Symmetries in magnetic phase transitions: I. The Landau-Ginzburg-Wilson Hamiltonian

1990 J. Phys. A: Math. Gen. 23 4399

(http://iopscience.iop.org/0305-4470/23/19/022)

J. Phys. A: Math. Gen. 23 (1990) 4399-4413. Printed in the UK

Symmetries in magnetic phase transitions: I. The Landau–Ginzburg–Wilson Hamiltonian

M K Peev†, J N Kotzev†, M I Aroyo†, P Kasperkovitz‡ and R Dirl‡

† Faculty of Physics, University of Sofia, A Ivanov Blvd 5, BG-1126 Sofia, Bulgaria
‡ Institut für Theoretische Physik, Technische Universität, Wiedner Hauptstrasse 8-10, A-1040 Wien, Austria

Received 29 March 1990

Abstract. The Landau-Ginzburg-Wilson Hamiltonian is a function that relates Landau's phenomenological theory of magnetic phase transitions to the quantum mechanics of a microscopic spin model. We study how the symmetry of the system under consideration manifests itself in these different descriptions of the thermodynamic properties (density operator, LGW Hamiltonian, other functions of the order parameters). The results of this discussion are used to comment on divergent opinions in the literature concerning the use of corepresentations in magnetic phase transitions.

1. Introduction

The Landau theory of phase transitions is a phenomenological theory based on some general assumptions [1]. The most fundamental assumption is that the equilibrium thermodynamic potential, which carries all information on the thermodynamic behaviour of the system, may be expressed in terms of a non-equilibrium thermodynamical potential (NETP) called Landau's free energy [2-4]. The latter depends on both the thermodynamic variables and some additional tensorial variables, the so-called order parameters. Another basic assumption of Landau is that the NETP is invariant under a group of transformations of the order parameters. It is believed that this group coincides with the symmetry group of the most regular phase ('high symmetry phase') [3-5]. Here the concept of phases is introduced by modelling the system as a quasi-classical system that admits a simple geometrical interpretation. For instance, a magnetic crystal is usually represented as a regular arrangement of localized atomic magnetic moments that transform like axial vectors [6].

Although the above-mentioned approach proves to be very useful in the analysis of experimental data [6-12] it still contains a certain amount of ambiguity. Especially the contradictory results obtained for magnetic phase transitions are well documented [4, 16-21]. These inconsistencies mainly originate from two problems that are still considered to be open questions. (i) What should be the symmetry group of the NETP for transitions between two magnetically ordered phases—the group of the higher-symmetry ordered phase [14-21] or that of the paramagnetic phase of the crystal [6-12]? (ii) What types of symmetry groups and representations (corepresentations) are to be used to get the right result? This problem is a consequence of the fact that the operation of time inversion that changes the sign of the magnetic order parameter can be represented either by a linear operator $\bar{\Theta}$ or by the antilinear Wigner operator

$\hat{\Theta}$ [22, 23]. While in the first case ordinary representation theory is appropriate [6-12] one has to use corepresentations of the magnetic group in the second case [13-20].

The aim of the present paper is to answer these questions. The solution proposed here emerged from the view that in deriving the properties of the Landau free energy one has to go back to the fundamental equations of statistical physics, i.e. to the partition function of a quantum system specified by a Hilbert space and a Hamilton operator $\hat{H}$. This is a particular generalization of Landau's ideas to quantum mechanical systems (see [1], section 147). We especially clarify the transformation properties of the Landau-Ginzburg-Wilson (LGW) Hamiltonian which links the canonical density operator (and thus the Hamilton operator of the system) to Landau's free energy.

The paper is organized as follows. In section 2 we introduce the LGW Hamiltonian Φ for a general spin system, considering especially various sets of parameters as the domain of this function. In section 3 the invariance properties of Φ are derived from the symmetry group of the Hamilton operator. In section 4 we consider also other functions defined on the same set of thermomagnetic variables. We then discuss in more detail the relation between the symmetry group of the Hamilton operator and that of the LGW Hamiltonian, paying special attention to the operations of time reversal and complex conjugation. These general considerations are illustrated with the example of a magnetic crystal in section 6 and our conclusions are summarized in section 7. In an appendix it is outlined under which conditions the quantum mechanical system is completely determined by the function Φ.

2. Definition of the Landau-Ginzburg-Wilson Hamiltonian

We consider a magnetic system with Hamiltonian

$$\hat{H} = \sum_{i,\xi,j,\eta} J_{i,j}^{\xi,\eta} \hat{S}_i^\xi \hat{S}_j^\eta \tag{1}$$

where i, j are labels of the localized spins and $\hat{S}_i^\xi$ are the Cartesian components of the spin at a given site; for Ising models the summation over ξ, η reduces to a single term. The partition function is

$$Z = \operatorname{Tr} \exp(-\beta \hat{H}) \qquad \beta = \frac{1}{k_B T} \tag{2}$$

and the equilibrium free energy takes the form

$$F = -\beta^{-1} \ln Z. \tag{3}$$

The projection of the total magnetic moment of the system into a direction specified by two angles ϕ, θ or the corresponding unit vector

$$\boldsymbol{n}(\phi, \theta) = (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta) \tag{4}$$

is

$$\hat{M}(\phi, \theta) = \mu_B \sum_i g_i \sum_\xi n^\xi(\phi, \theta) \hat{S}_i^\xi \tag{5}$$

here μ_B is the Bohr magneton and g_i is the g-factor of the ith particle. This operator is related to the z component of the total magnetic moment by a unitary transformation corresponding to a rotation in three-dimensional space:

$$\begin{aligned}\hat{R}(\phi, \theta, \psi)\hat{M}^z\hat{R}(\phi, \theta, \psi)^\dagger &= \hat{R}(\phi, \theta, \psi)\hat{M}(0, 0)\hat{R}(\phi, \theta, \psi)^\dagger \\ &= \sum_\xi n^\xi(\phi, \theta)\hat{M}^\xi = \hat{M}(\phi, \theta).\end{aligned} \tag{6}$$

In this equation the operator $\hat{R}(\phi, \theta, \psi)$ is the usual rotation operator parametrized by the Euler angles ϕ, θ, ψ

$$\hat{R}(\phi, \theta, \psi) = \exp(-i\phi\hat{S}^z)\exp(-i\theta\hat{S}^y)\exp(-i\psi\hat{S}^z) \tag{7}$$

$$\hat{S}^\xi = \sum_i \hat{S}_i^\xi. \tag{8}$$

As the rotation operators are unitary, all operators $\hat{M}(\phi, \theta)$ have the same spectrum as the operator $\hat{M}^z$. In the following we assume that the g-factors coincide for all spins contributing to $\hat{M}^z$ so that the magnetic moment is proportional to the total spin.

