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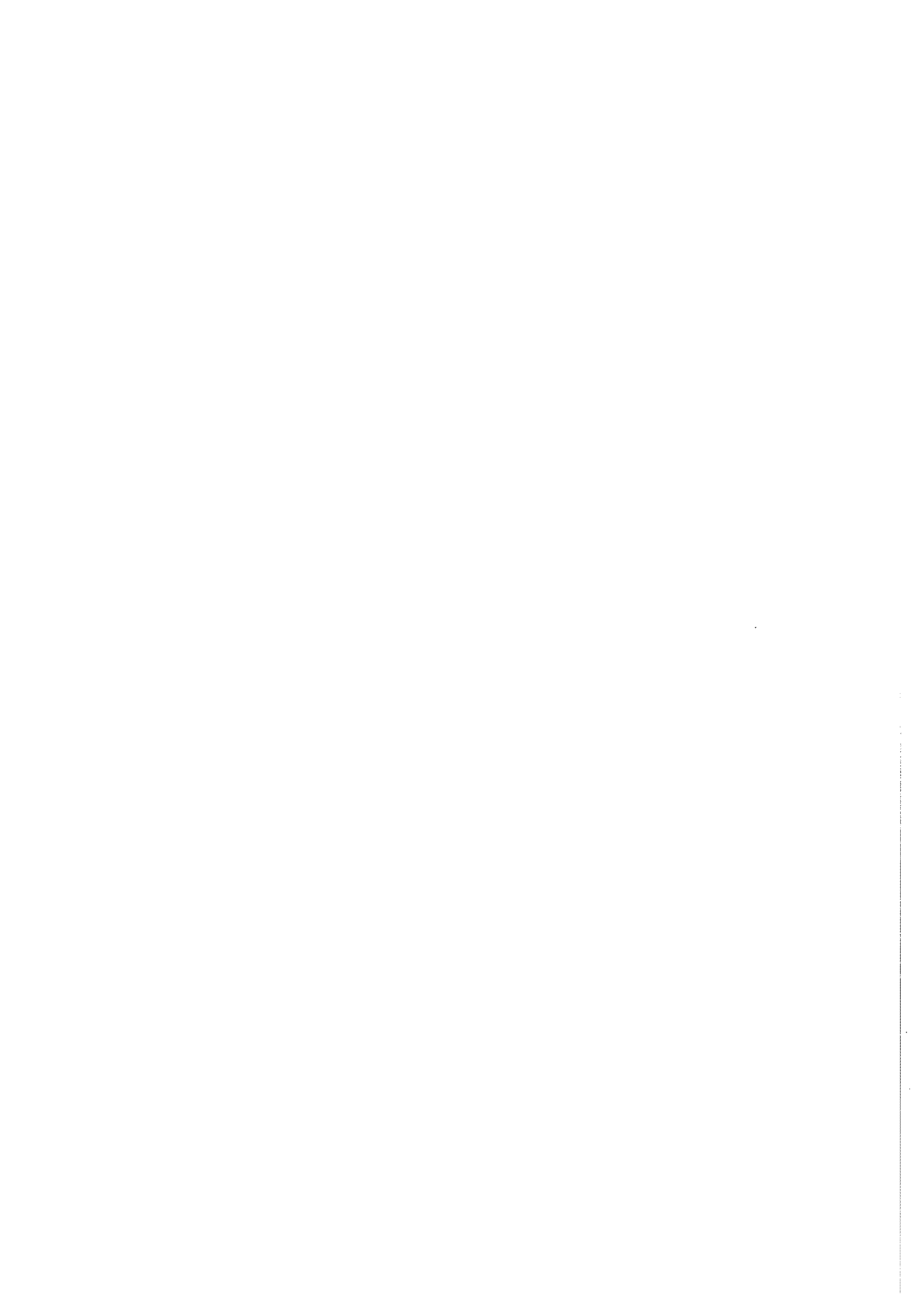
A Two-State Atom in a Solid: thermodynamic properties and the magnetic neutron scattering cross-section

