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ELECTRON-ELECTRON PARITY NON-CONSERVATION

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A B S T R A C T

We present a number of tensor identities, that we consider should be available for future work, they are obtained by a full tensor expansion of the parity non-conserving electron-electron interaction both in terms of a contact interaction and in terms of distributed operators.

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0.1 Introduction

As part of the calculation of the parity non-conserving electron-electron interaction in Samarium presented by Gongora (1986). We have expressed the various operators in terms of spherical tensors. These operators contain a δ -function of the separation r of the two particles as well as the momentum $p=-i\nabla$ and odd operators α , β . Since the derivations are quite lengthy we decided to present the expressions obtained so that they should be available for future work.

The parity non-conserving electron-electron interaction (H_{ee}), has been obtained relativistically in terms of a δ -function or contact interaction by Bouchiat and Bouchiat (1974), Sushkov and Flambaum (1978) and has been studied in terms of distributed operators by Hiller et al. (1978). In the latter form the matrix elements that previously contained the position δ -function now involve the electron wavefunctions over a full range of interparticle separations. One hopes in this way to obtain more accurately results with the available wavefunctions. In the case of a local potential the two forms should give identical results and we incorporated this as a numerical test on the correctness of the angular momentum calculations. We used Dirac wavefunctions throughout and obtained the same numerical results from the two forms - the results of this calculation are available in Gongora (1984).

In part II we start by presenting the full tensor expansion of H_{ee} corresponding to a contact interaction. In part III we move into the form of H_{ee} that is expressed in terms of distributed operators. Explicit expressions for the angular momentum relations used are presented in Judd (1963). We quote the main steps of the work by Hiller et al. (1978), but the interested reader is refer to their paper for more details.

0.2 PNC e-e CONTACT INTERACTION

The form we used for the PNC e-e interaction is;

$$H_{ee} = - \sum_{i \neq j} \frac{G_F}{4\sqrt{2}} (1 - 4\sin^2\theta_W) [\gamma_i^5 + \gamma_j^5 - \alpha_i \cdot \sigma_j - \sigma_i \cdot \alpha_j] \delta^3(\underline{r}_i - \underline{r}_j) \quad (1)$$

where G_F the Fermi constant, γ^5 and α are the Dirac matrices we used the convention of Bjorken and Drell (1964), and the σ are the Pauli matrices. We start by re-expressing the vector δ -function as a scalar product of tensors as given by Brink and Satchler (1968);

$$\delta(\underline{r}_i - \underline{r}_j) = \frac{1}{4\pi r_i^2} \delta(r_{ij}) \sum_k (2k+1) C_i^k \cdot C_j^k \quad (2)$$

which separates the radial and angular parts of this function, leaving the radial part contained in the scalar δ -function, the modified spherical harmonics obey the normalization given in Judd (1963).

When we combine equations (1) and (2) some terms contain a scalar product of two tensors of the same rank k which is defined by Judd (1963) as;

$$c_i^k \cdot c_j^k = \sum_q (-)^q c_{i-q}^k c_{j+q}^k \quad (3)$$

The rest are a combination of scalar products of tensors of rank 1 and rank k which can be recoupled in terms of i and j , by the use of a 6-j symbol we obtain;

$$\sigma_i \cdot \sigma_j \quad c_i^k \cdot c_j^k = \sum_{kq} (-)^{k+q+k+1} \left\{ \sigma_i c_i^k \right\}_q^k \left\{ \sigma_j c_j^k \right\}_{-q}^k \quad (4)$$

so equation (1) finally is written as;

$$H_{ee} = - \sum_{i \neq j} \frac{G_F}{4\sqrt{2}} (1-4\sin^2\theta_w) \sum_k (2k+1) [r_i^s + r_j^s] \left\{ \sum_q (-)^q c_{i-q}^k c_{j+q}^k \right.$$

$$= \sum_{\kappa Q} (-)^{K+K+Q+1} \left\{ \sigma_i c_{i,\kappa} \right\}_Q^K \left\{ \sigma_j c_{j,\kappa} \right\}_{-Q}^K \left\{ \frac{\delta r_{ij}}{4\pi r_{ij}^2} \right\} \quad (5)$$

0.3 H_{ee} IN TERMS OF DISTRIBUTED OPERATORS

We concentrate now on an alternative form of the initial operator H_{ee} , in which the position δ -function has been re-expressed in terms of equivalent distributed operators.

