Semiclassical approximations to 3j- and 6j-coefficients for quantum-mechanical coupling of angular momenta*

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(Received 21 April 1975)

The coupling of angular momenta is studied using quantum mechanics in the limit of large quantum numbers (semiclassical limit). Uniformly valid semiclassical expressions are derived for the 3j (Wigner) coefficients coupling two angular momenta, and for the 6j (Racah) coefficients coupling three angular momenta. In three limiting cases our new expressions reduce to those conjectured by Ponzano and Regge. The derivation involves solving the recursion relations satisfied by these coefficients, by a discrete analog of the WKB method. Terms of the order of the inverse square of the quantum numbers are neglected in the derivation, so that the results should be increasingly accurate for larger angular momenta. Numerical results confirm this asymptotic convergence. Moreover, the results are of a useful accuracy even at small quantum numbers.

I. INTRODUCTION

3j- and 6j-coefficients describe the quantum mechanical coupling of two and three angular momentum states, respectively. Classically this coupling corresponds to the addition of angular momentum vectors. For larger angular momenta the classical concept of vector addition becomes increasingly valid; so that in the limit of very large quantum numbers 3j- and 6j-coefficients should have an interpretation in terms of classical vector diagrams (Figs. 1a, 2a, 3a). One can expect that in this semiclassical limit 3j- and 6j-coefficients can be expressed as simple functions of the geometric variables which describe the classical angular momentum addition. Such a functional relationship between angular momentum coupling coefficients and classical vector diagrams has been suggested, on the basis of heuristic arguments, by Ponzano and Regge.[1] It is one aim of this paper to give a rigorous derivation for the expressions of Ponzano and Regge as the asymptotic (WKB) solutions of the recursion equations which define 3j- and 6j-coefficients.

For certain quantum mechanically allowed 3j- and 6j-coefficients, classical vector diagrams do not exist. For example, the classical angular momenta associated with some 6j-coefficients cannot be connected to give a vector tetrahedron as in Fig. 3a, and such cases are called classically forbidden. Thus, the quantum number domains of the angular momentum coupling coefficients are to be separated into classically allowed and classically forbidden regions. Interestingly enough, the algebraic definition of the geometric variables (volume and dihedral angles of the 6j-tetrahedron, etc.) can be continued from the classical domain of quantum numbers to the nonclassical domains. Accordingly, Ponzano and Regge stated three different expressions for 3j- and 6j-coefficients valid in either the classical domain, the nonclassical domain or at the boundary between these two domains. These expressions do not, however, smoothly connect with each other, and lacking a systematic derivation of their results Ponzano and Regge were not able to correct this deficiency.

Miller,[2] starting from the correspondence relations of classical and quantum mechanics, recently derived a semiclassical expression for 3j-coefficients restricted to the classically allowed domain of quantum numbers. Miller's result is identical with the corresponding expression of Ponzano and Regge giving, thus, support to the supposition that Ponzano and Regge's formulas are amenable to a rigorous derivation. We have, in fact, found such derivation and present it here. The route we have taken for this derivation will be outlined now.

One may recall that semiclassical expressions for quantum mechanical wavefunctions can be determined as asymptotic solutions of the Schrödinger second order differential equation by means of the WKB approximation. The 3j- and 6j-coefficients are the solutions of certain linear recursion equations which, as we have shown,[3] provide the most efficient and stable algorithm for their evaluation even for very large quantum numbers. The important role of these recursion equations in determining, except for overall factors, the angular momentum coupling coefficients had been well known in the early days of quantum mechanics[4] but sank into oblivion after the advent of group theory and the following derivation of closed expressions of 3j- and 6j-coefficients by Wigner[5] and Racah.[6] The three term recursion equations can be formally written as second order *difference* equations which are closely related to the second order differential equations which result from the Schrödinger equation for wavefunctions. In view of this relationship, it seems reasonable to attempt a derivation of the semiclassical formulas for 3j- and 6j-coefficients as the asymptotic (WKB) solutions of their recursion equations. To this purpose we extended the WKB theory from differential to difference equations and this yields then the semiclassical expressions of Ponzano and Regge.