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Abstract

A model of an atom in a magnetic solid is used to investigate theoretically features expected in the cross-section for the magnetic scattering of neutrons by the atom. The atom is assumed to have two nondegenerate states, which are envisaged to be two states in a crystal-field energy level scheme that are very well separated in energy from all higher states, and subjected to a Weiss molecular field. It is shown that the thermodynamic quantities that determine the weights attached to elastic and inelastic scattering events obey a sum rule. It can be exploited to give the temperature dependence of the weights given, say, the separation in energy of the crystal field levels and the critical temperature below which there is a spontaneous magnetic moment. A small value of the ratio of the energy separation and critical temperature leads to properties that are significantly different from those of an ion in a Weiss molecular field and not subjected to a crystal-field potential.



1. Introduction

The magnetic properties of some materials are tolerably described, in the first instance, in terms of the individual constituent magnetic atoms, perturbed by their local environments, instead of a more complicated scenario that involves all the unpaired electrons from all the atoms. Empirical evidence shows that, many materials which contain atoms from the rare earth series in the Periodic Table belong to this class of magnetic materials, and the finding can be understood on the grounds that the unpaired electrons occupy an f-shell which has a relatively small radius, i.e. f-electrons are highly localized and do not meander throughout the material. In the localized model of a magnetic material the environment of an atom is treated as a perturbation on the f-electron states. The components of the perturbation have a range of strengths, and they are treated accordingly. For rare earth materials it is often adequate to neglect all perturbations other than the electrostatic field created by the ligand ions (crystal-field potential) and the magnetic field produced by neighbouring magnetic ions [1]. The magnetic field is usually represented by a Weiss molecular field which is proportional to the atomic magnetic moment.

Two recent reports of the findings from interpretations of experimental investigations of a Tb compound [2] and Pr compounds [3] conclude that the magnetic properties of the rare earth ions, to a large extent, can be described in terms of just two energy states. These are two states from a plethora of crystal-field states, and they differ in energy by a very small amount, Δ , when compared to the energy of the next state in the crystal-field energy level scheme. Both teams of investigators used the neutron scattering experimental technique. The main purpose of this paper is to derive the neutron scattering cross-section for a two-state system, and provide an interpretation of its main features. To this end, the temperature dependence of the thermodynamic quantities that determine the weights of elastic and inelastic scattering events are obtained. The method used is different from the standard mean-field method for calculating thermodynamic quantities, and it is akin to the method used to derive the spherical model from the Heisenberg spin Hamiltonian [4].

Our model is derived from an isolated, two-state magnetic system, described by the Hamiltonian H_0 . To this is added a Weiss molecular field energy, V , that is meant to

represent the interaction of the system H_0 with its magnetic environment. As normal, V is proportional to the total angular momentum of the atom, \mathbf{J} . With our method of calculating the thermodynamic properties of $(H_0 + V)$ the strength of the Weiss molecular field is not explicit in the cross-section, and the two parameters in the model are Δ and the temperature, T_c , at which the spontaneous magnetic moment, μ_0 , as a function of increasing temperature, reaches the value zero. The two states of $(H_0 + V)$ are separated by an energy, ε , that varies with the temperature, and its maximum value is achieved at zero temperature. However, at this temperature and for $\Delta \ll T_c$ the weight attached to the inelastic event, in which the system is excited in energy by an amount ε , is very small compared to the weight attached to the inelastic events at a temperature $T = T_c$ at which $\varepsilon = \Delta$.

