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Quasi-classical formalism for Ising model algebras

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Abstract. A quasi-classical formalism is developed for spin algebras characteristic of Ising models, that is, an algebra in which all elements commute. Spin operators and their products are mapped onto continuous variables while traces are re-expressed as integrals over these variables.

1. Introduction

A few years ago (Kaplan and Summerfield 1969, Kaplan 1971), a quasi-classical spin formalism was developed which allows the exact quantum spin dynamics of physical systems to be expressed in the language of continuous variables. The continuous variables are unit vectors $\Omega_i (i = 1, 2, ..., N)$, one for each particle spin. In essence, spin matrices are replaced by functions of continuous variables while spin traces are identified with integrals of some function of these variables. This quasi-classical formalism is a generalization to spin theory of methods (Wigner 1932, Moyal 1949, Groenewold 1946) which have been developed for position and momentum variables beginning with Wigner's work in 1932.

These latter phase space methods have been extensively studied by Agarwal and Wolf (1970) who have shown their connection to the Sudarshan (1963a, b) and Glauber (1963) coherent state representation. Using spin coherent states (Radcliffe 1971), Kutzner (1973) has developed a phase space representation for spin systems which is closely related to the quasi-classical spin formalism of Kaplan and Summerfield. A review of the key concepts of the quasi-classical method for systems with both spin and position-momentum variables has been given by Mirkovitch and Summerfield (1973). These quasi-classical methods provide a natural framework for going to the classical limit of quantum theory. By this we mean that such a framework allows one to obtain by perturbation theory quantum corrections to classical spin problems which are exactly solvable, such as the one-dimensional isotropic Heisenberg model (Fisher 1964) and Ising model (Thompson 1968). For example, the classical theory provides the zeroth approximation and perturbation in the reciprocal of the spin quantum number S provides the first-order correction to the classical theory.

The quasi-classical formalism presented by Kaplan and Summerfield was for matrix algebras satisfying the commutation relations

$$[S_{\mu}, S_{\nu}] = \mathrm{i} \epsilon_{\mu\nu\alpha} S_{\alpha},$$

where $\epsilon_{\mu\nu\alpha}$ is the totally antisymmetric three-tensor. Such a formalism can be applied, for example, in the study of the Heisenberg model (Chang *et al* 1971, Chang and

Summerfield 1971, Ebara and Tanaka 1974, Harrigan and Jones 1973[†]). Our purpose in this paper is to outline the quasi-classical spin formalism for matrix algebras which contain only *commutin*'g matrices. We have in mind matrices characterizing Ising models. Thus when we refer to operators in the succeeding parts of this paper, we shall mean such commuting matrices. The formalism presented here is applied to the one-dimensional Ising model with arbitrary spin in a separate communication (Bowden and Kaplan 1976). This application provides a uniform treatment for all values of spin including the classical limit.

Our presentation proceeds as follows: in § 2 we introduce the general mapping procedures for a single particle of spin S. The associated spin operator is denoted by S^{z} . In § 3 we present the formulae for computing traces and in § 4 we give the generalization to many-particle systems.

2. General formalism

In this section we state and verify the mapping rules for a spin-S algebra formed by a spin operator S^z , an identity operator I, and arbitrary functions of the spin operator for which we use the notation $A(S^z)$. The mappings for S^z and I are given by (we denote mappings by arrows, \rightarrow)

$$S^{z} \to S\Omega \equiv S_{W}(\Omega) \tag{1}$$

and

$$I \to 1 \equiv I_{\rm W}(\Omega), \tag{2}$$

where S is the spin quantum number and Ω is a continuous variable with a range (-1, +1). We call the function into which the operator has been mapped the 'Wigner equivalent' function. Thus S_W and I_W are the 'Wigner equivalent' functions for the operators S^z and I.

To obtain the mappings of functions of S^z we employ a building up principle which can be stated as follows. If $A_W(\Omega)$ and $B_W(\Omega)$ are the Wigner equivalents of two arbitrary operators $A(S^z)$ and $B(S^z)$, then the Wigner equivalent of the product, $A(S^z)B(S^z)$, is obtained by the rule

$$(AB)_{W}(\Omega) = A_{W}(\Omega)GB_{W}(\Omega), \tag{3}$$

where the left-right differential operator (Groenewold 1946) G is given by

$$G = 1 + \sum_{k=1}^{2S} \frac{(2S-k)!}{(2S)!k!} \frac{\tilde{d}^{k}}{d\Omega^{k}} (1-\Omega^{2})^{k} \frac{\tilde{d}^{k}}{d\Omega^{k}}.$$
 (4)

(The arrows indicate directions of differentiation.)

