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Solving spin-1 problems using spin-1/2 methods

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It is shown how many problems involving aspects of spin-1 matrix algebra may be handled in a way analogous to the spin-1/2 algebra of the Pauli matrices. A number of examples of the main point are given in illustration.

INTRODUCTION

When one must illustrate spin effects in relativistic or nonrelativistic quantum-mechanical systems, most examples use spin-½, when possible, for simplicity because the algebra of the Pauli spin matrices σ_i ($i = 1, 2, 3$) allows reduction of spin matrix products to, at most, linear combinations of σ_i, and in addition permits straightforward unitary transformations to the most simple forms. In detail, the Pauli matrices have the anticommutation relations

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij} \tag{1}$$

as well as the usual commutation relations ($\sigma = 2\mathbf{S}$, where $\mathbf{S}$ are spin-½ spin matrices)

$$\sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon_{ijk}\sigma_k \tag{2}$$

(summing over repeated indices) which combine to give

$$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k. \tag{3}$$

Equation (3) leads to such diverse applications as unitary transformations of the Dirac equation,[1] and "derivation" of the electron's magnetic moment.[2]

It is the purpose of this paper to derive the algebraic equations for spin-1 analogous to Eq. (3) in a way that does not depend on a specific matrix representation of the spin-1 spin matrices, and to then illustrate by a number of specific examples how such algebraic equations may be used to simplify and sometimes solve spin-1 problems in a manner that is completely analogous to spin-½ considerations involving the Pauli matrix algebra.

In the next section the general idea of the derivation of the algebraic relations is outlined for any spin, and then the detailed results given for spin-1. This section is followed by several examples involving spin-1 Hamiltonians and other operators in which the spin-1 algebraic relations are used to good advantage.

SPIN-1 ALGEBRA

Because there exists the well-known 2×2 matrix representation of the Pauli matrices, all their properties may be found by explicit matrix algebra, in particular, Eqs. (1) and (3) may easily be discovered, and since the matrices correspond to spin-½, no higher products need be considered. The simplest spin-1 matrix representation is 3×3, and already in this case it becomes difficult to "discover" useful algebraic relations, particularly since one needs to look at triple products of spin matrices. It is, therefore, important to be able to derive Eq. (3) and its higher spin generalizations in a representation independent way.[3]

One solution to this question is to utilize the transformation properties of spin matrices and their products when they are subject to continuous Lorentz transformations (rotations and pure velocity transformations). A general Lorentz transformation of the coordinate four-vector X_μ (Greek indices run from 1 to 4) is written

$$X'_\mu = a_{\mu\nu}X_\nu, \tag{4}$$

$$a_{\mu\nu}a_{\mu\rho} = \delta_{\nu\rho}, \tag{5}$$

where $X_4 \equiv it$ (the speed of light being the velocity unit) and a_{ij}, ia_{4j}, ia_{j4}, and a_{44} are real numbers. For the symmetric, traceless covariantly defined spin tensor $\tilde{S}_{\mu\nu\rho}\cdots$ of rank $2s$ (spin s integer or half-integer), the corresponding transformation rule is[4]

$$(e^{i\tau\cdot\mathbf{S}})^\dagger\tilde{S}_{\mu\nu\rho\cdots}(e^{-i\tau\cdot\mathbf{S}}) = a_{\mu\alpha}a_{\nu\beta}a_{\rho\gamma}\cdots\tilde{S}_{\alpha\beta\gamma\cdots}, \tag{6}$$

where $\mathbf{S}$ are now the spin matrices for any spin and where τ are three complex parameters that define the particular Lorentz transformation. For example, for a pure Lorentz transformation (no rotation) with relative velocity $\mathbf{V}$

$$\tau = i\tanh^{-1}(v)\hat{\mathbf{V}}, \tag{7}$$

$$a_{ij} = \delta_{ij} + (\gamma - 1)\hat{V}_i\hat{V}_j, \qquad \gamma = 1/(1 - V^2)^{1/2}, \tag{8}$$