In the neutron scattering cross-section the weight of the elastic event is μ_0^2 , and the weight of the inelastic events, apart from the detailed-balance factor, is the isothermal susceptibility, χ . We find that the quantity $(\mu_0^2 + T\chi)$ is a constant (T is the temperature in units of Boltzmann's constant) that depends solely on the angular momenta (spin and orbital) of the magnetic atom. For $T \geq T_c$ one has $\mu_0 = 0$ and the susceptibility depends on temperature in the manner of the Curie-Weiss law. Below T_c the value of μ_0 , and hence χ , depends on the energy-separation parameter Δ . The dependence is very pronounced when the separation is small compared to T_c , and it disappears in the opposite extreme.

2. Model

The isolated atom, described by H_0 , has two nondegenerate states $|j\rangle$ with $j = 1, 2$, that are chosen to be purely real. With these states the diagonal matrix elements of the total angular momentum, \mathbf{J} , are zero.

The wave functions and energies of the two states of $(H_0 + V)$ can be written in terms of the corresponding quantities for H_0 . Since V is proportional to \mathbf{J} only its off-diagonal matrix elements are different from zero. The separation of the two energy levels of $(H_0 + V)$ is,

$$\varepsilon = \sqrt{(\Delta^2 + (2\langle 1|V|2\rangle))^2}, \quad (2.1)$$

where Δ is the corresponding quantity for the system described by H_0 .

To calculate the neutron cross-section, which is treated in the next section, we need the matrix elements of \mathbf{J} . Let us label the two states of $(H_0 + V)$ by the letters a and b . We find,

$$\left. \begin{array}{l} E_a \\ E_b \end{array} \right\} = \frac{1}{2} (E_1 + E_2 \pm \varepsilon) \quad (2.2)$$

in which $(E_1 - E_2) = \Delta$. The matrix elements of J_x and J_y are assumed to be zero, i.e. the components of \mathbf{J} perpendicular to the axis of quantization, the z -axis, are quenched by the crystal field; it is argued in §6 that, this assumption does not bear on our main findings. The matrix elements required to calculate the cross-section are found to be,

$$\langle a|J_z|a\rangle = -\langle b|J_z|b\rangle = \langle 1|J_z|2\rangle \{1 - (\Delta/\varepsilon)^2\}^{1/2},$$

and, (2.3)

$$\langle a|J_z|b\rangle = \langle 1|J_z|2\rangle (\Delta/\varepsilon).$$

The matrix element of the angular momentum operators between the two states of H_0 , $\langle 1|J_z|2\rangle$, can be expressed in terms of other parameters in the model, as we will demonstrate.

Here, it remains to specify V . A Weiss molecular-field description of the magnetic environment is provided by the choice,

$$V = \lambda \cdot \mathbf{J}, \quad (2.4)$$

where λ is a coupling parameter. In our treatment of the thermodynamic properties of the system, given in §4, the coupling parameter makes no explicit appearance in the thermodynamic quantities that enter the neutron cross-section.

3. Neutron Scattering Cross-Section

The magnetic neutron cross-section is derived from the so-called dipole approximation to the magnetic-scattering amplitude. In this approximation the cross-section, in units of 0.29 barns, is,

$$\frac{d^2\sigma}{d\Omega dE'} = \left(\frac{k'}{k}\right) \left\{\frac{1}{2} g F(\mathbf{K})\right\}^2 \sin^2 \theta \sum_{\mu, \mu'} p_{\mu} \langle \mu | J_z | \mu' \rangle \langle \mu' | J_z | \mu \rangle \delta(\omega + E_{\mu} - E_{\mu'}). \quad (3.1)$$

Here, $\mathbf{K} = (\mathbf{k} - \mathbf{k}')$ is at an angle θ to the axis of quantization, which we have labelled the z -axis. The vector \mathbf{K} is the change in the wave vector of the neutron created by the scattering event, and ω is the concomitant change in the energy ($\hbar = 1$) of the neutron. The delta function in (3.1) expresses the conservation of energy for a scattering event. The labels μ, μ' refer to the states of $(H_0 + V)$, g is the Landé factor, and $F(\mathbf{K})$ is the atomic form factor. The quantity p_{μ} is the Boltzmann population factor for the state labelled μ , and $\sum p_{\mu} = 1$.

