Frame Transformations for Fermions

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Abstract

The analog to the Legendre addition theorem is found for half-integral angular momentum using frame transformations for rotor states.
I. INTRODUCTION

The Legendre addition theorem for spherical harmonics applies to the coupling of two particles with equal orbital angular momentum $\ell$ to give total orbital angular momentum of zero. If we denote the spherical angles of particle one by $(1) = (\theta_1, \phi_1)$, and of particle two by $(2) = (\theta_2, \phi_2)$, then the addition theorem for spherical harmonics becomes

$$\sqrt{4\pi/(2\ell + 1)} \sum_m (-1)^m \psi_{-m}^I(1)\psi_m^I(2) = \psi_0^I(\bar{I}),$$

where $(\bar{I}) \equiv (\bar{\theta}_1, \bar{\phi}_1)$ are the body coordinates of particle one with respect to particle two. The addition theorem represents a transformation from lab coordinates $(1)$ and $(2)$ to body coordinates $(\bar{I})$ called a *frame transformation*. The addition theorem is symmetric with respect to exchange of coordinates $(1)$ and $(2)$ or, equivalently, $(\bar{I})$ and $(\bar{2})$. Because the total angular momentum in the lab frame is zero, the left and right hand sides of the equation are rotational invariants.

It is interesting that the only attribution of this addition theorem to Legendre found by the authors in the current literature is in the book by Whittaker and Watson which was initially published in 1902 [1,2]. Today, the addition theorem for spherical harmonics is derived without any reference given to Legendre because it is so widely known and so easily proven. For example, the well known book by Rose [3] on angular momentum theory gives two proofs of the addition theorem without references.

When the two coupled orbital angular momenta are not equal, so that the total angular momentum is not zero, a generalized addition theorem or frame transformation can still be derived for rotor states as shown by Chang and Fano [4]. Indeed, the addition theorem of Legendre is a special case of the frame transformation for rotor states. Frame transformations are used to transform from a weakly coupled basis in which two particles move nearly independently to a strongly coupled one in which one of the particles ‘follows’ the other. In effect, we transform from the lab frame in the weakly coupled case to the body frame in the strongly coupled case. Frame transformations were used by Chang and Fano for diatomic molecules in which an electron was weakly coupled to the molecular frame at large distances but strongly coupled nearby. Their frame transformations theory was put on a firm group theoretical footing using the representation theory of rotors with the systematic treatment of inversions and molecular symmetries by Harter, et al [5]. We will follow the
latter treatment here. However, in this work what is called the strongly coupled basis was called the Born-Oppenheimer Approximate (BOA) basis in [5]. Frame transformation theory uses the standard matrix relations of rotor states given by Casimir [6]. For a detailed exposition of rotor representation theory in physics, we refer the reader to the books by Biedenharn and Louck [7] and Harter[8] and the references therein.

Surprisingly, after nearly two hundred years, there is no analogous addition theorem when the coupled angular momenta are equal and half-integral which occurs for spin one-half particles. That is, in the above equation, what happens when we replace integral \( \ell \) by half-integral \( j \) so that the wavefunctions are no longer spherical harmonics? The left hand side of (1.1) will still be a rotational invariant. However, on the right hand side \( \psi^j_0(1) \) is not defined because \( j \) is half-integral and the body-axis projection is half-integral as well and cannot be zero. Is there, then, an analogous addition theorem for half-integral \( j \)?

The purpose of this work is to extend the addition theorem for spherical harmonics and the frame transformations for rotor states to the case of half-integral angular momentum coupling. This would correspond to the coupling of two particles which have both integral orbital angular momentum \( \ell \) and intrinsic spin one-half angular momentum \( \frac{1}{2} \). That is, we will consider the angular momentum coupling of two fermions in the \( j - j \) coupling limit which is useful for atomic and nuclear shell theory. We give frame transformations for the general case of the coupling of unequal half-integral angular momentum states and then the corresponding addition theorem for the coupling of equal half-integral angular momentum states which is special case of these frame transformations. Below, in order to make this presentation self-contained, we first rederive the spin zero frame transformation relations of Chang and Fano [4] and the addition theorem of Legendre [1], using the formalism of Harter, et al [5] before proceeding to their spin one-half analogs.

