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Extension of the Dirac identity

D J Klein

Department of Marine Sciences, Texas A&M University at Galveston, Galveston, Texas 77553, USA

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Abstract. A constructive proof is presented to show that, for any permutation P on spin space, $P+P^{-1}$ can be expressed as a linear combination of spin-operator products $\Pi\, s_m \cdot s_n$ with all the particle indices m, n in a product distinct.

1. Introduction

In many fermion systems the exchange of the particle spin is of importance (Dirac 1929) as in atomic (Van Vleck and Sherman 1935, Corson 1951, Harter 1971), nuclear (Harter 1971, Biedenharn 1963), and solid state (Herring 1963, Klein and Seitz 1973) problems. Then the Dirac identity (see these references and also Schrödinger (1941), Corson (1948), Lezuo (1972) and Partensky (1972) for extensions in other directions) relating spin operators and transpositions, i.e., two-particle permutations, is of use. Generalisations (see the references already cited) of this original result can describe effective m-body interactions with $m \geqslant 3$. One such case (Herring 1963, Klein and Seitz 1973) arises in the higher orders of degenerate perturbation expansions for the Heisenberg exchange interaction models; indeed, the extensions of the Dirac identity considered here are applicable to such a problem where the full Schrödinger Hamiltonian is spin-free and time-reversal invariant.

We are concerned with a spin space composed from N-fold tensor products of two-state spinors

$$\gamma^N : \{|\sigma_1 \otimes \sigma_2 \otimes \ldots \otimes \sigma_N\rangle;\ \sigma_i = \alpha \text{ or } \beta,\ \ i = 1 \text{ to } N\}. \tag{1.1}$$

Permutations P in the symmetric group $\mathscr{S}_N$ act on the particle indices, and we denote a cyclic permutation carrying n to 1 and i to $i+1$, $i = 1$ to $n-1$, by $(12\ldots n)$. Then the *Dirac identity* relates a transposition to the usual spin operators, as s_i for particle i,

$$(12) = 2s_1 \cdot s_2 + \tfrac{1}{2} \tag{1.2}$$

which is easily proven by comparing the actions of the left- and right-hand sides on the basis kets of γ^2. Similarly, one can establish

$$(123)+(132) = (12)+(23)+(31)-1, \tag{1.3}$$

a result which is (Herring 1963, Klein and Seitz 1973) only slightly less well known, and which expresses the sum $(123)+(132)$ of permutations in terms of spin operators, if (1.2) is substituted in for the transpositions on the right of (1.3). Here extensions of these relations involving more general permutations are to be established.

We let

$$X \equiv \sum_P x_P P \tag{1.4}$$

denote an element of the group algebra $\mathscr{A}_N$ of $\mathscr{S}_N$, with the x_P being scalars, $P \in \mathscr{S}_N$. If all the x_P are real, then X is *real.* We define a type of average

$$\langle X \rangle \equiv \tfrac{1}{2} \sum_P (x_P P + x_P^* P^{-1}) \tag{1.5}$$

termed the *Hermitian part* of X. Then in theorem 1 it is shown that for a real $X \in \mathscr{A}_N$, its Hermitian part can be expressed as a (real) linear combination of involutary (i.e., self-inverse) permutations. Since a transposition is the only cycle which is its own inverse, we see that the set $\mathscr{I}_N$ of involutary permutations consists of the identity and those $\tau \in \mathscr{S}_N$ which are products of disjoint transpositions. Thus using (1.2) every $\langle X \rangle$, for $X \in \mathscr{A}_N$ a real X, is expressed in terms of spin operators. The method of proof is largely constructive and is utilised to give explicit expressions for the $\langle P \rangle$ with P a representative of each class of $\mathscr{S}_5$. A second theorem establishes the situations under which $\mathscr{I}_N$ forms a basis to the real part of $\langle \mathscr{A}_N \rangle$.