Using the results of the previous section one finds for (3.1) the result,

$$\frac{d^2\sigma}{d\Omega dE'} = \left(\frac{k'}{k}\right) \left\{\frac{1}{2} F(\mathbf{K}) \sin \theta\right\}^2 \left\{\mu_0^2 \delta(\omega) + \frac{1}{2} \omega \chi \{1 + n(\omega)\} [\delta(\omega + \varepsilon) + \delta(\omega - \varepsilon)]\right\}. \quad (3.2)$$

The weights of the elastic and inelastic contributions to the cross-section are thermodynamic quantities. First, the weight of the purely elastic line is proportional to μ_0^2 where μ_0 is the magnetic moment of the atom. The inelastic processes, which contribute when the energy of the neutron changes in the scattering event by $\pm \varepsilon$, contain the standard detailed - balance factor,

$$\omega[1 + n(\omega)] = \omega / \{1 - \exp(-\omega / T)\}, \quad (3.3)$$

where T is the temperature (in units of Boltzmann's constant). The thermodynamic quantity, χ , is the magnetic susceptibility.

For the thermodynamic quantities we find the expressions,

$$\mu_0 = g \langle 1 | J_z | 2 \rangle \{1 - (\Delta / \epsilon)^2\}^{1/2}, \quad (3.4)$$

and,

$$\chi = g^2 \langle 1 | J_z | 2 \rangle^2 (2 / \epsilon) (\Delta / \epsilon)^2 \tanh(\epsilon / 2T). \quad (3.5)$$

A few comments about μ_0 and χ are appropriate at this juncture. The magnetic moment vanishes at the temperature, T_c , at which the energy separation $\epsilon = \Delta$. The temperature dependence of μ_0 is one of the subjects of the next section. It can be shown that, using (3.4) and (5.1), for example,

$$g \langle J_z \rangle = -\mu_0 \tanh(\epsilon / 2T). \quad (3.6)$$

This admits the interpretation that μ_0 is the local magnetic moment, of an isolated ion, and $g \langle J_z \rangle$ is the bulk magnetic moment. The difference between the two moments is created by thermal fluctuations, which vanish at zero temperature. Regarding the susceptibility its presence in the cross-section is required by the general theory of scattering, or equivalently linear response theory [5]; one knows from the theory that the frequency sum-rule in $(1/\omega)$ applied to the inelastic events in the cross-section gives the isothermal susceptibility (apart from a factor 2). Finally, let us note that the structure of the cross-section (3.2) is quite independent of the method used to estimate the thermodynamic quantities, which is taken up in the next sections. Of course, the structure of (3.2) does reflect the properties assumed of our model, and notably the existence of two magnetic states and the absence of processes involving the transverse components of the angular momentum, cf. §6.

4. Thermodynamic Properties

We will determine the thermodynamic properties of the system by calculating the thermal average value of $\mathbf{J}\cdot\mathbf{J}$ and equating this to $J(J+1)$. The outcome of the exercise is an equation from which we can calculate the temperature dependence of μ_0 and χ .

Average values of products of J_α are readily obtained from the partition function by differentiating it the requisite number of times with respect to λ_α . From the second derivative of the partition function we find,

$$g^2 \langle J_z^2 \rangle = (\mu_0^2 + T\chi) = g^2 J(J+1), \quad (4.1)$$

where μ_0 and χ are defined in (3.4) and (3.5) and the final equality arises because for our model system we have $\langle J_x^2 \rangle = \langle J_y^2 \rangle = 0$. Looking at the cross-section (3.2) one sees that (4.1) admits an interpretation as a sum rule on the relative weights of the elastic and inelastic scattering events.

