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The generalised drone-fermion method and the semi-invariant approach for spin systems

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Abstract. An analysis is carried out in order to establish for spin systems the formal connection between a recent generalisation of the drone-fermion method and semi-invariant techniques (such as employed by Vaks, Larkin and Pikin). A linked cluster expansion in terms of the semi-invariants of any time-ordered cumulant spin average is proved as a consequence of the usual linked cluster theorem for fermion operators. The most important semi-invariants are evaluated for any spin value S given by $(2S+1)=2^n$, $n=1,2,3,\ldots$, using a diagrammatic induction procedure based on conventional diagrammatic rules for fermion operators. The ultimate diagrammatic rules in both methods are shown to be equivalent.

1. Introduction

In a recent paper (Psaltakis and Cottam 1980, hereafter referred to as I) the authors have generalised the usual spin $S=\frac{1}{2}$ drone-fermion representation (Mattis 1965, Spencer 1968) to any spin value S satisfying

$$(2S+1)=2^n \qquad (n=1,2,3,\ldots). \tag{1.1}$$

This representation assigns two drone-fermion states to each physical spin state, and so effectively allows both Wick's theorem and the linked cluster theorem to be employed in a conventional diagrammatic perturbation technique. Explicitly, the representation can be expressed as (see I)

$$S^z=\sum_{m=1}^{n}2^{m-1}(c_m^+c_m-\tfrac{1}{2}), \tag{1.2}$$

$$S^+=\sum_{m=1}^{n}A_m^n(\phi c_m)^+(\phi c_{m-1})\ldots(\phi c_1), \tag{1.3}$$

$$S^-=\sum_{m=1}^{n}A_m^n(\phi c_1)^+\ldots(\phi c_{m-1})^+(\phi c_m), \tag{1.4}$$

where

$$\phi=d+d^+ \tag{1.5}$$

and c_m $(m=1,2,\ldots,n)$ and d are mutually anticommuting fermion operators. The positive definite operators A_m^n are given by

$$A_m^n=\left[4^{n-1}-\left(\sum_{k=m+1}^{n}2^{k-1}(c_k^+c_k-\tfrac{1}{2})\right)^2\right]^{1/2} \qquad (m=1,2,\ldots,n). \tag{1.6}$$

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The purpose of this paper is to establish the formal connection between the generalised drone-fermion method and the semi-invariant techniques of Stinchcombe *et al* (1963) and Vaks *et al* (1968), as applied to the Heisenberg model of a ferromagnet. The central concept in the latter techniques is that of the semi-invariants, which are defined as unperturbed time-ordered cumulant averages of spin operators. As shown in § 2 of this paper, this kind of average appears naturally also within the context of the drone-fermion method and corresponds to n-point vertex functions. The linked cluster expansion of any time-ordered cumulant spin average in terms of these vertex functions follows as a direct consequence of the usual linked cluster theorem for fermion operators (Abrikosov *et al* 1965). One of the main problems of the theory consists in the actual evaluation of the semi-invariants. In the technique of Vaks *et al* (1968) this is achieved, for any spin value S, by a set of diagrammatic rules derived from a generalisation of Wick's theorem to spin operators. A clear exposition of this procedure was given by Izyumov and Kassan-Ogly (1970). Nevertheless, as shown in § 3, for spin values given by (1.1) one need employ only the usual Wick theorem for fermion operators and its resulting diagram technique (Abrikosov *et al* 1965) to evaluate the most useful semi-invariants.

In § 4 a general discussion of the results is given, together with a summary of the ultimate diagrammatic rules for developing the perturbation expansion of any time-ordered cumulant spin average or of the free energy of the system.

2. Semi-invariants as n-point vertex functions

The Heisenberg Hamiltonian $\mathscr{H}$ for a ferromagnetic insulator can be written as $\mathscr{H}=\mathscr{H}_0+\mathscr{H}_1$ where $\mathscr{H}_0$ and $\mathscr{H}_1$ are respectively the Zeeman and Heisenberg terms:

$$\begin{aligned}\mathscr{H}_0&=-h\sum_i S_i^z,\\ \mathscr{H}_1&=-\tfrac{1}{2}\sum_{ij} v(r_{ij})[S_i^+S_j^-+S_i^zS_j^z].\end{aligned}\tag{2.1}$$

Denoting by $\tilde{S}^\alpha(\tau)$ and $S^\alpha(\tau)$ the Heisenberg representations of the spin operator S^α ($\alpha=+,-,z$), with respect to the Hamiltonians $\mathscr{H}$ and $\mathscr{H}_0$ respectively, we may write for the time-ordered average of any pair of spin operators the following equation (Abrikosov *et al* 1965):

$$\langle\mathscr{T}[\tilde{S}_1^{\alpha_1}(\tau_1)\tilde{S}_2^{\alpha_2}(\tau_2)]\rangle=\frac{\langle\mathscr{T}[S_1^{\alpha_1}(\tau_1)S_2^{\alpha_2}(\tau_2)\sigma(\beta)]\rangle_0}{\langle\sigma(\beta)\rangle_0}\tag{2.2}$$

where $\mathscr{T}$ is the Wick time-ordering operator, the σ matrix is given by

$$\sigma(\beta)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\dots\int_0^\beta d\tau_n\,\mathscr{T}[\mathscr{H}_1(\tau_1)\dots\mathscr{H}_1(\tau_n)]\tag{2.3}$$

and the brackets $\langle\dots\rangle$ and $\langle\dots\rangle_0$ denote thermal averages with respect to $\mathscr{H}$ and $\mathscr{H}_0$ respectively. For spin value S given by (1.1) we may use (1.2)–(1.4) to express the spin operators in (2.2) in terms of the fermion operators $c_n, \dots, c_1, d$. However, noting that $\mathscr{H}_0$ in (2.1) is diagonal in the number operators $c_m^+c_m$, we may apply the linked cluster theorem for fermion operators (Abrikosov *et al* 1965) to rewrite (2.2) as

