{1-a_2}m_2) = bg_0(m_1,m_2) \ , \qquad (1.6)$$

which implies that the second derivatives of g_0 will tend to zero for $m_1,m_2 \to 0$, so that for (small) $\Pi_1 \neq 0$, $\Pi_2 \neq 0$, the behaviour of $f(h_1,h_2)$ for small h_1,h_2 will be dominated by the term $\frac{1}{2}\Pi_1 m_1^2 + \frac{1}{2}\Pi_2 m_2^2$.

The general treatment in the previous chapter leads to the following conclusions:

i) If $\Pi_1 > 0$, $\Pi_2 > 0$, the system with free energy (1.3) will have a critical point at $h_1=h_2=0$. Depending on the magnitude of b, Π_1, Π_2, there may be four regimes I, II, III, IV, characterized by different sets of critical exponents, as described in appendix E of chapter III.

ii) If one of the coefficients Π_1 or Π_2 is negative, the critical point at $m_1=m_2=0$ of the reference system is unstable and a neighbourhood of $m_1=m_2=0$ will not be reached. There will be first-order transitions which may terminate in classical critical points.

These features will be made more explicit using the linear model of Schofield to describe the reference system. This model will be defined in section 2; in section 3 we investigate the effects of critical-exponent renormalization in the case of positive Π_1 and Π_2 . In section 4 the first-order transitions and classical critical points are treated in some detail for negative Π_2, the special case that $\Pi_1 < 0$, $\Pi_2 > 0$ is treated in section 5.

2. The linear Schofield model.

This model has been introduced in ref. 1, cf. also ref. 2, to give a simple description of systems satisfying the homogeneity property (1.5). The model describes rather accurately several magnetic and fluid systems, cf. e.g. refs. 3, 4 and also, for a review of experimental results, refs. 5, 6.

In this section we give a slightly modified, but equivalent, description which is convenient in view of the Legendre transform (1.2). Other variants and extensions of the linear model [7),8)], which have been used in the description of critical phenomena, will not be taken into consideration here.

According to the Schofield parametrization and eqs. (1.5), (1.6), the function g_0 and its first and second derivatives can be expressed in terms of the variables b and θ, with $b > 0$, $-1 \leq \theta \leq 1$, i.e.

$$g_0(m_1,m_2) = G(\theta)b \ , \tag{2.1}$$

$$h_i^* = \partial g_0/\partial m_i = H_i(\theta)b^{a_i} \ , \quad i=1,2 \ , \tag{2.2}$$

$$k_{ij} = \partial^2 g_0/\partial m_i \partial m_j = K_{ij}(\theta)b^{a_i+a_j-1} \ , \quad i,j=1,2 \ . \tag{2.3}$$

Here the variables b and θ, for $-1 < \theta < 1$, are defined by the parametrization

$$m_i = M_i(\theta)b^{1-a_i} \ , \quad i=1,2 \ . \tag{2.4}$$

For $\theta=\pm1$, (corresponding to a first-order transition at $h_2^*=0$ below the critical temperature of the reference system), m_1 and m_2 satisfy

$$\begin{aligned} m_1 &= M_1(-1)b^{1-a_1} = M_1(1)b^{1-a_1}, \\ M_2(-1)b^{1-a_2} &\leq m_2 \leq M_2(1)b^{1-a_2}. \end{aligned} \tag{2.5}$$

In the (restricted) linear model it is assumed that

$$M_1(\theta) = \mu_1(\theta^2-\theta_1^2), \quad M_2(\theta) = \mu_2\theta \ , \quad K_{11}(\theta) = \kappa \ , \tag{2.6}$$

where μ_1, μ_2, κ, θ_1^2 are positive constants. Furthermore, for a_i, i=1,2, it is assumed that

$$\tfrac{1}{2} < a_i < 1 \ , \quad 1+a_1 < 2a_2 \ , \tag{2.7}$$

corresponding to the conditions $0 < \alpha < 1$ and $1 < \gamma < 2$ for the critical exponents of the reference system.

The other functions of θ can now be determined using the relations

$$\sum_{j=1}^{2} (1-a_j)K'_{ij}(\theta)M_j(\theta) = \sum_{j=1}^{2} (a_i+a_j-1)K_{ij}(\theta)M'_j(\theta) \ , \tag{2.8}$$

$$a_iH_i(\theta) = \sum_{j=1}^{2} (1-a_j)K_{ij}(\theta)M_j(\theta) \ , \tag{2.9}$$

$$G(\theta) = \sum_{i=1}^{2} (1-a_i)H_i(\theta)M_i(\theta) \ , \tag{2.10}$$

which follow from (2.1)-(2.4). (The primes denote derivatives with respect to θ).

From (2.7) and (2.8) we have

$$K_{12}(\theta) = -\frac{2(2a_1-1)}{2a_2+a_1-2}\frac{\mu_1\kappa}{\mu_2}\theta \ , \tag{2.11}$$

$$K_{22}(\theta) = \frac{2(1-a_1)(2a_1-1)}{(2a_2-1)(2a_2+a_1-2)}\frac{\mu_1^2\theta_1^2\kappa}{\mu_2^2}(1+s\theta^2) \ , \tag{2.12}$$

with

$$s = \frac{2a_2+3a_1-3}{2a_2-a_1-1} \ , \tag{2.13}$$

and therefore, cf. (2.9),

$$H_1(\theta) = n_1(\theta^2-\theta_2^2) \ , \tag{2.14}$$

$$H_2(\theta) = n_2\theta(\theta_3^2-\theta^2) \ , \tag{2.15}$$

with

$$n_1 = \frac{2a_2-a_1-1}{2a_2+a_1-2}\mu_1\kappa \ , \tag{2.16}$$

$$n_2 = \frac{2(2a_1-1)(2a_2-a_1-1)}{(2a_2+a_1-2)(4a_2-3)}\frac{\mu_1^2\kappa}{\mu_2} \ , \tag{2.17}$$

$$\theta_2^2 = \frac{(1-a_1)(2a_2+a_1-2)}{a_1(2a_2-a_1-1)}\theta_1^2 \ , \tag{2.18}$$

$$\theta_3^2 = \frac{(1-a_1)(4a_2-3)}{(2a_2-1)(2a_2-a_1-1)}\theta_1^2 \ . \tag{2.19}$$

Taking into account that the largest value of θ^2 will occur for $H_2(\theta) = 0$ below the critical temperature, we have

$$\theta_3^2 = 1 \tag{2.20}$$

and therefore

$$\theta_1^2 = \frac{(2a_2-1)(2a_2-a_1-1)}{(1-a_1)(4a_2-3)} \ , \tag{2.21}$$

$$\theta_2^2 = \frac{(2a_2-1)(2a_2+a_1-2)}{a_1(4a_2-3)} \ , \tag{2.22}$$

$$n_2\mu_2 = \frac{2(2a_1-1)}{4a_2-3}n_1\mu_1 \ . \tag{2.23}$$

Then finally K_{11}, K_{12} and K_{22} can be rewritten

$$K_{11}(\theta) = \frac{2a_2+a_1-2}{2a_2-a_1-1}\,\frac{n_1}{\mu_1} = \kappa, \tag{2.24}$$

$$K_{12}(\theta) = \frac{-2(2a_1-1)}{2a_2-a_1-1}\,\frac{n_1}{\mu_2}\,\theta\ , \tag{2.25}$$

$$K_{22}(\theta) = \frac{n_2}{\mu_2}\,(1+s\theta^2)\ . \tag{2.26}$$

Here the coefficients n_1, n_2, μ_1, μ_2 satisfy the relation (2.23) and s is defined by (2.13).

From eq. (1.3) the free energy $f(h_1,h_2)$ as a function of the external fields h_1 and h_2 can be expressed as

$$f(h_1,h_2) = \min_{m_1,m_2 \in J} \left[g_0(m_1,m_2) - \sum_{i=1}^{2} (h_i^* m_i + \tfrac{1}{2}\Pi_i m_i^2) \right], \tag{2.27}$$

where J denotes the set of values m_1,m_2 satisfying the implicit equations

$$h_i = h_i^* + \Pi_i m_i\ ,\quad i=1,2\ , \tag{2.28}$$

with the functions $h_i^* = \partial g_0/\partial m_i$, cf. (2.2). In terms of the variables b,θ these values m_1,m_2 can be paramatrized by (2.4), or correspond to $h_2^*=0$ and satisfy (2.5). Accordingly, we have from (2.27), using (2.1), (2.2), (2.4), (2.5), (2.9), (2.10),

$$f(h_1,h_2) = \min\,\{f_1(h_1,h_2),\ f_2(h_1,h_2)\}\ . \tag{2.29}$$

Here

$$f_1(h_1,h_2) = \min_{b,\theta \in J_1} \left[-\,b \sum_{i=1}^{2} (a_i H_i(\theta) M_i(\theta) + \tfrac{1}{2}\Pi_i M_i^2(\theta)\, b^{1-2a_i}) \right], \tag{2.30}$$

in which J_1 denotes the set of solutions b,θ, $(b>0,\ \theta^2<1)$, satisfying

$$h_i = b^{a_i}(H_i(\theta) + \Pi_i M_i(\theta) b^{1-2a_i})\ ,\quad i=1,2, \tag{2.31}$$

and

$$f_2(h_1,h_2) = \min_{b \in J_2} \left[-\,b(a_1 H_1(1) M_1(1) + \tfrac{1}{2}\Pi_1 M_1^2(1)\, b^{1-2a_1}) - \tfrac{1}{2}h_2^2/\Pi_2 \right], \tag{2.32}$$

where J_2 denotes the set of solutions b satisfying

$$h_1 = b^{a_1}(H_1(1) + \Pi_1 M_1(1)\, b^{1-2a_1})\ . \tag{2.33}$$

In (2.32) the minimum over m_2 has been taken explicitly. The relation

$$m_2 = -\,\partial f_2/\partial h_2 = h_2/\Pi_2 \tag{2.34}$$

is identical to the relation between the magnetization and the external magnetic field under the influence of demagnetizing effects, (the demagnetizing factor D corresponding to Π_2). We therefore refer to the solutions involging J_2 as solutions of the demagnetizing phase. Note that f_2 can only contribute to the minimum in (2.29) if Π_2 is positive. (For negative Π_2, the stability condition that the susceptibility is positive is not satisfied, and solutions involving J_2 can then be ignored). In the following the solutions involving J_1 will also be called solutions of the normal phase.