2. Setting up the proof

The method of proof of the following three lemmas and theorem 1 are all of a similar type. First we note the identity

$$\langle P + \tau P \tau^{-1} \rangle = \langle \tau \langle \tau P + P \tau \rangle \rangle \qquad P \in \mathscr{S}_N,\ \tau \in \mathscr{I}_N. \tag{2.1}$$

Next suppose that there is a sequence

$$\tau_1, \tau_2, \ldots, \tau_z \tag{2.2}$$

of an odd number z of involutary permutations and corresponding sequence

$$P_0 \equiv P \qquad P_j \equiv \tau_j P_{j-1} \tau_j^{-1} \qquad j = 1 \text{ to } m,\ P \in \mathscr{S}_N \tag{2.3}$$

such that

$$\langle P_z \rangle = \langle P \rangle. \tag{2.4}$$

Then, utilising (2.1), we find

$$\langle P \rangle = \tfrac{1}{2} \sum_{j=1}^{z} (-1)^j \langle P_{j-1} + P_j \rangle = \tfrac{1}{2} \sum_{j=1}^{z} (-1)^j \langle \tau_j \langle \tau_j P_{j-1} + P_{j-1} \tau_j \rangle \rangle. \tag{2.5}$$

In the following we find that with the appropriate choices for the τ_i, $i = 1$ to z, and $P_0 = P$ the identity of (2.5) yields recurrence relations for $\langle P \rangle$ in terms of 'simpler' $\langle Q \rangle$. Thus the overall proof will be inductive starting with the results of (1.2) and (1.3) and expressing more and more 'complicated' $\langle P \rangle$ in terms of 'simpler' $\langle Q \rangle$ already known to be expressible in terms of $\tau \in \mathscr{I}_N$. When this is done we say P is *reducible*, and the heirarchical ordering for *complexity* is indicated implicitly in the proofs. Also we shall use, without making any special note, the fact that if $\tau \in \mathscr{I}_N$ and $P \in \mathscr{S}_N$ are disjoint, then $\langle \tau P \rangle = \tau \langle P \rangle$.

Lemma 1. If $P \in \mathscr{S}_6$, then $\langle P \rangle$ is reducible.

Proof. Equation (1.3) has established the result if P is a three-cycle. The remaining four non-trivial classes are considered as separate cases.

First case, $P = (1234)$. We choose a sequence

$$\tau_1 = (34),\ \tau_2 = (24),\ \tau_3 = (14)$$

for which $z = 3$ is odd and

$$P_0 = (1234),\ P_1 = (1243),\ P_2 = (1423),\ P_3 = (1234) = P.$$

Then (2.5) becomes

$$\langle(1234)\rangle = \tfrac{1}{2}\langle(34)\langle(123)+(124)\rangle - (24)\langle(314)+(312)\rangle + (14)\langle(123)+(423)\rangle\rangle.$$

Using (1.3) the inner brackets over three-cycles may be converted to scalars and transpositions, which in turn are multiplied by a τ_i, whence (1.3) may again be utilised. For example, in the first part of the above equation

$$\begin{aligned}\langle(34)\langle(123)\rangle\rangle &= \langle(34)\{(12)+(23)+(13)-1\}\rangle\\ &= \langle(12)(34)+(243)+(143)-(34)\rangle\\ &= (12)(34)+\tfrac{1}{2}\{(24)+(43)+(32)+(14)+(43)+(31)-2\}-(34).\end{aligned}$$

Thus $\langle(1234)\rangle$ is reduced to a sum over scalars, transpositions and disjoint products of two transpositions.

Second case, $P = (12345)$. We choose a sequence

$$\tau_1 = (23)(45),\ \tau_2(25)(14),\ \tau_3 = (12)(34)$$

for which $z = 3$ is odd and

$$P_0 = (12345),\ P_1 = (13254),\ P_2 = (43521),\ P_3 = (34512) = P.$$

Then (2.5) becomes

$$\begin{aligned}\langle(12345)\rangle = \tfrac{1}{2}\langle&(23)(45)\langle(135)+(124)\rangle - (25)(14)\langle(324)+(135)\rangle\\ &+(12)(34)\langle(135)+(245)\rangle\rangle.\end{aligned}$$

Here the three-cycles in the inner brackets are reducible to scalars and transpositions, which when multiplied by the τ_i yield three- or four-cycles, which are in their turn reducible. Thus (12345) is reducible.