$$\langle\mathcal{T}[\tilde{S}_1^{\alpha_1}(\tau_1)\tilde{S}_2^{\alpha_2}(\tau_2)]\rangle = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1'\ldots\int_0^\beta d\tau_n'\langle\mathcal{T}[S_1^{\alpha_1}(\tau_1)S_2^{\alpha_2}(\tau_2)\mathcal{H}_1(\tau_1')\ldots\mathcal{H}_1(\tau_n')]\rangle_0^{\prime\mathrm{con}} \tag{2.4}$$

where $\langle\ldots\rangle_0^{\prime\mathrm{con}}$ denotes an average in which only connected contractions with respect to the integration variables $\tau_1',\ldots,\tau_n'$ are taken into account. From (2.4) we can easily conclude that

$$\langle\mathcal{T}[(\tilde{S}_1^{\alpha_1}(\tau_1)-\langle\tilde{S}_1^{\alpha_1}(\tau_1)\rangle)(\tilde{S}_2^{\alpha_2}(\tau_2)-\langle\tilde{S}_2^{\alpha_2}(\tau_2)\rangle)]\rangle = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1'\ldots\int_0^\beta d\tau_n'\,\langle\mathcal{T}[S_1^{\alpha_1}(\tau_1)S_2^{\alpha_2}(\tau_2)\mathcal{H}_1(\tau_1')\ldots\mathcal{H}_1(\tau_n')]\rangle_0^{\mathrm{con}} \tag{2.5}$$

where now the average $\langle\ldots\rangle_0^{\mathrm{con}}$ takes into account connected contractions with respect to all τ-variables appearing inside it. Equation (2.5) is readily generalised for τ-ordered averages of a product of a larger number of spin operators. In that case the left-hand side of (2.5) will in general be the cumulant part of the average.

Using the fact that $\mathcal{H}_1$, equation (2.1), is expressed in terms of the spin operators $S_i^{\alpha_i}$, we see that the right-hand side of (2.5) is expanded in terms of τ-ordered averages of the form $\langle\mathcal{T}(\Pi_{i=1}^n S_i^{\alpha_i}(\tau_i))\rangle_0^{\mathrm{con}}$ connected with interaction lines†. Diagrammatically such quantities, hereafter referred to as semi-invariants, correspond to n-point vertex functions and we shall denote them by

$$M_n^{\alpha_1\ldots\alpha_n}(\tau_1\boldsymbol{r}_1,\ldots,\tau_n\boldsymbol{r}_n)=\left\langle\mathcal{T}\left(\prod_{i=1}^n S_i^{\alpha_i}(\tau_i)\right)\right\rangle_0^{\mathrm{con}}. \tag{2.6}$$

Equation (2.6) can be written alternatively as

$$M_n^{\alpha_1\ldots\alpha_n}(\tau_1\boldsymbol{r}_1,\ldots,\tau_n\boldsymbol{r}_n)=\left\langle\left(\prod_{i=1}^n S_i^{\alpha_i}(\tau_i)\right)\right\rangle_0 - \sum_{m_1+m_2+\ldots+m_k=n} M_{m_1}^{\alpha_1\cdots}M_{m_2}^{\cdots}\ldots M_{m_k}^{\cdots\alpha_n} \tag{2.7}$$

where the second term on the right-hand side of (2.7), representing the sum of products of all possible semi-invariants of lower order, takes into account all disconnected contractions appearing now in the first term. In the form of (2.7), the semi-invariants are clearly unperturbed time-ordered cumulant spin averages, and coincide with the analogous quantities defined in the techniques of Stinchcombe *et al* (1963) and Vaks *et al* (1968). It is to be noted that although in the latter techniques a linked cluster expansion in terms of the semi-invariants, valid for any spin value S, can be proved using special considerations for spin operators, our proof, valid for any spin value given by (1.1), was based solely on the usual linked cluster theorem for fermion operators.

The Fourier component in the frequency–momentum representation of an nth-order semi-invariant is defined by

$$M_n^{\alpha_1\ldots\alpha_n}(\eta_1\boldsymbol{q}_1,\ldots,\eta_n\boldsymbol{q}_n)=\frac{1}{\beta^n}\int_0^\beta d\tau_1\ldots\int_0^\beta d\tau_n \times\sum_{\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n} M_n^{\alpha_1\ldots\alpha_n}(\tau_1\boldsymbol{r}_1,\ldots,\tau_n\boldsymbol{r}_n)\prod_{i=1}^n\exp(\mathrm{i}\eta_i\tau_i+\mathrm{i}\boldsymbol{q}_i\boldsymbol{r}_i) \tag{2.8}$$

† The same conclusion applies also to the perturbation expansion of $-\beta F$, where F is the free energy of the system.

where by convention we interpret η_i and $\boldsymbol{q}_i$ as the boson frequency and momentum *leaving* the α_ith vertex point. From the form of the unperturbed Hamiltonian $\mathscr{H}_0$ in (2.1), it follows that we have non-zero connected contractions in (2.6) only when $\boldsymbol{r}_1 = \ldots = \boldsymbol{r}_n$, and thus (2.8) can be written as

$$M_n^{\alpha_1 \ldots \alpha_n}(\eta_1 \boldsymbol{q}_1, \ldots, \eta_n \boldsymbol{q}_n) = N \delta_{\boldsymbol{q}_1 + \ldots + \boldsymbol{q}_n, 0} M_n^{\alpha_1 \ldots \alpha_n}(\eta_1, \ldots, \eta_n). \tag{2.9}$$

Here N is the number of lattice sites and

$$M_n^{\alpha_1 \ldots \alpha_n}(\eta_1, \ldots, \eta_n) = \frac{1}{\beta^n} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \left\langle \mathscr{T}\left(\prod_{i=1}^n S^{\alpha_i}(\tau_i) \right) \right\rangle_0 \prod_{i=1}^n \exp(\mathrm{i}\eta_i \tau_i)$$
$$- \sum_{m_1 + m_2 + \ldots + m_k = n} M_{m_1}^{\alpha_1 \ldots} M_{m_2}^{\ldots} \ldots M_{m_k}^{\ldots \alpha_n}. \tag{2.10}$$