3. Critical-exponent renormalization.

In this section we discuss the case that

$$\Pi_1 > 0, \quad \Pi_2 > 0 . \tag{3.1}$$

Then the function between brackets in the right-hand side of (1.3) is a convex function of m_1, m_2. As a consequence the value of m_1, m_2 at which the infimum occurs is uniquely determined for each h_1, h_2 and there are no first-order transitions. The free energy $f(h_1, h_2)$ has a critical point for b=0, or

$$h_1 = h_2 = 0. \tag{3.2}$$

A. Demagnetizing phase.

For $h_1 > 0$ and $|h_2| \leqslant h_D$, with

$$h_D = \Pi_2 M_2(1)\, b^{1-a_2}, \quad M_2(1) = -M_2(-1) , \tag{3.3}$$

b is the solution of (2.33), there is a demagnetizing phase, cf. (2.34), (2.5). The second derivatives

$$\chi_{ij} = -\partial^2 f/\partial h_i \partial h_j \tag{3.4}$$

of the free energy (1.3) in this phase are given by

$$\chi_{11} = \left\{\frac{a_1 H_1(1)}{(1-a_1)M_1(1)}\, b^{2a_1-1} + \Pi_1\right\}^{-1} ,$$
$$\chi_{12} = 0, \quad \chi_{22} = \Pi_2^{-1} , \tag{3.5}$$

i.e. the magnetic susceptibility χ_{22} is constant.

In the two regimes (i) and (ii), such that

$$\text{(i)}\quad b^{2a_1-1} \gg \Pi_1 \,, \qquad \text{(ii)}\quad b^{2a_1-1} \ll \Pi_1 \,, \tag{3.6}$$

the second derivative χ_{11} can be described by

$$\chi_{11}^{(i)} = \frac{(1-a_1)M_1(1)}{a_1H_1(1)}\, b^{1-2a_1}, \quad \chi_{11}^{(ii)} = \frac{1}{\Pi_1}\left\{1 - \frac{a_1H_1(1)}{\Pi_1(1-a_1)M_1(1)}\, b^{2a_1-1}\right\} . \tag{3.7}$$

In regime (i) we have, cf. (2.33),

$$\chi_{11} \simeq \chi_{11}^{(i)} \simeq \frac{(1-a_1)M_1(1)}{a_1H_1(1)} \left(\frac{h_1}{H_1(1)}\right)^{-\alpha} , \quad (\alpha = \frac{2a_1-1}{a_1}) , \tag{3.8}$$

$$h_D \simeq \Pi_2M_2(1) \left(\frac{h_1}{H_1(1)}\right)^{\beta} , \quad (\beta = \frac{1-a_2}{a_1}) . \tag{3.9}$$

In regime (ii), however,

$$\chi_{11} \simeq \chi_{11}^{(ii)} \simeq \frac{1}{\Pi_1} \left\{1 - \frac{a_1H_1(1)}{\Pi_1(1-a_1)M_1(1)} \left(\frac{h_1}{\Pi_1M_1(1)}\right)^{\frac{\alpha}{1-\alpha}} \right\} , \tag{3.10}$$

$$h_D \simeq \Pi_2M_2(1) \left(\frac{h_1}{\Pi_1M_1(1)}\right)^{\frac{\beta}{1-\alpha}} . \tag{3.11}$$

In (3.10) and (3.11) we have a Fisher renormalization [9] for the critical exponents α and β, describing the specific heat and the boundary of the demagnetizing phase.

More specifically, χ_{11} can be approximated by χ_{11}^{A}, A = (i),(ii), with precision λ, $0 < \lambda \ll 1$, if the condition

$$(1-\lambda)\chi_{11} < \chi_{11}^{A} < (1+\lambda)\chi_{11} \tag{3.12}$$

is satisfied. Eq. (3.12) is equivalent to

$$b^{2a_1-1} > \frac{\Pi_1(1-a_1)M_1(1)}{a_1H_1(1)}\, \frac{1}{\lambda} , \quad \text{for } A = \text{(i)} , \tag{3.13}$$

$$b^{2a_1-1} < \frac{\Pi_1(1-a_1)M_1(1)}{a_1H_1(1)}\, \sqrt{\lambda} , \quad \text{for } A = \text{(ii)} . \tag{3.14}$$

B. Normal phase.

Outside the demagnetizing phase, the second derivatives of the free energy (1.3) are given by

$$\underline{\underline{\chi}} = (\underline{\underline{k}} + \underline{\underline{\Pi}})^{-1}$$

$$= \left[(K_{11}(\theta)b^{2a_1-1} + \Pi_1)(K_{22}(\theta)b^{2a_2-1} + \Pi_2) - K_{12}^2(\theta)b^{2a_1+2a_2-2}\right]^{-1} \times$$

$$\times \begin{pmatrix} \Pi_2 + K_{22}(\theta)b^{2a_2-1} & -K_{12}(\theta)b^{a_1+a_2-1} \\ -K_{12}(\theta)b^{a_1+a_2-1} & \Pi_1 + K_{11}(\theta)b^{2a_1-1} \end{pmatrix}, \qquad (3.15)$$

in which b and θ satisfy (2.4), and

$$\underline{\underline{\chi}} = \begin{pmatrix} \chi_{11} & \chi_{12} \\ \chi_{12} & \chi_{22} \end{pmatrix}, \quad \underline{\underline{k}} = \begin{pmatrix} k_{11} & k_{12} \\ k_{12} & k_{22} \end{pmatrix}, \quad \underline{\underline{\Pi}} = \begin{pmatrix} \Pi_1 & 0 \\ 0 & \Pi_2 \end{pmatrix} \qquad (3.16)$$

Starting from (3.15) we can distinguish between four different regimes:

$$\begin{array}{lll} \text{I.} & b^{2a_1-1} \gg \Pi_1, & b^{2a_2-1} \gg \Pi_2, \\ \text{II.} & b^{2a_1-1} \ll \Pi_1, & b^{2a_2-1} \gg \Pi_2, \\ \text{III.} & b^{2a_1-1} \gg \Pi_1, & b^{2a_2-1} \ll \Pi_2, \\ \text{IV.} & b^{2a_1-1} \ll \Pi_1, & b^{2a_2-1} \ll \Pi_2. \end{array} \qquad (3.17)$$

The susceptibility in these four regimes can be described by matrices $\underline{\underline{\chi}}^A$, with A = I,II,III, IV, which have a homogeneous singular part $\underline{\underline{\chi}}_s^A$, i.e.

$$\chi^A_{s,ij}(h_1,h_2) \sim b^{1-a_i^A-a_j^A}, \quad \text{for } h_i \sim b^{a_i^A}, \quad (i,j=1,2,\ A=\text{I,II,III,IV}). \qquad (3.18)$$

Eq. (3.18) leads to the critical exponents

$$\alpha_A = 2 - \frac{1}{a_1^A}, \quad \beta_A = \frac{1-a_2^A}{a_1^A}, \quad \gamma_A = \frac{2a_2^A-1}{a_1^A}, \quad \Delta_A = \frac{a_2^A}{a_1^A}, \quad \delta_A = \frac{a_2^A}{1-a_2^A}. \qquad (3.19)$$

The matrices $\underline{\underline{\chi}}^A$ are given by:

I.

$$\underline{\underline{\chi}}^I = \underline{\underline{k}} = \{K_{11}(\theta)K_{22}(\theta) - K_{12}^2(\theta)\}^{-1} \begin{pmatrix} K_{22}(\theta)b^{1-2a_1} & -K_{12}(\theta)b^{1-a_1-a_2} \\ -K_{12}(\theta)b^{1-a_1-a_2} & K_{11}(\theta)b^{1-2a_2} \end{pmatrix}, \qquad (3.20)$$

which is the susceptibility matrix of the reference system. Eq. (3.20) has the form (3.18), with unrenormalized critical exponents, i.e. $a_1^I=a_1$, $a_2^I=a_2$, and

$$\alpha_I = \alpha,\quad \beta_I = \beta,\quad \gamma_I = \gamma,\quad \Delta_I = \Delta,\quad \delta_I = \delta\ . \tag{3.21}$$

II.

$$\underline{\underline{\chi}}^{II} = \begin{pmatrix} \Pi_1^{-1} - \Pi_1^{-2}\{K_{11}(\theta) - K_{12}^2(\theta)K_{22}^{-1}(\theta)\}b^{2a_1-1} & -\Pi_1^{-1}K_{12}(\theta)K_{22}^{-1}(\theta)b^{a_1-a_2} \\ -\Pi_1^{-1}K_{12}(\theta)K_{22}^{-1}(\theta)b^{a_1-a_2} & K_{22}^{-1}(\theta)b^{1-2a_2} \end{pmatrix}. \tag{3.22}$$

In this case we have eq. (3.18) with $a_1^{II} = 1-a_1$, $a_2^{II} = a_2$, leading to the critical exponents, cf. (3.19),

$$\alpha_{II} = -\frac{\alpha}{1-\alpha}\ ,\quad \beta_{II} = \frac{\beta}{1-\alpha}\ ,\quad \gamma_{II} = \frac{\gamma}{1-\alpha}\ ,\quad \Delta_{II} = \frac{\Delta}{1-\alpha}\ ,\quad \delta_{II} = \delta. \tag{3.23}$$

The exponents (3.23) correspond to the Fisher renormalization [9] of critical exponents, see also chapter III for further references to the literature. The specific heat has a cusp, $(\alpha_{II} < 0)$, the susceptibility diverges, $(\gamma_{II} > 0)$, and the mixed derivative χ_{12}^{II} diverges also, since $a_2 > a_1$, cf. (2.7).

