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Propagator for quantum systems involving spin–orbit coupling

M Moshinsky[1] **and E Sadurní**

Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México DF, Mexico

E-mail: moshi@fisica.unam.mx and sadurni@fisica.unam.mx

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Abstract

In the present paper we compute the propagator of a quantum mechanical system whose Hamiltonian consists of two commuting terms, the spin–orbit coupling being one of them. We assume that the propagator corresponding to the first part can be cast into a closed form. A detailed treatment is given when such term is set as the simple harmonic oscillator. Some applications are also included.

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1. Introduction

In the study of transient phenomena in quantum mechanics the concept of propagator is of vital importance. Furthermore, the existence of a closed form of such propagator leads immediately to the possibility of analysing many effects in an exact way. Our objective is to compute the propagator corresponding to idealized systems which can be physically realized in the study of atomic nuclei, as well as in quasi-relativistic systems such as those described by the Pauli Hamiltonian or by Hamiltonians emerging from a Foldy–Wouthuysen transformation (for applications to compound systems see Hamiltonians (25) and (28) in [1]). In particular, we will focus on the explicit form of the propagator corresponding to a Hamiltonian written as an exactly solvable part plus the spin–orbit term.

We have organized this paper as follows. In section 2 we observe that for spherically symmetric problems the complete Hamiltonian commutes with the spin–orbit part. Therefore we express the complete propagator as the action of a rotation on the explicitly known kernel corresponding to the problem without coupling. Since the propagator for the harmonic oscillator lies in this category we study this example from the viewpoint of phase space symmetry in section 3. Section 4 is devoted to some applications. Transient effects due

[1] Member of El Colegio Nacional and Sistema Nacional de Investigadores.

to sudden interactions have been studied since long ago by Moshinsky, so we analyse the evolution of states due to the sudden introduction of spin–orbit coupling in section 4.1. The evolution of a translated Gaussian distribution for the harmonic oscillator and spin–orbit term is included in section 4.2. In section 4.3 we derive some formulae for special cases in connection with the spectral decomposition of our newly obtained propagator.

2. General Hamiltonian

Consider physical units such that $\hbar = 1$. We start with a time-independent Hamiltonian of the form

$$H = H_1 + H_2, \tag{1}$$

where the terms H_1 and H_2 commute but may depend on the same phase space variables. Now we look at the evolution operator and write

$$\exp(-\mathrm{i}Ht) = \exp(-\mathrm{i}H_1 t)\exp(-\mathrm{i}H_2 t). \tag{2}$$

Therefore, its propagator can easily be written as

$$K(x, x'; t) = \langle x|\exp(-\mathrm{i}Ht)|x'\rangle = \int \mathrm{d}x'' \langle x|\exp(-\mathrm{i}H_1 t)|x''\rangle\langle x''|\exp(-\mathrm{i}H_2 t)|x'\rangle, \tag{3}$$

or

$$\begin{aligned} K(x, x'; t) &= \int \mathrm{d}x'' \langle x|\exp(-\mathrm{i}H_2 t)|x''\rangle\langle x''|\exp(-\mathrm{i}H_1 t)|x'\rangle \\ &= \int \mathrm{d}x'' K_2(x, x''; t) K_1(x'', x'; t). \end{aligned} \tag{4}$$

The last expression is useful in the case when both propagators $K_1(x, x''; t)$, $K_2(x'', x'; t)$ are known explicitly with the remaining problem of performing an integration. The propagator K_2 can be written as

$$\langle x|\exp(-\mathrm{i}H_2 t)|x''\rangle = \exp\left(-\mathrm{i}tH_2\left(-\mathrm{i}\frac{\partial}{\partial x}, x\right)\right)\delta(x - x'') \tag{5}$$

and inserting back in (3) we obtain

$$K(x, x'; t) = \exp\left(-\mathrm{i}tH_2\left(-\mathrm{i}\frac{\partial}{\partial x}, x\right)\right)K_1(x, x'; t), \tag{6}$$

which is quite general. Equation (6) can also be written interchanging indices 1 and 2. From this point we reduce our treatment to the case $H_2 = \alpha\mathbf{L}\cdot\mathbf{S}$ and H_1 spherically symmetric so that $[H_1, H_2] = 0$. Then (6) becomes

$$K(\mathbf{r}, \mathbf{r}'; t) = \exp(-\mathrm{i}t\alpha\mathbf{L}\cdot\mathbf{S})K_1(\mathbf{r}, \mathbf{r}'; t), \tag{7}$$

where $\mathbf{L} = -\mathrm{i}\mathbf{r}\times\nabla$, i.e. its differential representation. The operator on the RHS of (7) has the form of a rotation of coordinates $\mathbf{r}$ in its functional representation though the parameters S_i are no longer numbers (or Euler angles) but operators. That we can call it a rotation comes from the fact that it is a unitary operator and we can find its finite-dimensional representation acting on spatial coordinates. In fact, there is no difficulty in proving the formula

$$\exp(\mathrm{i}\phi\mathbf{L}\cdot\mathbf{S})f(\mathbf{r}) = f(\exp(\phi\mathbf{M}\cdot\mathbf{S})\mathbf{r}) \tag{8}$$

for any (locally) analytic function f and non-commuting S_i. We have defined the vector of matrices $(\mathbf{M}_{ij})_k = \epsilon_{ijk}$, i.e. the antisymmetric generators of the rotation in their Cartesian representation where ϕ is regarded as real. The proof of (8) goes as follows.