We illustrate equations (2), (3) with a spin- $\frac{1}{2}$ system obeying the algebraic relation

$$(S^{z})^{2} = \frac{1}{4}I.$$
 (5)

In this $(S = \frac{1}{2})$ case we have from equation (1)

$$S_{\rm W} = \frac{1}{2}\Omega,\tag{6}$$

$$I_{\rm W} = 1, \tag{7}$$

[†]Harrigan and Jones employ coherent spin states.

and from (4)

$$G = 1 + \frac{\ddot{d}}{d\Omega} (1 - \Omega^2) \frac{\vec{d}}{d\Omega}.$$
 (8)

Substituting these expressions into equation (3), we have

$$[S^{z}S^{z}]_{W} = (\frac{1}{2}\Omega)G(\frac{1}{2}\Omega) = \frac{1}{4} \equiv \frac{1}{4}I_{W}$$
(9)

which shows that equation (5) is preserved under the mapping.

We must now verify that we have indeed obtained a one-to-one mapping of the algebra. By this we mean that if we have an algebraic equation of the form

$$A(S^{z})B(S^{z}) = C(S^{z})$$

$$\tag{10}$$

then our mapping rules guarantee that

$$A_{\mathbf{W}}GB_{\mathbf{W}} = C_{\mathbf{W}}.\tag{11}$$

We do this by considering the equations for the projection operators P_m ,

$$P_m P_{m'} = \delta_{mm'} P_{m'}. \tag{12}$$

We will show below that

$$[P_m]_{\mathsf{W}}G[P_{m'}]_{\mathsf{W}} = \delta_{mm'}[P_{m'}]_{\mathsf{W}}$$
(13)

with the mapping for P_m being given by

$$[P_m]_{\mathbf{W}} = \frac{1}{2^{2S}} [(1+\Omega)^{S+m} (1-\Omega)^{S-m} {2S \choose S+m},$$
(14)

where $\binom{2S}{m}$ is a binomial coefficient. First, however, we will show that the mapping given by equation (14) is in agreement with the mappings (1) and (2) of S^z and *I*. This is done by noting that the decompositions of *I* and S^z in terms of projection operators are

$$I = \sum_{m=-S}^{m=+S} P_m \tag{15}$$

and

$$S^{z} = \sum_{m=-S}^{m=+S} m P_{m}.$$
 (16)

Using the binomial theorem we find

$$\sum_{m=-S}^{+S} [P_m]_{\mathbf{W}} = \sum_{m=-S}^{+S} \frac{1}{2^{2S}} [(1+\Omega)^{S+m} (1-\Omega)^{S-m}] {\binom{2S}{S+m}} = 1$$
(17)

and

$$\sum_{n=-s}^{+s} m[P_m]_{W} = \sum_{m=-s}^{+s} \frac{m}{2^{2s}} [(1+\Omega)^{s+m} (1-\Omega)^{s-m}] {\binom{2s}{s+m}} = S\Omega, \quad (18)$$

so that the projection operator mapping is indeed compatible with that of the fundamental operators S^z and *I*. Since every operator can be decomposed into projection operators, the validity of equation (13) implies the validity of any equation of the form of equation (11) providing equation (10) is true. To prove equation (13) we first rewrite the Wigner equivalent of the projection operator in the form

$$[P_m]_{W} = \frac{1}{2^{2S}} [(1+\Omega)^{2S-\lambda} (1-\Omega)^{\lambda}] {\binom{2S}{2S-\lambda}}$$
(19)

and note that this is equivalent to

$$[P_m]_{W} = \frac{1}{\lambda!} \frac{1}{2^{2S}} \lim_{z \to 0} \frac{d}{dz^{\lambda}} [(z+1) + \Omega(1-z)]^{2S}$$
(20)

with $\lambda = S - m$. Thus we have

$$[P_{m}]_{W}G[P_{m'}]_{W} = \frac{1}{\lambda!\lambda'!} \frac{1}{[2^{2S}]^{2}} \lim_{\substack{z \to 0 \\ z' \to 0}} \frac{d}{dz^{\lambda}} \frac{d}{dz'^{\lambda'}} [(z+1) + \Omega(1-z)]^{2S} G[(z'+1) + \Omega(1-z')]^{2S},$$
(21)

where G is given by equation (4). Substituting G given by equation (4) into equation (21) and carrying out the left- and right-hand differentiations, we obtain

$$[P_m]_{\mathbf{W}}G[P_{m'}]_{\mathbf{W}} = \frac{2^{-4S}}{\lambda!\lambda'!} \lim_{\substack{z\to0\\z'\to0}} \frac{\mathrm{d}}{\mathrm{d}z^{\lambda}} \frac{\mathrm{d}}{\mathrm{d}z'^{\lambda'}} E(z, z', \Omega),$$
(22)

where

$$E(z, z', \Omega) = \sum_{k=0}^{2S} \frac{(2S)!}{(2S-k)!k!} \{ [z+1+\Omega(1-z)][z'+1+\Omega(1-z')] \}^{2S-k} \times [(1-\Omega^2)(1-z)(1-z')]^k.$$
(23)