III.

$$\underline{\underline{\chi}}^{III} = \begin{pmatrix} K_{11}^{-1}(\theta)b^{1-2a_1} & -\Pi_2^{-1}K_{12}(\theta)K_{11}^{-1}(\theta)b^{a_2-a_1} \\ -\Pi_2^{-1}K_{12}(\theta)K_{11}^{-1}(\theta)b^{a_2-a_1} & \Pi_2^{-1} - \Pi_2^{-2}\{K_{22}(\theta) - K_{12}^2(\theta)K_{11}^{-1}(\theta)\}b^{2a_2-1} \end{pmatrix}. \tag{3.24}$$

Eq. (3.24) has the form (3.18), with $a_1^{III} = a_1$, $a_2^{III} = 1-a_2$, and therefore we have

$$\alpha_{III} = \alpha,\quad \beta_{III} = \Delta,\quad \gamma_{III} = -\gamma,\quad \Delta_{III} = \beta,\quad \delta_{III} = 1/\delta, \tag{3.25}$$

corresponding to the renormalization found by Essam and Place [10]. The specific heat diverges, the susceptibility has a cusp and the mixed derivative tends to zero.

IV.

$$\underline{\underline{\chi}}^{IV} = \underline{\underline{\Pi}}^{-1} - \underline{\underline{\Pi}}^{-1}\cdot\underline{\underline{k}}\cdot\underline{\underline{\Pi}}^{-1}$$

$$= \begin{pmatrix} \Pi_1^{-1} - \Pi_1^{-2}K_{11}(\theta)b^{2a_1-1} & -(\Pi_1\Pi_2)^{-1}K_{12}(\theta)b^{a_1+a_2-1} \\ -(\Pi_1\Pi_2)^{-1}K_{12}(\theta)b^{a_1+a_2-1} & \Pi_2^{-1} - \Pi_2^{-2}K_{22}(\theta)b^{2a_2-1} \end{pmatrix}. \tag{3.26}$$

In this case we have a complete critical-exponent renormalization, i.e. $a_1^{IV} = 1-a_1$, $a_2^{IV} = 1-a_2$, and

$$\alpha_{IV} = -\frac{\alpha}{1-\alpha}\ ,\quad \beta_{IV} = \frac{\Delta}{1-\alpha}\ ,\quad \gamma_{IV} = -\frac{\gamma}{1-\alpha}\ ,\quad \Delta_{IV} = \frac{\beta}{1-\alpha}\ ,\quad \delta_{IV} = \frac{1}{\delta}\ , \tag{3.27}$$

and all second derivatives are finite.

We now investigate the conditions under which the susceptibility $\underline{\underline{\chi}}$ can be approximated by the susceptibility $\underline{\underline{\chi}}^A$, $A = I, II, III, IV$, with precision λ, $0 < \lambda \ll 1$, i.e.

$$(1-\lambda)\underline{\underline{\chi}} < \underline{\underline{\chi}}^A < (1+\lambda)\underline{\underline{\chi}} \quad , \tag{3.28}$$

where the inequality $\underline{\underline{A}} < \underline{\underline{B}}$ means that the matrix $\underline{\underline{B}} - \underline{\underline{A}}$ is positive definite. For the four regimes we obtain the following conditions from eq. (3.28), see appendix A for some details of the calculation,

$$\text{I.} \quad \lambda k_{11} - \Pi_1 > 0 \ ,$$

$$(\lambda k_{11} - \Pi_1)(\lambda k_{22} - \Pi_2) - \lambda^2 k_{12}^2 > 0 \ , \tag{3.29}$$

$$\text{II.} \quad \sqrt{\lambda}\Pi_1 - k_{11} > 0 \ ,$$

$$\lambda^2 \Pi_1^2 k_{22} \pm \lambda\{(\Pi_1 - k_{11})k_{12}^2 + k_{11}^2 k_{22} - \Pi_1^2 \Pi_2\} - \Pi_2 k_{11}^2 > 0 \ , \tag{3.30}$$

$$\text{III.} \quad \sqrt{\lambda}\Pi_2 - k_{22} > 0 \ ,$$

$$\lambda^2 \Pi_2^2 k_{11} \pm \lambda\{(\Pi_2 - k_{22})k_{12}^2 + k_{11} k_{22}^2 - \Pi_1 \Pi_2^2\} - \Pi_1 k_{22}^2 > 0 \ , \tag{3.31}$$

$$\text{IV.} \quad \sqrt{\lambda}\Pi_1 - k_{11} > 0 \ ,$$

$$(\sqrt{\lambda}\Pi_1 - k_{11})(\sqrt{\lambda}\Pi_2 - k_{22}) - k_{12}^2 > 0 \ . \tag{3.32}$$

For the calculations in the rest of this section, (and also in the following sections), it will be convenient to introduce a new variable

$$\rho = |\kappa/\Pi_1| b^{2a_1-1} \tag{3.33}$$

to describe the "distance" to the critical point and a new parameter

$$\Pi = \frac{\mu_2}{n_2} |\kappa/\Pi_1|^p \, \Pi_2 \ , \qquad p = \frac{2a_2-1}{2a_1-1} \ , \tag{3.34}$$

to characterize the relative magnitude of Π_1 and Π_2. The second derivatives of g_0 can then be expressed as, cf. (2.3), (2.24)-(2.26),

$$k_{11} = |\Pi_1|\rho \quad , \tag{3.35}$$

$$k_{12} = -|\Pi_1\Pi_2/\Pi|^{\frac{1}{2}} (s-t)^{\frac{1}{2}} \, \theta \rho^{\frac{1}{2}(p+1)} \ , \tag{3.36}$$

$$k_{22} = |\Pi_2/\Pi|(1+s\theta^2)\rho^p \ , \tag{3.37}$$

with s defined in (2.13) and

$$t = \frac{3-s}{1+s} \,. \tag{3.38}$$

Note that $s-t > 0$ in view of the conditions (2.7) imposed on a_1 and a_2.

Using (3.35)-(3.37), the conditions (3.29)-(3.32) can be written in terms of ρ, θ and Π, i.e.

I. $\lambda\rho - 1 > 0$,

$$(\lambda\rho-1)(\lambda\Pi^{-1}\rho^{p}-1) + (t\lambda\rho - s)\lambda\Pi^{-1}\rho^{p}\theta^{2} > 0 \,, \tag{3.39}$$

II. $\rho - \sqrt{\lambda} < 0$,

$$\begin{aligned} &(\rho^{2}+\lambda)(\lambda\Pi^{-1}\rho^{p}-1) + (t\rho^{2} + (s-t)\rho + s\lambda)\lambda\Pi^{-1}\rho^{p}\theta^{2} > 0 \,, \\ &(\rho^{2}-\lambda)(\lambda\Pi^{-1}\rho^{p}+1) + (t\rho^{2} + (s-t)\rho - s\lambda)\lambda\Pi^{-1}\rho^{p}\theta^{2} < 0 \,, \end{aligned} \tag{3.40}$$

III. $(\Pi^{-1}\rho^{p} - \sqrt{\lambda}) + s\Pi^{-1}\rho^{p}\theta^{2} < 0$,

$$\begin{aligned} &(\lambda\rho-1)(\Pi^{-2}\rho^{2p}+\lambda) + \left[(s-t)\lambda\rho + \{(s+t)\lambda\rho - 2s\}\Pi^{-1}\rho^{p}\right]\Pi^{-1}\rho^{p}\theta^{2} \\ &\qquad + s(t\lambda\rho - s)\Pi^{-2}\rho^{2p}\theta^{4} > 0 \,, \\ &(\lambda\rho+1)(\Pi^{-2}\rho^{2p}-\lambda) + \left[(s-t)\lambda\rho + \{(s+t)\lambda\rho + 2s\}\Pi^{-1}\rho^{p}\right]\Pi^{-1}\rho^{p}\theta^{2} \\ &\qquad + s(t\lambda\rho + s)\Pi^{-2}\rho^{2p}\theta^{4} < 0 \,, \end{aligned} \tag{3.41}$$

IV. $\rho - \sqrt{\lambda} < 0$,

$$(\rho-\sqrt{\lambda})(\Pi^{-1}\rho^{p} - \sqrt{\lambda}) + (t\rho - s\sqrt{\lambda})\Pi^{-1}\rho^{p}\theta^{2} > 0 \,. \tag{3.42}$$

We shall now investigate in particular for which values of ρ eqs. (3.39)-(3.42) are satisfied for all θ, $(0 \leq \theta^2 < 1)$, in the regimes I, II, III, IV. In that case one should always pass through such a regime in approaching the critical point within the normal phase.

