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Summation formulae for spherical spinors

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Abstract. The summation formulae for spinor spherical waves ($j=l\pm 1/2$), analogous to the well known summation formulae for ordinary spherical harmonics, are derived. The summation over magnetic quantum number gives a combination of unit and Pauli matrices with coefficients depending on the Legendre polynomials and their derivatives. Application to the full scattering solution of the Dirac equation is also described.

The purpose of this paper is to derive the summation formulae for spherical spinors, analogous to the well known summation formula for spherical harmonics (Edmonds 1959)

$$\sum_{m=-l}^{l} Y_{lm}^{*}(\hat{n}) Y_{lm}(\hat{q}) = \frac{2l+1}{4\pi} P_l(\hat{n}\cdot\hat{q}) \tag{1}$$

where $\hat{n}$ and $\hat{q}$ are two unit vectors. The spherical wavefunctions of a particle with spin $\frac{1}{2}$ and defined value of total angular momentum j (spherical spinors) can be written in the standard notation as (Berestetskii *et al* 1972, Rose 1957)

$$\Omega_{\kappa m}(\hat{n}) = \begin{bmatrix} \left(\dfrac{j+m}{2j}\right)^{1/2} Y_{lm-1/2}(\hat{n}) \\ \left(\dfrac{j-m}{2j}\right)^{1/2} Y_{lm+1/2}(\hat{n}) \end{bmatrix} \tag{2a}$$

for $j=l+\frac{1}{2}$, i.e. $\kappa=-l-1=-j-\frac{1}{2}$, and

$$\Omega_{\kappa m}(\hat{n}) = \begin{bmatrix} -\left(\dfrac{j-m+1}{2j+2}\right)^{1/2} Y_{lm-1/2}(\hat{n}) \\ \left(\dfrac{j+m+1}{2j+2}\right)^{1/2} Y_{lm+1/2}(\hat{n}) \end{bmatrix} \tag{2b}$$

for $j=l-\frac{1}{2}$, i.e. $\kappa=l=j+\frac{1}{2}$. The quantum number κ combines j and parity.

The full continuum solution of the Dirac equation (Darwin 1928) contains expressions of the type

$$\sum_{m} \Omega_{\pm\kappa m}(\hat{r}) \Omega_{\kappa m}^{\dagger}(\hat{p}) \tag{3}$$

where $\hat{r}$ is the unit radius vector and $\hat{p}$ is the unit vector in the direction of the particle's asymptotic momentum. To our knowlege no explicit summation formula of type (3) has been derived and it is the purpose of the present paper to fill this gap. A summation formula of this type proved to be very useful in the analysis of relativistic and retardation effects in photo-ionization (for the non-relativistic analysis of retardation effects see Bechler and Pratt 1989, 1990 and Cooper 1990, 1993).

Since expression (3) is a 2×2 matrix it can be written as

$$\sum_m \Omega_{\kappa m}(\hat{r})\Omega^{\dagger}_{\kappa m}(\hat{p}) = aI + \boldsymbol{b}\cdot\boldsymbol{\sigma} \tag{4}$$

where I is the unit matrix and $\boldsymbol{\sigma}$ are the Pauli matrices. Since both spherical spinors in (4) correspond to the same value of the orbital angular momentum and therefore have the same parity, the coefficient a is a scalar function of $\hat{p}\cdot\hat{r}$ and $\boldsymbol{b}$ is a pseudo-vector proportional to $\hat{p}\times\hat{r}$. Due to rotational invariance of (4) we can choose $\hat{p}$ as the direction of quantization without any limitations to the generality of final formulae. With this choice of quantizaiton axis only spherical harmonics Y_{lM} with $M=0$ in (2) contribute to (4). Using

$$Y_{l0}(\hat{p}) = \left(\frac{2l+1}{4\pi}\right)^{1/2} \qquad Y_{l0}(\hat{r}) = \left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\hat{p}\cdot\hat{r}) \tag{5}$$

we obtain from (2) and (5) for $\kappa=-j-\frac{1}{2}$

$$\sum_m \Omega_{\kappa m}(\hat{r})\Omega^{\dagger}_{\kappa m}(\hat{p}) = \begin{bmatrix} \frac{l+1}{4\pi} P_l(\hat{p}\cdot\hat{r}) & \left(\frac{l(l+1)}{4\pi(2l+1)}\right)^{1/2} Y_{l,-1}(\hat{r}) \\ \left(\frac{l(l+1)}{4\pi(2l+1)}\right)^{1/2} Y_{l,1}(\hat{r}) & \frac{l+1}{4\pi} P_l(\hat{p}\cdot\hat{r}) \end{bmatrix}. \tag{6}$$

