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## Simplified recursive algorithm for Wigner $3j$ and $6j$ symbols

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We present a highly accurate, *ab initio* recursive algorithm for evaluating the Wigner  $3j$  and  $6j$  symbols. Our method makes use of two-term, nonlinear recurrence relations that are obtained from the standard three-term recurrence relations satisfied by these quantities. The use of two-term recurrence relations eliminates the need for rescaling of iterates to control numerical overflows and thereby simplifies the widely used recursive algorithm of Schulten and Gordon. [S1063-651X(98)02506-9]

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The Wigner  $3j$  and  $6j$  symbols arise frequently in contexts involving the coupling of angular momenta in quantum mechanics and other applications of the rotation group. While one can utilize the explicit expressions of Wigner [1] and Racah [1] to calculate specific values of these quantities, computationally the direct approach is often impractical, especially for large quantum numbers. As has long been recognized, a convenient alternative numerical approach is to make use of the three-term recurrence relations [see Eq. (1)] satisfied by these quantities. In 1975, Schulten and Gordon (SG) [2] developed an *ab initio* recursive algorithm that has come to be widely used. A particular advantage of the SG method is that it produces, as the result of the same calculation, not just the value of a single  $3j$  or  $6j$  symbol, as is the case with the direct approach, but values for an entire *family* of symbols whereby one quantum number is allowed to range over its allowed values with the other parameters of the symbol held fixed. From a computational point of view, however, a limitation of the SG method is that it readily leads to numerical overflows. Existing implementations of the SG method are designed to test for the occurrence of overflows and periodically rescale the iterates so as to keep them of a manageable magnitude to ensure numerical accuracy.

The purpose of this article concerns the limitation of the SG recursive method: overflows and the need for countermeasures. We show that this feature can be avoided entirely. Now, each of the  $3j$  or  $6j$  symbols  $f(j)$ ,  $g(m)$ , or  $h(j)$ , listed in Table I, separately obeys a recurrence relation of the form

$$X_\psi(n)\psi(n+1) + Y_\psi(n)\psi(n) + Z_\psi(n)\psi(n-1) = 0, \tag{1}$$

$$n_{\min} \leq n \leq n_{\max},$$

where  $\psi(n)$  signifies either  $f(j)$ ,  $g(m)$ , or  $h(j)$ , with the index  $n$  denoting  $j$  or  $m$  together with its allowed range of values,  $n_{\min} \leq n \leq n_{\max}$ . We also list in Table I the functions  $X_\psi$ ,  $Y_\psi$ , and  $Z_\psi$  that appear in the recurrence relation for each symbol, as well as the minimum and maximum values of the variable  $j$  or  $m$ . We propose to solve Eq. (1), a linear, three-term recurrence relation, by working with a pair of

*nonlinear, two-term* recurrence relations, each equivalent to Eq. (1), which are defined in terms of the ratios of successive values of  $\psi(n)$ . The first is given in terms of the ratios  $r_\psi(n) \equiv \psi(n)/\psi(n-1)$ ,

$$r_\psi(n) = \frac{-Z_\psi(n)}{Y_\psi(n) + X_\psi(n)r_\psi(n+1)}, \quad n \leq n_{\max} - 1. \tag{2}$$

Note that Eq. (2) defines a *backwards* recurrence scheme, where, since  $X_\psi(n_{\max}+1)=0$  for each of the symbols in Table I, the starting value  $r_\psi(n_{\max}) = -Z_\psi(n_{\max})/Y_\psi(n_{\max})$  is known. As an example, the version of Eq. (2) associated with the  $3j$  symbol  $f(j)$  is, using the information in Table I, given by  $r_f(j) = -(j+1)A(j)/[B(j) + jA(j+1)r_f(j+1)]$ . The second recurrence relation is defined in terms of the ratios  $s_\psi(n) \equiv \psi(n)/\psi(n+1)$ , which are suitable for forward iteration. In terms of these quantities, Eq. (1) is equivalent to