It follows from the definition of the spin operators $\hat{S}_i^z$ that the operator $\hat{M}^z$ has a pure point spectrum. Let its spectral decomposition be

$$\hat{M}^z = \sum_M M\hat{P}(M). \tag{9}$$

The projection operators $\hat{P}(M)$ that occur in this decomposition may be used to define a function Φ:

$$\Phi(M) = -\beta^{-1}\ln(\mathrm{Tr}\exp(-\beta\hat{H})\hat{P}(M)). \tag{10}$$

The function Φ is defined on a finite set of points M and is real valued since $\hat{H}$ and the projectors $\hat{P}(M)$ are Hermitean operators. Here and in most of the following discussion the dependence of Φ on β and $\hat{H}$ (or the exchange integrals $J_{i,j}^{\xi,\eta}$) is not shown explicitly. The resolution of unity in terms of the projection operators $\hat{P}(M)$

$$\sum_M \hat{P}(M) = \hat{1} \tag{11}$$

allows one to express the partition function in terms of Φ:

$$Z = \sum_M \exp(-\beta\Phi(M)). \tag{12}$$

The function Φ is known as the Landau-Ginzburg-Wilson (LGW) Hamiltonian. As will be shown elsewhere [24], this function is not only of interest in itself but can also be used to define another function $\tilde{\Phi}$ with the following properties: first, in the thermodynamic limit $\tilde{\Phi}$ becomes a continuous function of a continuous variable M ranging over the spectrum of the operator $\hat{M}^z$; second, one may set

$$F \approx \tilde{\Phi}(M_0) \tag{13}$$

where $\tilde{\Phi}(M_0)$ is the absolute minimum of $\tilde{\Phi}(M)$. For a Hamiltonian that admits a ferromagnetic transition, $\tilde{\Phi}(M)$ is nothing but the Landau free energy obtained through Landau's approximation [1] generalized to the quantum case [24, 25]. Although their analytic properties are quite different, the functions Φ and $\tilde{\Phi}$ have the same transformation properties under the transformations considered in the next section.

The definition of Φ is easily generalized from one magnetic moment, say $\hat{M}^z$, to a set of commuting moments $\hat{M}_l^z$. For such a set the common projection operators $\hat{P}(\boldsymbol{M})$ are labelled by vectors

$$\boldsymbol{M} = (M_1, M_2, \ldots) \tag{14}$$

and defined by the eigenvalue equations

$$\hat{M}_l^z \hat{P}(\boldsymbol{M}) = M_l \hat{P}(\boldsymbol{M}). \tag{15}$$

The label $l = 1, 2, \ldots$ distinguishes the subsystems into which the original system is divided. For a magnetic crystal consisting of localized spins it is assumed that both the number of subsystems and their size go to infinity in the thermodynamic limit (see section 4). In any case all spins contained in one subsystem are assumed to have identical g-factors ($g_i = g_l$, $M_i^\xi = \mu_B g_l S_i^\xi$).

A less straightforward generalization of the definition of Φ is obtained if the unit operator is decomposed in terms of projection operators that do not commute. Consider, for instance, the projection operators

$$\hat{P}(M, \phi, \theta) = \hat{R}(\phi, \theta, 0)\hat{P}(M)\hat{R}(\phi, \theta, 0)^{\dagger}. \tag{16}$$

The subspace into which the operator (16) projects is spanned by the eigenvectors of the operator $\hat{M}(\phi, \theta)$ belonging to the eigenvalue M. Because of (11), the identity

$$\hat{R}(0, \pi, 0)\hat{P}(M)\hat{R}(0, \pi, 0)^{\dagger} = \hat{P}(-M) \tag{17}$$

and the unitarity of the rotation operators,

$$\int \mathrm{d}\Omega \sum_{M \geqslant 0} \frac{2 - \delta_{M,0}}{4\pi} \hat{P}(M, \phi, \theta) = \hat{1}. \tag{18}$$

Replacing the operator $\exp(-\beta\hat{H})$ with $\exp(-\beta\hat{H})\hat{1}$ in the definition of the free energy and using the resolution (18), one obtains the following generalizations of (10) and (12):

$$\Phi(M, \phi, \theta) = -\beta^{-1} \ln\left(\operatorname{Tr} \exp(-\beta\hat{H}) \frac{2 - \delta_{M,0}}{4\pi} \hat{P}(M, \phi, \theta)\right) \tag{19}$$

$$Z = \int \mathrm{d}\Omega \sum_{M \geqslant 0} \exp(-\beta\Phi(M, \phi, \theta)). \tag{20}$$

If the system is very large it is to be expected that the function $\Phi(M, \phi, \theta)$ varies only slowly with the variable M. In such a case we may pass to a LGW Hamiltonian Φ', a function of three variables M^x, M^y, M^z ranging continuously within a sphere whose radius is given by the maximum value of M:

$$M = \sqrt{(M^x)^2 + (M^y)^2 + (M^z)^2} \qquad \phi = \tan^{-1}\left(\frac{M^y}{M^x}\right) \qquad \theta = \cos^{-1}\left(\frac{M^z}{M}\right) \tag{21}$$

$$\Phi(M, \phi, \theta) = \Phi'(M^x, M^y, M^z). \tag{22}$$

For $M^x = M^y = M^z = 0$ this definition of Φ' is unique only if the values $\Phi(0, \phi, \theta)$ coincide for all angles. It should be noted that no assumptions on the continuity of Φ' are needed if one is only interested in discussing the transformation properties of this function; for that purpose one simply substitutes the expressions (21) for the variables of Φ in order to obtain the new function Φ'. Clearly this construction may be performed for each subsystem if the original system is divided into several parts.

It is obvious that there exist infinitely many different resolutions of the unity each of which can be used to define a LGW Hamiltonian. In any case the resulting function contains more information than the partition function because Z can be computed from Φ. On the other hand, the LGW Hamiltonian contains, in general, less detailed information on the interaction of the magnetic moments than the Hamilton operator does; the conditions under which the two descriptions of the system are fully equivalent are discussed in the appendix.

Which of the many possible resolutions of unity is preferable depends on the further steps of the calculation. For instance, the choice of a special resolution may be justified by its utility in an approximate calculation of the free energy. In that respect a necessary condition for a LGW Hamiltonian to be useful is that its absolute minimum at low temperatures occurs for those parameters that label the subspace spanned by the groundstate(s) of the system. As can be seen from the representations (12) and (20) of the partition function, a restriction of the domain of Φ to a neighbourhood of this point means that the original state space is reduced to a small part of it. This implicitly defines a new system which should approximate the original one at low temperatures. In the appendix we illustrate these ideas with the example of two spins of magnitude $\frac{1}{2}$, for both the Ising and the Heisenberg interactions.

There are two more guiding principles for the definition of the LGW Hamiltonian. If the partition function is expressed in terms of this function we arrive at a quasiclassical description of the quantum system. In this picture the states are specified by the labels of the projectors occurring in the resolution of unity. It gives more insight into the physical behaviour of the system if these labels are not just some useful mathematical entities but refer to quantities that are, at least in principle, measurable. The labels M and M, ϕ, θ meet this requirement since they are related to the measurement of the spin in a given direction. In addition to these considerations, one would like to see the symmetry properties of the quantum system also in the quasiclassical picture; this topic is discussed in detail in the next section.