Let $R := \mathrm{e}^{\mathbf{M}\cdot\mathbf{S}\phi}$ and $U := \mathrm{e}^{\mathrm{i}\mathbf{L}\cdot\mathbf{S}\phi}$. For any analytical function f we have

$$\begin{aligned} f(R\mathbf{r}) &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \frac{\partial^n f}{\partial \phi^n}\bigg|_{\phi=0} = \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \left(\frac{\partial r_i'}{\partial \phi} \frac{\partial}{\partial r_i'} \right)^n f(\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}} \\ &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \left(\frac{\partial (R\mathbf{r})_i}{\partial \phi}\bigg|_{\phi=0} \frac{\partial}{\partial r_i'} \right)^n f(\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}} \\ &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \left((\mathbf{M}_{ji})_k S_k \mathbf{r}_i \frac{\partial}{\partial r_j} \right)^n f(\mathbf{r}) \\ &= \sum_{n=0}^{\infty} \frac{(\mathrm{i}\phi)^n}{n!} \left(-\mathrm{i}\epsilon_{ijk} r_i \frac{\partial}{\partial r_j} S_k \right)^n f(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{L}\cdot\mathbf{S}\phi} f(\mathbf{r}) = U f(\mathbf{r}), \end{aligned} \tag{9}$$

so the chain rule is sufficient to prove (8), regardless of the group structure of S_i. Note, however, that the result of the operation $R\mathbf{r}$ is spin dependent while the product r^2 is preserved.

With (8) in mind, the general form of our propagator reads

$$K(\mathbf{r}, \mathbf{r}'; t) = K_1(\exp(-t\alpha\mathbf{M}\cdot\mathbf{S})\mathbf{r}, \mathbf{r}'; t), \tag{10}$$

and the complete propagator K is known explicitly as K_1 has been assumed to be so. We must point out, however, that for (10) to be of any use it is necessary to compute $\exp(-t\alpha\mathbf{M}\cdot\mathbf{S})\mathbf{r}$ explicitly. This will be done in the appendix. Another way to confirm (10) is by looking at the propagator equation

$$\left\{ H(-\mathrm{i}\nabla, \mathbf{r}, \mathbf{S}) - \mathrm{i}\frac{\partial}{\partial t} \right\} K(\mathbf{r}, \mathbf{r}'; t) = -\mathrm{i}\delta^3(\mathbf{r} - \mathbf{r}')\delta(t), \tag{11}$$

noting that

$$\alpha\mathbf{L}\cdot\mathbf{S} - \mathrm{i}\frac{\partial}{\partial t} = \exp(-\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t)\left(-\mathrm{i}\frac{\partial}{\partial t}\right)\exp(\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t) \tag{12}$$

and

$$\exp(-\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t) H_1(\mathbf{p}, \mathbf{r}) \exp(\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}) = H_1(\mathbf{p}, \mathbf{r}), \tag{13}$$

(11) is equivalent to

$$\exp(-\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t)\left\{ H_1(-\mathrm{i}\nabla, \mathbf{r}) - \mathrm{i}\frac{\partial}{\partial t} \right\} \exp(\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t) K(\mathbf{r}, \mathbf{r}'; t) = -\mathrm{i}\delta^3(\mathbf{r} - \mathbf{r}')\delta(t), \tag{14}$$

and can also be written as

$$\begin{aligned} \left\{ H_1(-\mathrm{i}\nabla, \mathbf{r}) - \mathrm{i}\frac{\partial}{\partial t} \right\} K(\exp(\alpha\mathbf{M}\cdot\mathbf{S}t)\mathbf{r}, \mathbf{r}'; t) &= -\mathrm{i}\exp(\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t)\delta^3(\mathbf{r} - \mathbf{r}')\delta(t) \\ &= -\mathrm{i}\delta^3(\mathbf{r} - \mathbf{r}')\delta(t), \end{aligned} \tag{15}$$

the last equality coming from $f(t)\delta(t) = f(0)\delta(t)$. Finally, (15) implies

$$K_1(\mathbf{r}, \mathbf{r}'; t) = K(\exp(t\alpha\mathbf{M}\cdot\mathbf{S})\mathbf{r}, \mathbf{r}'; t), \tag{16}$$

which is equivalent to result (10). Let us remark that a generalization of this method may be established by considering the addition of a Hamiltonian with the generators of its symmetry in scalar product with some constant operators.

3. The propagator of the harmonic oscillator with spin–orbit coupling from phase space symmetry

Consider units $\hbar = 1$ and for simplicity choose $\bar{m} = 1/2$, $\omega = 2$ for the mass and frequency of the oscillator. The Hamiltonian of our problem is

$$H = \mathbf{p}^2 + \mathbf{r}^2 + \alpha \mathbf{r} \times \mathbf{p} \cdot \mathbf{S}, \tag{17}$$

$\mathbf{S}$ being any spin. The phase space symmetry of this problem is easily described by applying a linear (spin-dependent) canonical transformation to $\mathbf{r}$ and $\mathbf{p}$, i.e.

$$\begin{pmatrix} \mathbf{r}' \\ \mathbf{p}' \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \mathbf{r} \\ \mathbf{p} \end{pmatrix}, \tag{18}$$

with $D\tilde{A} - C\tilde{B} = I$, $B\tilde{A} = A\tilde{B}$, $C\tilde{D} = D\tilde{C}$. For the symmetry of the oscillator we require the matrix in (18) to be an element of $O(6)$. The invariance of the spin–orbit term admits a transformation of the spin $\mathbf{S}' = R\mathbf{S}$ with R an element of $O(3)$, while the orbital angular momentum is transformed into

$$\mathbf{r}' \times \mathbf{p}' = (A\mathbf{r} + B\mathbf{p}) \times (C\mathbf{r} + D\mathbf{p}) = R(\mathbf{r} \times \mathbf{p}). \tag{19}$$

The last equality is satisfied for all $\mathbf{r}$, $\mathbf{p}$ iff A, B, C, D are all proportional to R. This is written as

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} \alpha R & \beta R \\ \gamma R & \delta R \end{pmatrix}. \tag{20}$$