II. SPIN ZERO PARTICLES (BOSONS)

A. Weakly Coupled Basis

We let particle one have orbital angular momentum \( l_1 \) and particle two have orbital angular momentum \( l_2 \) and assume that the interaction between them is such that the total angular momentum \( L = l_1 + l_2 \) is conserved. We may write the total angular momen-
tum wavefunction as a product wavefunction of the spherical harmonics using the Wigner coupling coefficients such that

$$\Psi_{\ell_1 \ell_2}^{LM}(weak) = \sum_{m_1, m_2} C_{m_1 m_2}^{\ell_1 \ell_2 L} \psi_{m_1}^{\ell_1}(1) \psi_{m_2}^{\ell_2}(2), \quad (2)$$

where the condition $m_1 + m_2 = M$ on such sums is understood implicitly. We call this wavefunction the weakly coupled basis which is appropriate if the two particles are not strongly coupled. However, if the two particles are strongly coupled so that one particle ‘follows’ the other, then it is better to transform to the moving frame of one of the particles, say, particle two. Such a transformation is called a frame transformation. In order to effect such a transformation it is necessary to use rotor wavefunctions.

B. Strongly Coupled Basis and Rotor States

We let particle two define the body frame so that the body $\bar{z}$-axis is at spherical angles $(\theta_2, \phi_2)$ with respect to the lab z-axis and corresponds to Euler angles $(\theta_2, \phi_2, \gamma_2)$ where $\gamma_2$ is an arbitrary rotation about the body $\bar{z}$-axis. We use the standard rotor wavefunctions [5-8] such that

$$\psi_{m_2}^{\ell_2}(2) \equiv \sqrt{(2\ell_2 + 1)/4\pi} D_{m_2}^{l_2}(2). \quad (3)$$

We may now transform the particle one wavefunction into this body frame using

$$\psi_{m_1}^{\ell_1}(1) = \sum_{m_1'} D_{m_1 m_1'}^{l_1*}(2) \psi_{m_1'}^{l_1}(\bar{1}). \quad (4)$$

Note that the Euler angle $\gamma_2$ is superfluous in (3) but not in (1). Physically in (1) $m_1$ is the projection of the angular momentum along the lab z-axis, whereas $m_1'$ is the projection of the angular momentum along the body $\bar{z}$-axis as defined by particle two. In (3) we have $m_2' = 0$, so the projection of the angular momentum along the body $\bar{z}$-axis is zero. This is necessary because a point particle can have no orbital angular momentum about an axis through it. The same would be true if (3) represented the wavefunction about the axis of a diatomic molecule as was the case considered by Chang and Fano [4].

We may now rewrite (2) so that
\[
\Psi_{\ell_1 \ell_2}^{LM}(weak) = \sqrt{(2\ell_2 + 1)/4\pi} \sum_{m_1, m_2, m'_1} C_{m_1m_2 M}^{\ell_1 \ell_2 L} D_{m_1m'_1}^{l_1 \ast}(2) D_{m_20}^{l_2 \ast}(2) \psi_{m'_1}^{l_1}(\bar{1}). \tag{5}
\]