$$s_\psi(n) = \frac{-X_\psi(n)}{Y_\psi(n) + Z_\psi(n)s_\psi(n-1)}, \quad n \geq n_{\min} + 1, \tag{3}$$

where, since  $Z_\psi(n_{\min})=0$ , the starting value is known,  $s_\psi(n_{\min}) = -X_\psi(n_{\min})/Y_\psi(n_{\min})$ . The numerical advantage of making such transformations on Eq. (1) is that  $r_\psi(n)$  and  $s_\psi(n)$  maintain values of order unity throughout the iteration, which eliminates the possibility of overflows. The reason for considering separate backward and forward iteration schemes pertains to issues of numerical stability that are discussed below. Before delving into these issues, however, it will be instructive to illustrate the use of Eqs. (2) and (3).

We illustrate the use of Eqs. (2) and (3) upon assuming that the  $\psi(n)$  remain nonzero throughout the allowed range. We first employ a backward iteration on Eq. (2) from  $n = n_{\max}$  down to  $n = n_{\text{mid}} + 1$ , where  $n_{\text{mid}}$  is some convenient midpoint, e.g.,  $n_{\text{mid}} = \frac{1}{2}(n_{\min} + n_{\max})$ . One will thus have generated the sequence of iterates  $r_\psi(n_{\max}), r_\psi(n_{\max} - 1), \dots, r_\psi(n_{\text{mid}} + 1)$ . It is then straightforward to obtain  $\psi(n)$  for  $n_{\text{mid}} + 1 \leq n \leq n_{\max}$ ,

$$\psi(n_{\text{mid}} + k) = \psi(n_{\text{mid}}) \prod_{p=1}^k r_\psi(n_{\text{mid}} + p),$$

TABLE I. Parameters for, and constituents of, the three-term recurrence relations satisfied by the  $3j$  and  $6j$  symbols, as represented by Eq. (1). In each case, all parameters except the variable  $j$  or  $m$  are held fixed. Also listed are the normalization condition and sign convention for each symbol. We use the notation of Ref. [2].

$3j$ or $6j$ symbol ( $\psi$ )	$f(j)=\begin{pmatrix} j & j_2 & j_3 \\ -m_2-m_3 & m_2 & m_3 \end{pmatrix}$	$g(m)=\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m & -m-m_1 \end{pmatrix}$	$h(j)=\begin{pmatrix} j & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{pmatrix}$
Variable	$j$	$m$	$j$
$X_\psi$	$jA(j+1)$	$C(m+1)$	$jE(j+1)$
$Y_\psi$	$B(j)$	$D(m)$	$F(j)$
$Z_\psi$	$(j+1)A(j)$	$C(m)$	$(j+1)E(j)$
	$A(j)=\{[j^2-(j_2-j_3)^2][(j_2+j_3+1)^2-j^2] \times [j^2-(m_2+m_3)^2]\}^{1/2}$	$C(m)=[(j_2-m+1)(j_2+m) \times (j_3-m-m_1+1) \times (j_3+m+m_1)]^{1/2}$	$E(j)=[\{j^2-(j_2-j_3)^2 \times [(j_2+j_3+1)^2-j^2] \times [j^2-(l_2-l_3)^2 \times [(l_2+l_3+1)^2-j^2]\}^{1/2}$
Functions	$B(j)=(2j+1)[(m_2+m_3) \times \{j_2(j_2+1)-j_3(j_3+1)\} - (m_2-m_3)j(j+1)]$	$D(m)=j_2(j_2+1)+j_3(j_3+1) - j_1(j_1+1) - 2m(m+m_1)$	$F(j)=(2j+1)\{j(j+1)[-j(j+1) + j_2(j_2+1)+j_3(j_3+1) - 2l_1(l_1+1)+l_2(l_2+1) \times [j(j+1)+j_2(j_2+1) - j_3(j_3+1)]+l_3(l_3+1) \times [j(j+1)-j_2(j_2+1) + j_3(j_3+1)]\}$
End points	$j_{\min}=\max( j_2-j_3 , m_2+m_3)$ $j_{\max}=j_2+j_3$	$m_{\min}=\max(-j_2, -j_3-m_1)$ $m_{\max}=\min(j_2, j_3-m_1)$	$j_{\min}=\max( j_2-j_3 , l_2-l_3)$ $j_{\max}=\min(j_2+j_3, l_2+l_3)$
Normalization	$\sum_{j=j_{\min}}^{j_{\max}} (2j+1)f^2(j)=1$	$(2j_1+1)\sum_{m=m_{\min}}^{m_{\max}} g^2(m)=1$	$(2l_1+1)\sum_{j=j_{\min}}^{j_{\max}} (2j+1)h^2(j)=1$
Sign	$\text{sgn}[f(j_{\max})]=(-1)^{j_2-j_3+m_2+m_3}$	$\text{sgn}[g(m_{\max})]=(-1)^{j_2-j_3-m_1}$	$\text{sgn}[h(j_{\max})]=(-1)^{j_2+j_3+l_2+l_3}$