The thermal average in (2.10) is taken with respect to the density operator

$$\rho_0 = \exp(\beta h S^z) / \mathrm{Tr}[\exp(\beta h S^z)]. \tag{2.11}$$

Equations (2.9)–(2.11) show that the problem of evaluating the semi-invariants reduces to a single-site one. In § 3 we proceed in the evaluation of these quantities with the help of the usual diagrammatic rules for fermion operators (Abrikosov *et al* 1965). For this purpose we define the Green functions

$$C_m^0(\tau) = \langle \mathscr{T}[c_m(\tau) c_m^+(0)] \rangle_0, \qquad D^0(\tau) = \langle \mathscr{T}[\phi(\tau)\phi(0)] \rangle_0. \tag{2.12}$$

Fourier transforms can be defined in the usual way (see I), and the corresponding Fourier coefficients are given by

$$C_m^0(\alpha) = (\mathrm{i}\alpha + 2^{m-1} h)^{-1}, \qquad D^0(\alpha) = 2(\mathrm{i}\alpha)^{-1}, \tag{2.13}$$

where $\mathrm{i}\alpha$ is an imaginary fermion frequency. In a diagrammatic representation $-(1/\beta) C_m^0(\alpha)$ and $-(1/\beta) D^0(\alpha)$ will be drawn as a solid line (with index m) and a broken line respectively, as in I. The semi-invariant $M_n^{\alpha_1 \ldots \alpha_n}(\eta_1, \ldots, \eta_n)$ will be equal to the sum of all connected diagrams, in the frequency representation, that can be formed from the vertices $\alpha_1, \ldots, \alpha_n$.

3. Evaluation of the semi-invariants

In this section detailed considerations of the structure of the diagrams forming the semi-invariants lead to an inductive procedure for their evaluation in terms of the generalised drone-fermion representation. By this means all semi-invariants up to fourth order are evaluated for any spin value S given by (1.1). In the evaluation we distinguish three classes of semi-invariants: longitudinal, transverse and mixed, according to the type of vertices involved.

3.1. Longitudinal semi-invariants

These are formed only from (z)-type vertices. The lowest-order longitudinal semi-invariant is $M_1^z(\eta_1)$ and from (2.11) we have simply

$$M_1^z(\eta_1) = \delta_{\eta_1, 0} R_0 \tag{3.1}$$

where

$$R_0 = \langle S^z \rangle_0 = \sum_{m=1}^{n} 2^{m-1}(f_m - \tfrac{1}{2}) \tag{3.2}$$

and

$$f_m = \langle c_m^+ c_m \rangle_0 = [\exp(-2^{m-1}\beta h) + 1]^{-1}. \tag{3.3}$$

It is a matter of elementary transformations to show that, for the corresponding spin value S given by (1.1), R_0 can be written as

$$R_0 = (S + \tfrac{1}{2}) \coth[(S + \tfrac{1}{2})\beta h] - \tfrac{1}{2} \coth(\tfrac{1}{2}\beta h) \tag{3.4}$$

as expected. Let us consider now a general $(\lambda + 1)$-order longitudinal semi-invariant, $(\lambda \geq 1)$. From the discussion following (2.13) and the form of the S^z operator, (1.2), we conclude that

$$M_{\lambda+1}^{zz\ldots z}(\eta_1, \ldots, \eta_{\lambda+1}) = \sum_{m=1}^{n} (2^{m-1})^{\lambda+1} \lambda! P_{\lambda+1}^{zz\ldots z}(m) \tag{3.5}$$

where $P_{\lambda+1}^{zz\ldots z}(m)$ is represented diagrammatically in figure 1. The factorial $\lambda!$ in (3.5) takes into account all diagrams similar to that of figure 1 which result from making all possible permutations of λ vertices (one vertex has to be regarded as fixed). Applying the usual diagrammatic rules for fermion operators, we obtain

$$P_{\lambda+1}^{zz\ldots z}(m) = (-1)\delta_{\eta_1,0} \ldots \delta_{\eta_{\lambda+1},0} \sum_{\alpha} \left(-\frac{1}{\beta} C_m^0(\alpha)\right)^{\lambda+1}. \tag{3.6}$$

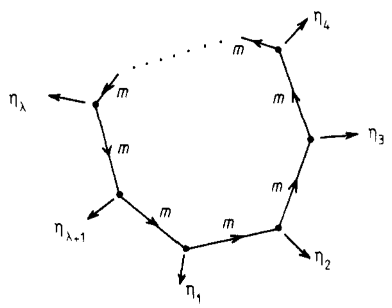

Figure 1. Definition of $P_{\lambda+1}^{zz\ldots z}(m)$ in the evaluation of $M_{\lambda+1}^{zz\ldots z}(\eta_1, \ldots, \eta_{\lambda+1})$.

The frequency summation in (3.6) can be readily performed, and after substituting the result into (3.5) we find that

$$M_{\lambda+1}^{zz\ldots z}(\eta_1, \ldots, \eta_{\lambda+1}) = \delta_{\eta_1,0} \ldots \delta_{\eta_{\lambda+1},0} \sum_{m=1}^{n} (2^{m-1})^{\lambda+1} \left[\left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)^{\lambda} \frac{1}{\mathrm{e}^x + 1}\right]_{x=-2^{m-1}\beta h}. \tag{3.7}$$

Denoting by $R_0^{[\lambda]}$ the λth derivatives of R_0 with respect to βh, and using (3.2) and (3.3), equation (3.7) can be rewritten as

$$M_{\lambda+1}^{zz\ldots z}(\eta_1, \ldots, \eta_{\lambda+1}) = \delta_{\eta_1,0} \ldots \delta_{\eta_{\lambda+1},0} R_0^{[\lambda]}. \tag{3.8}$$

3.2. *Transverse semi-invariants*

These are formed from pairs of (+), (−) vertices. The lowest-order transverse semi-invariant $M_2^{+-}(\eta_1, \eta_2)$ can be expressed as

$$M_2^{+-}(\eta_1, \eta_2) = \sum_{m=1}^{n} \langle (A_m^n)^2 \rangle_0 P_2^{+-}(m) \tag{3.9}$$

where $P_2^{+-}(m)$ is defined in figure 2*a*. The term $\langle (A_m^n)^2 \rangle_0$ in the above expression takes into account all possible connected and disconnected contractions between the fermion operators of A_m^n, (1.6), appearing in the representation of S^+, (1.3), with the corresponding operators appearing in the representation of S^-, (1.4). The factorisation of the diagrammatic contributions shown in (3.9) is more easily understood in the τ representation. In this representation we shall have a term $\langle \mathscr{T}[A_m^n(\tau_1) A_m^n(\tau_2)] \rangle_0$ which for any τ_1, τ_2 is equal to $\langle (A_m^n)^2 \rangle_0$. Thus, transforming to the frequency representation, this term will appear just as a multiplicative factor. It is worth emphasising that all diagrams summed in (3.9) are connected because $P_2^{+-}(m)$ in figure 2*a* is connected.