Denoting by θ the angle between $\hat{p}$ and $\hat{r}$ and by φ the azimuthal angle of $\hat{r}$ in the plane perpendicular to $\hat{p}$ we have

$$Y_{l,\pm1}(\hat{r}) = \mp\left[\frac{(2l+1)(l-1)!}{4\pi(l+1)!}\right]^{1/2} \sin\theta P'_l(\hat{p}\cdot\hat{r}) \exp(\pm i\varphi) \tag{7}$$

where P'_l denotes the derivative of the Legendre polynomial with respect to its argument. Using (7) and (6) we can easily find the coefficients a and $\boldsymbol{b}$ in (4)

$$a = \frac{l+1}{4\pi} P_l(\hat{p}\cdot\hat{r}),\ \boldsymbol{b} = \frac{i}{4\pi} P'_l(\hat{p}\cdot\hat{r})(\hat{p}\times\hat{r}) \tag{8}$$

where we have used $\hat{r}=(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. For $\kappa=-j-\frac{1}{2}$ $(j=l+\frac{1}{2})$ we have therefore

$$\sum_m \Omega_{\kappa m}(\hat{r})\Omega^{\dagger}_{\kappa m}(\hat{p}) = \frac{l+1}{4\pi} P_l(\hat{p}\cdot\hat{r}) + \frac{i}{4\pi} P'_l(\hat{p}\cdot\hat{r})(\hat{p}\times\hat{r})\cdot\boldsymbol{\sigma}. \tag{9a}$$

Proceeding along similar lines we find for $\kappa=j+\frac{1}{2}$ $(j=l-\frac{1}{2})$

$$\sum_m \Omega_{\kappa m}(\hat{r})\Omega^{\dagger}_{\kappa m}(\hat{p}) = \frac{l}{4\pi} P_l(\hat{p}\cdot\hat{r}) - \frac{i}{4\pi} P'_l(\hat{p}\cdot\hat{r})(\hat{p}\times\hat{r})\cdot\boldsymbol{\sigma}. \tag{9b}$$

The other two summation formulae for spherical spinors read

$$\sum_m \Omega_{-\kappa m}(\hat{r})\Omega^\dagger_{\kappa m}(\hat{p}) = \frac{1}{4\pi} P'_l(\hat{p}\cdot\hat{r})\hat{p}\cdot\sigma - \frac{1}{4\pi} P'_{l+1}(\hat{p}\cdot\hat{r})\hat{r}\cdot\sigma \qquad (10a)$$

for $\kappa = -j - \frac{1}{2}$ and

$$\sum_m \Omega_{-\kappa m}(\hat{r})\Omega^\dagger_{\kappa m}(\hat{p}) = -\frac{1}{4\pi} P'_l(\hat{p}\cdot\hat{r})\hat{p}\cdot\sigma + \frac{1}{4\pi} P'_{l+1}(\hat{p}\cdot\hat{r})\hat{r}\cdot\sigma \qquad (10b)$$

for $\kappa = j + \frac{1}{2}$. Expressions (10) are pseudo-scalars since parities of $\Omega_{-\kappa m}$ and $\Omega_{\kappa m}$ are different.

To show a possible application we use (9) and (10) in the partial wave expansion of the full scattering solution of the Dirac equation in the form used by Pratt *et al* (1973) and Scofield (1989) to describe the photoeffect.