$$1 \leq k \leq n_{\max} - n_{\text{mid}}. \quad (4)$$

Of course, the value of  $\psi(n_{\text{mid}})$  is presently unknown; it will be determined shortly through normalization. We now iterate Eq. (3) from  $n=n_{\min}$  up to  $n=n_{\text{mid}}-1$ ; this produces the iterates  $s_\psi(n_{\min}), s_\psi(n_{\min}+1), \dots, s_\psi(n_{\text{mid}}-1)$ . From these quantities we obtain  $\psi(n)$  for  $n_{\min} \leq n \leq n_{\text{mid}}-1$ ,

$$\psi(n_{\text{mid}}-k) = \psi(n_{\text{mid}}) \prod_{p=1}^k s_\psi(n_{\text{mid}}-p),$$

$$1 \leq k \leq n_{\text{mid}} - n_{\min}. \quad (5)$$

With the combined equations (4) and (5), we have thus determined the  $\psi(n)$  up to an unknown multiplicative factor  $\psi(n_{\text{mid}})$ . The magnitude of this factor is readily determined by imposing the normalization conditions given in Table I. We then utilize the phase information listed in Table I to completely determine  $\psi(n)$  for all  $n$ . As an example, we show in Fig. 1 the result of applying this simple algorithm to obtain the family of  $3j$  symbols,

$$f(j) = \begin{pmatrix} j & 100 & 60 \\ -15 & 70 & -55 \end{pmatrix},$$

which remains nonzero over the allowed range  $40 \leq j \leq 160$ .

The  $3j$  and  $6j$  symbols, of course, can and do vanish for selected values of their parameters. If, say,  $\psi(n_0) \equiv 0$ ,  $r_\psi(n_0+1)$  and  $s_\psi(n_0-1)$  are undefined. We must therefore modify the above algorithm to account for this possibility, and we will be guided by the following observations. Examining Fig. 1, we note the resemblance between  $f(j)$  and a one-dimensional bound quantum eigenstate. This is a generic feature of the  $3j$  and  $6j$  symbols; we use  $f(j)$  merely as an illustration. Now, it is known, from the semiclassical theory of the  $3j$  and  $6j$  symbols [3], that the range of allowed quantum numbers,  $n_{\min} \leq n \leq n_{\max}$ , can be divided into the following subranges: a ‘‘classical’’ region  $n_I \leq n \leq n_{II}$  and two complementary ‘‘nonclassical’’ regions  $n_{\min} \leq n < n_I$  and  $n_{II} < n \leq n_{\max}$ . The classical region is defined as the set of quantum numbers for which it is possible to construct a vector diagram showing the coupling of the angular momentum vectors; in the nonclassical regimes, such vector diagrams do not exist [4]. The limits of the classical region,  $n_I$  and  $n_{II}$ ,