Proceeding in the evaluation of $M_2^{+-}(\eta_1, \eta_2)$, we shall prove first by induction that

$$P_2^{+-}(m) = \delta_{\eta_1+\eta_2,0}[f_m(1-f_{m-1}) \ldots (1-f_1) - (1-f_m) f_{m-1} \ldots f_1] \frac{1}{\beta(h - \mathrm{i}\eta_1)}. \tag{3.10}$$

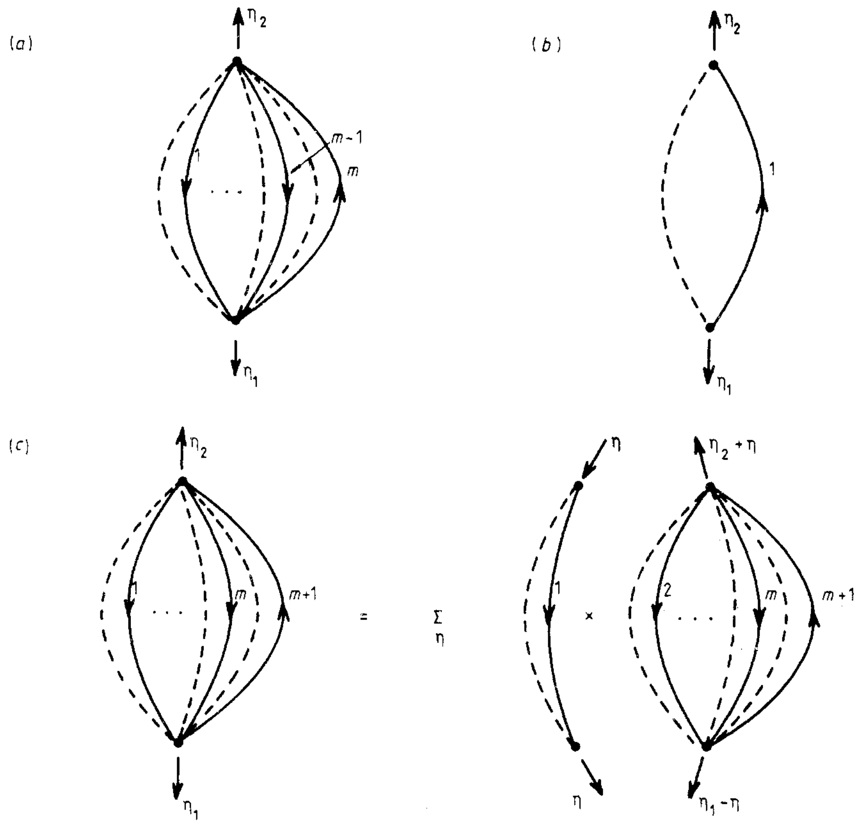

Figure 2. Evaluation of $M_2^{+-}(\eta_1, \eta_2)$: (*a*) $P_2^{+-}(m)$; (*b*) $P_2^{+-}(1)$; (*c*) $P_2^{+-}(m+1)$ as a convolution.

For $m = 1$ figure $2a$ reduces to figure $2b$, and it can be verified directly that

$$P_2^{+-}(1) = \delta_{\eta_1+\eta_2,0}(-1+2f_1)\frac{1}{\beta(h-\mathrm{i}\eta_1)}. \tag{3.11}$$

Thus (3.10) is valid for $m = 1$. We assume now its validity for a given m and consider the $m+1$ case. As shown in figure $2c$, the $m+1$ diagram can be considered as a frequency convolution of two diagrams, the first of which is just $P_2^{+-}(1)$ of figure $2b$, whilst the second has the same structure as $P_2^{+-}(m)$ of figure $2a$ but with each C_j^0 line replaced by C_{j+1}^0. Noting that the above replacement is equivalent to replacing h by $2h$ (see equation (2.13)), we may use the assumption of induction and (3.11) to write

$$P_2^{+-}(m+1) = \delta_{\eta_1+\eta_2,0}(-1+2f_1)[f_{m+1}(1-f_m)\ldots(1-f_2)-(1-f_{m+1})f_m\ldots f_2]$$
$$\times\frac{1}{\beta^2}\sum_\eta \frac{1}{2h-\mathrm{i}\eta_1+\mathrm{i}\eta}\,\frac{1}{h+\mathrm{i}\eta}. \tag{3.12}$$

The frequency summation in (3.12) can be readily performed, and after some re-arrangement we obtain

$$P_2^{+-}(m+1) = \delta_{\eta_1+\eta_2,0}[f_{m+1}(1-f_m)\ldots(1-f_1)-(1-f_{m+1})f_m\ldots f_1]\frac{1}{\beta(h-\mathrm{i}\eta_1)}. \tag{3.13}$$

Thus (3.10) is valid also for the $m+1$ case and the proof of it is completed by induction. Substituting (3.10) into (3.9) and using the algebraic identity (A1.1) of appendix 1, we obtain finally the expression

$$M_2^{+-}(\eta_1, \eta_2) = \delta_{\eta_1+\eta_2,0}2R_0/\beta(h-\mathrm{i}\eta_1). \tag{3.14}$$

It is worth mentioning that the result of equation (3.14) can alternatively be derived by working in the τ representation. Nevertheless, we have chosen to follow the rather lengthy induction procedure because it can straightforwardly be adapted to the evaluation of the mixed semi-invariants, as illustrated in the next subsection.