Using the relations,
\[
\sum_{m_1, m_2} C_{m_1m_2 M}^{\ell_1 \ell_2 L} D_{m_1m'_1}^{l_1 \ast}(2) D_{m_20}^{l_2 \ast}(2) = C_{m'_10 m_1}^{\ell_1 \ell_2 L} D_{MM'}^{l_1 \ast}(2), \tag{6}
\]
we find the frame transformations for spin zero particles:
\[
\Psi_{\ell_1 \ell_2}^{LM}(weak) = \sqrt{(2\ell_2 + 1)/4\pi} \sum_{m'_1} C_{m'_10 m_1}^{\ell_1 \ell_2 L} D_{MM'}^{l_1 \ast}(2) \psi_{m'_1}^{l_1}(\bar{1}) \tag{7}
\]
\[
= \sqrt{(2L + 1)/4\pi} \sum_{m'_1} (-1)^{l_1-m'_1} C_{m'_1-m'_0}^{L \ell_1 \ell_2} D_{MM'}^{l_1 \ast}(2) \psi_{m'_1}^{l_1}(\bar{1})
\]
\[
= \sum_{m'_1} (-1)^{l_1-m'_1} C_{m'_1-m'_0}^{L \ell_1 \ell_2} \Psi_{l_1 \ell_2 m'_1}^{LM}(strong),
\]
where we define the strongly coupled basis to be
\[
\Psi_{\ell_1 \ell_2 m'_1}^{LM}(strong) = \sqrt{(2L + 1)/4\pi} D_{MM'}^{l_1 \ast}(2) \psi_{m'_1}^{l_1}(\bar{1}). \tag{8}
\]

In the strongly coupled basis we couple the total angular momentum \(L\) to that of particle one \(l_1\) to get the orbital angular momentum of particle two \(l_2\). This is equivalent to angular momentum subtraction where \(L - l_1 = l_2\). The rotor wavefunction \(D_{MM'}^{l_1 \ast}(2)\) has total angular momentum quantum number \(L\) and carries the particle one orbital angular momentum projection \(m'_1\) along its body \(\bar{z}\)-axis.

If we let the total angular momentum be zero, \(L = 0\), so that \(M = m'_1 = 0\) and \(\ell_1 = \ell_2 \equiv \ell\), we find
\[
\sum_{m} C_{-m m 0}^{\ell \ell 0} \psi_{m}^{l}(1) \psi_{m}^{l}(2) = (-1)^{l} \psi_{0}^{l}(\bar{1})/\sqrt{4\pi},
\]
or the addition theorem for spherical harmonics, namely, the Legendre addition theorem for spin zero particles:
\[
\sqrt{4\pi/(2\ell + 1)} \sum_{m} (-1)^{m} \psi_{-m}^{l}(1) \psi_{m}^{l}(2) = \psi_{0}^{l}(\bar{1}). \tag{9}
\]
Note that while in the lab frame the total angular momentum $L$ is zero, in the body frame the total angular momentum is $l$. The total angular momentum is not conserved in the body frame because it is not an inertial frame. However, the projection of the angular momentum along both the lab $z$-axis and the body $\bar{z}$-axis is zero. We now wish to derive the equivalent addition theorem for a system in which both particles have spin one-half in addition to their orbital angular momenta. Below, we will derive the frame transformations for total angular momentum $J$ and then let $J = 0$ to derive the analogous addition theorem for two spin one-half particles.

III. SPIN ONE-HALF PARTICLES (FERMIONS)

A. Weakly Coupled Basis

We now let the two particles have spin one-half in addition to their angular momentum using the $j - j$ coupling scheme. Particle one has total angular momentum $j_1 = l_1 + \frac{1}{2}$, particle two has total angular momentum $j_2 = l_2 + \frac{1}{2}$, and the total angular momentum of the two particles is $J = j_1 + j_2$. The weakly coupled basis using $j - j$ coupling now becomes

$$
\Psi^{JN\ell_1\ell_2}_{j_1j_2}(weak) = \sum_{n_1, n_2} C_{n_1 n_2}^{\ell_1 \ell_2} J \psi_{n_1}(1) \psi_{n_2}(2)
$$

We could equally well have used $L - S$ coupling instead of $j - j$ coupling to prove the relations below, although the derivation is more difficult. Note that in the sums above the sums on $m_1, \sigma_1$ are restricted by the condition $m_1 + \sigma_1 = n_1$ and the sums on $m_2, \sigma_2$ are restricted by the condition $m_2 + \sigma_2 = n_2$.