3. Invariance properties of the LGW Hamiltonian

Consider a LGW Hamiltonian of the form $\Phi(M_1, \phi_1, \theta_1; M_2, \phi_2, \theta_2; \dots)$ where the subscripts refer to 'identical' parts of the system, i.e. to subsystems for which the eigenvalues of the operators S_l^z and their degeneracies coincide. As is evident from (19), the function Φ depends both on the Hamiltonian $\hat{H}$ (and β) and on the projection operators $\hat{P}_l(M_l, \phi_l, \theta_l)$. Each of these projection operators may be represented as [26]

$$\hat{P}_l(M_l, \phi_l, \theta_l) = c(0, M_l)\hat{1} + \sum_{n=1}^{2S} c(n, M_l)[\hat{S}_l(\phi_l, \theta_l)]^n \tag{23}$$

where S is the maximum eigenvalue of $\hat{S}_l^z$

$$c(n, M_l) = c(n, M_l)^* \tag{24}$$

and

$$\begin{aligned}\hat{S}_l(\phi_l, \theta_l) &= \hat{R}_l(\phi_l, \theta_l, \psi_l)\hat{S}_l^z\hat{R}_l(\phi_l, \theta_l, \psi_l)^+ \\ &= \sum_{\xi} n^{\xi}(\phi_l, \theta_l)\hat{S}_l^{\xi} = \boldsymbol{n}(\phi_l, \theta_l) \cdot \hat{\boldsymbol{S}}_l.\end{aligned} \tag{25}$$

The subscript l of the rotation operators indicates that they are of the form (7) but related to the spin operators S_l^ξ of the subsystem.

To make all these dependences more explicit we change the notation as follows:

$$\Phi(M_1, \phi_1, \theta_1; M_2, \phi_2, \theta_2; \ldots)$$
$$\to \Phi(\hat{H}; M_1, \boldsymbol{n}(\phi_1, \theta_1) \cdot \boldsymbol{S}_1; M_2, \boldsymbol{n}(\phi_2, \theta_2) \cdot \boldsymbol{S}_2; \ldots). \tag{26}$$

It follows from the definition of the LGW Hamiltonian, equation (19) generalized for a decomposition of the system into identical subsystems, and the commutation relations

$$[S_l^\xi, S_{l'}^\zeta] = 0 \quad \text{for } l \neq l' \tag{27}$$

that Φ is a symmetric function of the arguments referring to different subsystems. That is, if the N-tuple $P1, P2, \ldots$ is obtained from the N-tuple $1, 2, \ldots$ by a permutation P then

$$\Phi(\hat{H}; M_1, \boldsymbol{n}(\phi_1, \theta_1) \cdot \boldsymbol{S}_1; M_2, \boldsymbol{n}(\phi_2, \theta_2) \cdot \boldsymbol{S}_2; \ldots)$$
$$= \Phi(\hat{H}; M_{P1}, \boldsymbol{n}(\phi_{P1}, \theta_{P1}) \cdot \boldsymbol{S}_{P1}; M_{P2}, \boldsymbol{n}(\phi_{P2}, \theta_{P2}) \cdot \boldsymbol{S}_{P2}; \ldots). \tag{28}$$

Furthermore, the representation (23) of the projection operators entails that

$$\Phi(\hat{W}\hat{H}\hat{W}^{-1}; M_1, \boldsymbol{n}(\phi_1, \theta_1) \cdot \hat{W}\hat{\boldsymbol{S}}_1\hat{W}^{-1}; M_2, \boldsymbol{n}(\phi_2, \theta_2) \cdot \hat{W}\hat{\boldsymbol{S}}_2\hat{W}^{-1}; \ldots)$$
$$= \Phi(\hat{H}; M_1, \boldsymbol{n}(\phi_1, \theta_1) \cdot \hat{\boldsymbol{S}}_1; M_2, \boldsymbol{n}(\phi_2, \theta_2) \cdot \hat{\boldsymbol{S}}_2; \ldots) \tag{29}$$

for every unitary operator $\hat{W}(\hat{W}^{-1} = \hat{W}^\dagger)$.

A formally identical relation is obtained if one considers antiunitary operators instead of unitary ones. Let $u_1, u_2, \ldots$ be elements of the Hilbert space, $c_1, c_2, \ldots$ be complex numbers, and $\hat{A}$ be an antiunitary operator; then

$$\hat{A}(c_1 u_1 + c_2 u_2) = c_1^*(\hat{A}u_1) + c_2^*(\hat{A}u_2) \tag{30}$$

$$\langle \hat{A}u_1, \hat{A}u_2 \rangle = \langle u_2, u_1 \rangle = \langle u_1, u_2 \rangle^*. \tag{31}$$

These equations imply that the states $\hat{A}u_\sigma$ form an orthonormal basis of the Hilbert space if the states u_σ form such a basis. Therefore

$$\begin{aligned}
\operatorname{Tr} \exp(-\beta\hat{H})\hat{P}_l(M_1, \phi_1, \theta_1) \ldots
&= \sum_\sigma \langle u_\sigma, \mathrm{e}^{-\beta\hat{H}} \hat{P}_l(M_1, \phi_1, \theta_1) \ldots u_\sigma \rangle \\
&= \sum_\sigma \langle u_\sigma, \mathrm{e}^{-\beta\hat{H}} \hat{P}_l(M_1, \phi_1, \theta_1) \ldots u_\sigma \rangle^* \\
&= \sum_\sigma \langle \hat{A}u_\sigma, \hat{A}\, \mathrm{e}^{-\beta\hat{H}} \hat{P}_l(M_1, \phi_1, \theta_1) \ldots u_\sigma \rangle \\
&= \sum_\sigma \langle \hat{A}u_\sigma, \hat{A}\, \mathrm{e}^{-\beta\hat{H}} \hat{A}^{-1}\hat{A}\hat{P}_l(M_1, \phi_1, \theta_1) \ldots \hat{A}^{-1}\hat{A}u_\sigma \rangle \\
&= \operatorname{Tr} \hat{A} \exp(-\beta\hat{H})\hat{A}^{-1}\hat{A}\hat{P}_l(M_1, \phi_1, \theta_1) \ldots \hat{A}^{-1}.
\end{aligned} \tag{32}$$

Since β and the coefficients $c(n, M_l)$ are real numbers, the action of the antiunitary operator $\hat{A}$ may be transferred to the operators $\hat{H}$ and $\hat{S}_l(\phi_l, \theta_l)$, respectively; this finally gives relation (29) with $\hat{W} = \hat{A}$.