To be specific, we shall assume here and in the following that the gap exponent satisfies

$$\Delta > \frac{3}{2} \,, \tag{3.43}$$

so that $t > 0$.

<u>Regime I</u>: From (3.39) we have the condition:

$$\begin{aligned} &g_1(\rho) < 0, \quad \text{if } \rho > \frac{s}{t\lambda} \\ &g_1(\rho) > 1, \quad \text{if } \frac{1}{\lambda} < \rho < \frac{s}{t\lambda} \,, \end{aligned} \tag{3.44}$$

with

$$g_1(\rho) \equiv - \frac{(\lambda\rho-1)(\lambda\Pi^{-1}\rho^p - 1)}{(t\lambda\rho-s)\lambda\Pi^{-1}\rho^p} . \tag{3.45}$$

From (3.44) it follows that

$$\rho > \left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} , \quad \text{if } \left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} > \frac{s}{t\lambda} ,$$

$$\rho > \rho_1 \qquad , \quad \text{if } \left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} < \frac{s}{t\lambda} , \tag{3.46}$$

with ρ_1 the solution of

$$g_1(\rho) = 1, \quad \max \left\{ \frac{1}{\lambda} , \left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} \right\} < \rho < \frac{s}{t\lambda} . \tag{3.47}$$

Regime II: Eq. (3.40) for all θ with $0 \leqslant \theta^2 < 1$ implies

$$\rho - \sqrt{\lambda} < 0, \quad \lambda\Pi^{-1}\rho^p - 1 > 0, \quad g_2(\rho) < 0 , \tag{3.48}$$

with

$$g_2(\rho) \equiv \rho^2 - \lambda + \left\{(t+1)\rho^2 + (s-t)\rho - (s+1)\lambda\right\}\lambda\Pi^{-1}\rho^p . \tag{3.49}$$

From the first and second inequality in (3.48), we have

$$\Pi < \lambda^{\frac{1}{2}p+1} , \quad \left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} < \rho < \sqrt{\lambda} . \tag{3.50}$$

Eq. (3.50) ensures that we have a regime II for $\theta=0$. In order to have this regime for all values of θ, we must require that

$$g_2\left(\left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} \right) < 0 , \tag{3.51}$$

which leads to the condition

$$\left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} < A_2 , \tag{3.52}$$

with

$$A_2 \equiv \tfrac{1}{2}(t+2)^{-1} \left[\left\{(s-t)^2 + 4(s+2)(t+2)\lambda\right\}^{\frac{1}{2}} - (s-t)\right] \simeq \frac{s+2}{s-t}\lambda , \ (\lambda << 1). \tag{3.53}$$

Then for all values of ρ satisfying

$$\left(\frac{\Pi}{\lambda}\right)^{\frac{1}{p}} < \rho < \rho_2 , \tag{3.54}$$

where $\rho_2 < \sqrt{\lambda}$ is the positive solution of

$$g_2(\rho) = 0 , \tag{3.55}$$

we have regime II for all θ. Note that for small λ the condition (3.52) for Π for all $0 \leqslant \theta^2 < 1$ is much more stringent than (3.50) for Π, if $\theta=0$.

Regime III: From eq. (3.41) for $\theta=0$ it follows that

$$\Pi^{-1}\rho^p - \sqrt{\lambda} < 0 , \quad \lambda\rho - 1 > 0 , \tag{3.56}$$

or

$$\Pi > \lambda^{-p+\frac{1}{2}} , \quad \frac{1}{\lambda} < \rho < (\Pi\sqrt{\lambda})^{\frac{1}{p}} . \tag{3.57}$$

If we require regime III for all θ, then the first and second inequality in eq. (3.41) follow from the third one and eq. (3.56). It is therefore sufficient to require that

$$g_3(\rho) < 0 , \tag{3.58}$$

with

$$g_3(\rho) \equiv -\lambda(\lambda\rho+1) + (s-t)\lambda\rho\Pi^{-1}\rho^p + \{(s+1)(t+1)\lambda\rho + (s+1)^2\}(\Pi^{-1}\rho^p)^2 . \tag{3.59}$$

If now

$$g_3(\tfrac{1}{\lambda}) < 0 , \tag{3.60}$$

i.e.

$$\Pi^{-1}\lambda^{-p} < A_3 , \tag{3.61}$$

with

$$A_3 \equiv \tfrac{1}{2}(s+1)^{-1}(s+t+2)^{-1}\left[\{(s-t)^2 + 8(s+1)(s+t+2)\lambda\}^{\frac{1}{2}} - (s-t)\right] \simeq \frac{2}{s-t}\lambda , \quad (\lambda \ll 1), \tag{3.62}$$

then there is a regime III for all values $0 \leqslant \theta^2 < 1$, if

$$\frac{1}{\lambda} < \rho < \rho_3 , \tag{3.63}$$

where $\rho_3 > \frac{1}{\lambda}$ is the solution of

$$g_3(\rho) = 0 . \tag{3.64}$$

Again condition (3.61) for $0 \leqslant \theta^2 < 1$ is much stronger than (3.57) for $\theta=0$.

Regime IV: From eq. (3.42) we have

$$\rho < \sqrt{\lambda}, \quad g_4(\rho) > 1 , \tag{3.65}$$

with

$$g_4(\rho) \equiv - \frac{(\rho-\sqrt{\lambda})(\Pi^{-1}\rho^p - \sqrt{\lambda})}{(t\rho-s\sqrt{\lambda})\Pi^{-1}\rho^p} . \tag{3.66}$$

Therefore we have the condition

$$\rho < \rho_4 \ , \tag{3.67}$$

where ρ_4 is the smallest positive solution of

$$g_4(\rho) = 1 \ . \tag{3.68}$$

As a conclusion, there are regimes I and IV for all positive values of Π, (Π_1 being positive), cf. (3.46), (3.67), whereas regimes II and III occur for sufficiently small and sufficiently large Π resp., cf. (3.52), (3.61).

4. Negative Π_2.

In this section we investigate the case that $\Pi_2 < 0$. We first note that the infimum in (1.3) can only occur at a point (m_1, m_2) such that the matrix of second derivatives of the function between brackets [...] is positive. This gives the stability condition

$$\begin{aligned} &k_{11} + \Pi_1 > 0 \ , \\ &(k_{11} + \Pi_1)(k_{22} + \Pi_2) - k_{12}^2 > 0 \ , \end{aligned} \tag{4.1}$$

which can be expressed in terms of ρ and θ, cf. (3.35)-(3.37),

$$\rho + \operatorname{sgn} \Pi_1 > 0 \ , \tag{4.2}$$

$$(\rho + \operatorname{sgn} \Pi_1)(1 + \Pi\rho^{-p}) + (t\rho + s \operatorname{sgn} \Pi_1)\theta^2 > 0 \ . \tag{4.3}$$

Furthermore, for $\Pi < 0$ there is no demagnetizing phase and the external fields as given by (2.31) can be expressed as

$$\tilde{h}_1 \equiv \eta_1^{-1} |\kappa/\Pi_1|^{a_1/(2a_1-1)} h_1 = \rho^{a_1/(2a_1-1)} \{(\theta^2 - \theta_2^2) + \tfrac{1}{2}(1+s) \operatorname{sgn} \Pi_1 (\theta^2 - \theta_1^2)\rho^{-1}\} , \tag{4.4}$$

$$\tilde{h}_2 \equiv \eta_2^{-1} |\kappa/\Pi_1|^{a_2/(2a_1-1)} h_2 = \theta\rho^{a_2/(2a_1-1)} \{(1-\theta^2) + \Pi\rho^{-p}\} \ . \tag{4.5}$$

A. Π_1 positive.

We consider first the case that $\operatorname{sgn} \Pi_1 = 1$, $\Pi < 0$.

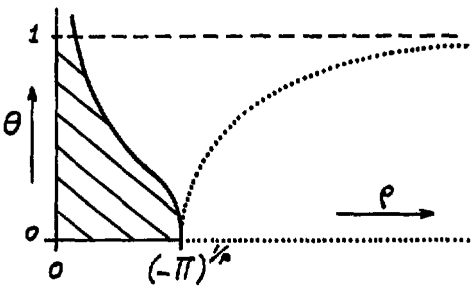

Fig. 1. Stability curve and the curve $\tilde{h}_2=0$ in the ρ,θ-plane for $\Pi_1 > 0$, $\Pi_2 < 0$.

In fig. 1, the drawn curve is the stability curve

$$\theta^2 = -\frac{(\rho+1)(1+\Pi\rho^{-p})}{t\rho+s}, \tag{4.6}$$

and the shaded area is the unstable region of the ρ,θ-plane. (It can easily be shown from (4.6) that $\partial\theta^2/\partial\rho < 0$ for the stability curve.) The dotted curve is the curve $\tilde{h}_2=0$, given by, cf. (4.5),

$$\theta=0 \text{ and } \theta^2 = 1+\Pi\rho^{-p}, \quad \rho > (-\Pi)^{\frac{1}{p}} . \tag{4.7}$$

For $\theta > 0$ we have $m_2 = \mu_2\theta > 0$, and the infimum in (1.3) must be realized at a positive value of h_2. The condition $\tilde{h}_2 > 0$ implies $\theta^2 < 1+\Pi\rho^{-p}$, corresponding to the region enclosed by the dotted curve in fig. 1, and a curve $\tilde{h}_2 = c$, with $c > 0$, lies in the stable part of the ρ,θ-plane.