The recursion equations determine the angular momentum coupling coefficients over a discrete domain of quantum numbers. Classical angular momenta vary over a continuous domain of values. According to the correspondence of classical and quantum mechanics one expects that the semiclassical expressions of 3j- and 6j-coefficients can be defined over continuous domains also. In fact, we have found that the asymptotic solutions of the 3j- and 6j-recursion equations viewed as functions of continuous variables obey asymptotically certain differential equations. Hence, the semiclassical $3j$- and $6j$-coefficients can also be understood as the WKB solutions of these second order differential equations in order to account for the continuous variation of the angular momenta in the semiclassical limit. If one employs the uniform WKB approximation to these differential equations, one obtains the $3j$- and $6j$-coefficients in terms of Airy function formulas which are uniformly valid over the entire domain of quantum numbers and, thus, present considerable improvement in accuracy, over the expressions given by Ponzano and Regge.

In Sec. 2 we will present the recursion equations of $3j$- and $6j$-coefficients, and show that in the semiclassical limit these equations are connected algebraically with classical vector diagrams. In Sec. 3 we derive the WKB solutions for second order difference equations, and demonstrate that these solutions also asymptotically satisfy associated differential equations. In Sec. 4 we apply the WKB approximation to obtain the semiclassical $3j$-coefficients in analytic form. In Sec. 5 these calculations are repeated to derive the semiclassical $6j$-coefficients. Finally, we compare in Sec. 6 the exact and the semiclassical values of $3j$- and $6j$-coefficients and demonstrate their convergence for large quantum numbers.

II. SEMICLASSICAL RECURSION EQUATIONS FOR 3j-COEFFICIENTS

The Wigner $3j$-coefficients define the algebra of the quantum mechanical addition of angular momenta.[7] For a classical mechanical system with two internal angular momenta $\mathbf{J}_2$ and $\mathbf{J}_3$ the resulting total angular momentum is uniquely determined as $\mathbf{J}_1 = \mathbf{J}_2 + \mathbf{J}_3$. Quantum mechanically, it is not possible to specify for the angular momenta $\mathbf{J}_2$ and $\mathbf{J}_3$ simultaneously all three Cartesian vector components, but at most one component. If the z-components m_2 and m_3 are thought to be specified the system is said to be prepared in the internal angular momentum state $|j_2 m_2\rangle\, |j_3 m_3\rangle$. The relative orientation of the angular momenta $\mathbf{J}_2$ and $\mathbf{J}_3$ in the x, y plane, measured by an angle η_1 is then necessarily undetermined, each angle η_1 being equally likely. Hence, the total angular momentum $|\mathbf{J}_1|$ can assume a variety of values depending on the relative orientations η_1 of $\mathbf{J}_2$ and $\mathbf{J}_3$. This situation is depicted by the classical vector diagram in Fig. 1a.

The system under consideration may also be prepared in a particular total angular momentum state $|(j_2, j_3)j_1 m_1\rangle$. For a system prepared in such a fashion the components of the angular momenta $\mathbf{J}_2$ and $\mathbf{J}_3$ have fixed projections along $\mathbf{J}_1$. The remaining components of $\mathbf{J}_2$ and $\mathbf{J}_3$, perpendicular to $\mathbf{J}_1$, are then necessarily undetermined. This situation is illustrated by the classical vector diagram in Fig. 2a. In particular, the z-components of $\mathbf{J}_2$ and $\mathbf{J}_3$ can take on a variety of values, depending on the orientation Θ_1 of $\mathbf{J}_2$ and $\mathbf{J}_3$ in a plane perpendicular to $\mathbf{J}_1$. Because of the randomness of the orientations of $\mathbf{J}_2$ and $\mathbf{J}_3$, each angle Θ_1 is equally likely.