Now let $\hat{W}$ be a unitary or antiunitary operator with the following properties:

$$\hat{W}\hat{H}\hat{W}^{-1} = \hat{H} \tag{33}$$

$$\hat{W}\boldsymbol{n}(\phi_l, \theta_l) \cdot \hat{\boldsymbol{S}}_l\hat{W}^{-1} = \boldsymbol{n}(\phi_l', \theta_l') \cdot \hat{\boldsymbol{S}}_{Pl}. \tag{34}$$

In (34) the permutation $P: l \rightarrow Pl$ and the relation between the angles ϕ_l, θ_l and ϕ'_l, θ'_l depend on the transformation under consideration. Equation (33) expresses that $\hat{W}$ is a symmetry transformation of the Hamiltonian $\hat{H}$ while (34) shows that the projection operators used to define the LGW Hamiltonian Φ are permuted under this transformation. If these equations hold true they entail the following symmetry relation of Φ:

$$\begin{aligned}\Phi(\hat{H}; M_1, \boldsymbol{n}(\phi_1, \theta_1) \cdot \hat{\boldsymbol{S}}_1; \ldots) &= \Phi(\hat{H}; M_1, \boldsymbol{n}(\phi'_1, \theta'_1) \cdot \hat{\boldsymbol{S}}_{P1}; \ldots) \\ &= \Phi(\hat{H}; M_{Q1}, \boldsymbol{n}(\phi'_{Q1}, \theta'_{Q1}) \cdot \hat{\boldsymbol{S}}_1; \ldots).\end{aligned} \tag{35}$$

In this equation Q is the inverse of the permutation P:

$$Q(Pl) = P(Ql) = l. \tag{36}$$

It should be noted that this argument cannot be reversed in general. Even if Φ satisfies a symmetry relation of the form (35) and we know an operator $\hat{W}$ that performs the transformation (34), we can only conclude from (29) that the LGW Hamiltonians for the Hamilton operators $\hat{H}$ and $\hat{W}^{+}\hat{H}\hat{W}$ coincide. From this a coincidence of the two Hamilton operators can only be deduced if there exists a one-to-one correspondence between Φ and $\hat{H}$ (see the appendix).

The symmetry transformations of the Hamiltonian form a group whose irreducible (co)representations determine the (non-accidental) degeneracies of the eigenvalues. These degeneracies are of essential importance for the form of the partition function and hence for the thermodynamics of the system. Usually certain symmetry properties of the Hamiltonian $\hat{H}$ are obvious from its definition (1) and they admit in most cases a simple geometrical interpretation. In order to transfer all these symmetries to the LGW Hamiltonian Φ it is essential to choose the set of projection operators, i.e. the domain of Φ, in such a way that relation (34) is satisfied for all the known symmetry operations $\hat{W}$.

The symmetry transformations considered in the following are composed of three operations which we now study in more detail.

Rotation of spins. Let $\hat{W}$ be the rotation operator (7) where the sum in (8) extends over all spins in the system. Geometrically this corresponds to a transformation where the vectors attached to each site are rotated about parallel axes by the same angle. Because of the commutation relations of the spin operators

$$\hat{R}(\phi, \theta, \psi)\boldsymbol{n}(\phi_l, \theta_l) \cdot \hat{\boldsymbol{S}}_l \hat{R}(\phi, \theta, \psi)^{-1} = \boldsymbol{n}(\phi'_l, \theta'_l) \cdot \hat{\boldsymbol{S}}_l \tag{37}$$

where

$$\boldsymbol{n}(\phi'_l, \theta'_l) = \mathscr{D}(\phi, \theta, \psi)\boldsymbol{n}(\phi_l, \theta_l) \tag{38}$$

$$\mathscr{D}(\phi, \theta, \psi) = \mathscr{D}_z(\phi)\mathscr{D}_y(\theta)\mathscr{D}_z(\psi) \tag{39}$$

$$\mathscr{D}_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathscr{D}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{40}$$

Note that the matrices (39) and (40) form a real three-dimensional representation of the rotation group.

Using again the more concise notation of the preceding paragraph, we therefore obtain the following implication:

$$[\hat{H}, \hat{R}(\phi, \theta, \psi)] = 0 \Rightarrow \Phi(M_1, \phi_1, \theta_1; \ldots) = \Phi(M_1, \phi'_1, \theta'_1; \ldots). \tag{41}$$

Here the relation between the angles ϕ_l, θ_l and ϕ'_l, θ'_l is given by (4), and (38)-(40). These relations are easily generalized if the Hamiltonian is invariant under individual rotations of the spins about certain axes, as is the case for all Ising models.

Permutations of spins. Originally the sites where the spins are localized have been labelled by an index $i \in \{1, \ldots, N\}$. We assume for simplicity that all the spins are identical, i.e. the operators $\hat{S}_i^z$ all have the same (non-degenerate) eigenvalues σ. A natural basis of the Hilbert space is then given by the common eigenstates of these operators. For each permutation $P: i \to Pi$ there exists a unitary operator $\hat{U}(P)$ defined by

$$\hat{U}(P) u_{\sigma_1, \ldots, \sigma_N} = u_{\sigma_{Q1}, \ldots, \sigma_{QN}} \tag{42}$$

where again $Q = P^{-1}$. Equation (42) implies

$$\hat{U}(P) \hat{S}_i^\xi \hat{U}(P)^{-1} = \hat{S}_{Pi}^\xi. \tag{43}$$

At the start of this section it was assumed that the system can be divided into identical subsystems. This implicitly means that the index i can be replaced by a pair of indices l, n with

$$l \in \{1, \ldots, N_1\} \qquad n \in \{1, \ldots, N_2\} \qquad N_1 N_2 = N. \tag{44}$$

A permutation $P: l, n \to l', n'$ transforms subsystems into subsystems if l' depends only on l and P but not on n ($l' = Pl$). For these permutations

$$\hat{U}(P) \hat{S}_l^\xi \hat{U}(P)^{-1} = \hat{S}_{Pl}^\xi \tag{45}$$

and

$$[\hat{H}, \hat{U}(P)] = 0 \Rightarrow \Phi(M_1, \phi_1, \theta_1; \ldots) = \Phi(M_{Q1}, \phi_{Q1}, \theta_{Q1}; \ldots). \tag{46}$$

Time reversal. This is the most interesting transformation because it is the consequences of this symmetry that gave rise to divergent opinions and contradictory results in the literature. Consider the time reversal operator $\hat{\Theta}$ introduced by Wigner (see, e.g., [22]). This antiunitary operator reverses all spins

$$\hat{\Theta} \hat{S}_i^\xi \hat{\Theta}^{-1} = -\hat{S}_i^\xi. \tag{47}$$

As a consequence

$$\hat{\Theta} \boldsymbol{n}(\phi_l, \theta_l) \cdot \hat{\boldsymbol{S}}_l \hat{\Theta}^{-1} = -\boldsymbol{n}(\phi_l, \theta_l) \cdot \hat{\boldsymbol{S}}_l = \boldsymbol{n}(\bar{\phi}_l, \bar{\theta}_l) \cdot \hat{\boldsymbol{S}}_l \tag{48}$$

where

$$\bar{\phi} = \phi + \pi \qquad \bar{\theta} = \pi - \theta. \tag{49}$$

As the exchange integrals $J_{i,j}^{\xi,\zeta}$ are real numbers, $\hat{\Theta}$ is a symmetry operation of all Hamiltonians of the form (1) and the implication for the LGW Hamiltonian Φ is

$$[\hat{H}, \hat{\Theta}] = 0 \Rightarrow \Phi(M_1, \phi_1, \theta_1; \ldots) = \Phi(M_1, \bar{\phi}_1, \bar{\theta}_1; \ldots). \tag{50}$$

The symmetry properties of Φ for a Hamiltonian that is invariant under a combination of the three operations considered above may be deduced from (41), (46) and (50).