Following Hiller et al. (1978), we start with a Hamiltonian;

$$H = \sum_i c (\alpha_i \cdot p_i + \beta m_i c) + U^{\text{tot}} \quad (6)$$

where U^{tot} contains a sum of electron-electron and electron-nucleus parity conserving interactions as well as central field $U(r_i)$. The Breit interaction is not included in this approximation.

We write equation (1) in the following form;

$$\begin{aligned} H_{ee} &= \sum_{i \neq j} c_{ee} (\gamma_i^5 + \gamma_j^5) (1 - \alpha_i \cdot \alpha_j) \delta r_{ij} \\ &= \sum_{i \neq j} c_{ee} P_{ij} \delta r_{ij} \end{aligned} \quad (7)$$

where $C_{ee} = -(G_F/4\sqrt{2})(1-4\sin^2\theta_W)$ for this operator. Lengthy algebraic manipulations (Hiller et al.(1978)) then allows one to express the matrix element of (7) between states of opposite parity $|\alpha\rangle$ and $|\beta\rangle$, eigenstates of H , in terms of distributed operators;

$$\begin{aligned} H_{\alpha\beta} &= C_{ee} \langle \alpha | P_{ij} \delta r_{ij} | \beta \rangle \\ &= i \frac{C_{ee}}{4\pi} \left[\frac{\epsilon_\alpha - \epsilon_\beta}{c} \langle \alpha | h | \beta \rangle + 2i \langle \alpha | (P-Q) | \beta \rangle \right. \\ &\quad \left. - \frac{1}{c} \langle \alpha | [u^{\text{tot}}, h] | \beta \rangle \right] \end{aligned} \quad (8)$$

where;

$$h = \frac{1}{2} \sum_{i \neq j} h_{ij} = \frac{1}{2} \sum_{i \neq j} (\sigma_i - \sigma_j) \cdot f_{ij} + i (\sigma_i \times \sigma_j) \cdot f_{ij} \quad (9.1)$$

$$P = \frac{1}{2} \sum_{i \neq j} P_{ij} = \frac{1}{2} \sum_{i \neq j} \alpha_i \cdot f_{ij} \times p_i - \alpha_j \cdot f_{ij} \times p_j \quad (9.2)$$

$$\begin{aligned} Q = \frac{1}{2} \sum_{i \neq j} Q_{ij} &= \frac{1}{2} \sum_{i \neq j} i (\alpha_i \cdot \sigma_j f_{ij} \cdot p_i - \alpha_j \cdot \sigma_i f_{ij} \cdot p_j \\ &\quad + \alpha_j \cdot f_{ij} \sigma_i \cdot p_j - \alpha_i \cdot f_{ij} \sigma_j \cdot p_i) \end{aligned} \quad (9.3)$$

$$f_{ij} = \frac{f}{r^3} = \frac{f_i - f_j}{r^3} = - \nabla_i \left(\frac{1}{|f_i - f_j|} \right) \quad (9.4)$$

Equation (8) differs from theirs by a factor of c , because our Hamiltonian is in atomic units while theirs is in relativistic units.

As the above equations are expressed in terms of the function f we make use of its known expression in tensor form as given by Judd (1963);

$$f_{ij} = \frac{1}{2} \sum_{i \neq j} \sum_k \frac{(-)^k}{\sqrt{3!}} \left[\frac{r_i^{k-1}}{r_j^{k+1}} [k(2k-1)(2k+1)]^{1/2} [c_i^{k-1} c_j^k]^{(1)} \theta(r_j - r_i) + \right. \\ \left. \frac{r_j^k}{r_i^{k+2}} [(k+1)(2k+1)(2k+3)]^{1/2} [c_i^{k+1} c_j^k]^{(1)} \theta(r_i - r_j) \right] \quad (10)$$

where the first term corresponds to $r_i < r_j$ and the second to $r_i > r_j$.