In the paramagnetic phase, obtained at temperatures in excess of T_c , at which μ_0 is zero, (4.1) provides the result,

$$\chi = g^2 J(J+1)/T, \quad T \geq T_c. \quad (4.2)$$

This susceptibility is a factor of three larger than the susceptibility of a free ion, and the difference is a consequence of the action of the crystal-field potential. At zero temperature the susceptibility obtained from (3.4) is,

$$\chi = 2g^2 \langle |J_z|2 \rangle^2 (\Delta^2 / \epsilon^3), \quad T = 0. \quad (4.3)$$

The saturation value of the magnetic moment follows from (4.1), namely,

$$\mu_o = g \sqrt{J(J+1)}, T = 0. \quad (4.4)$$

It is of interest to compare (4.3) with the value of the susceptibility at T_c . To this end it is useful to introduce some reduced variables. Let $x = (\Delta/2T_c)$ and $y = (J(J+1)/\langle 1 | J_z | 2 \rangle^2)$, which are related by,

$$y = (\tanh x) / x \leq 1. \quad (4.5)$$

This relation follows from (4.1) evaluated for $T = T_c$. Writing $\chi = \chi(T)$, the ratio of the susceptibilities $T = 0$ and $T = T_c$ is,

$$\{\chi(0) / \chi(T_c)\} = (1 - y)^{3/2} / (xy). \quad (4.6)$$

In the limit $x \ll 1$,

$$\{\chi(0) / \chi(T_c)\} \rightarrow 0.192 \quad x^2,$$

and this means, for the case in hand, that the weight of the inelastic contribution to the cross-section is relatively weak at a temperature small compared to T_c . For $T = 0$ and $x \rightarrow 0$ one finds that the energy separation is independent of Δ and it achieves the value $\varepsilon = 2T_c\sqrt{3}$.

To calculate thermodynamic quantities in the range of temperatures up to T_c it proves useful to introduce a third reduced variable, $z = (\varepsilon/2T_c)$. The sum rule (4.1) expressed in terms of the reduced variables is,

$$y = 1 + (x/z)^2 \{(\tau/z) \tanh(z/\tau) - 1\}, \quad (4.7)$$

where $\tau = (T/T_c)$. The magnetic moment is obtained from (3.4) using the values of y and $(\Delta/\varepsilon) = (x/z)$, and the corresponding value of the susceptibility follows immediately from (4.1). By way of an illustration, Table 1 contains values of $\mu_o/\{g\sqrt{J(J+1)}\}$, $\chi(T)/\chi(T_c)$ and (Δ/ε) as a function of (T/T_c) for the particular case $x = (\Delta/2T_c) = 0.30$.

Looking at the values in Table 1 of μ_0 it is evident that they are significantly different from those obtained from a standard mean-field method. To quantify this observation we include in the table values of m that satisfy the mean-field equation.

$$m = \tanh(m / \tau) . \quad (4.8)$$

The moment μ_0 vanishes as T approaches T_c with a power-law dependence namely,

$$\mu_0 \propto (1 - \tau)^{1/2}, \tau \rightarrow 1,$$

and m possesses the same temperature dependence. The difference between μ_0 and m is in the amplitude factors, and for μ_0 we find that this strongly depends on the value of $x = (\Delta/2T_c)$, for small values of x . In the latter case,

$$\mu_0^2 \propto \left\{ 1 - (\Delta / \varepsilon)^2 \right\} / y = (5 / x^2)(1 - \tau). \quad (4.9)$$

Hence, a small value of x enhances the magnitude of μ_0 , for a given value of τ . In the opposite extreme, $x \rightarrow \infty$, we find that μ_0 is independent of x . The corresponding values of χ are obtained from (4.1). A small value of x reduces χ , and enhances μ_0 , and we find for $x \ll 1$ and τ close to unity,

$$\chi(T) = \chi(T_c) \{ 1 - 5(1 - \tau) / x^2 \}. \quad (4.10)$$

For large values of x the susceptibility is independent of x , at the same level of approximation in $(1 - \tau)$.