Since in a stable part of the ρ,θ-plane the variable $\tilde{h}_1$ must change monotonically on a curve $\tilde{h}_2 = c$, there cannot be a first-order transition for positive $\tilde{h}_2$. In fact, if $\tilde{h}_1$ has a stationary point P on a curve with $\tilde{h}_2 = c$, the curves with constant $\tilde{h}_1$ and $\tilde{h}_2$ resp. must touch at the point P and P must lie on the stability curve, since, (in the m_1,m_2-plane), cf. (2.28),

$$\left.\frac{dh_1}{dm_1}\right|_{h_2} = \frac{\partial h_1}{\partial m_2}\left[\left.\frac{dm_2}{dm_1}\right|_{h_2} - \left.\frac{dm_2}{dm_1}\right|_{h_1}\right] = \frac{(k_{11}+\Pi_1)(k_{22}+\Pi_2) - k_{12}^2}{k_{22}+\Pi_2} . \tag{4.8}$$

Consider now the value $\tilde{h}_2 = 0$. If $\theta=0$ and ρ decreases from ∞ to $(-\Pi)^{1/p}$, then $\tilde{h}_1$ increases from $-\infty$ to $\tilde{h}_{1c}$, with

$$\tilde{h}_{1c} = -(-\Pi)^{a_1/(2a_2-1)} \{\theta_2^2 + \tfrac{1}{2}(1+s) \operatorname{sgn} \Pi_1\theta_1^2(-\Pi)^{-1/p}\} . \tag{4.9}$$

On the branch with $\theta\neq0$, $\tilde{h}_1$ increases from $\tilde{h}_{1c}$ to ∞, if ρ increases from

$(-\Pi)^{1/p}$ to ∞.

For $\tilde{h}_1 > \tilde{h}_{1c}$, we have $\theta > 0$, if $\tilde{h}_2 \downarrow 0$, and $\theta < 0$, if $\tilde{h}_2 \uparrow 0$; there is a spontaneous magnatization and a first-order transition when we pass through $\tilde{h}_2 = 0$. The point $\rho = (-\Pi)^{1/p}$, $\theta=0$, or $\tilde{h}_1 = \tilde{h}_{1c}$, $\tilde{h}_2 = 0$, is a classical critical point. As $g_0(m_1,m_2)$ is analytic in a neighbourhood of this point, the free energy (1.3) around this point can be found from a Landau expansion.

B. Π_1 negative.

We now consider the case that sgn $\Pi_1 = -1$, $\Pi < 0$. From (4.2) and (4.3) we have the conditions

$$\rho > 1 , \tag{4.10}$$

$$\theta^2 > \frac{(\rho-1)(-1 - \Pi\rho^{-p})}{t\rho - s} , \quad \text{if } \rho > \frac{s}{t} , \tag{4.11}$$

$$\theta^2 < \frac{(\rho-1)(1 + \Pi\rho^{-p})}{s - t\rho} , \quad \text{if } \rho < \frac{s}{t} . \tag{4.12}$$

(i) If $-\Pi > (s/t)^p$, then (4.12) gives instability for $\rho < s/t$ and the stability curve is determined by (4.11). This stability curve has $\partial\theta^2/\partial\rho < 0$, so that this case is analogous to the case of positive Π_1 in subsection A. (Note that on the stability curve in this case $\theta^2 \to \infty$ for $\rho \downarrow s/t$.)

(ii) If $-\Pi < (s/t)^p$, then (4.11) is trivially satisfied and the stability curve is determined by (4.12). We first consider the case that $-\Pi < \{\frac{1}{2}(s+1)\}^{2p}$.

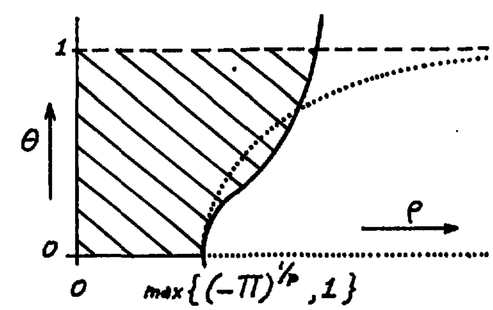

Fig. 2. Stability curve and curve $\tilde{h}_2 = 0$ in the ρ,θ-plane for $\Pi_1 < 0$, $-\Pi < \{\frac{1}{2}(s+1)\}^{2p}$.

In fig. 2 the shaded area is again the unstable part of the ρ,θ-plane. Note that in this case the dotted curve $\tilde{h}_2 = 0$ has a second intersection point, (with $\theta > 0$), with the stability curve. In fact, the intersection points can be found from eqs. (4.7) and (4.12) with equality sign. We find

$$\theta=0, \quad \text{or } \rho = (s+1)/(t+1) = \{\tfrac{1}{2}(s+1)\}^2 , \tag{4.13}$$

so that there is an intersection point with $\theta > 0$, if and only if

$$-\Pi < \{\tfrac{1}{2}(s+1)\}^{2p} . \tag{4.14}$$

In that case a curve $\tilde{h}_2 = c$ passes through an unstable portion of the ρ,θ-plane for sufficiently small $c > 0$. As a consequence, there are first-order transitions for sufficiently small $|\tilde{h}_2|$.

On the other hand, if (4.14) is not satisfied, i.e. if $\{\tfrac{1}{2}(s+1)\}^{2p} < -\Pi < (s/t)^p$, we also have $\partial\theta^2/\partial\rho > 0$ on the stability curve, but now the curves $\tilde{h}_2 = c$, with $c > 0$, lie in the stable region of the ρ,θ-plane, and there are no first-order transitions.

We now investigate the case (4.14) in more detail. From (4.5) and (4.12) with equality sign it follows that $\tilde{h}_2$ on the stability curve is given by

$$\tilde{h}_2 = \rho^{a_2/(2a_1-1)}(1+\Pi\rho^{-p})^{\frac{3}{2}}(\rho-1)^{\frac{1}{2}}\{(s+1) - (t+1)\rho\}(s-t\rho)^{-\frac{3}{2}} , \tag{4.15}$$

so that

$$\frac{\partial\tilde{h}_2}{\partial\rho} = \tilde{h}_2\rho^{-1}\left[\frac{a_2}{2a_1-1} + \frac{\{(s+3) - (t+3)\rho\}(s-t)\rho}{2\{(s+1) - (t+1)\rho\}(s-t\rho)(\rho-1)} - \frac{3}{2}\,\frac{p\Pi}{\rho^p+\Pi}\right]. \tag{4.16}$$

The function between brackets in the right-hand side of (4.16) is monotonically decreasing in ρ for

$$\max\,\{(-\Pi)^{1/p},\ 1\} \ < \rho \ < \tfrac{1}{4}(s+1)^2 . \tag{4.17}$$

Values of $\rho > \tfrac{1}{4}(s+1)^2$ are not of interest, since we can restrict ourselves to $\tilde{h}_2 > 0$. To see the monotonicity we introduce the variable

$$x = \frac{s-t\rho}{\rho-1} , \tag{4.18}$$

and the function between brackets in (4.16) can be written as

$$\phi(x) = a_2/(2a_1-1) + \psi(x) - \frac{3}{2}\,p\Pi\left[\{(s+x)/(t+x)\}^p + \Pi\right]^{-1} , \tag{4.19}$$

with

$$2(s-t)\psi(x) = \frac{(x-3)(s+x)(t+x)}{x(x-1)} = (1-st) + x - \frac{8}{x-1} + \frac{3st}{x} , \tag{4.20}$$

so that

$$2(s-t)\,\frac{d\psi}{dx} = \frac{8x^2 + (x-1)^2(x^2-3st)}{x^2(x-1)^2} > 0, \qquad (4.21)$$

using that $x > 1$ and $st = 3-s-t < 3$. Therefore $\phi(x)$ is an increasing function of x for $\Pi < 0$. For $x \downarrow 1$, $(\rho \uparrow \frac{1}{4}(s+1)^2)$, we have $\phi(x) \to -\infty$ and for $\rho \downarrow \max\{(-\Pi)^{1/p}, 1\}$, $\phi(x) \to +\infty$.

As a consequence there is one and only one value ρ_c in the interval (4.17) satisfying $\phi(x) = 0$, so that

$$\frac{\partial \tilde{h}_2}{\partial \rho}(\rho_c) = 0 \; . \qquad (4.22)$$

Eq. (4.22) implies that on the stability curve $\tilde{h}_2$ increases from 0 to $\tilde{h}_{2c} = \tilde{h}_2(\rho_c)$, if ρ increases from $\max\{(-\Pi)^{1/p}, 1\}$ to ρ_c; $\tilde{h}_2$ decreases from $\tilde{h}_{2c}$ to 0, if ρ increases from ρ_c to $\frac{1}{4}(s+1)^2$. Thus for all values $0 < \tilde{h}_2 < \tilde{h}_{2c}$, the curve at constant $\tilde{h}_2$ contains a part lying in the unstable region of the ρ,θ-plane and there must be first-order transitions at constant $\tilde{h}_2$. For $\tilde{h}_2 > \tilde{h}_{2c}$ the curve at constant $\tilde{h}_2$ lies in the stable region of the ρ,θ-plane implying that there is no first-order transition. Qualitatively the phase diagram in $\tilde{h}_1,\tilde{h}_2$-space is given in the figures 3a and 3b.