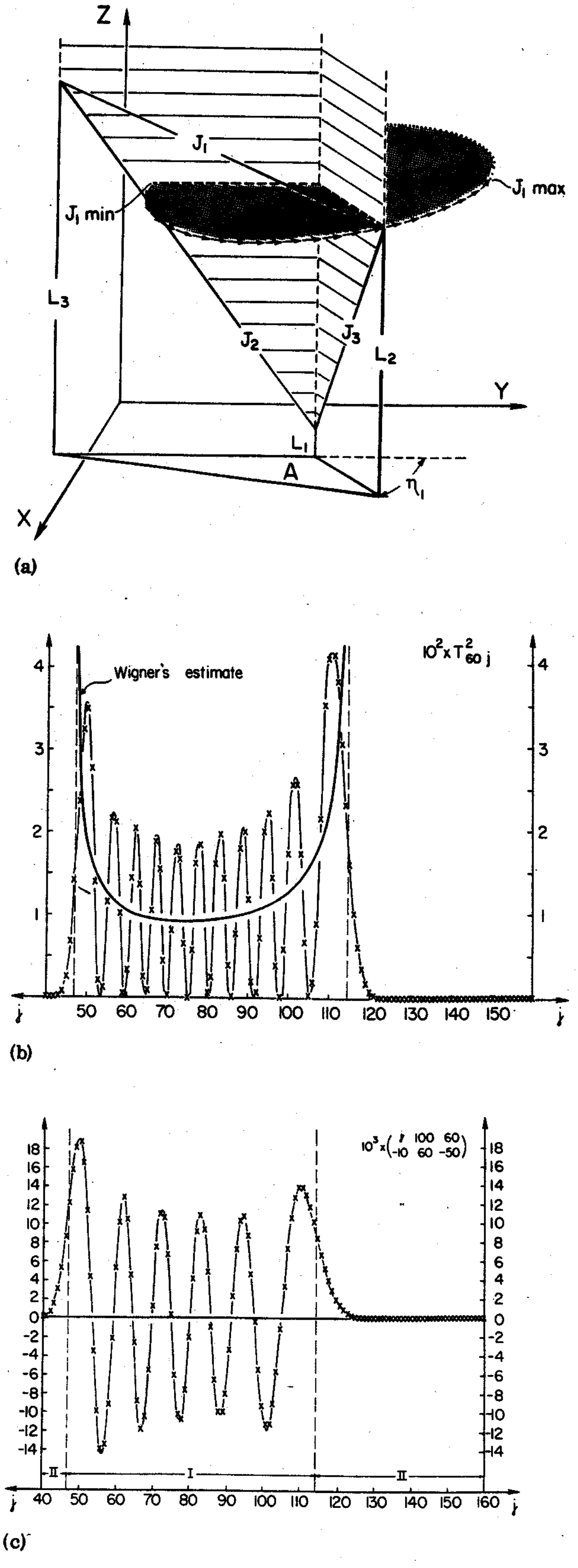

FIG. 1. The series of $3j$-coefficients $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$, $j_1 \min \le j_1 \le j_1 \max$, in (c) and the corresponding manifold of classical angular momentum vector diagrams $\mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 = 0$ $(J_i = j_i + \frac{1}{2},\ J_{iz} = m_i)$ generated by rotation around the shaded circle in (a). The quantum mechanical probability distribution $(2j_1+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2$ for the occurrence of the classical vector diagrams in (a) are compared in (b) with Wigner's semiclassical estimate $(2j_1+1)/4\pi A$.