In principle, the next higher-order transverse semi-invariant M_4^{+-+-} can be derived in a similar manner to M_2^{+-}, but it is more convenient to make use of the relation

$$M_4^{+-+-}(\eta_1, \eta_2, \eta_3, \eta_4) = [M_3^{+-z}(\eta_1, \eta_4, \eta_3+\eta_2)$$
$$+M_3^{+-z}(\eta_3, \eta_4, \eta_1+\eta_2)]\frac{M_2^{+-}(-\eta_2, \eta_2)}{R_0}. \tag{3.15}$$

The quantity M_3^{+-z} appearing in (3.15) is a mixed semi-invariant which is defined and evaluated in the next subsection, giving

$$M_3^{+-}(\eta_1, \eta_2, \eta_3) = 2\delta_{\eta_1+\eta_2+\eta_3,0}\left(-\frac{R_0}{\beta^2(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)}+\frac{R_0'}{\beta(h-\mathrm{i}\eta_1)}\delta_{\eta_3,0}\right). \tag{3.16}$$

The justification of (3.15) is most easily accomplished using general properties of spin operators (Izyumov and Kassan-Ogly 1970) together with our definition of the semi-invariants, as shown in appendix 2. Combining (3.14)–(3.16), we obtain the result

$$M_4^{+-+-}(\eta_1, \eta_2, \eta_3, \eta_4)$$
$$= 4\delta_{\eta_1+\eta_2+\eta_3+\eta_4,0}\left(-\frac{R_0(2h-\mathrm{i}\eta_1-\mathrm{i}\eta_3)}{\beta^3(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)(h-\mathrm{i}\eta_3)(h+\mathrm{i}\eta_4)}\right.$$
$$\left.+\frac{R_0'}{\beta^2(h-\mathrm{i}\eta_1)(h-\mathrm{i}\eta_3)}(\delta_{\eta_2+\eta_3,0}+\delta_{\eta_3+\eta_4,0})\right). \tag{3.17}$$

3.3. Mixed semi-invariants

The mixed semi-invariants involve both (z)-type vertices and pairs of $(+)$, $(-)$ vertices. In their evaluation it is convenient to isolate those parts which correspond to zero outgoing frequency at the (z) vertex points. These parts can be more easily expressed via the identity

$$\frac{\partial}{\partial(\beta h)}M_n^{\alpha_1\ldots\alpha_n}(\eta_1,\ldots,\eta_n) = M_{n+1}^{\alpha_1\ldots\alpha_n z}(\eta_1,\ldots,\eta_n,0). \tag{3.18}$$

An elementary proof of (3.18) valid for any spin value S is given in appendix 3 of this paper. For an alternative proof we refer to Stinchcombe *et al* (1963). Within the context of the drone-fermion method, equation (3.18) has a simple diagrammatic interpretation also discussed in appendix 3. Using (3.18), the mixed semi-invariant M_3^{+-z} can be expressed as

$$M_3^{+-z}(\eta_1,\eta_2,\eta_3) = (1-\delta_{\eta_3,0})M_3^{+-z}(\eta_1,\eta_2,\eta_3\neq 0)+\delta_{\eta_3,0}\,\partial M_2^{+-}(\eta_2,\eta_2)/\partial(\beta h). \tag{3.19}$$

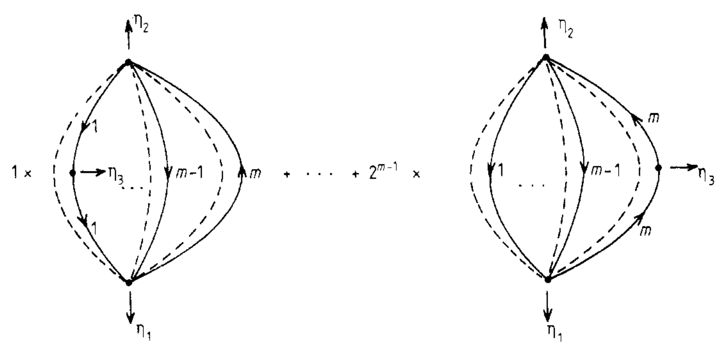

Figure 3. Definition of $P_3^{+-z}(m)$ in the evaluation of $M_3^{+-z}(\eta_1, \eta_2, \eta_3\neq 0)$.

Thus we need only consider the diagrams contributing to $M_3^{+-z}(\eta_1,\eta_2,\eta_3\neq 0)$. Noting that contractions of a $c_{m'}^+(\tau_3)c_{m'}(\tau_3)$ operator with $A_{m''}^n(\tau_1)A_{m''}^n(\tau_2)$ are τ-independent in the τ representation, and hence proportional to $\delta_{\eta_3,0}$ in the frequency representation, we conclude that

$$M_3^{+-z}(\eta_1,\eta_2,\eta_3\neq 0) = \sum_{m=1}^{n}\langle(A_m^n)^2\rangle_0 P_3^{+-z}(m). \tag{3.20}$$

Here $P_3^{+-z}(m)$ is defined as the series of diagrams of figure 3 which can be obtained from that of figure 2a by attaching a (z) vertex point on each of the $C_{m'}^0$ lines in turn

$(m'=1,2,\ldots,m)$ and including the appropriate weighting factors that result from (1.2). By an induction proof similar to that of (3.10), one can show that for $\eta_3\neq 0$

$$P_3^{+-z}(m)=\delta_{\eta_1+\eta_2+\eta_3,0}\left(-\frac{f_m(1-f_{m-1})\ldots(1-f_1)-(1-f_m)f_{m-1}\ldots f_1}{\beta^2(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)}\right). \tag{3.21}$$

Combining (3.19)–(3.21) and using (3.14) and the identity (A1.1), we obtain the expression for $M_3^{+-z}(\eta_1,\eta_2,\eta_3)$ already quoted in (3.16).