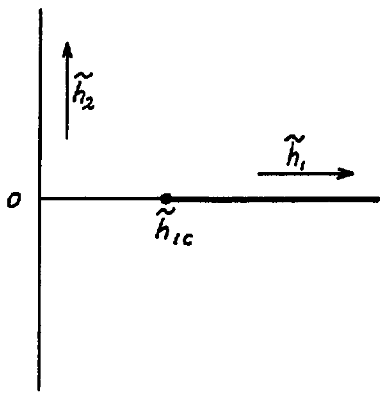

Fig. 3a

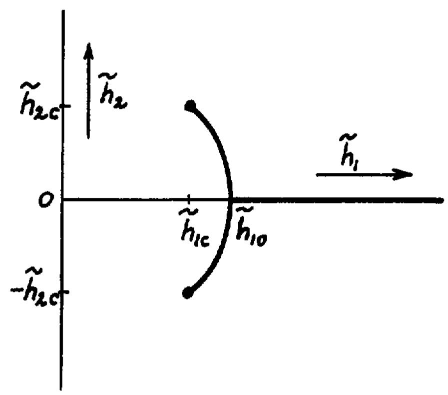

Fig. 3b

Phase diagrams in the $\tilde{h}_1,\tilde{h}_2$-plane for negative Π(or Π_2). Fig. 3a is characteristic for $\Pi_1 > 0$, $\Pi < 0$, or $\Pi_1 < 0$, $\Pi < -\{\frac{1}{2}(s+1)\}^{2p}$. In fig. 3b we have $\Pi_1 < 0$, $-\{\frac{1}{2}(s+1)\}^{2p} < \Pi < 0$.

From fig. 3b we note that $\tilde{h}_1(\rho_c) < \tilde{h}_{1o}$, where $\tilde{h}_{1o}$ is the $\tilde{h}_1$-value of the triple point corresponding to the first-order transition at $\tilde{h}_2 \to 0$. This can be seen from the inequality

$$\tilde{h}_1(\rho_c) < h_1(\tfrac{1}{4}(s+1)^2) < \tilde{h}_{1o} , \tag{4.23}$$

which can be derived easily taking into account that $\tilde{h}_1(\rho)$ on the stability curve has a minimum at $\rho = \rho_c$ and that $\rho = \frac{1}{4}(s+1)^2$ in the intersection point with $\theta \neq 0$ of the curve $\tilde{h}_2 = 0$ and the stability curve.

5. The case $\Pi_1 < 0$, $\Pi_2 > 0$.

In this section we investigate the possibility of first-order transitions in the case $\Pi_1 < 0$, $\Pi_2 > 0$. Since Π_2 is positive, we must also take into account the solutions of (2.33) corresponding to the demagnetizing phase. The second derivatives of the free energy in this phase are given by (3.5), but now with $\Pi_1 < 0$. The stability condition is $\chi_{11} > 0$, or

$$\frac{b^{2a_1-1}}{|\Pi_1|} > \frac{(1-a_1)M_1(1)}{a_1 H_1(1)} , \tag{5.1}$$

which in view of the parametrization (3.33), cf. also (2.6), (2.14), (2.21), (2.22), (2.24), can be expressed as

$$\rho > \kappa \frac{(1-a_1)(1-\theta_1^2)\mu_1}{a_1(1-\theta_2^2)\eta_1} = \tfrac{1}{4}(s+1)^2 . \tag{5.2}$$

On the other hand, the boundary of the demagnetizing phase, cf. (3.3), is given by

$$\tilde{h}_D \equiv \eta_2^{-1}|\kappa/\Pi_1|^{a_2/(2a_1-1)}\, h_D = \Pi\rho^{(1-a_2)/(2a_1-1)} , \tag{5.3}$$

so that $\tilde{h}_D$ is an increasing function of ρ. Eqs. (5.2) and (5.3) imply that for all values $\tilde{h}_2$ with

$$|\tilde{h}_2| < \tilde{h}_{Dc} \equiv \Pi\{\tfrac{1}{4}(s+1)^2\}^{(1-a_2)/(2a_1-1)} , \tag{5.4}$$

there must be a first-order transition to the demagnetizing phase. In fact the intersection point of a curve with $\tilde{h}_2 = c$, $0 < c < \tilde{h}_{Dc}$, in the normal phase $(0 \leqslant \theta^2 < 1)$ with the boundary of the demagnetizing phase $(\theta^2 = 1)$ occurs at a value ρ smaller than $\frac{1}{4}(s+1)^2$ and therefore in the unstable part of the demagnetizing phase, cf. (5.2).

Furthermore, first-order transitions at $\tilde{h}_2 = c$, $(c>0)$, can arise if the curve $\tilde{h}_2 = c$ in the normal phase contains a part lying in the unstable region of the ρ,θ-plane. To investigate this in more detail we consider the stability conditions (4.10)-(4.12). For positive Π eq. (4.11) is trivial and the stability curve is given by

$$1 + \Pi\rho^{-p} = \frac{s-t\rho}{\rho-1}\,\theta^2 \,, \tag{5.5}$$

i.e. for larger values of θ^2 (with $\theta^2 < 1$), the point (ρ,θ) is a stable solution. For fixed $\Pi>0$, the behaviour of the stability curve in the ρ,θ-plane is slightly more complicated than in the preceding section, but a detailed treatment is not necessary in order to derive for which values of $\tilde{h}_2$ there should occur a first-order transition. The behaviour of $\tilde{h}_2$ on the stability curve is given by eq. (4.15) but now for Π positive. Note that $\tilde{h}_2$ is positive on the stability curve for the values ρ satisfying $1 < \rho < \frac{1}{4}(s+1)^2$, which implies that for all intersection points of the stability curve with $\theta^2 = 1$, we must have

$$\tilde{h}_2 < \tilde{h}_{Dc} \,, \tag{5.6}$$

as $\tilde{h}_2 = \tilde{h}_D$ is an increasing function of ρ.

We shall now prove that for sufficiently small values of $\Pi>0$ there is one and only one maximum $\tilde{h}_{2c}(\Pi)$ of $\tilde{h}_2$ lying on the stability curve with $\theta^2 < 1$. This implies that for all values $\tilde{h}_2$, satisfying

$$|\tilde{h}_2| < \tilde{h}_{2c}(\Pi) \,, \tag{5.7}$$

there is a first-order transition. To prove eq. (5.7) and to determine the critical field $\tilde{h}_{2c}(\Pi)$ we first note that the extrema on the stability curve are determined by $\phi(x) = 0$, where $\phi(x)$ has been defined by (4.19). The condition $\phi(x) = 0$ defines a function $\Pi(x)$ which is given by

$$q - 2\psi(x) = 3p\left[1 + \Pi(x)\{(t+x)/(s+x)\}^p\right]^{-1} \,, \tag{5.8}$$

$$q = \frac{s+3}{s-1} \,. \tag{5.9}$$

On the other hand we must have $\theta^2 < 1$ and from (5.5) and (5.8) we find the inequality

$$q - 2\psi(x) > 3px^{-1} \,. \tag{5.10}$$

The function $q-2\psi$ can be written, cf. (4.20),

$$(s-t)(q-2\psi) = \frac{3(s-t)q}{x} - \frac{(x-3)^3}{x(x-1)} \,, \tag{5.11}$$

so that (5.10) is equivalent to

$$3(s-t)(p-q) + \frac{(x-3)^3}{x-1} < 0 \, . \tag{5.12}$$

Since s>t and p>q, eq. (5.12) is satisfied for

$$1 < x < x_0 < 3 \, , \tag{5.13}$$

where x_0 is the solution of (5.12) with equality sign,

$$x_0 = 3 - (L-9)^{\frac{1}{3}}\{(\sqrt{L}+3)^{\frac{1}{3}} - (\sqrt{L}-3)^{\frac{1}{3}}\} \, , \tag{5.14}$$

$$L = 9 + (s-t)(p-q) \, . \tag{5.15}$$

It can now be proved that $\Pi(x)$, defined by (5.8), is an increasing function of x in the interval (5.13). From (5.8) we have

$$\frac{d\Pi(x)}{dx} = p\left(\frac{s+x}{t+x}\right)^p \{(s+x)(t+x)(s-t)(q-2\psi)\}^{-1}\eta(x), \tag{5.16}$$

with

$$\eta(x) = 6(s+x)(t+x)(s-t)\,\frac{d\psi}{dx} - \{3p - (q-2\psi)\}(s-t)^2(q-2\psi) \, . \tag{5.17}$$

Using the inequalities (5.10) and (5.12) we find

$$\eta(x) > 6(s-t)(s+x)(t+x)\,\frac{d\psi}{dx} - (x-1)\{(s-t)(q-2\psi)\}^2$$

$$= \frac{3(s-t)q(x-3)^2(3x-1)}{x(x-1)} - \frac{(x-3)^4(x^2-10x+3)}{x(x-1)^2} > \frac{2x(x-3)^4}{(x-1)^2} > 0 \, . \tag{5.18}$$

Also, the function $\theta^2(x)$ defined by

$$3p(q - 2\psi(x))^{-1} = x\theta^2(x) \, , \tag{5.19}$$

obtained from (5.5) and (5.8), increases monotonically from 0 to 1, if x increases from 1 to x_0, since

$$\frac{d\theta^2(x)}{dx} = \frac{2x(x-3)^2\theta^4(x)}{3(s-t)p(x-1)^2} \geq 0 \, . \tag{5.20}$$