Orthogonality is fulfilled when the proportionality factors are trigonometric functions, i.e. $\alpha^2 + \beta^2 = \gamma^2 + \delta^2 = 1$ and $\alpha\gamma + \beta\delta = 0$. Therefore, the most general canonical transformation leaving H invariant is

$$\begin{pmatrix} \cos\phi R & \sin\phi R \\ -\sin\phi R & \cos\phi R \end{pmatrix} \tag{21}$$

for any real ϕ. The spatial matrix elements of the corresponding unitary transformation U satisfy a well-known equation written in (36.21) of [2]. The general solution for a transformation of the form (21) is given by

$$\langle \mathbf{r}|U|\mathbf{r}'\rangle = (2\pi \sin\phi)^{-3/2} \exp\left(\frac{-\mathrm{i}}{2}\{(r^2 + r'^2)\cot\phi - 2\csc\phi (R\mathbf{r}) \cdot \mathbf{r}'\}\right), \tag{22}$$

and we are interested in the explicit form of the functions $\phi(t)$, $R(t)$. When U is the evolution operator, the LHS of (22) is the propagator of our problem and is also a solution of the equation

$$\left\{H - \mathrm{i}\frac{\partial}{\partial t}\right\} \langle \mathbf{r}|U|\mathbf{r}'\rangle = -\mathrm{i}\delta^3(\mathbf{r} - \mathbf{r}')\delta(t). \tag{23}$$

For $\mathbf{r} \neq \mathbf{r}'$ this equation becomes homogeneous. The replacement of (22) and (17) in (23) leads to first and second spatial as well as time derivatives of $\langle \mathbf{r}|U|\mathbf{r}'\rangle$, which are in turn $\langle \mathbf{r}|U|\mathbf{r}'\rangle$ multiplied by a polynomial in the variables r^2, r'^2 and rr'. Thus, $\mathbf{r} \neq \mathbf{r}'$ in (23) gives rise to a set of homogeneous equations for the coefficients of our polynomial. The equations emerging from terms which do not contain rr' turn out to be equivalent and so we write only the equation corresponding to the coefficient of r'^2

$$-\frac{1}{2}\frac{\partial \cot\phi}{\partial t} + \csc^2\phi = 0 \tag{24}$$

with solution $\frac{\partial\phi}{\partial t} = -2$. The coefficient of rr' yields

$$\alpha \csc\phi R_{lj}\epsilon_{ijk}S_k + \frac{\partial}{\partial t}(\csc\phi R^{-1})_{il} - 2\cot\phi\csc\phi (R^{-1})_{il} = 0, \tag{25}$$

after adopting the sum convention over the index $j = 1, 2, 3$. Using the solution of (24), (25) can be reduced to

$$-\alpha \mathbf{M} \cdot \mathbf{S} = \frac{\partial R}{\partial t} R^{-1} \tag{26}$$

with solution $R = \exp(-\alpha \mathbf{M} \cdot \mathbf{S} t)$. The integration constant is set equal to unity so that R is in effect a rotation. Returning to our general solution (22) with these results we find that

$$K(\mathbf{r}, \mathbf{r}'; t) = \langle \mathbf{r} | U | \mathbf{r}' \rangle = K_{\text{oscillator}}(R\mathbf{r}, \mathbf{r}'; t), \tag{27}$$

where the actual formula for $K_{\text{oscillator}}$ can be found in [4]. We write the complete expression restoring the frequency ω and mass $\bar{m}$,

$$K(\mathbf{r}, \mathbf{r}'; t) = \left(\frac{\bar{m}\omega}{2\pi \mathrm{i} \sin \omega t} \right)^{\frac{3}{2}} \exp \left(\frac{\mathrm{i}\bar{m}\omega}{2} \{ (r^2 + r'^2) \cot \omega t - 2 \csc \omega t (\mathrm{e}^{-\alpha \mathbf{M} \cdot \mathbf{S} t} \mathbf{r}) \cdot \mathbf{r}' \} \right). \tag{28}$$

Thus, we have arrived at the sought propagator satisfying (10) by following a different path. More than confirming our earlier results, this example has been worked out to illustrate that the direct study of phase space symmetries may lead to a closed expression for $K(\mathbf{r}, \mathbf{r}'; t)$.

4. Applications

4.1. The spin–orbit coupling as a sudden perturbation

Before studying a direct application of our propagator (10), we analyse the sudden introduction of the spin–orbit coupling in order to compare it with the case in which such a term is absent. Let us consider a system which is described by a Hamiltonian H_1 for all times $t < 0$ and $H_1 + \alpha \mathbf{L} \cdot \mathbf{S}$ for $t > 0$. Suppose that such a system is found to be in the eigenstate ϕ_n at negative times. Assuming $[H_1, \mathbf{L} \cdot \mathbf{S}] = 0$ as usual, we address to the question of what is the evolution of the state after the spin–orbit coupling is applied. To this end, we denote the state ϕ_n by a ket of the orbital angular momentum in direct product with a spinor, i.e. $|l, m_l\rangle |s, m_s\rangle$. This in turn can be expanded in terms of kets of the total angular momentum j which are the eigenstates of the system at positive times,

$$|l, m_l\rangle |s, m_s\rangle = \sum_{j=|l-s|}^{l+s} \sum_{m=-j}^{j} \langle j, m | l, m_l, s, m_s \rangle |j, m, s, l\rangle. \tag{29}$$

In order to find the ket at time $t > 0$, we apply the corresponding propagator $U = \exp -\mathrm{i}(H_1 + \alpha \mathbf{L} \cdot \mathbf{S})t$ to both sides of (29) and find

$$U|n, l, m_l\rangle |s, m_s\rangle = \sum_{j=|l-s|}^{l+s} \sum_{m=-j}^{j} \langle j, m | l, m_l, s, m_s \rangle \, \mathrm{e}^{-\mathrm{i}E_{n,j,s,l}t} |n, j, m, s, l\rangle, \tag{30}$$

with $E_{n,j,s,l}$ the eigenvalues of $H_1 + \alpha \mathbf{L} \cdot \mathbf{S}$. Since the sum is finite, (30) is a closed result. The probability density exhibits interference between the different j's. For the ground state $l = 0$ we observe no transient effect.

We can also state in general that any sudden perturbation introducing a finite spectrum and commuting with H_1 gives rise to interference (30) with the appropriate coefficients.