$$a_{i4} = -a_{4i} = i\gamma V_i, \tag{9}$$

$$a_{44} = \gamma. \tag{10}$$

By separately considering infinitesimal pure rotations and pure Lorentz transformations, all the elements of the spin tensor for a particular spin may be derived starting from $\tilde{S}_{44\cdots4}$ which must be a multiple of the identity matrix. The results for the lower elements are

$$\tilde{S}_{44\cdots4} = (i)^{2S}, \tag{11}$$

$$\tilde{S}_{4\cdots4j} = (i)^{2S-1}S_j/S, \tag{12}$$

$$\tilde{S}_{4\cdots4jk} = [(i)^{2S-2}/S(2S-1)]\{S_jS_k + S_kS_j - S\delta_{jk}\}. \tag{13}$$

By combining the specializations found from Eq. (6) for infinitesimal rotations and pure Lorentz transformations, the generalization of Eq. (3) may be derived, valid for any integer or half-integer spin.[5] The concern in the present paper is for the spin-1 algebra and it is given below.

In terms of the spin-1 spin tensor $\tilde{S}_{\mu\nu}$ and spin matrices S_i, the spin-1 algebraic relations following from Eq. (6) are

$$\tilde{S}_{ik}S_j = (-i/2)\{\delta_{ij}\tilde{S}_{4k} + \delta_{jk}\tilde{S}_{4i} + \epsilon_{jil}\tilde{S}_{lk} + \epsilon_{jkl}\tilde{S}_{il}\} \tag{14}$$

with

$$\tilde{S}_{44} = -1, \qquad \tilde{S}_{4j} = iS_j, \qquad \tilde{S}_{jk} = S_jS_k + S_kS_j - \delta_{jk}. \tag{15}$$

Substitution of Eq. (15) in Eq. (14) yields the spin-1 equation

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$$S_iS_jS_k + S_kS_jS_i = \delta_{ij}S_k + \delta_{jk}S_i. \quad (16)$$

Equation (16) is the spin-1 analog of Eq. (3) and may be used to reduce products of spin-1 matrices. Examples of Eq. (16) are the relations

$$(S_1^3) = S_1, \qquad S_1S_2S_1 = 0, \qquad S_1S_2S_3 + S_3S_2S_1 = 0. \quad (17)$$

Another common example is the characteristic equation for spin-1 matrices

$$(\mathbf{S}\cdot\hat{\mathbf{e}})^3 = \mathbf{S}\cdot\hat{\mathbf{e}}, \quad (18)$$

where $\hat{\mathbf{e}}$ is a unit vector with commuting components.

The applications of Eq. (16) are given in the next sections which involve generalizations of the characteristic equation, Eq. (18), and unitary and similarity transformations of Hamiltonians and other operators.

CHARACTERISTIC EQUATION APPLICATIONS

Suppose that both sides of Eq. (16) are contracted with the "minimal electromagnetic coupling" momentum operator $\boldsymbol{\pi} = \mathbf{P} - q\mathbf{A}$ for charge q and vector potential $\mathbf{A}$. Then one obtains

$$(\mathbf{S}\cdot\boldsymbol{\pi})^3 = \alpha\mathbf{S}\cdot\boldsymbol{\pi} + q\mathbf{B}\cdot\boldsymbol{\pi} \quad (19)$$

using the definition

$$\alpha \equiv \boldsymbol{\pi}\cdot\boldsymbol{\pi} - 2q\mathbf{S}\cdot\mathbf{B} \quad (20)$$

and

$$[\pi_i, \pi_j]_- = iq\epsilon_{ijk}B_k \quad (21)$$

for a constant magnetic field $\mathbf{B}$. Equation (19) is the generalization of Eq. (18) with $\hat{\mathbf{e}} = \hat{\mathbf{P}}$ to the external magnetic field case. The operator α commutes with $\mathbf{S}\cdot\boldsymbol{\pi}$ as well as π^2 and $\mathbf{S}\cdot\mathbf{B}$ and is very useful in problems involving a constant external magnetic field.