B. Strongly Coupled Basis and Rotor States

We now transform to the body $\bar{z}$-axis of particle two. In addition to (3) and (4) for transformations of the orbital wavefunctions, we also have the following transformations for the spin wavefunctions:
\[ \chi_{\tilde{\sigma}_2}(2) \equiv \sum_{\sigma'_2} D_{\sigma_2 \sigma'_2}(2), \]  

(11)

and

\[ \chi_{\tilde{\sigma}_1}(1) = \sum_{\sigma'_1} D_{\sigma_1 \sigma'_1}(2) \chi_{\tilde{\sigma}_1}(1). \]  

(12)

The spin functions \( \chi_{\tilde{\sigma}_2}(2) \) in (11) have the proper normalization as shown below. It is interesting to compare (3) with (11). In (3) we see that the body component of \( \psi_{m_2}(2) \) is \( m'_2 = 0 \), whereas in (11) we see that the body component of \( \chi_{\tilde{\sigma}_2}(2) \) is a linear combination of the possible components \( \sigma'_2 = -\frac{1}{2} \) and \( \sigma'_2 = +\frac{1}{2} \). This means that, physically, there is an equal likelihood of finding \( \sigma'_2 \) to be \( -\frac{1}{2} \) or \( +\frac{1}{2} \) about an arbitrary body axis. Indeed, we may use (3) and (11) as the actual definitions of \( \psi_{m_2}(2) \) and \( \chi_{\tilde{\sigma}_2}(2) \), respectively, in order to properly specify the lab and body components of orbital and spin angular momentum. In this sense any other definition would be incomplete.

Using the relations

\[ \sum_{m_1, \sigma_1} C_{m_1 \sigma_1 n_1}^{j_1} D_{m_1 m'_1}(2) D_{\sigma_1 \sigma'_1}^{j_1}(2) = C_{m'_1 \sigma'_1 n'_1}^{j_1} D_{n_1 n'_1}(2), \]  

(13)

where \( m'_1 + \sigma'_1 = n'_1 \) and

\[ \sum_{m_2, \sigma_2} C_{m_2 \sigma_2 n_2}^{j_2} D_{m_2 \sigma'_2}(2) D_{\sigma_2 \sigma'_2}^{j_2}(2) = C_{0 \sigma'_2 \sigma'_2}^{j_2} D_{n_2 \sigma'_2}(2), \]  

(14)

we find

\[ \Psi_{J_{1J_{2}}, \ell_1 \ell_2}(weak) = \sqrt{(2\ell_2 + 1)/4\pi} \sum_{n_1, n_2, \sigma_2, \sigma'_2} C_{n_1 n_2 J}^{j_1 j_2} D_{n_1 n'_1}(2) D_{n_2 \sigma_2}(2) \]  

\[ \times \sum_{m'_1, \sigma'_1} C_{m'_1 \sigma'_1 n'_1}^{j_1} \psi_{m_1}(\tilde{1}) \chi_{\tilde{\sigma}_1}(1). \]

It is important to note that the sum on \( m'_1, \sigma'_1 \) is restricted by the condition \( m'_1 + \sigma'_1 = n'_1 \).