4.2. Evolution of a Gaussian distribution

Now we study the evolution of a specific state ψ as the initial condition for the harmonic oscillator with the spin–orbit coupling. Let such state be given by

$$\psi(\mathbf{r}, 0) = \phi(\mathbf{r})\chi := A\, \mathrm{e}^{-\frac{1}{2}\omega(\mathbf{r}-\mathbf{r}_0)^2} \chi, \tag{31}$$

with χ being any spinor and A the appropriate normalization factor. The spatial part of ψ is merely a translation of the ground state of the ordinary harmonic oscillator of frequency ω and mass $\bar{m} = 1$. It is well known (see [3] for applications to the deuteron in a uniform electrostatic field) that the translated Gaussian distribution undergoes an oscillatory behaviour about the origin. When we compute

$$\int \mathrm{d}^3 r'' K_{\text{oscillator}}(\mathbf{r}, \mathbf{r}''; t)\phi(\mathbf{r}'') = \phi(\mathbf{r}, t), \tag{32}$$

we obtain a probability density

$$|\phi(\mathbf{r}, t)|^2 = |A|^2\, \mathrm{e}^{-\omega(\mathbf{r}-\cos(\omega t)\mathbf{r}_0)^2}. \tag{33}$$

In view of result (27), the initial condition (31) evolves as

$$\psi(\mathbf{r}, t) = \int \mathrm{d}^3 r'' K_{\text{oscillator}}(\mathrm{e}^{\alpha \mathbf{M}\cdot\mathbf{S}t}\mathbf{r}, \mathbf{r}''; t)\psi(\mathbf{r}''), \tag{34}$$

and the probability density gives

$$\begin{aligned} |\psi(\mathbf{r}, t)|^2 &= |A|^2 \chi^{\dagger} \exp(-\omega(\mathrm{e}^{\alpha \mathbf{M}\cdot\mathbf{S}t}\mathbf{r} - \cos(\omega t)\mathbf{r}_0)^2)\chi \\ &= |A|^2 \chi^{\dagger} \exp(-\omega(\mathbf{r} - \cos(\omega t)\, \mathrm{e}^{-\alpha \mathbf{M}\cdot\mathbf{S}t}\mathbf{r}_0)^2)\chi. \end{aligned} \tag{35}$$

Therefore, the spin–orbit coupling gives rise to a periodical transformation of the direction in which the vibration takes place. Actually, the resemblance of that transformation with a rotational motion of $\mathbf{r}_0$ can be easily understood when we replace the magnetic moment proportional to the spin $\mathbf{S}$ by a constant magnetic field $\mathbf{B}$. The propagator becomes

$$K(\mathbf{r}, \mathbf{r}'; t) = K_{\text{oscillator}}(\mathrm{e}^{\alpha \mathbf{M}\cdot\mathbf{B}t}\mathbf{r}, \mathbf{r}'; t). \tag{36}$$

When (36) is applied to the initial state $\phi(\mathbf{r})$ we get a density

$$|\phi(\mathbf{r}, t)|^2 = |A|^2 \exp(-\omega(\mathbf{r} - \cos(\omega t)\, \mathrm{e}^{-\alpha \mathbf{M}\cdot\mathbf{B}t}\mathbf{r}_0)^2), \tag{37}$$

which truly undergoes a rotational motion in $\mathbf{r}_0$ as is expected for a charged particle in a magnetic field.

4.3. Spectral decomposition and summation formulae

Now we indicate how to write the spectral decomposition for (10) and exploit its properties. Let $H_1\phi_{\{N\}} = E^{(1)}_{\{N\}}\phi_{\{N\}}$ be the time-independent Schroedinger equation satisfied by eigenfunctions with quantum numbers $\{N\}$. When H_1 is spherically symmetric we can separate the eigenstates as

$$\phi_{\{N\}} = R_{nl}(r)Y_l^m(\hat{r})\, \mathrm{e}^{-\mathrm{i}E^{(1)}_{nl}t} \tag{38}$$

for some radial functions R_{nl} specified by the problem. Y_l^m are spherical harmonics and $\hat{r}$ is the unit vector in the direction of $\mathbf{r}$. The propagator of H_1 is written as

$$K_1(\mathbf{r}, \mathbf{r}'; t) = \sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} R_{nl}(r)R_{nl}(r')Y_l^m(\hat{r})Y_l^{m*}(\hat{r}')\, \mathrm{e}^{-\mathrm{i}E^{(1)}_{nl}t}. \tag{39}$$

The spin–orbit coupling introduces a modification of the wavefunctions and energies of the system:

$$(H_1 + \alpha\mathbf{L}\cdot\mathbf{S})\psi_{\{N\}} = \left(E^{(1)}_{\{N\}} + E^{(2)}_{\{N\}}\right)\psi_{\{N\}} = E_{\{N\}}\psi_{\{N\}}, \tag{40}$$

$E^{(2)}_{\{N\}} = E^{(2)}_{jls} = \frac{\alpha}{2}(j(j+1) - l(l+1) - s(s+1))$ being the eigenvalues of $\alpha\mathbf{L}\cdot\mathbf{S}$. The wavefunction is given by

$$\psi_{\{N\}} = R_{nl}(r)\mathcal{Y}^m_{jls}(\hat{r})\, \mathrm{e}^{-\mathrm{i}E_{njls}}, \tag{41}$$

with restrictions $-j \leqslant m \leqslant j$ and $|l-s| \leqslant j \leqslant l+s$. $\mathcal{Y}^m_{jls}$ are spinorial spherical harmonics. The complete propagator has a spectral decomposition

$$K(\mathbf{r},\mathbf{r}';t) = K_1(\mathrm{e}^{\alpha \mathbf{M}\cdot\mathbf{S}t}\mathbf{r},\mathbf{r}';t) = \sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{j=|l-s|}^{l+s}\sum_{m=-j}^{j} R_{nl}(r)R_{nl}(r')\mathcal{Y}^m_{jls}(\hat{r})\big[\mathcal{Y}^m_{jls}(\hat{r}')\big]^{\dagger}\,\mathrm{e}^{-\mathrm{i}E_{njls}t}. \tag{42}$$

Equation (42) is a closed expression for an infinite sum. Such an expression can be used to obtain new formulae for series of special functions.