A. Eigenvalues of $\mathbf{S}\cdot\boldsymbol{\pi}$

The eigenvalue equation is

$$\mathbf{S}\cdot\boldsymbol{\pi}\psi = b\psi \quad (22)$$

for eigenfunctions ψ and eigenvalues b. Repeated application of $\mathbf{S}\cdot\boldsymbol{\pi}$ and the utilization of Eq. (19) yields

$$\{\alpha\mathbf{S}\cdot\boldsymbol{\pi} + qP_3B\}\psi = b^3\psi, \quad (23)$$

where $\mathbf{B}$ has been chosen to be in the z direction. This leads to the cubic equation

$$b^3 - \alpha b - qP_3b = 0, \quad (24)$$

where the eigenfunction ψ has been chosen to be the simultaneous eigenfunction of the mutually commuting Hermitian operators $\mathbf{S}\cdot\boldsymbol{\pi}$, α, and P_3. Equation (24) is in a form for solution by standard methods.[6]

B. Eigenvalues of the Sakata-Taketani Hamiltonian

The Sakata-Taketani Hamiltonian for a relativistic spin-1 charged particle[7] of mass m and anomalous g factor $\mathcal{H}$ interacting with a constant external magnetic field has the form

$$H_{\rm ST} = \{m + \alpha/2m\}\sigma_3 + \{\alpha/2m - (\mathbf{S}\cdot\boldsymbol{\pi})^2/m\}i\sigma_2 + (qBS_3/2m)(1 - \mathcal{H})(\sigma_3 + i\sigma_2). \quad (25)$$

As has been shown[8] and will be reviewed in a later section of this paper, Eq. (25) may be transformed in the special case $\mathcal{H} = 1$ (corresponding to a g factor of 2) to the more convenient form

$$H'_{\rm ST} = \{m^2 + \alpha - (qBP_3/m^2)\mathbf{S}\cdot\boldsymbol{\pi}\}^{1/2}\sigma_3. \quad (26)$$

Representing the energy eigenvalue of $H^1_{\rm ST}$ by E, one sees that by squaring and reorganizing, Eq. (26) can be reorganized to

$$\mathbf{S}\cdot\boldsymbol{\pi}\psi = (m^2/qBP_3)\{\alpha - m^2 - E^2\}\psi \quad (27)$$

which has the same form as Eq. (22) and so may be solved by using the same methods to obtain the $\mathcal{H} = 1$ eigenvalues of Eq. (25).

NONRELATIVISTIC HAMILTONIANS AND OTHER OPERATORS APPLICATIONS

A particularly useful set of algebraic relations arises when one defines the following set of spin-1 matrices

$$\Sigma_1 \equiv S_1^2 - S_2^2, \qquad \Sigma_2 \equiv S_1S_2 + S_2S_1, \qquad \Sigma_3 \equiv S_3. \quad (28)$$

Using Eq. (16) one may show that the Σ_i matrices have the algebra

$$\Sigma_1^2 = \Sigma_2^2 = \Sigma_3^2 = S_3^2, \quad (29)$$

$$\Sigma_i\Sigma_j + \Sigma_j\Sigma_i = 2\sigma_{ij}S_3^2, \quad (30)$$

$$\Sigma_i\Sigma_j - \Sigma_j\Sigma_i = 2i\epsilon_{ijk}\Sigma_k, \quad (31)$$

which combine to give

$$\Sigma_i\Sigma_j = \delta_{ij}S_3^2 + i\epsilon_{ijk}\Sigma_k \quad (32)$$

exactly the same algebra as the Pauli spin matrix algebra of Eq. (3).

Several examples are given below in which the Σ_i matrices appear in spin-1 Hamiltonians and other operators. Because of Eq. (16), many simplifications occur and the problems become similar to spin-$^1/_2$ problems.