4. Representations of the symmetry group

The symmetry group of the Hamiltonian is defined as the group of all unitary/antiunitary operators $\hat{W}$ that commute with $\hat{H}$. In principle this is an extremely large group but, as pointed out previously, only a rather small subgroup of it is known from the beginning. If we want to discuss the symmetry properties of the LGW Hamiltonian even this group $\mathscr{G}_0$ has to be restricted in general to a subgroup $\mathscr{G}$ because the operators $\hat{W}$ have to satisfy relations of the form (34) in addition to (33). Each transformation $\hat{W} \in \mathscr{G}$ yields a relation of the form

$$\Phi'(\boldsymbol{M}) = \Phi'(\mathscr{D}(\hat{W})\boldsymbol{M}) \tag{51}$$

here $\boldsymbol{M} = (M_1^x, M_1^y, M_1^z, M_2^x, \ldots)$ is a vector with $3N_1$ components and $\mathscr{D}(\hat{W})$ is a real orthogonal matrix of dimension $3N_1$ whose form is evident from (41), (46) and (50):

$$\mathscr{D}(\hat{R}(\phi, \theta, \psi)) = \mathscr{E}(N_1) \otimes \mathscr{D}(\phi, \theta, \psi) \tag{52}$$

$$\mathscr{D}(\hat{U}(P)) = \mathscr{P} \otimes \mathscr{E}(3) \qquad \mathscr{P}_{l,l'} = \delta_{Ql,l'} \tag{53}$$

$$\mathscr{D}(\hat{\Theta}) = -\mathscr{E}(3N_1). \tag{54}$$

In these equations $\mathscr{E}(d)$ is the unit matrix of dimension d and

$$(\mathscr{A} \otimes \mathscr{B})_{pr,qs} = \mathscr{A}_{p,q}\mathscr{B}_{r,s}. \tag{55}$$

It follows from the form of the matrices (52)-(54) that

$$\hat{W}_3 = \hat{W}_2 \hat{W}_1 \Rightarrow \mathscr{D}(\hat{W}_3) = \mathscr{D}(\hat{W}_2)\mathscr{D}(\hat{W}_1). \tag{56}$$

This means that the matrices $\mathscr{D}(\hat{W})$ form a real orthogonal representation of the group $\mathscr{G}$. This representation is in general not a faithful one because all transformations $\hat{W}$ that commute with the joint projection operators $\hat{P}(\boldsymbol{M}) = \hat{P}(M_1, \phi_1, \theta_1; \ldots)$ are represented by the unit matrix $\mathscr{E}(3N_1)$. If the parameters M which label the projection operators are embedded into a Euclidean space of dimension $3N_1$ the matrices $\mathscr{D}$ may be considered as linear transformations of this real vector space. This construction shows how a group $\mathscr{G}$ of symmetry operators in the Hilbert space of the quantum mechanical problem is related to a group $\mathscr{G}_1$ that consists of linear operators in a real parameter space and is a homomorphic image of $\mathscr{G}$.

It is possible to extend the definition of the LGW Hamiltonian Φ by allowing the argument to vary over the whole real vector space (or a compact subset). In addition, we may also consider other functions defined on the same domain; they occur when the LGW Hamiltonian is written as a sum of several terms (see, e.g., the appendix) or if the exchange integrals are varied for a given system of spins. The transformations $\mathscr{D}(\hat{W})$ of the common domain of definition can be used to define transformations $\bar{W}$ in the set of considered functions:

$$(\bar{W}\Psi)(\boldsymbol{M}) = \Psi(\mathscr{D}(\hat{W})^{-1}\boldsymbol{M}). \tag{57}$$

This relation resembles the way a rotation operator in Hilbert space is assigned to a rotation in the Euclidean space on which the wavefunctions are defined. However, in deriving further formal analogies between the functions considered here and wavefunctions in a quantum mechanical problem, one has to keep in mind several concepts that are included in the definition of a quantum mechanical Hilbert space $\mathscr{H}_{\mathrm{QM}}$: (i) the elements are *complex-valued* functions or vectors; (ii) $\mathscr{H}_{\mathrm{QM}}$ is a *linear space* over the complex number field; (iii) $\mathscr{H}_{\mathrm{QM}}$ is *invariant* under the considered group of linear/antilinear operators; (iv) these operators are unitary/antiunitary in the sense of the scalar product defined in $\mathscr{H}_{\mathrm{QM}}$. It is exactly these properties that allow one to simplify the eigenvalue problem of the Hamilton operator by using the results of (ordinary) representation theory. If we want to exploit this (or a modified) theory also in the quasiclassical picture used here we first have to make more assumptions on the functions that are taken into account.

First we have to decide whether these functions should be real- or complex-valued. All LGW Hamiltonians, both exact and approximate ones, are obviously real functions but there do not exist any principal reasons to exclude complex-valued auxiliary functions. If such functions are included it is natural to embed them into a complex linear space $\mathscr{C}_{\mathrm{QCL}}$ (QCL = quasiclassical). In this space the operator of complex conjugation is defined through

$$(\bar{K}\Psi)(\boldsymbol{M})=\Psi(\boldsymbol{M})^{*}. \tag{58}$$

This antilinear operator must not be confused with the linear operator $\bar{\Theta}$

$$(\bar{\Theta}\Psi)(\boldsymbol{M})=\Psi(-\boldsymbol{M}) \tag{59}$$

which reflects the effect of time reversal in the quasiclassical description of the system. As the equations expressing the invariance properties of the LGW Hamiltonian are all of the form

$$(\bar{W}\Phi)(\boldsymbol{M})=\Phi(\boldsymbol{M}) \tag{60}$$

it is also natural to choose $\mathscr{C}_{\mathrm{QCL}}$ in such a way that this space is invariant under all transformations $\bar{W}$. There is no need to introduce a scalar product if $\mathscr{C}_{\mathrm{QCL}}$ is of finite dimension and the group $\mathscr{G}_1$ is compact; these two conditions suffice to allow for the use of all the familiar results of representation theory. The group represented in $\mathscr{C}_{\mathrm{QCL}}$ is the symmetry group of the LGW Hamiltonian

$$\mathscr{G}_2\times \mathrm{K}=\mathscr{G}_2'\times \boldsymbol{\Theta}\times \mathrm{K}. \tag{61}$$

The group $\mathscr{G}_2$ is a homomorphic image of $\mathscr{G}_1$, the homomorphism depending on the functions included in $\mathscr{C}_{\mathrm{QCL}}$, and $\boldsymbol{\Theta}$ and K are the groups generated by $\bar{\Theta}$ and $\bar{K}$, respectively. The group $\mathscr{G}_2\times \mathrm{K}$ is a 'grey' antiunitary group, so that the corresponding theory of corepresentations has to be used.