In what follows we restrict to the case $s = 1/2$, $S_i = \sigma_i/2$ and $H_1 = (\mathbf{p}^2 + \omega^2\mathbf{r}^2)/2$. The complete propagator reads

$$K(\mathbf{r},\mathbf{r}';t) = \sum_{l=0}^{\infty}\sum_{n=0}^{\infty} R_{nl}(r)R_{nl}(r')\exp\left(-\mathrm{i}\omega\left(2n+l+\frac{3}{2}\right)t\right)\sum_{j=|l-\frac{1}{2}|}^{l+\frac{1}{2}}\sum_{m=-j}^{j}\mathcal{Y}^m_{jl\frac{1}{2}}(\hat{r}) \times\big[\mathcal{Y}^m_{jl\frac{1}{2}}(\hat{r}')\big]^{\dagger}\exp\left(-\mathrm{i}\frac{\alpha}{2}t\left(j(j+1)-l(l+1)-\frac{3}{4}\right)\right). \tag{43}$$

In the last expression we find a sum of the radial (Gaussian–Laguerre) functions over n. By examining the propagator for a radial harmonic oscillator written in [4, p 225], we have

$$\sum_{n=0}^{\infty} R_{nl}(r)R_{nl}(r')\,\mathrm{e}^{-\mathrm{i}\omega(2n+l+3/2)t} = \frac{\omega\sqrt{rr'}}{\mathrm{i}\sin\omega t}\exp\left(\frac{\mathrm{i}\omega}{2}\{r^2+r'^2\}\cot\omega t\right)I_{l+1/2}\left(\frac{\omega r r'}{\mathrm{i}\sin\omega t}\right), \tag{44}$$

with I_k the modified Bessel function of order k. Result (44) can be replaced in the radial part of (43). We also find in (43) the sum of the angular functions

$$K_l := \sum_{j=|l-\frac{1}{2}|}^{l+\frac{1}{2}}\sum_{m=-j}^{j}\mathcal{Y}^m_{jl\frac{1}{2}}(\hat{r})\big[\mathcal{Y}^m_{jl\frac{1}{2}}(\hat{r}')\big]^{\dagger}\exp\left(-\mathrm{i}\frac{\alpha}{2}t\left(j(j+1)-l(l+1)-\frac{3}{4}\right)\right), \tag{45}$$

whose direct computation can be a bit lengthy but rewarding. First let us recall that the spinorial angular functions are given by

$$\mathcal{Y}^m_{j=l\pm\frac{1}{2},l,\frac{1}{2}} = \pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}\,Y_l^{m-\frac{1}{2}}\chi_+ + \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}\,Y_l^{m+\frac{1}{2}}\chi_-, \tag{46}$$

$\chi_\pm$ being the canonical basis for the $s = 1/2$ spinors. We find useful the definitions

$$\lambda(l, j=l-1/2) := -(l+1), \qquad \lambda(l, j=l+1/2) := l \tag{47}$$

$$K_l^{\pm} := \sum_m \mathrm{e}^{-\mathrm{i}\alpha\lambda(l,l\pm\frac{1}{2})t/2}\begin{pmatrix}\pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}\,Y_l^{m-\frac{1}{2}}\\ \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}\,Y_l^{m+\frac{1}{2}}\end{pmatrix}\left(\pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}\,Y_l^{m-\frac{1}{2}*},\ \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}\,Y_l^{m+\frac{1}{2}*}\right) \tag{48}$$

so that an additional sum over upper and lower sings must be made to obtain

$$K_l = K_l^+ + K_l^-. \tag{49}$$

It is convenient to redefine the index of summation for the total angular momentum projection. Let $\mu = m - \frac{1}{2}$ for $j = l + \frac{1}{2}$ and $\mu = m + \frac{1}{2}$ for $j = l - \frac{1}{2}$ so that $\mu = -l-1, \ldots, l$ for $j = l + \frac{1}{2}$ and $\mu = -l+1, \ldots, l$ for $j = l - \frac{1}{2}$. The two parts of K_l are now

$$K_l^+ = \sum_{\mu=-l-1}^{l} \frac{\mathrm{e}^{-\mathrm{i}\alpha l t/2}}{2l+1} \times \begin{pmatrix} (l+\mu+1) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & \sqrt{l+\mu+1}\sqrt{l-\mu}\, Y_l^{\mu}(\hat{r}) Y_l^{\mu+1 *}(\hat{r}') \\ \sqrt{l-\mu}\sqrt{l+\mu+1}\, Y_l^{\mu+1}(\hat{r}) Y_l^{\mu *}(\hat{r}') & (l-\mu) Y_l^{\mu+1}(\hat{r}) Y_l^{\mu+1 *}(\hat{r}') \end{pmatrix}, \tag{50}$$

$$K_l^- = \sum_{\mu=-l+1}^{l} \frac{\mathrm{e}^{\mathrm{i}\alpha (l+1) t/2}}{2l+1} \times \begin{pmatrix} (l-\mu+1) Y_l^{\mu-1}(\hat{r}) Y_l^{\mu-1 *}(\hat{r}') & -\sqrt{l+\mu}\sqrt{l-\mu+1}\, Y_l^{\mu-1}(\hat{r}) Y_l^{\mu *}(\hat{r}') \\ -\sqrt{l+\mu}\sqrt{l-\mu+1}\, Y_l^{\mu}(\hat{r}) Y_l^{\mu-1 *}(\hat{r}') & (l+\mu) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \end{pmatrix}. \tag{51}$$

Each of the coefficients in the spinorial matrix can be generated by the action of differential operators on the angular functions. Using the differential representation for angular momenta

$$L_3 = -\mathrm{i}\frac{\partial}{\partial\phi}, \qquad L_{\pm} = -\mathrm{i}\,\mathrm{e}^{\pm \mathrm{i}\phi}\left(\pm \mathrm{i}\frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi}\right) \tag{52}$$

for the upper sign in (48), we have

$$K_l^+ = \sum_{\mu=-l-1}^{l} \frac{\mathrm{e}^{-\mathrm{i}\alpha l t/2}}{2l+1} \begin{pmatrix} (l+L_3+1) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & L_- Y_l^{\mu+1}(\hat{r}) Y_l^{\mu+1 *}(\hat{r}') \\ L_+ Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & (l-L_3+1) Y_l^{\mu+1}(\hat{r}) Y_l^{\mu+1 *}(\hat{r}') \end{pmatrix}. \tag{53}$$