Hence, for all values of Π satisfying

$$0 < \Pi < \Pi(x_0) = (x_0-1)\left(\frac{s+x_0}{t+x_0}\right)^p \, , \tag{5.21}$$

we have one and only one extremum $\tilde{h}_{2c}$ of $\tilde{h}_2$ on the stability curve. It can easily be shown that this extremum is a maximum. This is trivial if the stability curve (5.5) has only one intersection point with $\theta^2=1$, as $\tilde{h}_2 \to 0$, if $\rho\downarrow 1$. Consider now the case that Π is such that there is more than one intersection point. Let (ρ_c, θ_c) denote the position of the extremum of $\tilde{h}_2$ on the stability curve, and $(\rho_1, 1)$ the intersection point of the stability curve with $\theta^2=1$ for the largest value of ρ satisfying $\rho < \rho_c$. Furthermore, let the value of $\tilde{h}_2$ at (ρ_c, θ_c) be given by $\tilde{h}_{2c}$ and the values of $\tilde{h}_2 = \tilde{h}_D$ in $(\rho_1, 1)$ and $(\rho_c, 1)$ by $\tilde{h}_a$ and $\tilde{h}_b$ resp. Then for all values $\theta \geqslant \theta_c$, we have at (ρ_c, θ), cf. (5.5),

$$\frac{\partial \tilde{h}_2}{\partial \theta} = \rho_c^{a_2/(2a_1-1)}(1 + \Pi\rho_c^{-p} - 3\theta^2) = \rho_c^{a_2/(2a_1-1)}(x_c\theta_c^2 - 3\theta^2) < 0 , \qquad (5.22)$$

and therefore $\tilde{h}_a < \tilde{h}_b < \tilde{h}_{2c}$. (5.23)

As a conclusion, we find that there is a value $\Pi = \Pi_s$, satisfying (5.21), so that first-order transitions occur at all values

$$|\tilde{h}_2| < \tilde{h}_{2c} , \quad \text{if } 0 < \Pi < \Pi_s ,$$
$$|\tilde{h}_2| < \tilde{h}_{Dc} , \quad \text{if } \Pi > \Pi_s , \qquad (5.24)$$

where the critical field $\tilde{h}_{2c} = \tilde{h}_{2c}(\Pi)$ is given by, cf. (4.5),

$$\tilde{h}_{2c} = (x_c - 1)\theta_c^3\{(s+x_c)/(t+x_c)\}^{a_2/(2a_1-1)} , \qquad (5.25)$$

x_c being the solution of $\Pi = \Pi(x_c)$, cf. (5.8), and $\theta_c = \theta(x_c)$, cf. (5.19), (or (5.5)); the critical field $\tilde{h}_{Dc} = \tilde{h}_{Dc}(\Pi)$ has been defined in (5.4). The value Π_s is given by $\Pi_s = \Pi(x_s)$, with x_s the solution of

$$\frac{(x-1)\theta^3(x)}{x\theta^2(x)-1} \left\{\frac{s+x}{t+x}\Big/\frac{s+1}{t+1}\right\}^{(1-a_2)/(2a_1-1)} = 1 , \qquad (5.26)$$

cf. (5.25) and the relation

$$\tilde{h}_{Dc} = (x_c\theta_c^2 - \left(\frac{s+x_c}{t+x_c}\right)^p \left(\frac{s+1}{t+1}\right)^{(1-a_2)/(2a_1-1)} , \qquad (5.27)$$

for $0 < \Pi < \Pi(x_0)$. Eq. (5.26) has only one solution x_s, since the left-hand side decreases monotonically from ∞, for $\Pi\downarrow 0$, to a value less than one, for $\Pi = \Pi(x_0)$, as $\theta^2(x_0) = 1$.

So far we have investigated for which values of $\tilde{h}_2$ there will be at least one first-order transition. A complete treatment of the phase diagram, however, would require a more elaborate analysis. In fact, at constant magnetic field, one may have: a second-order phase transition to the demagnetizing phase; a first-order transition in the normal phase followed by a second-order transition to the demagnetizing phase; a first-order transition from the normal phase to the demagnetizing phase; a first-order transition in the normal phase followed by a first-order transition to the demagnetizing phase. All first-order transitions terminate in classical critical points. For special values of Π there will be multicritical behaviour but these possibilities will not be analyzed further in this thesis.

Remarks.

i) It may be noted that the conclusions in this chapter are universal in the sense that they are independent of the specific values of a_1 en a_2, provided that the inequalities (2.7) and (3.43) are satisfied.

ii) A reference system in which the specific heat and the susceptibility have a cusp-like behaviour can also be taken into account. For example, if the reference free energy is given by

$$f_0(h_1^*,h_2^*) = \phi_0(h_1^*,h_2^*) - \tfrac{1}{2}\Lambda_1^{-1}h_1^{*2} - \tfrac{1}{2}\Lambda_2^{-1}h_2^{*2}, \tag{5.28}$$

where $\Lambda_1^{-1},\Lambda_2^{-1} > 0$ and ϕ_0 satisfies the homogeneity property (1.5) with $0 < a_i < \frac{1}{2}$, then the Legendre transform (1.4) can be evaluated to be

$$g_0(m_1,m_2) = \phi_0(\Lambda_1 m_1, \Lambda_2 m_2) + \tfrac{1}{2}\Lambda_1 m_1^2 + \tfrac{1}{2}\Lambda_2 m_2^2 , \tag{5.29}$$

apart from small correction terms. Eq. (5.29) leads to an expression for the reference free energy similar to (1.3), with Π_1 and Π_2 replaced by Λ_1 and Λ_2 resp. This implies that the considerations in section 3, and therefore also the Schofield model, may be used to describe a reference free energy with finite second derivatives. Furthermore, the critical properties of such a reference system are stable under small perturbations Π_i, as $|\Pi_i| << \Lambda_i$, see also section 7.4 and appendix G of chapter III for a more systematic discussion.

iii) A quadratic form depending only on m_1 and m_2 may be considered as an approximation to more general perturbations $P(m_1,m_2,h_1,h_2)$, depending on the external fields h_1 and h_2 as well, provided that the eigenvalues of the quadratic part are different from zero. Such perturbations can rise in a general way from constraints imposed on the reference system [9], cf. e.g. section 3 of chapter III. Important examples are e.g. the Baker-Essam model [11),12] for compressible Ising ferromagnets and the Syozi model [13] for Ising systems with bond-annealed impurities, see chapter III for a more complete discussion of the literature. However, if one of the eigenvalues of the quadratic part vanishes, one may have more complicated nulticritical behaviour, and further details of $P(m_1,m_2,h_1,h_2)$ can be essential for the critical properties, see e.g. ref. 14.

iv) The special case $\Pi_2=0$ has been previously investigated by Dohm and Kortman [15] using also a Schofield model for the reference system. For $\Pi_1>0$ there is a Fisher renormalization close to the critical point, for $\Pi_1<0$ there are first-order transitions for sufficiently small values of the magnetic field $\tilde{h}_2$ with a classical critical point at $\tilde{h}_{2c}(0)$. For $\Pi_1=0$ one has the critical behaviour of the reference system. A physical example is given by the tricritical point in compressible Ising ferromagnets, see e.g. refs. 15, 16.

Appendix A.

In this appendix we give an outline of the proof of eqs. (3.29)-(3.32), starting from the inequality (3.28). Eq. (3.28) is equivalent with the inequality

$$-\lambda(\underline{\underline{\chi}}^A)^{-1} < \underline{\underline{\chi}}^{-1} - (\underline{\underline{\chi}}^A)^{-1} < \lambda(\underline{\underline{\chi}}^A)^{-1} , \tag{A.1}$$

since $0 < \underline{\underline{A}} < \underline{\underline{B}} \Leftrightarrow 0 < \underline{\underline{B}}^{-1} < \underline{\underline{A}}^{-1}$. Eq. (3.29) is a direct consequence of (A.1), (with $(\underline{\underline{\chi}}^A)^{-1} = \underline{\underline{k}}$, $\underline{\underline{\chi}}^{-1} = \underline{\underline{k}}+\underline{\underline{\Pi}}$). Eq. (3.30) can be obtained from eq. (A.1), using that

$$(\underline{\underline{\chi}}^{II})^{-1} = \frac{1}{\Pi_1-k_{11}} \begin{pmatrix} \Pi_1^2 & \Pi_1 k_{12} \\ \Pi_1 k_{12} & k_{12}^2+k_{22}(\Pi_1-k_{11}) \end{pmatrix}$$

$$(\underline{\underline{\chi}}^{II})^{-1} - \underline{\underline{\chi}}^{-1} = \frac{1}{\Pi_1-k_{11}} \begin{pmatrix} k_{11}^2 & k_{11}k_{22} \\ k_{11}k_{22} & k_{12}^2-\Pi_2(\Pi_1-k_{11}) \end{pmatrix}. \tag{A.2}$$