This last term can, by the binomial expansion, be reduced to

$$E(z, z', \Omega) = 2^{2S} \sum_{k=0}^{2S} (1+\Omega)^{2S-k} (1-\Omega)^k (zz')^k {\binom{2S}{k}}.$$
 (24)

Substituting this last expression into equation (22), we obtain

$$[P_m]_{\mathbf{W}}G[P_{m'}]_{\mathbf{W}} = \delta_{mm'} \frac{1}{2^{2S}} [(1+\Omega)^{S+m} (1-\Omega)^{S-m}] {\binom{2S}{S+m}}$$
(25)

which is our desired result.

We close this section by giving the Wigner equivalents of several operators, namely,

$$[S^{z}S^{z}]_{W} = S^{2} \left(\Omega^{2} + \frac{1}{2S} (1 - \Omega^{2}) \right),$$
(26)

$$[S^{z}S^{z}S^{z}]_{W} = S^{3} \left[\Omega^{3} + \left(\frac{3}{2S} - \frac{1}{2S^{2}}\right) \Omega(1 - \Omega^{2}) \right].$$
(27)

These functions (and mappings of higher powers of S^{z}) are implicit in the mapping of $e^{iS^{z}}$:

$$[e^{iS^{2}\theta}]_{W} = (\cos\frac{1}{2}\theta + i\Omega\sin\frac{1}{2}\theta)^{2S},$$
(28)

where $e^{iS^{z_{\theta}}}$ is a rotation operator parametrized by the angle θ . It can be verified by direct

substitution that the group property of the rotation operator is indeed preserved under the mapping, i.e.,

$$[e^{iS^{z}\theta_{1}}]_{W}G[e^{iS^{z}\theta_{2}}]_{W} = [e^{iS^{z}\theta_{3}}]_{W},$$
(29)

where

$$\theta_3 = \theta_1 + \theta_2. \tag{30}$$

3. Traces

We expect that in this type of formalism the trace of an operator goes over into an integral over its Wigner equivalent. The rule for obtaining the trace of an arbitrary operator $A(S^z)$ from its Wigner equivalent $A_w(\Omega)$ is, for a particle of spin S,

Tr A(S^z) =
$$\frac{2S+1}{2} \int_{-1}^{1} A_{W}(\Omega) d\Omega.$$
 (31)

This can be seen by noting that if A is a projection operator P_m , then the left-hand side of equation (31) has value unity. However, from equation (14) the right-hand side of equation (31) has the same value since

$$\frac{2S+1}{2}\int_{-1}^{1} (P_m)_{\mathbf{W}} \,\mathrm{d}\Omega = \frac{2S+1}{2}\int_{-1}^{1} \binom{2S}{S+m} \frac{1}{2^{2S}} [(1+\Omega)^{S+m}(1-\Omega)^{S-m}] \,\mathrm{d}\Omega = 1.$$
(32)

Again, since an arbitrary operator can be decomposed into projection operators, equation (31) follows immediately.

The trace of the product of operators $A(S^z)$ and $B(S^z)$ is given by

$$\operatorname{Tr}\left[A(S^{z})B(S^{z})\right] = \frac{2S+1}{2} \int_{-1}^{1} A_{W}(\Omega) GB_{W}(\Omega) \,\mathrm{d}\Omega.$$
(33)

This can then be integrated by parts to obtain

$$\int_{-1}^{1} A_{\mathbf{w}}(\Omega) GB_{\mathbf{w}}(\Omega) d\Omega = \int_{-1}^{1} \left[\bar{G}A_{\mathbf{w}}(\Omega) \right] B_{\mathbf{w}}(\Omega) d\Omega = \int_{-1}^{1} A_{\mathbf{w}}(\Omega) \left[\bar{G}B_{\mathbf{w}}(\Omega) \right] d\Omega, \quad (34)$$

where \bar{G} is the right differential operator

$$\bar{G} = 1 + \sum_{k=1}^{2S} \frac{(2S-k)!}{(2S)!k!} (-1)^k \frac{\bar{d}^k}{d\Omega^k} (1-\Omega^2)^k \frac{\bar{d}^k}{d\Omega^k}.$$
(35)