The lower sign term yields

$$K_l^- = \sum_{\mu=-l+1}^{l} \frac{\mathrm{e}^{\mathrm{i}\alpha (l+1) t/2}}{2l+1} \begin{pmatrix} (l-L_3) Y_l^{\mu-1}(\hat{r}) Y_l^{\mu-1 *}(\hat{r}') & -L_- Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \\ -L_+ Y_l^{\mu-1}(\hat{r}) Y_l^{\mu-1 *}(\hat{r}') & (l+L_3) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \end{pmatrix}. \tag{54}$$

Here we can go further and re-express the sums

$$\sum_{\mu=-l-1}^{l} Y_l^{\mu+1} Y_l^{\mu+1 *} = \sum_{\mu=-l}^{l} Y_l^{\mu} Y_l^{\mu *}, \tag{55}$$

$$\sum_{\mu=-l+1}^{l} Y_l^{\mu-1} Y_l^{\mu-1 *} = \sum_{\mu=-l}^{l} Y_l^{\mu} Y_l^{\mu *} - Y_l^{l} Y_l^{l *}. \tag{56}$$

The extra term arising from (56) will vanish after applying the differential operators in (54). In this way the sums over μ in (53) and (54) are such that $\mu = -l, \ldots, l$ and we have

$$K_l^+ = \sum_{\mu=-l}^{l} \frac{\mathrm{e}^{-\mathrm{i}\alpha l t/2}}{2l+1} \begin{pmatrix} (l+L_3+1) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & L_- Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \\ L_+ Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & (l-L_3+1) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \end{pmatrix}, \tag{57}$$

$$K_l^- = \sum_{\mu=-l}^{l} \frac{\mathrm{e}^{\mathrm{i}\alpha (l+1) t/2}}{2l+1} \begin{pmatrix} (l-L_3) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & -L_- Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \\ -L_+ Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') & (l+L_3) Y_l^{\mu}(\hat{r}) Y_l^{\mu *}(\hat{r}') \end{pmatrix}. \tag{58}$$

Other useful relations are

$$\frac{2\mathrm{i}}{t}\frac{\partial\, \mathrm{e}^{-\frac{\mathrm{i}}{2}\alpha l t}}{\partial\alpha} = l\, \mathrm{e}^{-\frac{\mathrm{i}}{2}\alpha l t}$$
$$\frac{2\mathrm{i}}{t}\frac{\partial\, \mathrm{e}^{\frac{\mathrm{i}}{2}\alpha(l+1)t}}{\partial\alpha} = -(l+1)\, \mathrm{e}^{\frac{\mathrm{i}}{2}\alpha(l+1)t} \tag{59}$$
$$\mathbf{L}\cdot\mathbf{S} = \frac{1}{2}\begin{pmatrix} L_3 & L_- \\ L_+ & -L_3 \end{pmatrix}.$$

When these relations are used in (57) and (58), our expressions become

$$K_l^+ = \left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + 1\right]\sum_{\mu=-l}^{l}\frac{\mathrm{e}^{-\mathrm{i}\alpha l t/2}}{2l+1}Y_l^{\mu}(\hat{r})Y_l^{\mu *}(\hat{r}') \tag{60}$$

$$K_l^- = -\left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + 1\right]\sum_{\mu=-l}^{l}\frac{\mathrm{e}^{\mathrm{i}\alpha (l+1) t/2}}{2l+1}Y_l^{\mu}(\hat{r})Y_l^{\mu *}(\hat{r}'). \tag{61}$$

Adding the two parts we arrive at the sought result

$$K_l = \left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + 1\right]\sum_{\mu=-l}^{l}\frac{(\mathrm{e}^{-\mathrm{i}\alpha l t/2} - \mathrm{e}^{\mathrm{i}\alpha (l+1) t/2})}{2l+1}Y_l^{\mu}(\hat{r})Y_l^{\mu *}(\hat{r}') \tag{62}$$

$$= \left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + 1\right](-2\mathrm{i}\,\mathrm{e}^{\mathrm{i}\alpha t/4})\sin\left(\left(l+\frac{1}{2}\right)\alpha t/2\right)P_l(\cos\gamma), \tag{63}$$

P_l being the lth Legendre polynomial and γ the angle between $\hat{r}$ and $\hat{r}'$.

Two results can be derived from this formula. The first is achieved by the replacement of (63) and (44) in (43), leading to

$$K(\mathbf{r},\mathbf{r}';t) = \frac{\omega\sqrt{rr'}}{\mathrm{i}\sin\omega t}\exp\left(\frac{\mathrm{i}\omega}{2}\{r^2+r'^2\}\cot\omega t\right)\left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + 1\right](-2\mathrm{i}\,\mathrm{e}^{\mathrm{i}\alpha t/4})$$
$$\times\sum_{l=0}^{\infty}\sin\left(\left(l+\frac{1}{2}\right)\alpha t/2\right)P_l(\cos\gamma)I_{l+1/2}\left(\frac{\omega r r'}{\mathrm{i}\sin\omega t}\right), \tag{64}$$

and with the aid of (28) for $m = 1$, a cancellation of Gaussian factors is possible and we get a non-trivial formula for a series of Legendre, Fourier and Bessel functions (Pauli matrices also involved)

$$\left[\frac{2\mathrm{i}}{t}\frac{\partial}{\partial\alpha} + 2\mathbf{L}\cdot\mathbf{S} + \frac{1}{2}\right]\sum_{l=0}^{\infty}\sin\left(\left(l+\frac{1}{2}\right)\alpha t/2\right)P_l(\cos\gamma)I_{l+1/2}\left(\frac{\omega r r'}{\mathrm{i}\sin\omega t}\right)$$
$$= \frac{\mathrm{i}}{4\pi}\sqrt{\frac{\omega\,\mathrm{e}^{-\mathrm{i}\alpha t/2}}{2\pi i r r'\sin\omega t}}\exp(-\mathrm{i}\omega\csc\omega t\,(\mathrm{e}^{-\alpha\mathbf{M}\cdot\mathbf{S}t}\mathbf{r})\cdot\mathbf{r}'), \tag{65}$$

where the matrix elements of $\mathrm{e}^{-\alpha\mathbf{M}\cdot\mathbf{S}t}$ can be found in the appendix.