Third case, $P = (123456)$. We choose a sequence

$$\tau_1 = (56),\ \tau_2 = (46),\ \tau_3 = (36),\ \tau_4 = (26),\ \tau_5 = (16)$$

in which case $z = 5$ is odd, and (2.5) becomes

$$\begin{aligned}\langle(123456)\rangle = \tfrac{1}{2}\langle&(56)\langle(12346)+(12345)\rangle - (46)\langle(12365)+(12345)\rangle\\ &+(36)\langle(12645)+(12345)\rangle - (26)\langle(16345)+(12345)\rangle\\ &+(16)\langle(62345)+(12345)\rangle\rangle.\end{aligned}$$

Here the five-cycles in the inner brackets are reduced, the results multiplied by the τ_i, and these resultants reduced.

Fourth case, $P = (123)(456)$. We choose the sequence

$$\tau_1 = (14),\ \tau_2 = (25),\ \tau_3 = (36)$$

in which case $z=3$ is odd and (2.5) may be applied. The $\langle \tau_j P_{j-1} + P_{j-1}\tau_j \rangle$ involve six-cycles which are reduced, then multiplied by τ_i, and reduction via earlier cases again carried out.

Lemma 2. $\langle (12 \ldots n) \rangle$ is reducible for all n.

Proof. This lemma is already established for all $n \leqslant 6$. We now proceed by induction presuming the lemma is true for all $n < N$, and establish it for $\langle (123 \ldots N) \rangle$. We choose a sequence

$$\tau_1 = (23)(45), \ \tau_2 = (23), \ \tau_3 = (45).$$

Then $z = 3$ is odd, and (2.5) becomes

$$\begin{aligned} \langle (12345 \ldots) \rangle = \tfrac{1}{2} \langle (23)(45) \langle (135 \ldots) + (124 \ldots) \rangle - (23) \langle (1254 \ldots) + (1345 \ldots) \rangle \\ + (45) \langle (1234 \ldots) + (1235 \ldots) \rangle \rangle \end{aligned}$$

where ... here denotes the sequence from 6 up to N. Here the $(N-2)$- and $(N-1)$-cycles are reducible via the induction hypothesis. Multiplying these reduced forms by the τ_i we find two-cycles, three-cycles, four-cycles, products of two disjoint three-cycles, and disjoint products of all these with $\tau \in \mathscr{S}_N$. But using lemma 1 all these are reducible.

Lemma 3. If P is a product of disjoint three-cycles, then $\langle P \rangle$ is reducible.

Proof. Let P be an m-fold product of three-cycles

$$P \equiv \prod_{i=1}^{m} (3i-2, 3i-1, 3i)$$

and choose a sequence

$$\tau_1 = (1, 4, 7, \ldots, 3m-2), \ \tau_2 = (2, 5, 8, \ldots, 3m-1), \ \tau_3 = (3, 6, 9, \ldots, 3m).$$

Applying (2.5), we find that $(3m)$-cycles arise in the inner brackets. These are reducible via lemma 2; then multiplication by τ_i yields various $\langle Q \rangle$ reduced by lemma 1.

3. The main results

The technique and lemmas of the preceding section may be utilised to show the following theorem.

Theorem 1. For any $P \in \mathscr{S}_N$, $\langle P \rangle$ is a linear combination of involutary permutations of $\mathscr{S}_N$.

Proof. Starting from the results of the lemmas we proceed by induction, presuming that the theorem is true for all $P \in \mathscr{S}_N$ with the total number K of indices in disjoint m-cycles of $m \geqslant 3$ such that $K < M$; then we establish the theorem for the M-index case. We presume P is of a case not covered by the previous lemmas, so that P consists of two non-trivial disjoint pieces, one of which is an n-cycle with $n \geq 4$; we identify such a decomposition thus:

$$P = (12 \dots n)Q.$$

Now choose a sequence $\tau_1, \tau_2, \dots, \tau_z$ in the same way as was done for an n-cycle in lemmas 1 and 2. Then $P_z = P$, and we may apply (2.5) where for this τ sequence the Q part of P is left unaffected. Hence $\tau_j P_{j-1}$ and $P_{j-1}\tau_j$ involve a disjoint factor Q and a second factor moving fewer than n indices. Then the K values for $\tau_j P_{j-1}$ and $P_{j-1}\tau_j$ are less than M, and the $\langle \tau_j P_{j-1}\rangle$ and $\langle P_{j-1}\tau_j\rangle$ are reducible via the induction hypothesis. The $\tau_j\langle \tau_j P_{j-1} + P_{j-1}\tau_j\rangle$ give rise to sums of the same kinds of permutations which arise in lemmas 1 and 2 at a similar stage. Thus $\langle P\rangle$ is reducible.