Using

\[ C_{n'_1 \sigma'_2 (n'_1 + \sigma'_2)}^{j_1 j_2} D_{n'_1 + \sigma'_2}(2) = \sum_{n_1, n_2} C_{n_1 n_2 J}^{j_1 j_2} D_{n_1 n'_1}(2) D_{n_2 \sigma'_2}(2), \]
and

\[ \psi^{j_1}_{n_1'}(\mathbf{T}) \equiv \sum_{m_{n_1}' \sigma_{n_1}'} C^{j_1}_{m_{n_1}' \sigma_{n_1}'} \psi_{m_{n_1}'}^{j_1}(\mathbf{T}) \chi^{\frac{1}{2}}_{\sigma_{n_1}'}(\mathbf{T}) , \]  

we find the frame transformation for spin one-half particles:

\[ \Psi_{J_1 J_2}^{J N \ell_1 \ell_2}(\text{weak}) = \sqrt{(2\ell_2 + 1)/4\pi} \sum_{n_{1}'} \sum_{\sigma_{n_1}'} \sum_{\ell_{2}} C_{0 \sigma_{n_1}'}^{j_2} \sum_{n_{1}'} \sum_{\sigma_{n_1}'} ^{j_1} C_{n_{1}' \sigma_{n_1}'}^{j_2} J_{n_{1}', n_{1}'+\sigma_{n_1}'} D_{N,n_{1}'+\sigma_{n_1}'}^{J_{n_1}'}(2) \psi^{j_1}_{n_1} \]  

where we define the strongly coupled basis to be

\[ \Psi_{J_1 J_2}^{J N \ell_1 \ell_2}(\text{strong}) = \sqrt{(2J + 1)/4\pi} D_{N,n_{1}'+\sigma_{n_1}'}^{J_{n_1}'}(2) \psi^{j_1}_{n_1} \]  

The above should be compared with (7) and (5). In the strongly coupled basis we couple the total angular momentum \( J \) to that of particle one \( j_1 \) to get the orbital angular momentum of particle two \( j_2 \) corresponding to angular momentum subtraction \( J - j_1 = j_2 \). We then couple the angular momentum \( j_2 \) to the spin of particle two to get the orbital angular momentum of particle two \( l_2 \) corresponding to angular momentum subtraction \( l_2 = j_2 - \frac{1}{2} \). The rotor state with total angular momentum quantum number \( J \) carries the sum of angular momentum projections of particle one \( n_{1}' \) and particle two \( \sigma_{n} \) along its body \( \bar{z} \)-axis, where \( n_{1}' = m_{n_1} + \sigma_{n_1} \).

To derive the addition theorem for spin one-half particles we let \( J = 0 \), so that \( N = 0 \) and \( n_{1}' = -\sigma_{n} \). Then from (10), (16) and (17) letting \( j_1 = j_2 = j \) and \( n_1 = -n_2 = -n \), we find

\[ \sum_{n} C_{-n}^{j} \psi_{-n}(1) \psi_{n}(2) = \sum_{\sigma_{n}'} (-1)^{\frac{j-1}{2}} C_{-\sigma_{n}'}^{j} \psi_{-\sigma_{n}'}(2)/\sqrt{4\pi} , \]

or the addition theorem for spin one-half particles:

\[ \sqrt{4\pi/(2j + 1)} \sum_{n} (-1)^{j+n} \psi_{-n}(1) \psi_{n}(2) = (-1)^{j-\frac{1}{2}} \left\{ \frac{[\psi_{\frac{j}{2}}(\mathbf{T}) + \psi_{\frac{j}{2}}(\mathbf{T})]}{\sqrt{2}} \text{ for } \ell_2 = j + \frac{1}{2} \right\} , \]