A second result stemming out from (63) is as follows. Consider the spin–orbit coupling ($s = 1/2$) alone as the Hamiltonian of the system and whose propagator will be called the spin–orbit propagator. In such a case we have a spectral decomposition

$$K_{\mathrm{so}}(\mathbf{r},\mathbf{r}';t) := \langle\mathbf{r}|\,\mathrm{e}^{-\mathrm{i}\alpha\mathbf{L}\cdot\mathbf{S}t}|\mathbf{r}'\rangle$$
$$= \frac{\delta(r-r')}{r^2}\sum_{l=0}^{\infty}\sum_{j=l\pm\frac{1}{2}}\sum_{m=-j}^{j}\mathcal{Y}_{jl\frac{1}{2}}^{m}(\hat{r})\left[\mathcal{Y}_{jl\frac{1}{2}}^{m}(\hat{r}')\right]^{\dagger}\mathrm{e}^{-\mathrm{i}\alpha\lambda(l,j)t/2}, \tag{66}$$

and the use of definition (48) together with result (63) turns (64) into

$$K_{\rm so}(\mathbf{r},\mathbf{r}',t) = \frac{\delta(r-r')}{r^2}\left[\frac{2\mathrm{i}}{\alpha}\frac{\partial}{\partial t} + 2\mathbf{L}\cdot\mathbf{S} + 1\right](-2\mathrm{i}\,\mathrm{e}^{\mathrm{i}\alpha t/4})\sum_{l=0}^{\infty}\sin\left(\left(l+\frac{1}{2}\right)\alpha t/2\right)P_l(\cos\gamma). \tag{67}$$

It can be shown [5] that the sum over l in (67) is given by

$$\sum_{l=0}^{\infty}\sin\left(\left(l+\frac{1}{2}\right)\alpha t/2\right)P_l(\cos\gamma) = \mathrm{sign}(\sin(\alpha t/4))\frac{u[\cos(\gamma)-\cos(\alpha t/2)]}{\sqrt{2(\cos(\gamma)-\cos(\alpha t/2))}}, \tag{68}$$

where u is the unit step function. Thus we also have a closed expression for $K_{\rm so}$, equations (67) and (68).

5. Conclusions

We have succeeded in our attempt to obtain a closed expression of the propagator for spherically symmetric systems involving the spin–orbit coupling. As a result, kernel (10) was obtained and it resembles that of the symmetric problem alone, but with a rotational behaviour of one of its spatial variables which is given by equations (A.1) and (A.12) in the appendix. As remarked at the end of section 2, it is possible to generalize our method for systems involving certain (continuous) symmetries with interactions given by their corresponding generators.

Some applications were given though there could be many more. To summarize, the main results of section 4 consist of the evolution of states under sudden spin–orbit perturbation in (30), the evolution of Gaussian distributions given by (35) and formulae (65), (67) and (68) dealing with the case $s = 1/2$.

Appendix

Now we proceed to compute the matrix elements of $R = \mathrm{e}^{\xi\mathbf{M}\cdot\mathbf{S}}$ in three-dimensional space (ξ is any real parameter). This means that our results will be actually spinorial matrices. Such results will be sufficient to obtain the action of $\mathrm{e}^{\xi\mathbf{M}\cdot\mathbf{S}}$ on any three-dimensional vector. Let us start with the transformation

$$\mathbf{r}' = \mathrm{e}^{\xi\mathbf{M}\cdot\mathbf{S}}\mathbf{r}. \tag{A.1}$$

Since the components of $\mathbf{r}$ are also functions of the coordinates $r_1 = x, r_2 = y, r_3 = z$, we can write

$$x' = \mathrm{e}^{\mathrm{i}\xi\mathbf{L}\cdot\mathbf{S}}xI_s, \qquad y' = \mathrm{e}^{\mathrm{i}\xi\mathbf{L}\cdot\mathbf{S}}yI_s, \qquad z' = \mathrm{e}^{\mathrm{i}\xi\mathbf{L}\cdot\mathbf{S}}zI_s, \tag{A.2}$$

where $\mathbf{L}$ is the differential operator of angular momentum and $I_s = \sum_{m_s=-s}^{s}|s,m_s\rangle\langle s,m_s|$ is the identity in spin space. To compute each transformation in (A.2) the coordinates x, y, z should be expressed in terms of spherical harmonics and xI_s, yI_s, zI_s in terms of spinorial spherical harmonics by using the appropriate Clebsch–Gordan coefficients:

$$\begin{aligned} xI_2 &= \sqrt{\frac{2\pi}{3}}r\left(Y_1^{-1}-Y_1^1\right)\sum_{m_s=-s}^{s}|s,m_s\rangle\langle s,m_s| \\ &= \sqrt{\frac{2\pi}{3}}r\sum_{m_s=-s}^{s}\sum_{j=|1-s|}^{1+s}\sum_{m=-j}^{j}(\langle jm|1,-1,s,m_s\rangle - \langle jm|1,1,s,m_s\rangle)\mathcal{Y}_{j,1,s}^{m}\langle s,m_s|, \end{aligned} \tag{A.3}$$

$$yI_2 = \sqrt{\frac{2\pi}{3}}\mathrm{i}r\left(Y_1^{-1} + Y_1^1\right)\sum_{m_s=-s}^{s}|s, m_s\rangle\langle s, m_s| \tag{A.4}$$

$$= \sqrt{\frac{2\pi}{3}}\mathrm{i}r\sum_{m_s=-s}^{s}\sum_{j=|1-s|}^{1+s}\sum_{m=-j}^{j}(\langle jm|1, -1, s, m_s\rangle + \langle jm|1, 1, s, m_s\rangle)\mathcal{Y}_{j,1,s}^{m}\langle s, m_s|, \tag{A.5}$$

$$zI_2 = \sqrt{\frac{4\pi}{3}}rY_1^0\sum_{m_s=-s}^{s}|s, m_s\rangle\langle s, m_s|$$

$$= \sqrt{\frac{4\pi}{3}}r\sum_{m_s=-s}^{s}\sum_{j=|1-s|}^{1+s}\sum_{m=-j}^{j}\langle jm|1, 0, s, m_s\rangle\mathcal{Y}_{j,1,s}^{m}\langle s, m_s|. \tag{A.6}$$