$$\Psi_p(r) = 4\pi \sum_{\kappa m} \left[\Omega^\dagger_{\kappa m}(\hat{p})\phi \right] \mathrm{i}^l \exp(-\mathrm{i}\delta_\kappa) \begin{bmatrix} R_\kappa \Omega_{\kappa m}(\hat{r}) \\ \mathrm{i}S_\kappa \Omega_{-\kappa m}(\hat{r}) \end{bmatrix} \qquad (11)$$

wehre ϕ is a two component spinor describing the spin state of the continuum electron, δ_κ are the phase shifts and the R_κ, S_κ are radial functions. Denoting by $\varphi_p(r)$ and $\chi_p(r)$ the upper and lower component of $\Psi_p(r)$, respectively, we obtain, by virtue of (9) and (10)

$$\varphi_p(r) = \sum_{l=0}^{\infty} \mathrm{i}^l \exp(-\mathrm{i}\delta_l^{(-)}) R_l^{(-)}(r) \left[(l+1)P_l(\hat{p}\cdot\hat{r}) - \mathrm{i}P'_l(\hat{p}\cdot\hat{r})(\hat{r}\times\hat{p})\cdot\sigma \right] \varphi$$
$$+ \sum_{l=0}^{\infty} \mathrm{i}^l \exp(-\mathrm{i}\delta_l^{(+)}) R_l^{(+)}(r) \left[lP_l(\hat{p}\cdot\hat{r}) + \mathrm{i}P'_l(\hat{p}\cdot\hat{r})(\hat{r}\times\hat{p})\cdot\sigma \right] \varphi \qquad (12)$$

and

$$\chi_p(r) = \mathrm{i} \sum_{l=1}^{\infty} \mathrm{i}^l \exp(-\mathrm{i}\delta_l^{(-)}) S_l^{(-)}(r) \left[P'_l(\hat{p}\cdot\hat{r})\hat{p}\cdot\sigma - P'_{l+l}(\hat{p}\cdot\hat{r})\hat{r}\cdot\sigma \right] \varphi$$
$$-\mathrm{i} \sum_{l=1}^{\infty} \mathrm{i}^l \exp(-\mathrm{i}\delta_l^{(+)}) S_l^{(+)}(r) \left[P'_l(\hat{p}\cdot\hat{r})\hat{p}\cdot\sigma - P'_{l-1}(\hat{p}\cdot\hat{r})\hat{r}\cdot\sigma \right] \varphi. \qquad (13)$$

The summations in (12) and (13) are over the orbital angular momentum quantum number l with the indices $(-)$ and $(+)$ corresponding respectively, to negative $\kappa(j = l + \frac{1}{2})$ and positive $\kappa(j = l - \frac{1}{2})$. In the non-relativistic limit $\delta_l^{(-)} = \delta_l^{(+)} = \delta_l$, $R_l^{(-)} = R_l^{(+)} = R_l$ and for the upper component we obtain the usual non-relativistic partial wave series

$$\Psi_p(r) = \sum_{l=0}^{\infty} \mathrm{i}^l (2l+1) \exp(-\mathrm{i}\delta_l) R_l(r) P_l(\hat{p}\cdot\hat{r})\varphi. \qquad (14)$$

To find the non-relativistic limit of $\chi_p(r)$ we use the non-relativistic relations between radial functions

$$S_l^{(-)} = \frac{1}{2}\frac{\mathrm{d}R_l^{(-)}}{\mathrm{d}r} - \frac{1}{2}\frac{l}{r} R_l^{(-)} \qquad (15a)$$

$$S_l^{(+)} = \frac{1}{2}\frac{\mathrm{d}R_l^{(+)}}{\mathrm{d}r} + \frac{1}{2}\frac{l+1}{r} R_l^{(+)} \qquad (15b)$$

where $\hbar = c = 1$ and also the electron mass has been put equal to unity. Using (15) and the relations between Legendre polynomials and their derivatives we obtain, in the non-relativistic limit

$$\chi_p(r) = \frac{1}{2i}\sum_{l=0}^{\infty} i^l(2l+1)\exp(-i\delta_l)\frac{dR_l}{dr} \times \left(P_l(\hat{p}\cdot\hat{r})\boldsymbol{r}\cdot\boldsymbol{\sigma} + \frac{R_l}{r}P_l'(\hat{p}\cdot\hat{r})[\hat{p}\cdot\hat{\sigma} - (\hat{p}\cdot\hat{r})\hat{r}\cdot\boldsymbol{\sigma}]\right)\varphi. \tag{16}$$

It can be easily checked that (14) and (16) fulfill the well known relation between upper and lower components in the non-relativistic limit

$$\chi_p(r) = \frac{1}{2i}\boldsymbol{\sigma}\cdot\nabla\varphi_p(\boldsymbol{r}). \tag{17}$$

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