5. Mean-field method

It is to be noted that, in the previous treatment of the thermodynamic properties of our model no use is made of $\langle J_z \rangle$. Instead, thermodynamic properties are obtained from an

equation which is derived from $\langle \mathbf{J} \cdot \mathbf{J} \rangle = J(J+1)$. In this respect, the treatment of the thermodynamic properties is similar to the spherical model approximation for the static correlation functions of a Heisenberg magnet, while basing the thermodynamic properties on an equation for $\langle J_z \rangle$ using $\lambda \propto \langle J_z \rangle$ is the standard mean-field method [6]. Of course, the essential difference in the two methods is the assumption in the mean-field method that λ is proportional to $\langle J_z \rangle$, whereas in our method λ is not specified and it is not explicit in the values we derive for the magnetic moment and the susceptibility. The use of $\lambda \propto \langle J_z \rangle$ is physically motivated, scilicet the Weiss molecular field. For completeness, and to facilitate a comparison of the two methods, we briefly describe the standard mean-field method applied to our model system.

One easily finds,

$$\langle J_\alpha \rangle = - (2 / \varepsilon) \langle 1 | V | 2 \rangle \langle 1 | J_\alpha | 2 \rangle \tanh(\varepsilon / 2T). \quad (5.1)$$

For our model, the right-hand side vanishes for all Cartesian components except $\alpha = z$, and $\langle 1 | V | 2 \rangle = \lambda_z \langle 1 | J_z | 2 \rangle$. The standard mean-field method is obtained by taking λ_z to have the form,

$$\lambda_z = - \lambda_0 \langle J_z \rangle. \quad (5.2)$$

Using this relation in (5.1) yields an equation for the temperature dependence of the gap energy, namely,

$$\varepsilon = 2\lambda_0 \langle 1 | J_z | 2 \rangle^2 \tanh(\varepsilon / 2T). \quad (5.3)$$

This equation requires ε to vanish at a temperature which is larger than T_c . For $T = T_c$ one has $\varepsilon = \Delta$, and using these values in (3.5) and (5.3) we find [6],

$$g^2 = \lambda_0 \chi(T_c), \quad (5.4)$$

which determines the coupling parameter at T_c in terms of $\chi(T_c)$.

Other features of the mean-field method applied to our model are conveniently expressed in terms of the temperature, T_* , at which ε in (5.3) is zero. One finds,

$$T_* = \lambda_0 \langle 1 | J_z | 2 \rangle^2, \quad (5.5)$$

$$\varepsilon_0 = (\varepsilon / 2T_*) = \tanh(\varepsilon_0 T_* / T), \quad (5.6)$$

and (3.6) becomes,

$$\mu_0 = -g \langle J_z \rangle / \varepsilon_0. \quad (5.7)$$

Note that (5.5) implies that λ_0 is a constant which is independent of the temperature. At absolute zero $\varepsilon_0 = 1$. The temperature dependence of μ_0 obtained by the mean-field method is similar to that obtained by our method. In particular, (5.7) approaches zero at the critical temperature with the power-law dependence displayed in (4.9), and the only difference is that the factor 5 in (4.9) is replaced by the factor 3. While the two methods give similar values for μ_0 in the vicinity of T_c it is likely that our method and the mean-field method give significantly different values for the saturation moments, cf. (4.4) and (5.7).

To complete the physical picture on which the mean-field method rests we relate λ_0 to the strength of the exchange parameters in a Heisenberg interaction between spin operators, $\{\mathbf{S}_j\}$, located at sites labelled by the index j . Denoting the exchange parameter for two sites i and j by $I(i,j)$, which has the property $I(j,j) = 0$, the Heisenberg interaction is,

$$-\sum_{i,j} I(i,j) \mathbf{S}_i \cdot \mathbf{S}_j = - (g-1)^2 \sum_{i,j} I(i,j) \mathbf{J}_i \cdot \mathbf{J}_j, \quad (5.8)$$

and the mean-field energy parameter is [6],

$$\lambda_o = 2(g-1)^2 \sum_j I(i,j). \quad (5.9)$$

The results (5.4) and (5.9) relate the susceptibility, measured at T_c , to the strength of the exchange parameters.