We move now to the operator h , that contains on both terms the scalar product of two tensor operators, recoupling the Pauli matrices with the spherical harmonics of equation (10), we obtained for the first term;

$$(\sigma_i - \sigma_j) \cdot f_{ij} = \sum_k (-)^{k+1} \left[\frac{r_i^{k-1}}{r_j^{k+1}} [k(2k-1)(2k+1)]^{1/2} \left(\left\{ (\sigma_i c_i^{k-1})^k c_j^k \right\}_0^0 - \left\{ c_i^{k-1} (\sigma_j c_j^k)^{k-1} \right\}_0^0 \right) \right. \\ \left. + \frac{r_j^k}{r_i^{k+2}} [(k+1)(2k+1)(2k+3)]^{1/2} \left(\left\{ (\sigma_i c_i^{k+1})^k c_j^k \right\}_0^0 - \left\{ c_i^{k+1} (\sigma_j c_j^k)^{k+1} \right\}_0^0 \right) \right] \quad (11)$$

Where we have made an extra recoupling by means of a 6-j symbol in order to couple the operators acting on particle i together and independent of the ones acting on particle j, to make the full calculation easier. For the second term of (9.1) we expressed the cross product as a tensor of rank 1, and follow the same steps as for (11) obtaining;

$$\begin{aligned}
 i (\sigma_i \times \sigma_j) \cdot f_{ij} = \sum_R (-)^{k+1} \left\{ \frac{r_i^{k-1}}{r_j^{k+1}} [(2k-1)(2k+1)]^{1/2} \left[\sqrt{(k+1)} \left\{ (\sigma_i c_i^{k-1})^k (\sigma_j c_j^k)^k \right\}_0^0 + \sqrt{(k-1)} \left\{ (\sigma_i c_i^k)^{k-1} (\sigma_j c_j^k)^{k-1} \right\}_0^{(0)} \right] \right. \\
 \left. - \frac{r_j^k}{r_i^{k+2}} \sqrt{(2k+1)(2k+3)} \left[\sqrt{k} \left\{ (\sigma_i c_i^{k+1})^k (\sigma_j c_j^k)^k \right\}_0^{(0)} + \sqrt{(k+2)} \left\{ (\sigma_i c_i^{k+1})^{k+1} (\sigma_j c_j^k)^{k+1} \right\}_0^0 \right] \right\} \quad (12)
 \end{aligned}$$

Equations (11) and (12) are in terms of coupled tensors operators of rank zero, and sometimes, especially when reduced matrix elements are required it is better to work in terms of a product of tensors acting separately on particle i and j, this result is;

$$\begin{aligned}
 h = \frac{1}{2} \sum_{i \neq j} h_{ij} = \sum_R \sum_Q (-)^{Q+1} \left[\frac{r_i^{k-1}}{r_j^{k+1}} \sqrt{(2k-1)(2k+1)} \left(\frac{\sqrt{k}}{\sqrt{2k+1}} \left\{ (\sigma_i c_i^{k-1})_Q^k c_{j-Q}^k \right\} \right. \right. \\
 \left. \left. + \frac{\sqrt{k}}{\sqrt{2k-1}} \left\{ c_{i-Q}^{k-1} (\sigma_j c_j^k)_Q^{k-1} \right\} + \frac{\sqrt{k+1}}{\sqrt{2k+1}} \left\{ (\sigma_i c_i^{k-1})_Q^k (\sigma_j c_j^k)_{-Q}^k \right\} - \right. \\
 \left. \left. \frac{\sqrt{k-1}}{\sqrt{2k-1}} \left\{ (\sigma_i c_i^{k-1})_Q^{k-1} (\sigma_j c_j^k)_{-Q}^{k-1} \right\} \right) + \frac{r_j^k}{r_i^{k+2}} \sqrt{(2k+1)(2k+3)} \left(\frac{\sqrt{k+1}}{\sqrt{2k+1}} \left\{ (\sigma_i c_i^k)_Q^k c_{j-Q}^k \right\} + \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{\sqrt{k+1}}{\sqrt{2k+3}} \left\{ c_i^{k+1} (\sigma_j c_j^k)_{-Q}^{k+1} \right\} - \frac{\sqrt{k}}{\sqrt{2k+1}} \left\{ (\sigma_i c_i^{k+1})_Q^k (\sigma_j c_j^k)_{-Q}^k \right\} + \\
 & + \frac{\sqrt{k+2}}{\sqrt{2k+3}} \left\{ (\sigma_i c_i^{k+1})_Q^{k+1} (\sigma_j c_j^k)_{-Q}^{k+1} \right\} \Bigg] \quad (13)
 \end{aligned}$$