The evaluation of the next higher-order mixed semi-invariant M_4^{+-zz} proceeds along the same lines. Using (3.18) we may write

$$\begin{aligned}M_4^{+-zz}&(\eta_1,\eta_2,\eta_3,\eta_4)\\&=(1-\delta_{\eta_3,0})(1-\delta_{\eta_4,0})M_4^{+-zz}(\eta_1,\eta_2,\eta_3\neq 0,\eta_4\neq 0)\\&\quad+\delta_{\eta_3,0}\frac{\partial M_3^{+-z}(\eta_1,\eta_2,\eta_4)}{\partial(\beta h)}+\delta_{\eta_4,0}\frac{\partial M_3^{+-z}(\eta_1,\eta_2,\eta_3)}{\partial(\beta h)}\\&\quad-\delta_{\eta_3,0}\delta_{\eta_4,0}\frac{\partial^2 M_2^{+-}(\eta_1,\eta_2)}{\partial(\beta h)^2}.\end{aligned} \tag{3.22}$$

From arguments similar to those leading to (3.20) we conclude that

$$M_4^{+-zz}(\eta_1,\eta_2,\eta_3\neq 0,\eta_4\neq 0)=\sum_{m=1}^{n}\langle(A_m^n)^2\rangle_0 P_4^{+-zz}(m) \tag{3.23}$$

where $P_4^{+-zz}(m)$ is expressed diagrammatically in figure 4. We note that the diagrams of figure 4 can be formed from those of figure 3 by attaching the extra (z) vertex point in all possible topologically distinct positions and including the appropriate weighting factors. By an induction proof one can verify that for $\eta_3\neq 0$ and $\eta_4\neq 0$

$$\begin{aligned}P_4^{+-zz}(m)&=\delta_{\eta_1+\eta_2+\eta_3+\eta_4,0}\\&\quad\times\frac{[f_m(1-f_{m-1})\ldots(1-f_1)-(1-f_m)f_{m-1}\ldots f_1](2h-2\mathrm{i}\eta_1-\mathrm{i}\eta_3-\mathrm{i}\eta_4)}{\beta^3(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)(h-\mathrm{i}\eta_1-\mathrm{i}\eta_3)(h-\mathrm{i}\eta_1-\mathrm{i}\eta_4)}.\end{aligned} \tag{3.24}$$

Using (3.14) and (3.16), equations (3.22)–(3.24) may be combined to give

$$\begin{aligned}M_4^{+-zz}&(\eta_1,\eta_2,\eta_3,\eta_4)\\&=2\delta_{\eta_1+\eta_2+\eta_3+\eta_4,0}\left(\frac{R_0(2h-2\mathrm{i}\eta_1-\mathrm{i}\eta_3-\mathrm{i}\eta_4)}{\beta^3(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)(h-\mathrm{i}\eta_1-\mathrm{i}\eta_3)(h-\mathrm{i}\eta_1-\mathrm{i}\eta_4)}\right.\\&\quad\left.-\frac{R_0'}{\beta^2(h-\mathrm{i}\eta_1)(h+\mathrm{i}\eta_2)}(\delta_{\eta_3,0}+\delta_{\eta_4,0})+\frac{R_0''}{\beta(h-\mathrm{i}\eta_1)}\delta_{\eta_3,0}\delta_{\eta_4,0}\right)\end{aligned} \tag{3.25}$$

where the identity (A1.1) has been used once more.

4. Discussion

Once the evaluation of the semi-invariants is completed, the subsequent rules for developing the perturbation expansion of any time-ordered cumulant spin average or of the free energy of the system, using the generalised drone-fermion method, are

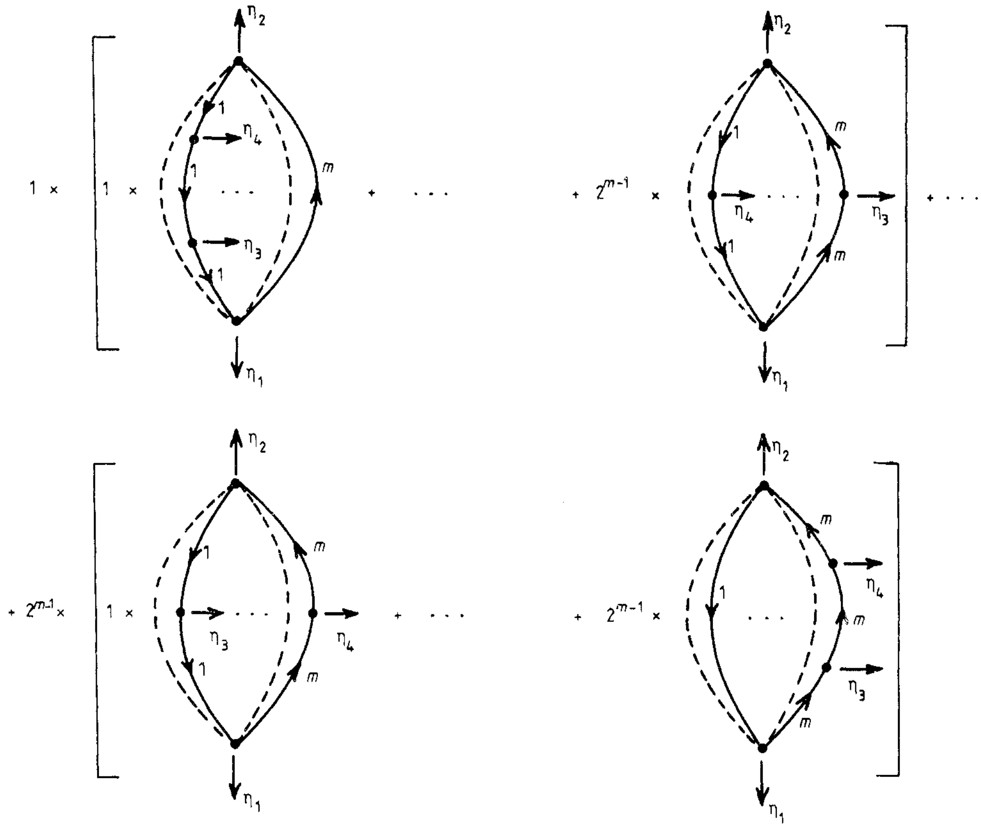

Figure 4. Definition of $P_4^{+-zz}(m)$ in the evaluation of $M_4^{+-zz}(\eta_1, \eta_2, \eta_3 \neq 0, \eta_4 \neq 0)$.

equivalent to those used in the semi-invariant technique of Vaks *et al* (1968), and may be summarised as follows.