6. Discussion

We have calculated the neutron cross-section for a magnetic ion that has two nondegenerate energy levels separated by an energy Δ . The environment of the ion exerts a Weiss molecular field and the potential is taken to be proportional to the total angular momentum, \mathbf{J} . The cross-section for this simple model can be calculated without approximation. The second aspect of our study is the calculation of the thermodynamic quantities in the cross-section, which are the weights attached to the elastic and inelastic scattering events. We have demonstrated that a sum rule for the weights, which is an exact statement, permits the calculation of the thermodynamic quantities in terms of Δ and the critical temperature, say. Moreover, the weights admit a physical interpretation; the weight attached to the elastic event is the square of the magnetic moment, and the corresponding quantity for inelastic events is the isothermal susceptibility.

The model can be viewed as an abstraction from a full crystal-field model, and it will be of value when Δ is small compared to the energy of the second excited state in the crystal-field energy level scheme. A case in point is the rare earth magnet studied by Staub et al. [2]. They estimate that the ratio of the energy of the second level to Δ is approximately 5.10^3 , and $x = (\Delta/2T_c) \sim 0.007$ where T_c is the temperature below which there is a spontaneous magnetic moment. For this set of parameters, we predict a separation in energy of the two states at zero temperature $\varepsilon = 1.64$ meV, which then decreases with increasing temperature, by a factor of 0.004, to its value $\varepsilon = \Delta$ at T_c . The small weight attached to the transition at zero temperature, which we find to be proportional to x^2 , and an instrument resolution larger than Δ contrive in the execution of the neutron-scattering experiment to render the transition unobservable. One of the compounds studied by Blaise et al. [3] might also be realistically described by our

model. For PrFe_2Ge_2 the ratio of the energy of the second level in the crystal-field scheme to Δ is ~ 14 , and $x = 0.37$. The interpretation of the scattering experiment provided by the authors is in accord on several fronts with our findings. For example, the weight attached to the transition with energy ε shows a substantial decrease in moving from the paramagnetic state down to $T = 0.2T_c$, and there is a concomitant increase in ε by a factor of three.

Regarding the magnetic moment one has the exact identity (3.6) that relates the bulk and local moments, from which one deduces $(-g \langle J_z \rangle / \mu_0) \leq 1$ and the equality is achieved at zero temperature. Physically the difference between the two moments can be ascribed to thermal fluctuations (absent in the classical limit). A very similar phenomenon is observed in the study of an isolated quantum harmonic oscillator, of interest in the interpretation of Mössbauer spectra, which has thermodynamic properties, e.g. Debye-Waller factor, that are different from those obtained for an assembly of oscillators. A physical interpretation of the ratio $(-g \langle J_z \rangle / \mu_0)$ can be made in terms of the average energy of $(H_0 + V)$. The latter, measured with respect to the midpoint of the two levels in H_0 which are separated by an energy Δ , is found to be,

$$-(\varepsilon / 2) \tanh (\varepsilon / 2T).$$

Referring back to the identity (3.6) one can therefore interpret the ratio of the magnetic moments as proportional to the variance in the average energy of the two states in $(H_0 + V)$.

