EXCHANGE OPERATORS IN SECOND QUANTIZATION FORMALISM*

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ABSTRACT

Using the representation of the generators of the U_4 group of supermultiplet theory in terms of creation and annihilation fermion operators, we express the exchange operators (Bartlett, Heisenberg, Majorana) in terms of the operators of spin and isospin and of the Casimir operator of the U_4 group (or equivalently, the Casimir operator of the associated $\mathfrak{U}_r$ group of orbital space). From these expressions, the eigenvalues for a long-range interaction with exchange follow trivially.

I. SECOND QUANTIZATION FORMULATION OF THE PROBLEM

A central two-body interaction with exchange effects is usually written as

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the operator

$$\sum_{i<j=1}^{n} (W + BP_{ij}^{\sigma} - HP_{ij}^{\tau} + MP_{ij}^{r})\, V(r_{ij}),$$

the parameters W, B, H and M specify a particular exchange mixture and are customarily normalized to unity, i.e. $W + B + H + M = 1$. In the limit of long range central force we can make the approximation of taking $V(r_{ij}) = -V_0$ (a constant), so we are left with the two-body interaction

$$I = -V_0 \sum_{a=0}^{3} A_a \sum_{i<j} P_{ij}^{(a)} \qquad (1)$$

($A_0 = W$, $A_1 = B$, $A_2 = -H$, $A_3 = M$), which is independent of the orbital coordinates of the particles since the exchange operators $P_{ij}^{(a)}$ depend only on the spin ($\vec{s}$) and isospin ($\vec{t}$) operators of a pair of particles. The explicit forms of the operators in (1) are [1]

$$P_{ij}^{(0)} = 1 \qquad \text{(Wigner)} \qquad (2a)$$

$$P_{ij}^{(1)} \equiv P_{ij}^{\sigma} = \tfrac{1}{2}(1 + 4\,\vec{s}_i \cdot \vec{s}_j) \qquad \text{(Bartlett)} \qquad (2b)$$

$$P_{ij}^{(2)} \equiv P_{ij}^{\tau} = \tfrac{1}{2}(1 + 4\,\vec{t}_i \cdot \vec{t}_j) \qquad \text{(Heisenberg)} \qquad (2c)$$

$$P_{ij}^{(3)} \equiv P_{ij}^{r} = -\tfrac{1}{4}(1 + 4\,\vec{s}_i \cdot \vec{s}_j)(1 + 4\,\vec{t}_i \cdot \vec{t}_j) \qquad \text{(Majorana)} \qquad (2d)$$

the eigenvalues of s_3 and t_3 being $\frac{1}{2}$, $-\frac{1}{2}$.

The second-quantized form of a general two-body interaction $\sum_{i<j} V_{ij}$ is[2]

$$\mathcal{V} = \frac{1}{2} \sum_{\rho_1 \rho_2} \sum_{\rho_1' \rho_2'} \langle \rho_1 \rho_2 | V_{12} | \rho_1' \rho_2' \rangle \{ b_{\rho_1}^+ b^{\rho_1'} b_{\rho_2}^+ b^{\rho_2'} - \delta_{\rho_2}^{\rho_1'} b_{\rho_1}^+ b^{\rho_2'} \} \tag{3}$$

b_ρ^+, $b^{\rho'}$ being, respectively, creation and annihilation fermion operators obeying the usual anticommutation rules, and ρ_i is an abridged notation for the quantum numbers of a state of the i^{th} particle: $\rho_i \equiv (\mu_i, \sigma_i, \tau_i)$ where $\mu_i = 1, 2, \ldots, r$ will characterize the orbital state, $\sigma_i = \pm \frac{1}{2}$ the spin state and $\tau_i = \pm \frac{1}{2}$ the isospin state. Now, if the interaction is independent of the orbital coordinates, as in (1), the summations over the indices μ in (3) can be performed immediately and we obtain for the second-quantized form of the operator I

$$\mathcal{I} = -V_0 \sum_{\alpha=0}^{3} A_\alpha \mathcal{P}^{(\alpha)} \tag{4}$$

with

$$\mathcal{P}^{(\alpha)} \equiv \frac{1}{2} \Sigma \langle \sigma_1 \tau_1, \sigma_2 \tau_2 | P_{12}^{(\alpha)} | \sigma_1' \tau_1', \sigma_2' \tau_2' \rangle \left\{ C_{\sigma_1 \tau_1}^{\sigma_1' \tau_1'} C_{\sigma_2 \tau_2}^{\sigma_2' \tau_2'} - \delta_{\sigma_2}^{\sigma_1'} \delta_{\tau_2}^{\tau_1'} C_{\sigma_1 \tau_1}^{\sigma_2' \tau_2'} \right\} \tag{5}$$