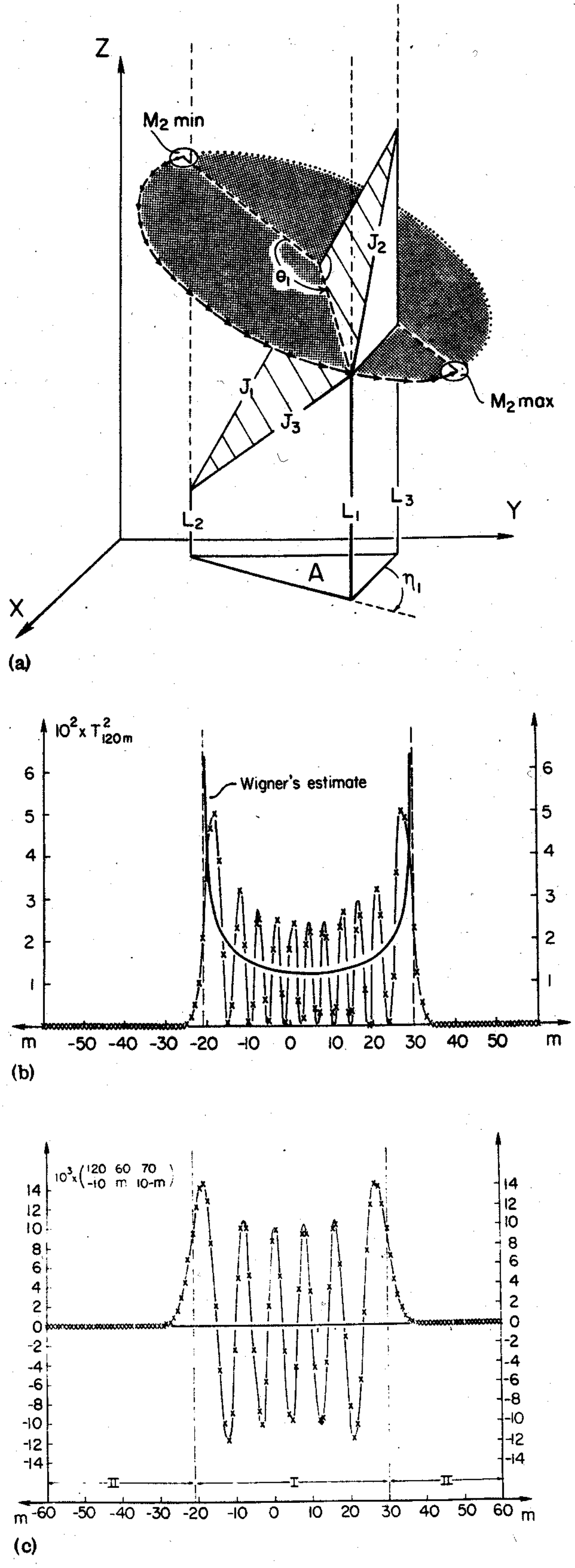

FIG. 2. The series of $3j$-coefficients $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$, $m_2\,\text{min} \leq m_2 \leq m_2\,\text{max}$, in (c) and the corresponding manifold of classical angular momentum vector diagrams $J_1 + J_2 + J_3 = 0$ ($J_i = j_i + \frac{1}{2}$, $J_{iz} = m_i$) generated by rotation around the shaded circle in (a). The quantum mechanical probability distribution $(2j_1+1)\begin{pmatrix} j_1 & j_2 & j_2 \\ m_1 & m_2 & m_3 \end{pmatrix}^2$ for the occurrence of the classical vector diagrams in (a) are compared in (b) with Wigner's semiclassical estimate $(2j_1+1)/4\pi A$.

The unitary transformation T between the representation $|j_2 m_2\rangle\,|j_3 m_3\rangle$ and $|(j_2,j_3)j_1 m_1\rangle$ of the system of two angular momenta

$$|j_2 m_2\rangle\,|j_3 m_1 - m_2\rangle = \sum_{j_1} T_{m_2 j_1}\,|(j_2,j_3)j_1 m_1\rangle \tag{1}$$

defines the $3j$-coefficients

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_2 & m_1 - m_2 \end{pmatrix} = (-1)^{j_2 - j_3 + m_1}\,[2j_1+1]^{-1/2}\,T_{m_2 j_1}. \tag{2}$$

T is customarily chosen real with the phase convention for its row vectors adopted as by Wigner. The squares $T_{m_2 j_1}{}^2$ of the elements of T are to be interpreted as the probability for a system prepared in the internal angular momentum state $|j_2 m_2\rangle\,|j_3 m_1 - m_2\rangle$ to be found in the total angular momentum state $|(j_2,j_3)j_1 m_1\rangle$ and, vice versa, as the probability for a system prepared in the total angular momentum state $|(j_2,j_3)j_1 m_1\rangle$ to be found in the internal angular momentum state $|j_2 m_2\rangle\,|j_3 m_1 - m_2\rangle$. On the basis of this interpretation Wigner established an approximate functional expression for $3j$-coefficients, using the classical vector diagrams in Figs. 1a and 2a. The probability that in Fig. 1a $j_1 \leq |\mathbf{J}_2 + \mathbf{J}_3| \leq j_1 + 1$, given by $T_{m_2 j_1}{}^2$, can be evaluated from the fact that each relative orientation η_1 of $\mathbf{J}_2$ and $\mathbf{J}_3$ is equally likely. Wigner found[5]

$$T_{m_2 j_1}{}^2 = (2j_1+1)/4\pi A \tag{3}$$

where A, the area of the triangle $\Delta(\mathbf{J}_1, \mathbf{J}_2, \mathbf{J}_3)$ projected onto the x, y plane, is given by the Cayley determinant

$$A^2 = -\frac{1}{16}\begin{vmatrix} 0 & J_1{}^2 - m_1{}^2 & J_2{}^2 - m_2{}^2 & 1 \\ J_1{}^2 - m_1{}^2 & 0 & J_3{}^2 - m_3{}^2 & 1 \\ J_2{}^2 - m_2{}^2 & J_3{}^2 - m_3{}^2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix}. \tag{4}$$