Now we move on to expressing the operator P , which is a symmetrical operator, so the different components of (9.2) are related by;

$$\alpha_j \cdot f_{ij} \times p_j = - (\alpha_i \cdot f_{ij} \times p_i)_{i \leftrightarrow j} \quad (14)$$

where $p_j = -i\nabla_j$ and its tensor form is given by Judd (1963), the appearance of p_j will require us to reduce the number of C_j appearing, when combined with f_{ij} in (9.2), for this purpose we use the equation;

$$(c^{k_1} c^{k_2})^k = \sqrt{2k+1} \begin{pmatrix} k_1 & k & k_2 \\ 0 & 0 & 0 \end{pmatrix} c^k$$

and follow the same procedure as with h_{ij} , to obtain;

$$\begin{aligned}
 \alpha_i \cdot f_{ij} \times p_i &= \sum_R \sum_Q \frac{(-)^Q}{\sqrt{2R+1}} \left[\sqrt{2k+1} \left((k+1) \frac{r_{i<}^{k-2}}{r_{j>}^{k+1}} - k \frac{r_{j<}^k}{r_{i>}^{k+3}} \right) \right. \\
 & \left(c_j^k [\alpha_i (c_i^k l_i)^k]_{-Q}^k \right) + \frac{r_{i<}^{k-2}}{r_{j>}^{k+1}} (2k+1) \sqrt{2k-1} \left(c_j^k [\alpha_i (c_i^k l_i)^{k-1}]_{-Q}^k \right) \\
 & \left. - \frac{r_{j<}^k}{r_{i>}^{k+3}} (2k+1) \sqrt{2k+3} \left(c_j^k [\alpha_i (c_i^k l_i)^{k+1}]_{-Q}^k \right) - \right]
 \end{aligned}$$

$$- \sqrt{k(k+1)(2k+1)} \left(\frac{r_{i<}^{k-1}}{r_{j>}^{k+1}} + \frac{r_{j<}^k}{r_{i>}^{k+2}} \right) \frac{\partial}{\partial r_i} c_{jQ}^k (\alpha_i c_i^k)^k_{-Q} \right] \quad (15)$$

changing in (15) $i \leftrightarrow j$ by (14) we obtained the corresponding expression for the second term of P_{ij} .

Finally we deal with the operator Q , and being also a symmetrical operator we have that;

$$- \alpha_j \cdot \sigma_i f_{ij} \cdot p_j + \alpha_j \cdot f_{ij} \alpha_i \cdot p_j = (\alpha_i \cdot \sigma_j f_{ij} \cdot p_i - \alpha_i \cdot f_{ij} \sigma_j \cdot p_i)_{i \leftrightarrow j} \quad (16)$$

Taking into account the (i) factor in equation (9.3) we obtained for the first term on the right hand side of (16);

$$\begin{aligned} i \alpha_i \cdot \sigma_j f_{ij} \cdot p_i &= \sum_{kQ} \sum_t (-)^{k+Q+t+1} \\ &\left\{ \sqrt{k(k+1)} \left(\frac{r_{i<}^{k-2}}{r_{j>}^{k+1}} + \frac{r_{j<}^k}{r_{i>}^{k+3}} \right) \left\{ \alpha_i (c_i^k)_t^k \right\}_Q^t \left\{ \sigma_j c_j^k \right\}_{-Q}^t \right. \\ &\left. - \left(k \frac{r_{i<}^{k-1}}{r_{j>}^{k+1}} - (k+1) \frac{r_{j<}^k}{r_{i>}^{k+2}} \right) \left(\frac{\partial}{\partial r_i} \right) \left\{ \alpha_i c_i^k \right\}_Q^t \left\{ \sigma_j c_j^k \right\}_{-Q}^t \right\} \end{aligned} \quad (17)$$

and using (16) we obtained the corresponding expression for $\alpha_j \cdot \sigma_i f_{ij} \cdot p_j$. For the second term of (16) we follow the same procedure as before but

because of the length of this calculation, we just give the final form of the operator which is;