Here the sum is over all repeated indices and the C operators are defined as

$$C_{\sigma\tau}^{\sigma'\tau'} = \sum_{\mu=1}^{r} b_{\mu\sigma\tau}^{+} b^{\mu\sigma'\tau'} \tag{6}$$

From the anticommutation rules of the fermion operators it can be deduced that the 16 operators $C_{\sigma\tau}^{\sigma'\tau'}$ have the commutation rules of the generators of a four-dimensional unitary group: U_4. Our purpose is to show that the exchange operators $\mathbb{P}^{(\alpha)}$ of (5) can be expressed in terms of the Casimir operators of both the group U_4 and its subgroup SU_2 (spin) x SU_2 (isospin). Once this has been done the eigenvalues of $\mathbb{P}^{(\alpha)}$ will follow immediately, and furthermore, $\mathcal{J}$ will be diagonal in a basis spanning an irreducible vector space of U_4 and whose rows are classified by the subgroup SU_2 x SU_2, i.e. in the basis

$$|[\tilde{b}_1 \tilde{b}_2 \tilde{b}_3 \tilde{b}_4]\,\beta\, SM_S\,,\, TM_t> \tag{7}$$

II. SECOND-QUANTIZED FORM OF THE EXCHANGE OPERATORS

Following Moshinsky and Nagel [3] we define 16 operators constructed by linear combination from the U_4 generators $C_{\sigma\tau}^{\sigma'\tau'}$:

$$\mathfrak{n} = \sum_{\sigma\tau}\sum_{\sigma'\tau'} (M_0)_{\sigma}^{\sigma'} (N_0)_{\tau}^{\tau'} C_{\sigma\tau}^{\sigma'\tau'} \equiv \sum_{\sigma\tau} C_{\sigma\tau}^{\sigma\tau} \tag{8a}$$

$$S_k = \tfrac{1}{2} \sum \sum (M_k)_{\sigma}^{\sigma'} (N_0)_{\tau}^{\tau'} C_{\sigma\tau}^{\sigma'\tau'} \tag{8b}$$

$$T_k = \tfrac{1}{2} \sum \sum (M_0)_{\sigma}^{\sigma'} (N_k)_{\tau}^{\tau'} C_{\sigma\tau}^{\sigma'\tau'} \tag{8c}$$

$$R_{jk} = \tfrac{1}{4} \sum \sum (M_j)_{\sigma}^{\sigma'} (N_k)_{\tau}^{\tau'} C_{\sigma\tau}^{\sigma'\tau'} \tag{8d}$$

where $j, k = 1, 2, 3$ refer to cartesian components, and

$$M_0 = N_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ M_1 = N_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ M_2 = N_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ M_3 = N_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the unit matrix and the Pauli matrices whose rows and columns are labeled by $\sigma, \sigma' = \frac{1}{2}, -\frac{1}{2}$ for the M's, and by $\tau, \tau' = \frac{1}{2}, -\frac{1}{2}$ for the N's. Among the commutations relations between the operators (8) one has

$$[S_j, S_k] = i \sum_l \epsilon_{jkl} S_l, \; [T_j, T_k] = i \sum_l \epsilon_{jkl} T_l, \; [S_j, T_k] = 0$$

so that S_1, S_2, S_3 are the generators of the subgroup SU_2 (spin) and T_1, T_2, T_3 are the generators of the subgroup SU_2 (isospin), of U_4.