We record the explicit formulae

$$(1234)+(1432)=(12)(34)-(13)(24)+(14)(23)+(24)+(13)-1$$

$$\begin{aligned}(12345)+(15432)&\\ =&(12)(34)+(12)(35)+(12)(45)+(13)(45)+(14)(23)+(15)(23)\\ &+(15)(24)+(15)(34)+(23)(45)+(25)(34)-(13)(24)-(13)(25)\\ &-(14)(25)-(14)(35)-(24)(35)-(12)-(23)-(34)\\ &-(45)-(15)+(13)+(14)+(24)+(25)+(35)-3. \end{aligned} \tag{3.1}$$

Higher-order formulae, for $P \in \mathcal{S}_N$, $n \geq 6$ can be obtained straightforwardly, albeit tediously, from the proofs leading to theorem 1.

Our final theorem is as follows.

Theorem 2. The real space spanned by the $\langle P\rangle$, $P \in \mathcal{S}_N$ has $\mathcal{I}_N$ as a basis so long as $N \leq 7$; for $N \geq 8$ $\mathcal{I}_N$ is overcomplete.

Proof. We let $e_{rs}^{[\alpha]}$ denote a real matrix basis element of the group algebra $\mathcal{A}_N$, where irreducible representations occurring on the spin space γ^N are labelled by two-rowed Young diagrams

$$[\alpha] = [\tfrac{1}{2}N + S, \tfrac{1}{2}N - S] \tag{3.2}$$

with S being the spin of the irreducible representation. Now

$$e_{rs}^{[\alpha]} = \frac{f^{[\alpha]}}{N!}\sum_P \Gamma_{sr}^{[\alpha]}(P^{-1})P$$

with $\Gamma_{sr}^{[\alpha]}$ identifying the s, r element of the $[\alpha]$ irreducible representation of dimension

$$f^{[\alpha]} = \frac{N!\,(2S+1)}{(\frac{1}{2}N+S+1)!\,(\frac{1}{2}N-S)!}.$$

Then a basis for the real space spanned by the $\langle P\rangle$, $P \in \mathcal{S}_N$, is clearly

$$\langle e_{rs}^{[\alpha]}\rangle = \tfrac{1}{2}(e_{rs}^{[\alpha]} + e_{sr}^{[\alpha]}) \qquad 1 \leq r \leq s \leq f^{[\alpha]}, [\alpha] \text{ ranging}$$

(presuming the irreducible representations are real). Now this space has dimension.

$$\sum_S \tfrac{1}{2} f^{[\alpha]}(f^{[\alpha]}+1). \tag{3.3}$$

But the number of elements in the set $\mathscr{I}_N$, which by theorem 1 spans this space, is

$$\sum_{S} n_{(\alpha)} \tag{3.4}$$

where $n_{(\alpha)}$ is the number of elements in the Sth involutary conjugacy class, specified by the partition

$$(\alpha) \equiv (2^{\frac{1}{2}N-S}, 1^{2S}) \tag{3.5}$$

with S ranging over the same values as the overall spin. Here

$$n_{(\alpha)} = \frac{N!}{(\frac{1}{2}N-S)!\,2^{\frac{1}{2}N-S}}$$

and the remarkable identity

$$n_{(\alpha)} = \tfrac{1}{2}f^{[\alpha]}(f^{[\alpha]}+1) \tag{3.6}$$

is readily checked to hold for the corresponding (α) and $[\alpha]$ of (3.2) and (3.5) with $N \leqslant 7$. For $N = 8$

$$n_{(\alpha)} \leqslant \tfrac{1}{2}f^{[\alpha]}(f^{[\alpha]}+1)$$

with the inequality holding for a couple of values of S. Hence (3.3) and (3.4) are identical for $N \leqslant 7$ while (3.4) exceeds (3.3) for $N \geqslant 8$, and the theorem is established.

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