$$\begin{aligned}
 -i \alpha_i \cdot f_{ij} \sigma_j \cdot p_i &= \sum_{R \in \mathbb{N}} (-)^{Q+1} \left\{ \frac{r_{i<}^{k-2}}{r_{j>}^{k+1}} \left(\frac{\sqrt{k(2k+1)(2k-3)(k-2)}}{(2k-1)} \right. \right. \\
 &\left. \left\{ [\alpha_i (c_i^{k-2} l_i)^{k-2}]_Q^{k-1} [\sigma_j c_j^k]_{-Q}^{k-1} \right\} + \frac{(2k+1)}{\sqrt{k(k-1)}} \left\{ [\alpha_i (c_i^k l_i)^{k-1}]_Q^{k-1} [\sigma_j c_j^k]_{-Q}^{k-1} \right\} \right. \\
 &+ \frac{\sqrt{(k+1)(2k-1)(2k+1)}}{\sqrt{k!}} \left\{ [\alpha_i (c_i^k l_i)^{k-1}]_Q^k [\sigma_j c_j^k]_{-Q}^k \right\} + \\
 &\left(\frac{\sqrt{k(R+1)}}{r_{j>}^{k+1}} \frac{r_{i<}^{k-2}}{\sqrt{k+1}} + \frac{\sqrt{k!}}{\sqrt{k+1}} \frac{r_{j<}^k}{r_{i>}^{k+3}} \right) \left\{ [\alpha_i (c_i^k l_i)^k]_Q^{k+1} [\sigma_j c_j^k]_{-Q}^{k+1} \right\} \\
 &+ \left(\frac{\sqrt{k+1}}{\sqrt{k!}} \frac{r_{i<}^{k-2}}{r_{j>}^{k+1}} - \frac{\sqrt{k}}{\sqrt{k+1}} \frac{r_{j<}^k}{r_{i>}^{k+3}} \right) \left\{ [\alpha_i (c_i^k l_i)^k]_Q^R [\sigma_j c_j^k]_{-Q}^R \right\} \\
 &+ \left(\frac{\sqrt{k+1}}{\sqrt{k!}} \frac{r_{i<}^{k-2}}{(2k-1) r_{j>}^{k+1}} + \frac{\sqrt{k(R+1)}}{\sqrt{k!}} \frac{r_{j<}^k}{r_{i>}^{k+3}} \right) \left\{ [\alpha_i (c_i^k l_i)^{k-1}]_Q^{k-1} [\sigma_j c_j^k]_{-Q}^{k-1} \right\} \\
 &+ \frac{r_{j<}^k}{r_{i>}^{k+3}} \left(\frac{\sqrt{(k+1)(2k+1)(2k+5)(k+3)}}{(2k+3)} \right) \left\{ [\alpha_i (c_i^{k+2} l_i)^{k+2}]_Q^{k+1} [\sigma_j c_j^k]_{-Q}^{k+1} \right\} \\
 &- \frac{(2k+1)}{\sqrt{(k+1)(k+2)}} \left\{ [\alpha_i (c_i^k l_i)^{k+1}]_Q^{k+1} [\sigma_j c_j^k]_{-Q}^{k+1} \right\} + \frac{\sqrt{k(2k+1)(2k+3)}}{\sqrt{k+1}} \left\{ [\alpha_i (c_i^k l_i)^{k+1}]_Q^k [\sigma_j c_j^k]_{-Q}^k \right\} \\
 &- \left[\frac{r_{i<}^{k-1}}{r_{j>}^{k+1}} (-) \frac{\sqrt{k(2k+1)(2k+3)(k-1)}}{(2k-1)} \right] \left\{ [\alpha_i c_i^{k-2}]_Q^{k-1} [\sigma_j c_j^k]_{-Q}^{k-1} \right\} \\
 &+ \left(k \frac{r_{i<}^{k-1}}{r_{j>}^{k+1}} - \frac{1}{(2k+3)} \frac{r_{j<}^k}{r_{i>}^{k+2}} \right) \left\{ [\alpha_i c_i^k]_Q^{k+1} [\sigma_j c_j^k]_{-Q}^{k+1} \right\} \\
 &+ \left(\frac{r_{i<}^{k-1}}{r_{j>}^{k+1}} + \frac{r_{j<}^k}{r_{i>}^{k+2}} \right) \left\{ (\alpha_i c_i^k)_Q^k (\sigma_j c_j^k)_{-Q}^k \right\}
 \end{aligned}$$

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