We can now return to equation (5) which gives the second-quantized version of the exchange operators $\mathbb{P}^{(\alpha)}$. For $\mathbb{P}^{(0)}$ we obtain from (2a) and (8a)

$$\mathbb{P}^{(0)} = \frac{1}{2} \sum_{\sigma\tau} C^{\sigma\tau}_{\sigma\tau} \left\{ \sum_{\sigma\tau} C^{\sigma\tau}_{\sigma\tau} - 1 \right\} = \frac{1}{2} \mathfrak{n} \{ \mathfrak{n} - 1 \} \tag{9}$$

For $\mathbb{P}^{(1)}$ we have

$$\mathbb{P}^{(1)} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \sum_{\sigma_1' \sigma_2'} \langle \sigma_1 \sigma_2 | P^{\sigma}_{12} | \sigma_1' \sigma_2' \rangle \sum_{\tau_1 \tau_2} \left\{ C^{\sigma_1' \tau_1}_{\sigma_1 \tau_1} C^{\sigma_2' \tau_2}_{\sigma_2 \tau_2} - \delta^{\sigma_1'}_{\sigma_2} \delta^{\tau_1}_{\tau_2} C^{\sigma_2' \tau_1}_{\sigma_1 \tau_1} \right\}$$

and since from (2b) the matrix element above has the value

$$\langle \sigma_1 \sigma_2 | P^{\sigma}_{12} | \sigma_1' \sigma_2' \rangle = \frac{1}{2} \delta^{\sigma_1'}_{\sigma_1} \delta^{\sigma_2'}_{\sigma_2} + 2 \sum_{k=1}^{3} \langle \sigma_1 | S^{(1)}_k | \sigma_1' \rangle \langle \sigma_2 | S^{(2)}_k | \sigma_2' \rangle$$

$$= \frac{1}{2} \delta^{\sigma_1'}_{\sigma_1} \delta^{\sigma_2'}_{\sigma_2} + \frac{1}{2} \sum_k (M_k)^{\sigma_1'}_{\sigma_1} (M_k)^{\sigma_2'}_{\sigma_2} \quad ,$$

we get finally

$$\mathfrak{p}^{(1)} = \tfrac{1}{4}\, \mathfrak{n}(\mathfrak{n} - 1) + \sum_{k=1}^{3} S_k S_k - \tfrac{3}{4}\, \mathfrak{n} \equiv \mathfrak{n}^2 - \mathfrak{n} + S^2 \tag{10}$$

where use has been made at an intermediate step of the fact that

$$\sum_k \sum_{\sigma_2} (M_k)^{\sigma_1}_{\sigma_2} (M_k)^{\sigma_2}_{\sigma_2'} = \sum_k (M_k M_k)^{\sigma_1}_{\sigma_2'} = 3\, \delta^{\sigma_1}_{\sigma_2'} \; .$$

For $\mathfrak{p}^{(2)}$ we obtain, by an entirely similar analysis

$$\mathfrak{p}^{(2)} = \tfrac{1}{4}\, \mathfrak{n}(\mathfrak{n} - 1) + \sum_{k=1}^{3} T_k T_k - \tfrac{3}{4}\, \mathfrak{n} \equiv \tfrac{1}{4}\, \mathfrak{n}^2 - \mathfrak{n} + T^2 , \tag{11}$$

and for $\mathfrak{p}^{(3)}$ we have

$$\mathfrak{p}^{(3)} = 2\, \mathfrak{n} - \tfrac{1}{2} \left[\tfrac{1}{4}\, \mathfrak{n}^2 + S^2 + T^2 + 4 \sum_{jk} R_{jk} R_{jk} \right] . \tag{12}$$

Now, if we define a tensor operator X_{qr} in U_4 by

$$X_{qr} = \sum_{\sigma\tau} \sum_{\sigma'\tau'} (M_q)^{\sigma}_{\sigma'} (N_r)^{\tau}_{\tau'} \, C^{\sigma'\tau'}_{\sigma\tau} \quad (q, r = 0, 1, 2, 3) \tag{13}$$

we find, by using the property of Pauli matrices

$$\sum_{q=0}^{3} (M_q)^{\sigma}_{\sigma'} (M_q)^{\sigma}_{\sigma'} = \sum_q (M_q \otimes M_q)^{\sigma\sigma}_{\sigma'\sigma'} = 2\,\delta^{\sigma}_{\sigma'}\,\delta^{\sigma}_{\sigma'}$$