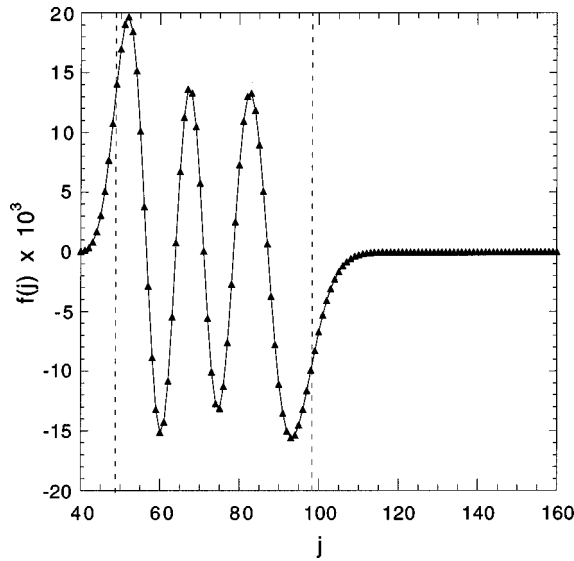


FIG. 1. Values for the family of  $3j$  symbols,  $f(j) = \binom{j}{15} \binom{100}{70} \binom{60}{-55}$ , over the entire range of allowed  $j$  values,  $40 \leq j \leq 160$ . In the classical region,  $j_I \leq j \leq j_{II}$ , where here  $j_I = 49$  and  $j_{II} = 98$  (shown as dashed lines),  $f(j)$  has an oscillatory character; in the nonclassical regions,  $f(j)$  decays monotonically. There are 25 orders of magnitude difference between the largest and smallest values in this family of  $3j$  symbols.

are determined as the roots of a certain determinant, known as the Cayley determinant [3]. For the parameters of Fig. 1, these are shown as dashed lines. The important point is that, in analogy with a bound eigenstate, in the classical region the  $3j$  and  $6j$  symbols have an oscillatory character, whereas in the nonclassical regions, they are monotonically decaying [3]. Depending on the width of the nonclassical regions, there can be many orders of magnitude difference between the smallest values of  $|\psi(n)|$  (found at  $n_{\max}$  and  $n_{\min}$ ) and the largest values, which occur in the classical region. In Fig. 1, for example, there are some 25 orders of magnitude difference between the largest and smallest values in this family of  $3j$  symbols.

These considerations are relevant for the following reasons. In numerical treatments of the one-dimensional Schrödinger equation, one employs the standard finite-difference approximation to replace the continuous differential equation by a three-term recurrence relation. We note that, conversely, as discussed in Ref. [2], the three-term recurrence relations satisfied by the  $3j$  and  $6j$  symbols can be shown to originate from eigenvalue problems. Now, as is well known, three-term recurrence relations possess two linearly independent solutions. If the desired physical solution of a recurrence relation is monotonically decreasing, as with the decay of  $\psi(n)$  in its nonclassical regions, it is simple to show that the other, linearly independent solution will be monotonically increasing. Indeed, the source of the numerical instability associated with three-term recurrence relations is that [5] if one attempts to calculate a decaying solution of the recurrence relation by *forward* iteration, the slightest round-off error will trigger the growth of the unwanted, linearly independent, diverging solution.

Therefore, in the nonclassical regions one must iterate the recurrence relation in the direction of increasing  $|\psi(n)|$  to avoid the instability. These are also just the regions where

overflows can develop. By contrast, in the classical region, where the solutions to the recurrence relation are oscillatory, there is no source of instability and one may safely iterate in either direction. The problem we seek to avoid in our ratio-based method is that of encountering an identically zero value of  $\psi$ . The zeros of  $\psi$ , however, if they occur, occur only in the classical region, where  $\psi(n)$  is oscillatory. We therefore adopt a hybrid approach. We utilize the two-term recurrence relations (2) and (3) in the respective nonclassical regions and the three-term recurrence relation (1) in the classical region.