Some of the properties of the operator \overline{G} are shown in the appendix. One of these is

$$\bar{G} = 1 + \sum_{k=1}^{2S} \left(\prod_{l=1}^{k} \left[L^2 - l(l-1) \right] \frac{(2S-k)!}{(2S)!k!} \right),$$
(36)

where the operator L^2 is given by

$$L^{2} \equiv -\frac{\mathrm{d}}{\mathrm{d}\Omega} (1 - \Omega^{2}) \frac{\mathrm{d}}{\mathrm{d}\Omega}.$$
(37)

Note that the eigenfunctions of L^2 are Legendre polynomials having eigenvalues l(l+1), i.e.,

$$L^{2}\mathbf{P}_{l}(\Omega) = l(l+1)\mathbf{P}_{l}(\Omega).$$
(38)

Obviously the eigenfunctions of \bar{G} are also Legendre polynomials. In the appendix the eigenvalues are shown to be [(2S-l)!(2S+l+1)!]/[(2S)!(2S+1)!], i.e.,

$$\bar{G}P_{l}(\Omega) = \frac{(2S-l)!(2S+l+1)!}{(2S)!(2S+1)!}P_{l}(\Omega).$$
(39)

To illustrate the above, consider a simple $S = \frac{1}{2}$ problem. Let

$$A = a_0 + a_1 S^z \tag{40}$$

and

$$B = b_0 + b_1 S^2. (41)$$

The Wigner equivalents of these operators are

 $A_{\rm W} = a_0 + \frac{1}{2}a_1\Omega \tag{42}$

and

$$B_{\mathbf{W}} = b_0 + \frac{1}{2}b_1\Omega. \tag{43}$$

In addition

$$\bar{G} = 1 + L^2. \tag{44}$$

From the rule (33), we obtain

$$\operatorname{Tr} AB = \int_{-1}^{1} \left[(1+L^2)(a_0 + \frac{1}{2}a_1\Omega) \right] (b_0 + \frac{1}{2}b_1\Omega) \, \mathrm{d}\Omega$$
$$= \int_{-1}^{1} \left[(a_0 + \frac{3}{2}a_1\Omega)(b_0 + \frac{1}{2}b_1\Omega) \, \mathrm{d}\Omega = 2(a_0b_0 + \frac{1}{4}a_1b_1).$$
(45)

4. Many-particle systems

The generalization to a system of N particles is straightforward. We have

$$S_i^z \to S\Omega_i = (S_i^z)_W, \qquad i = 1, \dots, N$$

$$(46)$$

and

$$I_i \to 1 = (I_i)_{\mathbf{W}}, \qquad i = 1, \dots, N.$$

$$(47)$$

The operators G and \overline{G} now are products of the G_i and \overline{G}_i of the individual particles, i.e.,

$$G = \prod_{i=1}^{N} G_i \tag{48}$$

and

$$\bar{G} = \prod_{i=1}^{N} \bar{G}_i,\tag{49}$$

where the G_i and \overline{G}_i are given by (cf equations (4) and (35))

$$G_i = 1 + \sum_{k=1}^{2S} \frac{(2S-k)!}{(2S)!k!} \frac{\overline{\partial}^k}{\partial \Omega_i^k} (1 - \Omega_i^2)^k \frac{\overline{\partial}^k}{\partial \Omega_i^k}$$
(50)

and

$$\bar{G}_i = 1 + \sum_{k=1}^{2S} \frac{(-1)^k (2S-k)!}{(2S)!k!} \frac{\vec{\delta}^k}{\partial \Omega_i^k} (1 - \Omega_i^2)^k \frac{\vec{\delta}^k}{\partial \Omega_i^k}.$$
(51)

Traces are now multiple integrals, i.e., for an arbitrary operator we have

$$\operatorname{Tr} A(S_1^z, S_2^z \dots S_N^z) = \left[\frac{1}{2}(2S+1)\right]^N \int \dots \int A_{\mathbf{w}}(\Omega_1, \Omega_2, \dots, \Omega_N) \, \mathrm{d}\Omega_1 \dots \, \mathrm{d}\Omega_N.$$
(52)