that

$$\sum_{qr} X_{qr} X_{qr} = 4 \sum_{\sigma\tau} \sum_{\sigma'\tau'} C^{\sigma'\tau'}_{\sigma\tau} C^{\sigma\tau}_{\sigma'\tau'} \equiv 4\,G(U_4) \tag{14}$$

where $G(U_4)$ is the Casimir operator of U_4, which has the property of being diagonal in a basis irreducible under U_4, i.e. in the basis (7). But from (13) and (8) we see that $X_{oo} = \mathfrak{n}$, $X_{ko} = 2\,S_k$, $X_{ok} = 2\,T_k$, and $X_{jk} = 4\,R_{jk}$, so we have the alternative expression

$$\sum_{qr} X_{qr} X_{qr} = \mathfrak{n}^2 + 4\,S^2 + 4\,T^2 + 16 \sum_{jk} R_{jk} R_{jk} \tag{15}$$

Equations (14) and (15) allow us to rewrite $\mathfrak{p}^{(3)}$ in the form

$$\mathfrak{p}^{(3)} = 2\,\mathfrak{n} - \tfrac{1}{2}\,G(U_4) \tag{16}$$

If in analogy with (6) we define r^2 operators

$$\mathfrak{C}^{\mu'}_{\mu} = \sum_{\sigma\tau} b^{+}_{\mu\sigma\tau}\, b^{\mu'\sigma\tau} \tag{17}$$

we can show, from their commutation relations, that they are the generators of an r-dimensional unitary group: $\mathcal{U}_r$. This group also has its Casimir operator $G(\mathcal{U}_r)$ and using (6) and (17) together with the commutation rules for b_ρ^+ and $b^{\rho'}$ we find this relation between the Casimir operators of the U_4 and $\mathcal{U}_r$ groups

$$G(U_4) = (4 + r)\, \mathfrak{n} - G(\mathcal{U}_r) \tag{18}$$

Combining the above results into equation (4) we arrive at the long-range exchange operator

$$\mathcal{J} = - V_0 \{ \tfrac{1}{2} W \mathfrak{n}(\mathfrak{n} - 1) + \tfrac{1}{4} (B - H)\, \mathfrak{n}(\mathfrak{n} - 4) + BS^2 - HT^2 - \tfrac{r}{2} M \mathfrak{n} + \tfrac{1}{2} MG(\mathcal{U}_r) \} \tag{19}$$

This operator is thus diagonal in the basis (7). The eigenvalues of $G(\mathcal{U}_r)$ are known to be [4]

$$Nr + \sum_{\mu=1}^{r} b_\mu (b_\mu - 2\mu + 1),$$

where N is the number of particles, and $[\, b_1\, b_2 \dots b_r]$ is the label for the irreducible representation of $\mathcal{U}_r$ which in Supermultiplet Theory must have a Young pattern conjugate to the pattern of the representation $|[\, \tilde{b}_1\, \tilde{b}_2\, \tilde{b}_3\, \tilde{b}_4]$ of U_4.

Finally one has the algebraic eigenvalue equation

$$\mathcal{J}\, |\, [\tilde{b}]\, \beta\, SM_S, TM_t > \; = \; - V_0 \; \{ \tfrac{1}{2} WN(N - 1) + \tfrac{1}{4} (B - H)\, N(N - 4)$$

$$+ BS(S+1) - HT(T+1) + \frac{1}{2} M \sum_{\mu=1}^{r} b_\mu^{\cdot}(b_\mu^{\cdot} - 2\mu + 1) \} | [\tilde{b}] \beta S M_s, T M_t > \tag{20}$$

III. CONCLUSION

The operator $\mathcal{S}$ with eigenvalues given in (20) for states $|[\tilde{b}]\beta S M_s, T M_t>$ represents then the exchange operator for a long-range interaction. It has been shown elsewhere[5] that a good model for an arbitrary central potential is a combination of an orbital pairing interaction ($\mathbb{P}$) plus a quadrupole-quadrupole interaction (Q^2), the interaction $\mathbb{P}$ taking account of the short-range correlations while Q^2 takes into account the long-range ones. Since our operator $\mathcal{S}$ could be applied in the long-range case, it is reasonable to consider that a long-range interaction with exchange could be described by $Q^2 \mathcal{S}$. Use has been made of this type of interaction in calculations with exchange effects in the 2s-ld shell[5].

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