A. Electric quadrupole moment Hamiltonian for spin-1

The interaction Hamiltonian for a spin-1 nucleus in a particular energy level and in an external electrostatic field gradient $\partial E_i/\partial X_j$ may be written utilizing the Wigner-Eckart theorem as[9]

$$H_{\rm INT} = -(Qq/4)(\partial E_i/\partial X_j)\{S_iS_j + S_jS_i\}, \quad (33)$$

where q is the charge and Q the size of the electric quadrupole moment. Because the external electric field $\mathbf{E}$ has zero divergence and zero curl at the position of the nucleus, its gradient tensor $\partial E_i/\partial X_j$ is symmetric and traceless and may, therefore, be chosen diagonal in principal axes. The standard form for the diagonal tensor is $-(qe/2)\mathrm{diag}(\eta - 1, -\eta - 1, 2)$ with all the other elements being zero. The parameters e and η specify the size and orientation of the field gradient. Substituting this form into Eq. (28) results in a simplified expression for $H_{\rm INT}$:

$$H_{\rm INT} = (q^2eQ/4)\{3S_3^2 - 2 + \eta\Sigma_1\}. \quad (34)$$

Because of the algebra of Eq. (32) one sees that S_3^2 commutes with all the Σ_i. One may, therefore, perform "rotations" on $\boldsymbol{\Sigma}\cdot\hat{\mathbf{e}}$ in Eq. (29) just as one may rotate $\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}$ in the spin-$^1/_2$ case. This particular problem, Eq. (29), simplifies if Σ_1 is "rotated" into Σ_3 because it will then be diagonal in the representation of spin-1 matrices which has $S_3 = \text{diag}(1, 0, -1)$ in units of $\hbar = 1$. The "rotation" is

$$RH_{\text{INT}}R^{\dagger} = (q^2eQ/4)\{3S_3^2 - 2 + nS_3\}, \qquad (35)$$

where

$$R = e^{(1/2)(S_3\Sigma_1/N)\theta} = \cos\theta/2 + (S_3\Sigma_1/N)\sin\theta/2 \qquad (36)$$

and

$$N^2 = -(S_3\Sigma_1)^2 = S_3^2, \qquad \theta = \pi/2. \qquad (37)$$

If, in addition to the electric quadrupole interaction, there is a magnetic dipole interaction, say $-(qB/2m)S_3$, a similar "rotation" of H_{INT} yields

$$H'_{\text{INT}} = \frac{q^2eQ}{4}\{3S_3^2 - 2\} + \frac{qB}{2m}\{1 - S_3^2\} + \left\{\left(\frac{qB}{2m}\right)^2 + \left(\frac{q^2eQn}{4}\right)^2\right\}^{1/2} S_3 \qquad (38)$$

which is diagonal in the same representation.

B. Asymmetrical rotor for spin-1

Consider the following general Hamiltonian

$$H = a + bS_3 + cS_1^2 + dS_2^2 + eS_3^2 + fS_1S_2 + gS_2S_1 \qquad (39)$$

with the coefficients restricted so that H is Hermitian. With the algebra of Eq. (32), one may rewrite the terms in Eq. (39) involving S_1 and S_2 to be linears combinations of Σ_1 and S_3^2. The results are

$$S_1^2 = 1 - S_3^2/2 + (1/2)\Sigma_1, \qquad (40)$$

$$S_2^2 = 1 - S_3^2/2 - (1/2)\Sigma_1, \qquad (41)$$

$$S_1S_2 = (1/2)\Sigma_2 + (i/2)S_3, \qquad (42)$$

$$S_2S_1 = (1/2)\Sigma_2 - (i/2)S_3. \qquad (43)$$

Thus H may be written in the following form:

$$H = a' + b'S_3 + c'\Sigma_1 + d'\Sigma_2 + e'S_3^2. \qquad (44)$$

Just as for the quadrupole Hamiltonian, H_{AR} may be "rotated" to a more convenient form in which it is manifestly diagonal. Defining the unitary operator

$$R = \exp[(1/2)S_3/N)\{c'\Sigma_1 + d'\Sigma_2\}\theta] \qquad (45)$$

with N now being defined by

$$N^2 = -\{S_3[c'\Sigma_1 + d'\Sigma_2]\}^2 = \{c'^2 + d'^2\}S_3^2, \qquad (46)$$

one may transform H into

$$H = RHR^{\dagger} = a' + e'S_3^2 + \{\cos\theta + (S_3/N)(c'\Sigma_1 + d'\Sigma_2)\sin\theta\} \times \{b'S_3 + c'\Sigma_1 + d'\Sigma_2\}. \qquad (47)$$