We wish to close this section with some remarks about the Wigner equivalent of the density matrix. This density function satisfies the Wigner equivalent of the Bloch equation

$$\frac{\mathrm{d}}{\mathrm{d}\beta} \left[\mathrm{e}^{-\beta H} \right]_{\mathrm{W}} = -H_{\mathrm{W}} G \left[\mathrm{e}^{-\beta H} \right]_{\mathrm{W}} \tag{53}$$

with a formal 'solution'

$$[\mathbf{e}^{-\boldsymbol{\beta}H}]_{\mathbf{W}} = \mathbf{e}^{-\boldsymbol{\beta}H_{\mathbf{W}}G}\mathbf{1},\tag{54}$$

where H_W is the Wigner equivalent of the Hamiltonian H and H_WG is a right differential operator. For an exchange interaction of the form

$$H = \sum_{i,j} J_{ij} S_i^z S_j^z$$
(55)

we have

$$H_{\mathbf{W}} = S^2 \sum_{i,j} J_{ij} \Omega_i \Omega_j \tag{56}$$

and

$$H_{\mathbf{W}}G = \sum_{i,j} J_{ij} \Theta_i \Theta_j \tag{57}$$

where the operator Θ_i is given by

$$\Theta_i = S\Omega_i + \frac{1}{2}(1 - \Omega_i^2) \frac{\partial}{\partial \Omega_i}.$$
(58)

Appendix

In this appendix we will prove by induction that

$$Q_{k} = \frac{d^{k}}{d\Omega^{k}} (1 - \Omega^{2})^{k} \frac{d^{k}}{d\Omega^{k}} = Q_{k-1}[k(k-1) - L^{2}]$$
(A.1)

which makes equation (36) self-evident. Employing the notation

$$A = d/d\Omega \tag{A.2}$$

and

$$T = 1 - \Omega^2, \tag{A.3}$$

we can express Q_k as

$$Q_{k} = A^{k} T^{k} A^{k} = A^{k-1} [A, T^{k-1}] T A^{k} + A^{k-1} T^{k-1} A T A A^{k-1}$$

= $A^{k-1} [A, T^{k-1}] T A^{k} + A^{k-1} [A T A, A^{k-1}] + A^{k-1} T^{k-1} A^{k-1} A T A.$ (A.4)

Since

$$ATA = -L^2 \tag{A.5}$$

the last term in equation (A.4) is $-Q_{k-1}L^2$. To complete the proof we must demonstrate that the first two terms yield $Q_{k-1}k(k-1)$. The two terms give

$$A^{k-1}T^{k-1}\{[A, T]A^{k}(k-1) + A[T, A^{k-1}]A\}$$

= $A^{k-1}T^{k-1}\Big[(k-1)\Big(\sum_{j=1}^{k} A_{1} \dots A_{j-1}[[A, T], A_{j}]A_{j+1} \dots A_{k} + A^{k}[A, T]\Big)$
+ $A\Big(\sum_{j=1}^{k-1} A_{1} \dots A_{j-1}[[T, A_{j}]], A_{j+1} \dots A_{k-1}A_{k}] + A^{k-1}[T, A]\Big)\Big], (A.6)$

where $A_j = A$. Collecting terms and noting that

$$[[A, T], A] = 2 \tag{A.7}$$

we find that the right-hand side of equation (A.6) becomes

$$A^{k-1}T^{k-1}\left(2A^{k-1}k(k-1)-2A^{k-1}\sum_{j=1}^{k-1}\sum_{j=j+1}^{k}1\right) = A^{k-1}T^{k-1}A^{k-1}k(k-1).$$
(A.8)

This proves the recursion equation (A.1) for the Q_k .

The representation for \overline{G} given by equation (36) can be used to extract its eigenvalues. That is, from equation (36)

$$\bar{G}P_{l}(\Omega) = \left(1 + \sum_{k=1}^{2S} \prod_{n=1}^{k} \left[L^{2} - n(n+1) \frac{(2S-k)!}{(2S)!k!}\right] P_{l}(\Omega) \\ = \left(1 + \sum_{k=1}^{2S} \prod_{n=1}^{k} \left[l(l+1) - n(n+1)\right] \frac{(2S-k)!}{(2S)!k!} \right) P_{l}(\Omega)$$

$$= \left(1 + \sum_{k=1}^{2S} \frac{(2l+k)!}{(l-k)!} \frac{(2S-k)!}{k!} \right) P_{l}(\Omega).$$
(A.9)

But from an identity due to Rothe as quoted by Gould (1969)

$$\sum_{k=0}^{n} \frac{x}{x+bk} \binom{x+bk}{k} \frac{y}{y+b(n-k)} \binom{y+b(n-k)}{n-k} = \frac{x+y}{x+y+bn} \binom{x+y+bn}{n}.$$
 (A.10)

Using equation (A.10) in equation (A.9) with x = l+1, b = 1, and y = 2S - l + 1, we get equation (39) almost immediately.

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