where we have evaluated the Wigner coupling coefficients. This should be compared to (9) for spin zero particles. Keep in mind that \( \psi_{\frac{j}{2}}(\mathbf{T}) \) and \( \psi_{\frac{j}{2}}(\mathbf{T}) \) on the right of (18) refer to \( j = j_1 \) and are given by (15). We may write these explicitly for \( \ell_1 = j + \frac{1}{2} \).
\[
\psi_j^\ell(T) = \sqrt{\frac{2j+3}{4j+4}} \psi_{j+\frac{1}{2}}^\ell(\mathbf{1}) \chi_{\frac{3}{2}}^\ell(T) - \sqrt{\frac{2j+1}{4j+4}} \psi_{j-\frac{1}{2}}^\ell(\mathbf{1}) \chi_{\frac{1}{2}}^\ell(T),
\]
\[
\psi_{j-1}^\ell(T) = -\sqrt{\frac{2j+3}{4j+4}} \psi_{j-\frac{1}{2}}^\ell(\mathbf{1}) \chi_{\frac{3}{2}}^\ell(T) + \sqrt{\frac{2j+1}{4j+4}} \psi_{j+\frac{1}{2}}^\ell(\mathbf{1}) \chi_{\frac{1}{2}}^\ell(T),
\]
and for \( \ell_1 = j - \frac{1}{2} \),
\[
\psi_j^{\ell_1}(T) = \sqrt{\frac{2j-1}{4j}} \psi_{j-\frac{1}{2}}^{\ell_1}(\mathbf{1}) \chi_{\frac{1}{2}}^{\ell_1}(T) + \sqrt{\frac{2j+1}{4j}} \psi_{j-\frac{1}{2}}^{\ell_1}(\mathbf{1}) \chi_{\frac{1}{2}}^{\ell_1}(T),
\]
\[
\psi_{j-1}^{\ell_1}(T) = \sqrt{\frac{2j-1}{4j}} \psi_{j-\frac{1}{2}}^{\ell_1}(\mathbf{1}) \chi_{\frac{1}{2}}^{\ell_1}(T) + \sqrt{\frac{2j+1}{4j}} \psi_{j-\frac{1}{2}}^{\ell_1}(\mathbf{1}) \chi_{\frac{1}{2}}^{\ell_1}(T).
\]

Thus (18) actually consists of four different cases corresponding to \( \ell_1 = j \pm \frac{1}{2} \) and \( \ell_2 = j \pm \frac{1}{2} \).

For interaction operators, such as the Coulomb interaction, which depend only on the relative coordinates \((\mathbf{1})\) between the two particles, it is much easier to evaluate matrix elements in \( j - j \) coupling using the strongly coupled basis on the right of (18).

We can derive a special case of (18) for pure spin states if we let \( \ell_1 = \ell_2 = 0 \) so that \( j = \frac{1}{2} \), \( \psi_j^\ell = \chi_{\frac{1}{2}}^\ell/\sqrt{4\pi} \), and \( \psi_{j-1}^\ell = \chi_{-\frac{1}{2}}^\ell/\sqrt{4\pi} \) on the left and right of (18). The addition theorem for spin states alone becomes:
\[
\left[ \chi_{\frac{1}{2}}^{\ell}(\mathbf{1}) \chi_{-\frac{1}{2}}^{\ell}(2) - \chi_{-\frac{1}{2}}^{\ell}(\mathbf{1}) \chi_{\frac{1}{2}}^{\ell}(2) \right]/\sqrt{2} = \left[ \chi_{\frac{1}{2}}^{\ell}(\mathbf{1}) - \chi_{-\frac{1}{2}}^{\ell}(\mathbf{1}) \right]/\sqrt{2}. \quad (19)
\]
This same equation may also be derived by substituting (11) and (12) directly on the left of (19) and using the spin one-half Wigner coupling coefficients. Note that from the definition of the spin functions in (11) we have
\[
\psi_0^\frac{1}{2} = \chi_0^\frac{1}{2}/\sqrt{4\pi} = \sum_{\sigma} D_{\sigma\sigma} \left( \frac{1}{2} \right)(2)/\sqrt{4\pi}, \quad (20)
\]
which has proper normalization for the rotational matrices.

The addition theorem for fermions above is antisymmetric with respect to exchange of particles (1) and (2) or, equivalently, \((\mathbf{1})\) and \((\mathbf{2})\). It is perhaps surprising that in the body frame the wavefunction appears as a linear combination of spin one-half particles although the total angular momentum is zero in the lab frame. However, only the lab frame is an inertial frame so that the angular momentum in the body frame need not be zero.
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