The most interesting case occurs when

$$\tan\theta = N/b'. \qquad (48)$$

Then the coefficients of Σ_1 and Σ_2 vanish and H' becomes

$$H' = a' + e'S_3^2 + [b'^2 + c'^2 + d'^2]^{1/2}S_3. \qquad (49)$$

The significance of the above Hamiltonian may be recognized by noting that the Hamiltonian for an asymmetrical rotor including quartic centrifugal distortion terms is[10]

$$H_{AR} = (1/2)\{S_1^2/I_1 + S_2^2/I_2 + S_3^2/I_3\} + (1/4)\sum_{ijkl}\tau_{ijkl}S_iS_jS_kS_l,$$

where $I_{1,2,3}$ are the principal moments of inertia of the rotor and τ_{ijkl} are distortion coefficients. It is clear that with the liberal use of Eq. (32), a very general form of H_{AR} may be put in the form of Eq. (39) and then diagonalized algebraically to the form of Eq. (49). Specifically, one may include all those terms $S_iS_jS_kS_l$ in the centrifugal distortion part of H_{AR} that do not contain an odd number of S_3 matrices.

C. Density matrix for a pure spin-1 state

The most general density matrix ρ for a spin-1 system is[11]

$$\rho = 1/3 + (1/2)\mathbf{P}\cdot\mathbf{S} + (1/4)Q_{ij}\{\tilde{S}_{ij} - (1/3)\delta_{ij}\}. \qquad (50)$$

The three parameters P_i and the five parameters Q_{ij} (note that Q_{ij} may be taken to be symmetric and traceless) describe a general spin-1 system[12] (called a mixed state, in general) in analogy to the density matrix for a general spin-½ system $\rho_{1/2} = (1/2)\{1 + \mathbf{P}\cdot\sigma\}$. For a pure state only four of the eight components of $\mathbf{P}$ and Q_{ij} are independent, and for a general mixed state all eight parameters are independent.[12]

A completely polarized state has $\mathbf{P} = (0, 0, 1)$ and $Q_{11} = Q_{22} = -1/3$, $Q_{33} = 2/3$. A completely aligned pure state has $\mathbf{P} = 0$ and $Q_{ij}Q_{ij} = 8/3$. In this case the four independent parameters can be chosen to be Q_{11}, Q_{22}, Q_{33}, and Q_{12}.

In both the completely polarized and the completely aligned cases, it is clear that only S_3^2 and Σ_i appear in the density matrix. This will also be ture for the specific mixed state with nonzero parameters P_3, Q_{11}, Q_{22}, Q_{33}, and Q_{12}. So the "rotation" technique may also be applied to these density matrices to bring them into diagonal form.

APPLICATIONS TO RELATIVISTIC HAMILTONIANS

A. Transformation of the Sakata-Taketani Hamiltonian

Referring again to Eq. (25) with $\mathcal{H} = 1$ so that the last term does not contribute, one may perform a similarity transformation[8] to obtain Eq. (26). This transformation can be considered the spin-1 analog of the Foldy-Wouthuysen transformation[13] for this particular Hamiltonian formulation of the relativistic spin-1 problem because Eq. (26) reduces directly in the small momentum approximation to the nonrelativistic Schrödinger equation. In detail the transformation operator is

$$S = e^{(1/2)\sigma_2\sigma_3\phi} = \cos\phi/2 + \sigma_2\sigma_3\sin\phi/2 \qquad (51)$$

which transforms H_{ST} from Eq. (25) into

$$SH_{\text{ST}}S^{-1} = \left[\cos\phi\left\{m + \frac{\alpha}{2m}\right\} - i\sin\phi\left\{\frac{\alpha}{2m} - \frac{(\mathbf{S}\cdot\pi)^2}{m}\right\}\right]\sigma_3 + \left[i\cos\phi\left\{\frac{\alpha}{2m} - \frac{(\mathbf{S}\cdot\pi)^2}{m}\right\} + \sin\phi\left\{m + \frac{\alpha}{2m}\right\}\right]\sigma_2. \qquad (52)$$