Eq. (3.31) follows, interchanging the subscripts 1 and 2 in (3.30). Finally, eq. (3.32) follows as a special case from the relations

$$0 < \underline{\underline{k}} < \sqrt{\lambda}\underline{\underline{\Pi}} \Leftrightarrow 0 < (-1)^{\ell+1}(\underline{\underline{\chi}}-\underline{\underline{\chi}}^{(\ell)}) < \lambda^{\frac{1}{2}(\ell+1)}\underline{\underline{\chi}}$$
$$\Leftrightarrow 0 < (-1)^{\ell+1}(\underline{\underline{\chi}}-\underline{\underline{\chi}}^{(\ell)}) < \lambda^{\frac{1}{2}(\ell-m)}(-1)^{m+1}(\underline{\underline{\chi}}-\underline{\underline{\chi}}^{(m)}) , \tag{A.3}$$

in which

$$\underline{\underline{\chi}}^{(\ell)} \equiv \underline{\underline{\Pi}}^{-1}\cdot\sum_{n=0}^{\ell} (-\underline{\underline{k}}\cdot\underline{\underline{\Pi}}^{-1})^n \tag{A.4}$$

is the "ℓ^{th}-order approximation" of $\underline{\underline{\chi}} = (\underline{\underline{k}}+\underline{\underline{\Pi}})^{-1}$. Eq. (A.3) can be proved easily using the identities

$$\underline{\underline{\Pi}}^{\frac{1}{2}}\cdot\underline{\underline{\chi}}\cdot\underline{\underline{\Pi}}^{\frac{1}{2}} = (\mathbb{1} + \underline{\underline{A}})^{-1}, \quad \underline{\underline{\Pi}}^{\frac{1}{2}}\cdot(\underline{\underline{\chi}}-\underline{\underline{\chi}}^{(\ell)})\cdot\underline{\underline{\Pi}}^{\frac{1}{2}} = (-1)^{\ell+1}(\mathbb{1} + \underline{\underline{A}})^{-1}\cdot\underline{\underline{A}}^{\ell+1}\ , \tag{A.5}$$

where $\underline{\underline{A}} = \underline{\underline{\Pi}}^{-\frac{1}{2}}\cdot\underline{\underline{k}}\cdot\underline{\underline{\Pi}}^{-\frac{1}{2}}$. Since $\underline{\underline{\chi}}^{(0)} = \underline{\underline{\Pi}}^{-1}$ and $\underline{\underline{\chi}}^{(1)} = \underline{\underline{\chi}}^{IV} = \underline{\underline{\Pi}}^{-1} - \underline{\underline{\Pi}}^{-1}\cdot\underline{\underline{k}}\cdot\underline{\underline{\Pi}}^{-1}$ we have from (A.3) that

$$\begin{aligned} 0 < \underline{\underline{k}} < \sqrt{\lambda}\underline{\underline{\Pi}} &\Leftrightarrow 0 < \underline{\underline{\chi}}-\underline{\underline{\chi}}^{IV} < \lambda\underline{\underline{\chi}} \\ &\Leftrightarrow 0 < \underline{\underline{\chi}}-\underline{\underline{\chi}}^{IV} < \sqrt{\lambda}(\underline{\underline{\Pi}}^{-1}-\underline{\underline{\chi}}) \Leftrightarrow 0 < \underline{\underline{\Pi}}^{-1} - \underline{\underline{\chi}} < \sqrt{\lambda}\underline{\underline{\chi}}\ . \end{aligned} \tag{A.6}$$

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SAMENVATTING.

Een belangrijk probleem in de statistische mechanica is de afleiding van thermodynamische eigenschappen van veeldeeltjessystemen, uitgaande van microscopische wisselwerkingen tussen de deeltjes. In veel gevallen is het voldoende om de vrije energie per deeltje te bepalen, waaruit de thermodynamische eigenschappen afgeleid kunnen worden. Deze eigenschappen zijn in het algemeen afhankelijk van de dracht van de wisselwerkingen tussen de deeltjes.

Een speciale klasse van veeldeeltjessystemen is de klasse van kortedrachtssystemen, waartoe o.a. de systemen behoren waarin de wisselwerking tussen de deeltjes een eindige dracht heeft, d.w.z. alleen verschillend van nul is als de afstand tussen de deeltjes niet te groot is. Voor kortedrachtssystemen heeft men bewezen dat de vrije energie per deeltje bestaat in de thermodynamische limiet. Een exacte berekening van de vrije energie in twee en meer dimensies is tot op heden niet gevonden, afgezien van een aantal uitzonderingsgevallen zoals bijvoorbeeld het tweedimensionale Ising model in afwezigheid van een magneetveld. De laatste jaren heeft men veel inzicht gekregen in het kwalitatieve gedrag van deze systemen door gebruik te maken van benaderingsmethoden. Zo heeft men bijvoorbeeld kunnen vaststellen dat veel kortedrachtsmodellen een (universeel) kritisch gedrag in de buurt van een faseovergang vertonen, waarbij het dominante singuliere deel van de vrije energie aan een homogeniteitseigenschap voldoet en een of meer susceptibiliteiten (tweede afgeleiden van de vrije energie) divergeren met welgedefinieerde kritische exponenten.

In de eerste twee hoofdstukken van dit proefschrift wordt een klasse van (quantummechanische) modelsystemen beschouwd, waarin behalve interacties van korte dracht ook (extreem) langedrachtswisselwerkingen kunnen voorkomen en meerdeeltjesinteracties van een gemengd karakter. Voor deze klasse wordt een exacte betrekking afgeleid, waarin de vrije energie uitgedrukt wordt met behulp van de Legendre getransformeerde g_0 van een referentiesysteem met uitsluitend kortedrachtswisselwerkingen en een (storings)term P die voortkomt uit de langedrachtsinteracties. In het geval dat men de vrije energie van het referentiesysteem exact kent, geeft deze betrekking ook de vrije energie van het systeem met langedrachtsinteracties exact. Maar ook als van het referentiesysteem alleen globale eigenschappen bekend zijn, bijvoorbeeld het asymptotische gedrag in de buurt van een kritisch punt, dan kunnen met behulp van deze betrekking algemene conclusies worden getrokken.

Bij het bewijs wordt gebruik gemaakt van de opsplitsing van P in een concaaf gedeelte Q en een convex gedeelte R. Voor concave P=Q is de relatie een generalisatie van een fundamenteel theorema van Bogoliubov Jr. Een eenvoudig bewijs van dit theorema (voor kwadratische Q) kan men vinden in hoofdstuk I. Het algemene bewijs voor willekeurige P en (quantummechanische) kortedrachtswisselwerkingen vereist een zorgvuldige behandeling van de thermodynamische limiet en wordt gegeven in hoofdstuk II.

In het derde hoofdstuk van dit proefschrift wordt aangetoond dat het kritische gedrag van een kortedrachtssysteem geheel van karakter verandert onder invloed van extreem langedrachtswisselwerkingen. In het bijzonder, als de functie P (sterk) convex is, zijn er geen eerste-orde faseovergangen (discontinuïteiten in eerste afgeleiden van de vrije energie), en is er een kritisch punt met susceptibiliteiten die een doornvormig (cusp-like) gedrag hebben met gerenormaliseerde kritische exponenten. Als het referentiesysteem een kritisch punt heeft met divergerende tweede afgeleiden en P (sterk) concaaf is in één richting, dan zijn er eerste-orde overgangen, die kunnen eindigen in een klassiek kritisch punt.

In de praktijk moet men echter rekening houden met het feit dat niet alle variabelen relevant zijn, d.w.z. op essentiële wijze bijdragen tot het kritische gedrag. Als voor P=0, d.w.z. in het referentiesysteem, één van de variabelen irrelevant is, dan behoeft dit nog niet in te houden dat dit ook voor P≠0 het geval is. Een algemene behandeling van dit soort problemen wordt in hoofdstuk III gegeven.

Analoge conclusies gelden ook voor kortedrachtssystemen waaraan zekere inherente beperkingen zijn opgelegd (constraints on hidden variables). Voor dergelijke systemen kan namelijk een betrekking afgeleid worden, die de vrije energie uitdrukt met behulp van de Legendre getransformeerde g_0 van het referentiesysteem en een (storings)term P, die in dat geval tevens afhangt van uitwendige koppelingsconstanten en/of -velden.

In het laatste hoofdstuk wordt een speciaal voorbeeld, met twee relevante variabelen m_1 en m_2, en met $P(m_1,m_2) = \frac{1}{2}\Pi_1 m_1^2 + \frac{1}{2}\Pi_2 m_2^2$, meer in detail uitgewerkt. Bij de beschrijving van het referentiesysteem wordt gebruik gemaakt van het lineaire model van Schofield.

STUDIEOVERZICHT.

Na in juni 1969 het eindexamen gymnasium β te hebben afgelegd aan het Charlois Lyceum in Rotterdam, begon ik in september van dat jaar natuur- en wiskunde te studeren aan de Rijksuniversiteit te Leiden. Het kandidaatsexamen natuurkunde en wiskunde met sterrenkunde legde ik af in juni 1973 en het doctoraalexamen natuurkunde met bijvak wiskunde in mei 1975. De experimentele stage werd doorlopen bij de werkgroep Thermometrie onder leiding van Dr. M. Durieux. In juni 1975 trad ik in dienst van de Stichting F.O.M. om bij de groep Theoretische Vaste Stof Fysica/Leiden, welke onder leiding van Prof.dr. P.W. Kasteleyn en Dr. H.W. Capel staat, het onderzoek te verrichten dat aan dit proefschrift ten grondslag ligt. De Stichting F.O.M. stelde mij in staat in 1976 aan de zomerschool over kritische verschijnselen en faseovergangen te Banff (Canada) deel te nemen.

Het eerste hoofdstuk kwam tot stand in nauwe samenwerking met Dr. P.A.J. Tindemans. Gedurende het gehele onderzoek heb ik mogen profiteren van de levendige interesse en de vele suggesties van Dr. J.H.H. Perk.

Het typewerk werd uitstekend verzorgd door mevrouw S. Hélant Muller-Soegies.