For our purposes, however, precisely *where* one draws the line between the classical and nonclassical regions is not crucial; all that is important is that we stop iterating with Eqs. (2) and (3) somewhere in the classical region, before we encounter a zero of  $\psi(n)$ . We will therefore adopt the following convention. In iterating Eqs. (2) and (3), starting from  $n_{\max}$  and  $n_{\min}$ , respectively, we note that both  $r_{\psi}(n)$  and  $s_{\psi}(n)$  initially maintain values less than unity. Only when we reach the first local extremum of  $\psi(n)$  do  $r_{\psi}$  and  $s_{\psi}$  first exceed unity. This provides a natural criterion for the locations of the boundaries and one that is simple to implement algorithmically. We will denote the values of  $n$  where  $r_{\psi}(n)$  and  $s_{\psi}(n)$  first exceed unity (having started from  $n_{\max}$  and  $n_{\min}$ ) by  $n_+$  and  $n_-$ , respectively. Specifically, we have  $r_{\psi}(n_+) > 1$ , but  $r_{\psi}(n_+ + 1) < 1$ .

The modifications of Eqs. (4) and (5) then become

$$\psi(n_+ + k) = \psi(n_+) \prod_{p=1}^k r_{\psi}(n_+ + p),$$

$$1 \leq k \leq n_{\max} - n_+, \quad (4')$$

and

$$\psi(n_- - k) = \psi(n_-) \prod_{p=1}^k s_{\psi}(n_- - p),$$

$$1 \leq k \leq n_- - n_{\min}, \quad (5')$$

where, as before,  $r_{\psi}$  and  $s_{\psi}$  are obtained from Eqs. (2) and (3), now for  $n_+ \leq n \leq n_{\max}$  and  $n_{\min} \leq n \leq n_-$ , respectively. At this point, we have the unknown quantities in Eqs. (4') and (5'),  $\psi(n_+)$  and  $\psi(n_-)$ . We can eliminate one of these unknowns in terms of the other as follows. Let us define two auxiliary sequences  $\Psi_-(n) \equiv \psi(n)/\psi(n_-)$  and  $\Psi_+(n) \equiv \psi(n)/\psi(n_+)$ . These quantities obviously satisfy the same three-term recurrence relation (1). One can then use Eq. (1) to iterate  $\Psi_-(n)$  in the forward direction starting from  $n = n_-$ , using the initial values  $\Psi_-(n_- - 1) = s_{\psi}(n_- - 1)$  and  $\Psi_-(n_-) = 1$ , up to some value of  $n$ ,  $n_c \leq n_+$ , say. (For convenience, we can take  $n_c = n_+$  if desired.) Likewise, we can use Eq. (4) to iterate  $\Psi_+(n)$  in the backward direction starting from  $n = n_+$ , using the initial values  $\Psi_+(n_+ + 1) = r_{\psi}(n_+ + 1)$  and  $\Psi_+(n_+) = 1$ , down to  $n = n_c$ . The value of  $\psi(n_c)$  derived from these two sequences must obviously be identical. This yields the connection between  $\psi(n_+)$  and  $\psi(n_-)$ ,  $\psi(n_-)/\psi(n_+) = \Psi_+(n_c)/\Psi_-(n_c)$ . Multiplying the  $\Psi_-(n)$  (which have now been evaluated unambiguously for  $n_{\min} \leq n \leq n_c$ ) by  $\psi(n_-)/\psi(n_+)$  thus leaves us with  $\Psi_+(n)$  for  $n_{\min} \leq n \leq n_{\max}$ ; i.e., we have determined  $\psi(n)$  up to the

unknown multiplicative factor  $\psi(n_+)$ . As before, we determine this factor by applying the normalization conditions and sign conventions given in Table I.

In conclusion, we have presented a recursive algorithm to compute the Wigner  $3j$  and  $6j$  symbols that simplifies the well-known SG method. Our method is based on the use of nonlinear, two-term recurrence relations that are obtained from the standard three-term recurrence relations obeyed by the  $3j$  and  $6j$  symbols. By eliminating the programming overhead of having to check for near overflows and keeping

track of rescaling factors, our algorithm provides a highly accurate, yet significantly simpler framework, with which to calculate these quantities.

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