A great simplification may be realized by choosing ϕ so that the coefficient of the σ_2 term is zero (assuming for this application that σ_3 is diagonal). This is accomplished with the choice

$$\tan\phi = -i\,\frac{\{\alpha/2m - (\mathbf{S}\cdot\boldsymbol{\pi})^2/m\}}{\{m + \alpha/2m\}}. \qquad (53)$$

The result is Eq. (26) which can then be subject to further analysis. In particular the nonrelativistic approximation in Eq. (26) leads to

$$H'_{\rm ST} \cong \{m + \alpha/2m\}\sigma_3 \qquad (54)$$

the upper components corresponding to the Schrödinger equation for a spin-1 particle with a g factor of 2 in a constant external magnetic field.

B. Energy eigenvalues of $H_{\rm ST}$ for arbitrary $\mathcal{H}$

By restricting the relativistic spin-1 particle described by Eq. (25) to move in the $x - y$ plane (perpendicular to $\mathbf{B} = B\hat{\mathbf{z}}$) the exact energy eigenvalues may be directly obtained. The first step is to reduce Eq. (25) with $P_3 = 0$ and $\boldsymbol{\pi} = \boldsymbol{\pi}_\perp = \mathbf{P}_\perp - q\mathbf{A}_\perp$ to a three-component form by choosing

$$\sigma_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The result is an equation for a three-component function ψ_u, the upper three components of the six-component Sakata-Taketani wave function, with the form

$$[m^2 + \alpha + (1 - \mathcal{H})qBS_3 + (1 - \mathcal{H})(qB/m^2)S_3(\mathbf{S}\cdot\boldsymbol{\pi}_\perp)^2]\psi_u = E^2\psi_u. \qquad (55)$$

Since

$$(\mathbf{S}\cdot\boldsymbol{\pi}_\perp)^2 = (1/2)\{\Sigma_1(\pi_1^2 - \pi_2^2) + \Sigma_2(\pi_1\pi_2 + \pi_2\pi_1)\} + (1 - S_3^2/2)\alpha + (1/2)qBS_3, \qquad (56)$$

one has [using Eq. (32)]

$$S_3(\mathbf{S}\cdot\boldsymbol{\pi}_\perp)^2 = (i/2)\{\Sigma_2(\pi_1^2 - \pi_2^2) - \Sigma_1(\pi_1\pi_2 + \pi_2\pi_1)\} + (1/2)\alpha S_3 + (1/2)qBS_3^2. \qquad (57)$$

Equation (55) becomes with this substitution

$$\Big[m^2 + \alpha + (1 - \mathcal{H})\frac{q^2B^2}{2m^2}S_3^2 + (1 - \mathcal{H})qB \times \left(1 + \frac{\alpha}{2m^2}\right)S_3 + (1 - \mathcal{H})\frac{qB}{2m^2}i\{\Sigma_2(\pi_1^2 - \pi_2^2) - \Sigma_1(\pi_1\pi_2 + \pi_2\pi_1)\}\Big]\psi_u = E^2\psi_u. \qquad (58)$$

Following the previous methods for "rotation" of the $\boldsymbol{\Sigma}\cdot\hat{\mathbf{e}}$ term to S_3, one may eliminate the Σ_1 and Σ_2 terms in Eq. (58). The result is the eigenvalues of Eq. (55) which are

$$E^2 = M^2 + \alpha + (1 - \mathcal{H})(q^2B^2/2m^2)S_3^2 + (1 - \mathcal{H})qB\{(1 + \alpha/2m^2)^2 - (\alpha^2 - q^2B^2)/4m^4S_3^2\}^{1/2}S_3. \qquad (59)$$

These eigenvalues are the same as those found by Tsai and co-workers[14] for the Proca theory.[15]

The same method works equally well for other relativistic formulations of the spin-1 problem.

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