It is often convenient to include in $\mathscr{C}_{\mathrm{QCL}}$ the linear functions

$$\Lambda_l^{\xi}(\boldsymbol{M})=M_l^{\xi}. \tag{62}$$

These functions form a basis of the ring of polynomial functions which are of interest for approximations of the LGW Hamiltonian. Linear functions are also needed if an interaction with an external magnetic field is added to the Hamilton operator (1). Because of (57), the functions (62) transform according to the representation $\mathscr{D}(\hat{W})$ under the action of the linear operators $\bar{W}$, so that $\mathscr{G}_2\cong\mathscr{G}_1$ in this case. There are two more interesting consequences. (i) The linear functions (62) and all their linear combinations transform like axial vectors under the (linear) operation of time reversal, i.e. $\bar{\Theta}\Lambda=-\Lambda$. Therefore if the LGW Hamiltonian is approximated by a polynomial in linear functions, no invariants of odd order can appear provided that the Hamilton operator commutes with Wigner's time reversal operator. (ii) The complex space spanned by the $3N_1$ functions (62) is invariant under the complex conjugation $\bar{K}$ and therefore a carrier space of a corepresentation of the symmetry group (61). If this corepresentation is decomposed into irreducible constituents (coirreps) then those of type II will occur with even multiplicity and those of type III in conjugated pairs. (We note in passing that an equivalent result is obtained if one considers only real functions from the outset and uses the corresponding representation theory [27]).

We close this section by pointing out that our conclusions on the admitted coirreps are equivalent to Kovalev's [5] use of 'odd physically irreducible representations' and to Toledano and Toledano's [6] use of 'odd physically irreducible corepresentations' (the latter terminology being to a certain extent misleading). They are, however, distinct from Cracknell's [7] use of corepresentations because he excludes the linear transformation $\bar{\Theta}$ from consideration and thus arrives at the incorrect result that in magnetic phase transitions there could exist odd invariants in the Landau expansion.

5. Symmetry groups of a magnetic crystal

In crystallography a crystal is represented by a structure, i.e. union of identical Bravais lattices. A model of a magnetic crystal is obtained by assigning a spin to each site where spins on crystallographically equivalent sites are assumed to have the same magnitude. This is an infinite system since a Bravais lattice consists of infinitely many points. A finite system is obtained by imposing 'periodic boundary conditions'. That is, one selects a subgroup $\mathscr{T}_{\mathrm{PB}}$ of the translation group $\mathscr{T}$ of the lattice which is generated by three large translations. Identifying all points that are connected by translations of $\mathscr{T}_{\mathrm{PB}}$, one ends up with a finite number of points, say N, that remain distinguishable. As the elements of $\mathscr{T}_{\mathrm{PB}}$ have no visible effect on the finite system, the non-trivial crystallographic transformations are no longer given by $\mathscr{S}$, the space group of the structure, but by its homomorphic image $\mathscr{S}_{\langle N\rangle} = \mathscr{S}/\mathscr{T}_{\mathrm{PB}}$. If the vector $\boldsymbol{a}$ is a point of the structure, which is also used as a label of one of the distinguishable points of the finite system, and $(R|\boldsymbol{t})$ an element of the space group $\mathscr{S}$, then the transformation of this point under the corresponding element $\langle R|\boldsymbol{t}\rangle \in \mathscr{S}_{\langle N\rangle}$ is given by the following relation:

$$\langle R|\boldsymbol{t}\rangle \boldsymbol{a} = R\boldsymbol{a} + \boldsymbol{t}(\text{modulo } \mathscr{T}_{\mathrm{PB}}). \tag{63}$$

In this purely geometrical picture crystal symmetry shows up in the way the N points are permuted; the transformation (63) corresponds to the permutation $P: i \to i'$ of section 3 and the transformation $\langle R^{-1}|-R^{-1}\boldsymbol{t}\rangle$ to the inverse permutation Q. In the corresponding model of a magnetic crystal this symmetry is reflected in the relations between the exchange integrals:

$$J^{\xi,\eta}_{\boldsymbol{a},\boldsymbol{b}} = \sum_{\xi',\eta'} R^{\xi,\xi'} R^{\eta,\eta'} J^{\xi',\eta'}_{\langle R^{-1}|-R^{-1}\boldsymbol{t}\rangle \boldsymbol{a}, \langle R^{-1}|-R^{-1}\boldsymbol{t}\rangle \boldsymbol{b}}. \tag{64}$$

Because of these symmetry relations there exists a group $\mathscr{S}_{(N)}$ of operators of the form $\hat{R}\hat{U}(P)$ (cf section 3) which is a symmetry group of the Hamiltonian (1) and, being isomorphic to the group $\mathscr{S}_{\langle N\rangle}$, is a homomorphic image of a space group $\mathscr{S}$. The Hamilton operator (1) is also invariant under the time reversal operator $\hat{\Theta}$ and may admit even more symmetry transformations such as collective or individual continuous rotations of spins, depending on the details of the interaction (Heisenberg, Ising, etc); in any case $S_{(N)} \times \boldsymbol{\Theta} \subseteq \mathscr{G}$.

To define the subsystems that are used in the definition of the LGW Hamiltonian we choose a subgroup $\mathscr{T}_{\langle N_2\rangle}$ of $\mathscr{T}_{\langle N\rangle} \cong \mathscr{T}/\mathscr{T}_{\mathrm{PB}}$. Next we select a vector $\boldsymbol{a}_1$ and define the set Σ_1 in the following way:

$$\boldsymbol{a} \in \Sigma_1 \Leftrightarrow \boldsymbol{a} = \boldsymbol{a}_1 + \boldsymbol{t} \text{ for some } \langle E|\boldsymbol{t}\rangle \in \mathscr{T}_{\langle N_2\rangle}. \tag{65}$$

The spins attached to the sites belonging to Σ_1 form the subsystem $l=1$. In a similar way the other $N_1 = N/N_2$ subsystems are introduced. For each set Σ_l there exists a stabilizer in $S_{\langle N \rangle}$ consisting of all 'visible' space group transformations which leave this set invariant. Each stabilizer obviously contains the group $\mathcal{T}_{\langle N_2 \rangle}$, and the intersection of the N_1 stabilizers reduces to this group if N_1 is sufficiently large. The space group transformations which map each subset Σ_l onto another subset $\Sigma_{l'}$ therefore form a group $\mathcal{S}_{\langle N_1 \rangle} \cong \mathcal{S}_{\langle N \rangle}/\mathcal{T}_{\langle N_2 \rangle}$ and the isomorphic group $\mathcal{S}_{\langle N_1 \rangle}$ of unitary operators transforms subsystems into subsystems. Those elements of $\mathcal{G}$, the symmetry group of the Hamilton operator, which satisfy this condition determine the invariance group $\mathcal{G}_1$ of the LGW Hamiltonian Φ (cf section 3). If we start with a Hamiltonian of the form (1) then the present construction shows that $\mathcal{G}_1$ contains at least a group isomorphic to $\mathcal{S}_{\langle N_1 \rangle} \times \Theta$, the first of these two groups reflecting the crystallographic symmetries of the underlying structure. The whole group is a grey magnetic group because of the presence of the second factor. Even if the interaction gives rise to transitions between ordered phases this does not change the symmetry of the LGW Hamiltonian, nor that of Landau's free energy. If the group of the higher-symmetry ordered phase is a black and white group it is a proper subgroup of $\mathcal{G}_1$. A physically interesting situation where $\mathcal{G}_1$ itself is a black and white magnetic group is found only in case that the microscopic Hamiltonian contains contributions from (effective) external magnetic fields.