(i) Draw all the appropriate connected diagrams formed by n-point vertex functions joined with interaction lines. Label the diagrams so that the total frequency and momentum are conserved at each n-point vertex function.

(ii) Associate a factor $NM_n^{\alpha_1 \ldots \alpha_n}(\eta_1, \ldots, \eta_n)$ with each n-point vertex function, where $\eta_1, \ldots, \eta_n$ are the boson frequencies leaving the vertex points $\alpha_1, \ldots, \alpha_n$ respectively.

(iii) Associate a factor $\beta J(\boldsymbol{q})/2N$ or $\beta J(\boldsymbol{q})/N$ with each interaction line carrying a momentum label $\boldsymbol{q}$ and joining a (+) to a (−) vertex point or two (z) vertex points respectively, where

$$v(r_{ij}) = \frac{1}{N} \sum_{\boldsymbol{q}} J(\boldsymbol{q}) \exp(-\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}_{ij}). \tag{4.1}$$

(iv) Associate a factor $1/p$ with each diagram, where p is its symmetry factor.

(v) Sum over all internal frequency and momentum labels within the restrictions imposed by (i).

So far in both techniques the parameter of smallness used to classify the diagrams has been $1/z$, where z is the number of spins interacting with any given spin. The rule for determining the $1/z$ dependence of any diagram is (Cottam and Stinchcombe 1970) that each independent momentum label which appears in an interaction line, and is eventually summed over, gives rise to a $1/z$ factor. The lowest-order $(1/z)^0$ renormalisation of the semi-invariants leads to the replacement in all expressions of the external field h by the self-consistent molecular field $\gamma = h + R_0 J(0)$. Explicitly this is accomplished in slightly different ways for each formalism. Within the context of the drone-fermion method, we renormalise to order $(1/z)^0$ the individual C_m^0 lines, essentially as in I, since the D^0 lines have no self-energy parts to this order. For the corresponding procedure followed in the semi-invariant technique we refer to Stinchcombe (1973). In the Vaks *et al* (1968) approach, the $(1/z)^0$ renormalisation is automatically incorporated in the formalism by including in the unperturbed Hamiltonian $\mathscr{H}_0$ the mean field part of the Heisenberg interaction.

The generalised drone-fermion method and the semi-invariant technique will clearly give rise to equivalent results. However, the former method is restricted to spin values given by (1.1). These, nevertheless, include all ferroelectrics described by a pseudo-spin Heisenberg model and many important ferromagnetic materials (e.g. Cr compounds for $S = \frac{3}{2}$ and Eu compounds for $S = \frac{7}{2}$).

Appendix 1.

Here we present the proof of the following useful algebraic identity:

$$\sum_{m=1}^{n} \langle (A_m^n)^2 \rangle_0 [f_m(1-f_{m-1}) \dots (1-f_1) - (1-f_m) f_{m-1} \dots f_1] = 2R_0. \tag{A1.1}$$

We start from the commutator relation

$$[S^+, S^-] = 2S^z \tag{A1.2}$$

which may be rewritten in terms of the drone-fermion representation (1.2)–(1.4) as

$$\begin{aligned}\sum_{m=1}^{n} (A_m^n)^2 [(\phi c_m)^+ (\phi c_{m-1}) \dots (\phi c_1)(\phi c_1)^+ \dots (\phi c_{m-1})^+ (\phi c_m) \\ - (\phi c_1)^+ \dots (\phi c_{m-1})^+ (\phi c_m)(\phi c_m)^+ (\phi c_{m-1}) \dots (\phi c_1)] \\ = 2 \sum_{m=1}^{n} 2^{m-1} (c_m^+ c_m - \tfrac{1}{2}).\end{aligned} \tag{A1.3}$$

In view of the identities $\phi^2 = 1$ and $c_m c_m^+ + c_m^+ c_m = 1$, equation (A1.3) is equivalent to

$$\begin{aligned}\sum_{m=1}^{n} (A_m^n)^2 [c_m^+ c_m (1 - c_{m-1}^+ c_{m-1}) \dots (1 - c_1^+ c_1) - (1 - c_m^+ c_m) c_{m-1}^+ c_{m-1} \dots c_1^+ c_1] \\ = 2 \sum_{m=1}^{n} 2^{m-1} (c_m^+ c_m - \tfrac{1}{2}).\end{aligned} \tag{A1.4}$$

The identity (A1.1) follows now from (A1.4) by taking the thermal average $\langle \dots \rangle_0$, with respect to ρ_0, of both sides and using (3.2), (3.3) as well as the fact that the operator $(A_m^n)^2$ depends only on $c_n^+ c_n, \dots, c_{m+1}^+ c_{m+1}$ (see (1.6)).

Appendix 2.

In this appendix we make use of an important identity for spin operators, established by Izyumov and Kassan-Ogly (1970), in order to justify equation (3.15). In fact, from equation (2.10) of their paper we have

$$\begin{aligned}\langle \mathcal{T}[S^+(\tau_1)S^-(\tau_2)S^+(\tau_3)S^-(\tau_4)]\rangle_0 &= 2G(\tau_2-\tau_3)\langle \mathcal{T}[S^+(\tau_1)S^-(\tau_4)S^z(\tau_3)]\rangle_0 \\ &\quad +2G(\tau_2-\tau_1)\langle \mathcal{T}[S^+(\tau_3)S^-(\tau_4)S^z(\tau_1)]\rangle_0 \end{aligned}\tag{A2.1}$$

where the G function is defined by

$$G(\tau-\tau')=\exp[h(\tau-\tau')]\begin{cases}[\exp(\beta h)-1]^{-1}, & \tau>\tau', \\ [1-\exp(-\beta h)]^{-1}, & \tau<\tau'.\end{cases}\tag{A2.2}$$

Using (3.14) one can easily verify the relation

$$M_2^{+-}(\tau_1,\tau_2)=2R_0G(\tau_2-\tau_1).\tag{A2.3}$$

From (A2.1), (A2.3) and our definition (2.7) for the M_4^{+-+-} and M_3^{+-z} semi-invariants in the τ representation, it follows that

$$\begin{aligned}M_4^{+-+-}(\tau_1,\tau_2,\tau_3,\tau_4) &= [M_3^{+-z}(\tau_1,\tau_4,\tau_3)M_2^{+-}(\tau_3,\tau_2) \\ &\quad +M_3^{+-z}(\tau_3,\tau_4,\tau_1)M_2^{+-}(\tau_1,\tau_2)]/R_0.\end{aligned}\tag{A2.4}$$

Equation (3.15) now is just the frequency representation of (A2.4).