Finally, let us consider what happens to our findings when we generalize the model by lifting the restriction that the transverse components of the angular momentum operator are quenched by the crystal field potential. Let the matrix elements $\langle 1 | J_\alpha | 2 \rangle$, with $\alpha = x, y$ or z , be different from zero. The sum rule (4.1) is changed only in so much as $\langle 1 | J_\alpha | 2 \rangle^2$ in μ_0^2 and χ is replaced by,

$$\sum_\alpha \langle 1 | J_\alpha | 2 \rangle^2.$$

Hence, in the discussion of thermodynamic properties that stem from the sum rule the variable y is,

$$y = J(J+1) / \sum_{\alpha} \langle 1 | J_{\alpha} | 2 \rangle^2.$$

Since this is the only change necessitated by the generalization of our model one concludes that the generalization does not change the thermodynamic properties. Next, we consider the change to the neutron scattering cross-section. In (3.1),

$$\sin^2 \theta \langle \mu | J_z | \mu' \rangle \langle \mu' | J_z | \mu \rangle,$$

is replaced by,

$$\sum_{\alpha, \beta} (\delta_{\alpha, \beta} - \hat{K}_{\alpha} \hat{K}_{\beta}) \langle \mu | J_{\alpha} | \mu' \rangle \langle \mu' | J_{\beta} | \mu \rangle,$$

in which \hat{K}_{α} is the α -component of the unit vector $\hat{\mathbf{K}} = \mathbf{K} / |\mathbf{K}|$. On carrying through the calculation of the cross-section the change with respect to (3.2) is that $\sin^2 \theta \langle 1 | J_z | 2 \rangle^2$ is replaced by,

$$\sum_{\alpha, \beta} (\delta_{\alpha, \beta} - \hat{K}_{\alpha} \hat{K}_{\beta}) \langle 1 | J_{\alpha} | 2 \rangle \langle 1 | J_{\beta} | 2 \rangle.$$

Now, the materials investigated are often in the form of powders, and not single crystals. In this case, it is appropriate to average the cross-section over the orientations of \mathbf{K} relative to the crystal axes. If the atomic form factor is independent of the direction of \mathbf{K} the orientational average amounts to no more than averaging the foregoing combination of matrix elements, and the answer is,

$$\frac{2}{3} \sum_{\alpha} \langle 1 | J_{\alpha} | 2 \rangle^2 = \frac{2}{3} J(J+1) / y.$$

We conclude that the thermodynamic properties of the cross-section are completely determined by the sum rule, which is the case with the simpler model we have used as a vehicle for our discussion in the preceding sections.

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Table 1

T/T_c	$\mu_o/g\sqrt{J(J+1)}$	$\chi(T)/\chi(T_c)$	(Δ/ϵ)
0.0	1.0 (1.0)	0.017	0.17
0.4	0.995 (0.986)	0.026	0.20
0.6	0.988 (0.907)	0.040	0.23
0.8	0.968 (0.711)	0.079	0.30
0.9	0.931 (0.525)	0.148	0.40
0.95	0.867 (0.379)	0.261	0.52
0.99	0.606 (0.173)	0.639	0.80

Various quantities are shown as a function of the reduced temperature (T/T_c). Results are for $x = 0.30$ for which $y = 0.97$. The results in brackets, alongside the results for the magnetic moment, are the reduced magnetic moment obtained by the standard mean-field method, equ (4.11).

References

1. Jensen, J. and Mackintosh, A. R. 1991 Rare Earth Magnetism, Structures and Excitations (Oxford: Clarendon Press).
2. Staub, U., Soderholm, L., Skanthakumar, S., and Antonio, M.R. 1995 Phys. Rev. **B52**, 9736.
3. Blaise, A., Fåk, B., Sanchez, J. P., Amoretti, G., Santini, P., Caciuffo, R., Schmitt, D., Malaman, B. and Venturini, G. 1995 J. Phys.: Condens. Matter **7**, 8317.
4. Eastwood, M. P. and Logan, D. E. 1995 Phys. Rev. **B52**, 9455.
5. Lovesey, S. W., 1987 Theory of Neutron Scattering from Condensed Matter, Vol. 2 (Oxford: Clarendon Press).
6. Elliott, R. J. and Gibson, A. F. 1974 An Introduction to Solid State Physics (London: Macmillan).