6. Conclusion

The present work was motivated by the contradictions in literature that are related to the transformation properties of the order parameters and the thermodynamic potential in the case of magnetic phase transitions. In order to clarify the concepts used in a theoretical description of these phenomena, we discussed in this paper the transformation properties of the Landau-Ginzburg-Wilson (LGW) Hamiltonian Φ. This function provides a quasiclassical description of a spin system which is more detailed than the description by means of an equilibrium thermodynamic potential; but compared to the microscopic quantum mechanical system from which Φ is obtained some details of the model are, in general, no longer fully transparent. The importance of Φ lies in the fact that (i) this function is uniquely determined by the Hamilton operator $\hat{H}$ and the choice of the variables (expectation values of magnetic moments); and (ii) a free energy of the Landau type may be obtained by approximating Φ in the neighbourhood of a point which characterizes a magnetic phase. While the second aspect will be discussed in more detail elsewhere [24], the definition of the LGW Hamiltonian and the resulting symmetry properties are considered in this paper. Taking the connection with Landau's free energy for granted, the transformation properties of Φ and other functions defined on the same order parameters are not only interesting in themselves but also of relevance for the Landau theory of magnetic phase transitions.

In our discussion we started from the quantum mechanical Hilbert space and a set of projection operators whose labels fixed the argument of the LGW Hamiltonian. The symmetry transformations of the Hamilton operator which are 'compatible' with the projection operators (for details see section 3) form a group $\mathcal{G}$ which includes the antiunitary operator of time inversion if no external magnetic field is present. These symmetry operators determine the invariance properties of Φ and the transformation properties of other functions defined on the same domain. This is a consequence of the fact that in the space of these functions a linear operator is related to each operator of the group $\mathscr{G}$; this results in a group $\mathscr{G}_1$ which is a homomorphic image of $\mathscr{G}$. It should be noted that in this construction the antilinear quantum mechanical operator of time inversion is mapped onto a linear operator whose action consists in reversing expectation values of all magnetic moments. The LGW Hamiltonian is invariant under $\mathscr{G}_1$, no matter which type of magnetic phase transition is considered in the following. The group $\mathscr{G}_1$ is a grey magnetic group in the absence of external magnetic fields, and a black and white one if such fields are present. Other real-valued functions, that are considered beside the LGW Hamiltonian, transform according to real (orthogonal) representations and the smallest representations of this kind are equivalent to the complex representations called 'physically irreducible' in the literature.

It is possible to also consider complex-valued functions of the order parameters and to introduce the antilinear operator of complex conjugation as additional symmetry operation of Φ. This results in a 'grey' antiunitary group of the form $\mathscr{G}_1 \times \mathrm{K}$ and the corresponding theory of corepresentations has to be used in this case. It is intended to discuss these two formally different but completely equivalent group theoretical approaches to magnetic phase transitions (representations over the field of real numbers—corepresentations of 'grey' groups) in the next paper of this series.

Acknowledgments

This work is part of the scientific and technical cooperation between Austria and Bulgaria (Project 1.22 of the Agreement 1988/89). Financial support for a research visit to Vienna is gratefully acknowledged. One of us (JNK) thanks Professor J L Birman for valuable discussions on these problems during his visit at the CCUNY. We are also very grateful to Professor D Hatch for useful comments and to N N Kortchev for drawing our attention to coherent spin states.

Appendix

In this appendix we discuss the relation between the Hamiltonian $\hat{H}$ and the LGW Hamiltonian Φ in more detail. We begin by investigating under which conditions the Hamilton operator is uniquely determined by the function Φ. It is sufficient to consider the functions (10) and (19), respectively, because all arguments are easily generalized for a system that is divided into several subsystems.

If the functions (10) coincide over the whole range of β for two Hamilton operators $\hat{H}_1$ and $\hat{H}_2$, $\hat{D}$ is the operator $\hat{H}_1 - \hat{H}_2$, and the function Δ is defined by

$$\Delta(M) = \mathrm{Tr}\,\hat{D}\hat{P}(M) \tag{66}$$

then this function vanishes identically. The point is whether or not $\Delta = 0$ implies $\hat{D} = \hat{0}$. Now, if $\Delta = 0$ for some operator $\hat{D}$ this relation remains true if we change the matrix elements that relate different values of M. Therefore the function (10) contains less information than the Hamiltonian if $\hat{H}$ is not of Ising type. Even then $\Phi(M)$ is an equivalent of $\hat{H}$ only in case that none of the eigenvalues M is degenerate:

$$\mathrm{Tr}\,\hat{P}(M) = 1 \text{ for all } M. \tag{67}$$

If the function (19) is considered instead of (10) then

$$\Delta(M, \phi, \theta) = \mathrm{Tr}\,\hat{D}\hat{P}(M, \phi, \theta) \tag{68}$$

and one has to find out when $\Delta = 0$ implies $\hat{D} = \hat{0}$. Here (67) is again found to be a necessary condition; this follows from the fact that if two eigenstates u_M and u'_M of $\hat{S}^z$ are orthogonal so are all the states $\hat{R}(\phi, \theta, 0)u_M$ and $\hat{R}(\phi', \theta', 0)u'_M$. However, (67) is also a sufficient condition for the LGW Hamiltonian (19) to contain exactly the same information as the Hamilton operator (1). To see this, note that (67) implies that the Hilbert space $\mathcal{H}$ is the carrier space of an irreducible representation D^S of SU(2). It is well known that in this case an operator $\hat{D}$ is already fixed by the values of the corresponding function Δ on that part of its domain where $M = S$ (these values of Δ are the expectation values of $\hat{D}$ for coherent spin states, see [29] and the references quoted therein).