Appendix 3.

In this appendix we give a proof of equation (3.18) valid for any spin value S. We consider only the case when the sum of the frequencies in (3.18) is zero, since otherwise both sides vanish identicaly. From (2.11) we have

$$\partial\rho_0/\partial(\beta h)=\rho_0 S^z-\rho_0\langle S^z\rangle_0\tag{A3.1}$$

and on taking the derivative with respect to βh of both sides of (2.10) we may write

$$\begin{aligned}\frac{\partial}{\partial(\beta h)}M_n^{\alpha_1\ldots\alpha_n}(\eta_1,\ldots,\eta_n) &= \frac{1}{\beta^{n+1}}\int_0^\beta d\tau_1\ldots\int_0^\beta d\tau_n\int_0^\beta d\tau\left\langle\mathcal{T}\left(\prod_{i=1}^n S^{\alpha_i}(\tau_i)S^z(\tau)\right)\right\rangle_0\prod_{i=1}^n\exp(i\eta_i\tau_i) \\ &\quad -\langle S^z\rangle_0\frac{1}{\beta^n}\int_0^\beta d\tau_1\ldots\int_0^\beta d\tau_n\left\langle\mathcal{T}\left(\prod_{i=1}^n S^{\alpha_i}(\tau_i)\right)\right\rangle_0\prod_{i=1}^n\exp(i\eta_i\tau_i) \\ &\quad -\frac{\partial}{\partial(\beta h)}\sum_{m_1+m_2+\ldots+m_k=n}M_{m_1}^{\alpha_1\ldots}M_{m_2}^{\ldots}\ldots M_{m_k}^{\ldots\alpha_n}.\end{aligned}\tag{A3.2}$$

In the first term of (A3.2) we have taken into account all possible orderings of the S^z operator with respect to the other operators. An additional term resulting from the dependence of the $S^\alpha(\tau)$ operators on βh can be easily shown to vanish under the assumption of zero frequency sum. Using (2.10), (3.1) and (3.2) equation (A3.2) can be written as

$$\frac{\partial}{\partial(\beta h)} M_n^{\alpha_1\ldots\alpha_n}(\eta_1,\ldots,\eta_n)$$
$$= \frac{1}{\beta^{n+1}} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \int_0^\beta \mathrm{d}\tau \left\langle \mathcal{T}\left(\prod_{i=1}^n S^{\alpha_i}(\tau_i) S^z(\tau) \right) \right\rangle_0 \prod_{i=1}^n \exp(\mathrm{i}\eta_i\tau_i)$$
$$- M_1^z(\eta=0)\left(M_n^{\alpha_1\ldots\alpha_n}(\eta_1,\ldots,\eta_n) + \sum_{m_1+m_2+\ldots+m_k=n} M_{m_1}^{\alpha_1\ldots} M_{m_2}^{\ldots} \ldots M_{m_k}^{\ldots\alpha_n} \right)$$
$$- \frac{\partial}{\partial(\beta h)} \sum_{m_1+m_2+\ldots+m_k=n} M_{m_1}^{\alpha_1\ldots} M_{m_2}^{\ldots} \ldots M_{m_k}^{\ldots\alpha_n}. \tag{A3.3}$$

For $n=1$ equation (3.18) is valid, as the right-hand side of (A3.3) will just be equal to $M_2^{\alpha_1 z}(\eta_1, 0)$. Assuming the validity of (3.18) for all semi-invariants of order smaller than or equal to $n-1$, we can easily conclude from (A3.3) that its right-hand side will be equal to $M_{n+1}^{\alpha_1\ldots\alpha_n z}(\eta_1,\ldots,\eta_n, 0)$, and so the proof of (3.18) is completed by induction.

Within the context of the generalised drone-fermion method, it is possible to give an alternative proof of (3.18) which assists in a simple diagrammatic interpretation. As mentioned at the end of § 2, the semi-invariant $M_n^{\alpha_1\ldots\alpha_n}(\eta_1,\ldots,\eta_n)$ consists of all connected diagrams that can be formed from the vertices $\alpha_1,\ldots,\alpha_n$. Thus its βh dependence results only from the C_m^0 lines, as the D^0 lines do not depend on βh, (2.13). We can easily verify that

$$\frac{\partial}{\partial(\beta h)}\left(-\frac{1}{\beta} C_m^0(\alpha)\right) = 2^{m-1}\left(-\frac{1}{\beta} C_m^0(\alpha)\right)^2. \tag{A3.4}$$

Diagrammatically, equation (A3.4) is represented in figure 5. We see that the effect of the derivative $\partial/\partial(\beta h)$ on each C_m^0 line is to create a (z) vertex point with zero outgoing frequency, and so (3.18) follows. This interpretation is also useful because it provides the link between the $(1/z)^0$ renormalisation procedure as achieved in the semi-invariant approach (Stinchcombe 1973) and the generalised drone-fermion method (I).

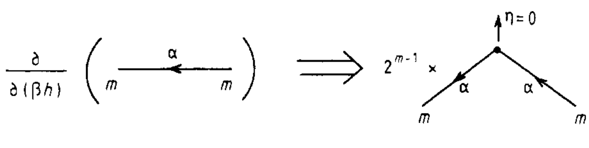

Figure 5. Diagrammatic representation of equation (A3.4).

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