The differential operator in (A.2) affects the spinorial spherical harmonic as

$$\mathrm{e}^{\mathrm{i}\xi\mathbf{L}\cdot\mathbf{S}}\mathcal{Y}_{jls}^{m} = \exp\left(\frac{\mathrm{i}\xi}{2}(j(j+1) - l(l+1) - s(s+1))\right)\mathcal{Y}_{jls}^{m}. \tag{A.7}$$

The functions $\mathcal{Y}$ can also be inverted in terms of canonical spinors and coordinates x, y, z:

$$\mathcal{Y}_{j,1,s}^{m} = \sum_{m_l', m_s'}\langle 1, m_l', s, m_s'|jm1s\rangle Y_1^{m_l'}|s, m_s'\rangle$$

$$= \sqrt{\frac{3}{2\pi}}\sum_{m_s'}\left\{\frac{1}{2}(\langle 1, -1, s, m_s'|jm1s\rangle - \langle 1, 1, s, m_s'|jm1s\rangle)x - \frac{\mathrm{i}}{2}(\langle 1, -1, s, m_s'|jm1s\rangle\right.$$

$$\left. + \langle 1, 1, s, m_s'|jm1s\rangle)y + \frac{1}{\sqrt{2}}\langle 1, 0, s, m_s'|jm1s\rangle z\right\}|s, m_s'\rangle. \tag{A.8}$$

Therefore, the successive replacement of (A.3), (A.5), (A.6), (A.7) and (A.8) in (A.2) gives the primed coordinates as linear combinations of x, y, z with spinorial matrices as coefficients

$$x' = \sum_{m_s, m_s', j, m}|s, m_s'\rangle\langle s, m_s|\,\mathrm{e}^{\frac{\mathrm{i}\xi}{2}(j(j+1)-s(s+1)-2)}(\langle jm|1, -1, s, m_s\rangle - \langle jm|1, 1, s, m_s\rangle)$$

$$\times\left\{\frac{1}{2}(\langle 1, -1, s, m_s'|jm1s\rangle - \langle 1, 1, s, m_s'|jm1s\rangle)x - \frac{\mathrm{i}}{2}(\langle 1, -1, s, m_s'|jm1s\rangle\right.$$

$$\left. + \langle 1, 1, s, m_s'|jm1s\rangle)y + \frac{1}{\sqrt{2}}\langle 1, 0, s, m_s'|jm1s\rangle z\right\}, \tag{A.9}$$

$$y' = \mathrm{i}\sum_{m_s, m_s', j, m}|s, m_s'\rangle\langle s, m_s|\,\mathrm{e}^{\frac{\mathrm{i}\xi}{2}(j(j+1)-s(s+1)-2)}(\langle jm|1, -1, s, m_s\rangle + \langle jm|1, 1, s, m_s\rangle)$$

$$\times\left\{\frac{1}{2}(\langle 1, -1, s, m_s'|jm1s\rangle - \langle 1, 1, s, m_s'|jm1s\rangle)x - \frac{\mathrm{i}}{2}(\langle 1, -1, s, m_s'|jm1s\rangle\right.$$

$$\left. + \langle 1, 1, s, m_s'|jm1s\rangle)y + \frac{1}{\sqrt{2}}\langle 1, 0, s, m_s'|jm1s\rangle z\right\}, \tag{A.10}$$

$$z' = \sqrt{2}\sum_{m_s, m_s', j, m}|s, m_s'\rangle\langle s, m_s|\,\mathrm{e}^{\frac{\mathrm{i}\xi}{2}(j(j+1)-s(s+1)-2)}\langle jm|1, 0, s, m_s\rangle$$

$$\times\left\{\frac{1}{2}(\langle 1, -1, s, m_s'|jm1s\rangle - \langle 1, 1, s, m_s'|jm1s\rangle)x - \frac{\mathrm{i}}{2}(\langle 1, -1, s, m_s'|jm1s\rangle\right.$$

$$\left. + \langle 1, 1, s, m_s'|jm1s\rangle)y + \frac{1}{\sqrt{2}}\langle 1, 0, s, m_s'|jm1s\rangle z\right\}, \tag{A.11}$$

which are the explicit transformations of **r**, rendered as finite sums. Finally, the matrix elements of the operator R can be read off from (A.9)–(A.11),

$$R_{lk} = (\mathrm{e}^{\xi \mathbf{M}\cdot\mathbf{S}})_{lk} = \sum_{m_s, m_s', j, m} |s, m_s'\rangle\langle s, m_s|\, \mathrm{e}^{\frac{\mathrm{i}\xi}{2}(j(j+1)-s(s+1)-2)} A_l B_k, \tag{A.12}$$

with

$$\begin{aligned} A_1 &= \langle jm|1, -1, s, m_s\rangle - \langle jm|1, 1, s, m_s\rangle \\ A_2 &= \mathrm{i}(\langle jm|1, -1, s, m_s\rangle + \langle jm|1, 1, s, m_s\rangle) \\ A_3 &= \sqrt{2}\langle jm|1, -0, s, m_s\rangle \end{aligned} \tag{A.13}$$

$$\begin{aligned} B_1 &= \frac{1}{2}(\langle 1, -1, s, m_s'|jm1s\rangle - \langle 1, 1, s, m_s'|jm1s\rangle) \\ B_2 &= \frac{-\mathrm{i}}{2}(\langle 1, -1, s, m_s'|jm1s\rangle + \langle 1, 1, s, m_s'|jm1s\rangle) \\ B_3 &= \frac{1}{\sqrt{2}}\langle 1, 0, s, m_s'|jm1s\rangle \end{aligned} \tag{A.14}$$

and this holds for any spin.

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