Next let us consider the form of the function $\Phi(M_1, \phi_1, \theta_1, \ldots)$ assuming that all the subsystems are irreducible and $\mu_B g_i = 1$ for all magnetic moments. Since the Hilbert space $\mathcal{H}$ is of finite dimension

$$\exp(-\beta\hat{H}) = d_0(\beta)\hat{1} + \sum_{k=1}^{K} d_k(\beta)\hat{H}^k \tag{69}$$

where the coefficients $d_k(\beta)$ are real and $K \leqslant \dim\mathcal{H}$ (the lower K is, the more degenerate the eigenvalues of $\hat{H}$ are). As the exchange integrals are symmetrical functions of the site indices,

$$J_{i,j}^{\xi,\eta} = J_{i,j}^{\eta,\xi} = \sum_{p=1}^{3} a_{i,j}^{p}(\boldsymbol{n}_{i,j}^{p})^{\xi}(\boldsymbol{n}_{i,j}^{p})^{\eta} \tag{70}$$

where the real numbers $a_{i,j}^p$ and the unit vectors $\boldsymbol{n}_{i,j}^p$ specify the interaction between the two magnetic moments. Therefore the operator $\hat{H}^k$ is a sum of terms each of which consists of $2k$ factors of the form $\boldsymbol{n}\cdot\hat{\boldsymbol{S}}$; here $\boldsymbol{n} = \boldsymbol{n}_{i,j}^p$, $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_i$ or $\hat{\boldsymbol{S}}_j$, and repetitions are allowed. To calculate the contribution of this term to the LGW Hamiltonian one has to take into account that

$$\hat{R}(\phi, \theta, 0)^{\dagger}\boldsymbol{n}\cdot\hat{\boldsymbol{S}}\hat{R}(\phi, \theta, 0) = \mathcal{D}(\phi, \theta, 0)^{-1}\boldsymbol{n}\cdot\hat{\boldsymbol{S}}. \tag{71}$$

Moreover,

$$\langle u_{SM}, (\boldsymbol{n}\cdot\hat{\boldsymbol{S}})^{\nu}u_{SM}\rangle = \sum_n \Pi_{\nu-2n}^{S,\nu}(M)P_{\nu-2n}(n_z) \tag{72}$$

where P_l is the usual Legendre polynomial. The function $\Pi_l^{S,\nu}$ is also a polynomial of degree l and parity $(-1)^l$:

$$\Pi_1^{S,1} = M \qquad \Pi_2^{S,2} = \tfrac{1}{3}[3M^2 - S(S+1)] \qquad \Pi_0^{S,2} = \tfrac{1}{3}S(S+1) \qquad \text{etc.} \tag{73}$$

If the parameters M_i^{ξ}, defined in section 2 through (21), are used as variables, one obtains (for $M_i > 0$)

$$\exp(-\beta\Phi'(M_1; \ldots)) = (2\pi)^{-N}\left(1 - \beta\sum_{i,\xi,j,\eta} J_{i,j}^{\xi,\eta} M_i^{\xi}M_j^{\eta} + \mathrm{O}(\beta^2)\right). \tag{74}$$

Equation (74) shows explicitly the one-to-one correspondence between the Hamilton operator and the LGW Hamiltonian provided that the variables are suitably chosen and the system is composed of irreducible spins (in the derivation of (74) this condition is used in (72)).

All these properties show up even in the simplest example: two interacting spins of magnitude $\frac{1}{2}$. For a Heisenberg interaction

$$\hat{H} = -4J\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \qquad e^{-\beta\Phi} = \frac{e^{-\beta J}}{8\pi^2}[(e^{2\beta J} + \cosh 2\beta J) + \sinh 2\beta J(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2)] \tag{75}$$

while for the corresponding Ising model

$$\hat{H} = -4JS_1^z S_2^z \qquad e^{-\beta\Phi} = \frac{1}{4\pi^2}[\cosh \beta J + \sinh \beta J(n_1^z n_2^z)]. \tag{76}$$

As the spins are irreducible all the symmetry properties of the Hamilton operators are reflected in the form of the LGW Hamiltonians. Moreover, in both examples the minimum of this function characterizes the ground states of the system. For the Heisenberg interaction this is located at $\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 = 1$; this corresponds to the states $\hat{R}(\phi, \theta, 0)u_{++}$ which span the subspace with $S = 1$. In the Ising model the minimum is obtained for $n_1^z n_2^z = 1$, i.e. for the states u_{++} and u_{--}.

References

[1] Landau L D and Lifshitz E M 1980 *Statistical Physics* 3rd edn (Oxford: Pergamon) part 1
[2] Gufan Yu M 1982 *Structural Phase Transitions* (Moscow: Nauka) (in Russian)
[3] Izyumov Yu A and Siromyatnikov V N 1984 *Phase Transitions and Crystal Symmetry* (Moscow: Nauka) (in Russian)
[4] Toledano J-C and Toledano P 1987 *The Landau Theory of Phase Transitions* (Singapore: World Scientific)
[5] Lyubarskii G Ya 1960 *The Application of Group Theory in Physics* (Oxford: Pergamon)
[6] Izyumov Yu A, Naish V E and Ozerov R P 1981 *Neutronography of Magnetics* (Moscow: Atomizdat) (in Russian)
[7] Dzyaloshinski I E 1957 *Sov. Phys.-JETP* **5** 1259 (*Zh. Eksp. Teor. Fiz.* **32** 1547)
[8] Kovalev O V 1963 *Sov. Phys.-Solid State* **5** 2309 (*Fiz. Tverd. Tela* **5** 1356)
[9] Kovalev O V 1965 *Sov. Phys.-Crystallography* **9** 665 (*Kristallografia* **9** 783)
[10] Sirotin Yu I 1963 *Sov. Phys.-Crystallography* **8** 195 (*Kristallografia* **8** 259)
[11] Bertaut E F 1968 *Acta Cryst.* A **28** 217
[12] Birman J L and Izyumov Yu A 1980 *Phys. Rev.* B **21** 1089
[13] Dimmock J O 1963 *Phys. Rev.* **130** 1337
[14] Cracknell A P 1971 *J. Phys. C: Solid State Phys.* **4** 2488
[15] Cracknell A P 1975 *Magnetism in Crystalline Materials* (Oxford: Pergamon)
[16] Cracknell A P, Lorenz J and Przistava J A 1976 *J. Phys. C: Solid State Phys.* **9** 1731
[17] Rudra P and Sikdar M K 1979 *J. Math. Phys.* **20** 1579
[18] Toledano P, Clin M and Hedoux M 1981 *Ferroelectrics* **35** 239
[19] Clin M, Hedoux M and Toledano P 1984 *Ferroelectrics* **54** 265
[20] Kocinski J and Osuch K 1987 *Phase Transitions* **10** 151
[21] Soliom J 1966 *Physica* **32** 1243
[22] Wigner E P 1959 *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (New York: Academic)
[23] Bradley C J and Cracknell A P 1972 *The Mathematical Theory of the Symmetry in Solids* (Oxford: Clarendon)
[24] Peev M K *et al* 1990 *Preprint*
[25] Zvesdin A K, Matveev B M, Muhin A A and Popov A I 1985 *Rare Earth Ions in Magnetically Ordered Crystals* (Moscow: Nauka)
[26] Torruella A J 1985 *J. Math. Phys.* **16** 1637
[27] Kasperkovitz P and Kahl G 1981 *J. Math. Phys.* **22** 2404
[28] Birman J L 1974 *Theory of Crystal Space Groups and Infra-Red and Raman Lattice Processes of Insulating Crystals* (Berlin: Springer)
[29] Klauder J R and Skagerstam B S 1985 *Coherent States* (Singapore: World Scientific)