Likewise, the probability for $m_2 \leq J_{2z} \leq m_2 + 1$ in Fig. 2a also given by $T_{m_2 j_1}{}^2$ can be evaluated by assuming that each angle Θ_1 is equally likely. The result is again (3).

In Figs. 1c and 2c the $3j$-coefficients $\begin{pmatrix} j_1 & 100 & 60 \\ -10 & 60 & -50 \end{pmatrix}$ and $\begin{pmatrix} 120 & 60 & 70 \\ -10 & m_2 & 10-m_2 \end{pmatrix}$ are plotted representing the quantum mechanical probability amplitudes corresponding to the classical angular momentum coupling depicted by Figs. 1a and 2a. Figures 1b and 2b present the associated probabilities $T_{m_2 j_1}{}^2$ for a comparison with the Wigner expression (3). One can see that Eq. (3) does not really approximate individual $3j$-coefficients, but does provide an approximation for the average taken over a few neighboring $3j$-coefficients. Our aim now is to show how Wigner's estimate can be refined to give more accurate expressions for individual $3j$-coefficients.

The $3j$-coefficients in Figs. 1c and 2c are determined except for an overall constant factor as solutions of recursion equations. The coupling coefficients in Fig. 1c associated with the classical angular momentum diagram in Fig. 1a obey the recursion equation[3]

$$(j_1+1)\,a(j_1)\begin{pmatrix} j_1-1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix} - (2j_1+1)\,b(j_1)$$

$$\times \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix} + j_1 a(j_1+1)\begin{pmatrix} j_1+1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix} = 0 \tag{5a}$$

where

$$a(j_1) = \{[(j_2+j_3+1)^2 - j_1^2][j_1^2-(j_2-j_3)^2][j_1^2-m_1^2]\}^{1/2}, \tag{5b}$$

$$b(j_1) = 2j_1(j_1+1)m_2 + [j_1(j_1+1)+j_2(j_2+1)-j_3(j_3+1)]m_1. \tag{5c}$$

The coupling coefficients in Fig. 2c associated with the classical angular momentum diagram in Fig. 2a are the solution of[3]

$$c(m_2,m_3)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2-1 & m_3+1\end{pmatrix} + d(m_2,m_3)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix}$$

$$+\,c(m_2+1,m_3-1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1\end{pmatrix} = 0 \tag{6a}$$

where

$$c(m_2,m_3) = [(j_2-m_2+1)(j_2+m_2)(j_3+m_3+1)(j_3-m_3)]^{1/2}, \tag{6b}$$

$$d(m_2,m_3) = j_2(j_2+1) + j_3(j_3+1) - j_1(j_1+1) + 2m_2m_3. \tag{6c}$$

In the limit of large angular momentum quantum numbers recursion equations (5) and (6) are algebraically connected with the classical vector diagrams in Figs. 1a and 2a. To demonstrate this asymptotic connection, one may multiply the quantum numbers j_i and m_i by a parameter λ assumed to be large such that all terms in Eqs. (5) and (6) of order $O(\lambda^{-2})$ and smaller may be neglected. Let us apply this approximation to Eq. (5) first. The length of a classical angular momentum vector corresponding to the quantum number λj_i is $\lambda J_i = \lambda j_i + \frac{1}{2}$ (in units $\hbar$). Substituting this in (5b) gives

$$a(j_1) = 4F(\lambda J_1 - \tfrac{1}{2},\ \lambda J_2, \lambda J_3)P(\lambda J_1 - \tfrac{1}{2},\ \lambda m_1)$$

where

$$F(a,b,c) = \tfrac{1}{4}[(a+b+c)(-a+b+c)(a-b+c)(a+b-c)]^{1/2}$$

is the area of a triangle $\Delta(a,b,c)$ and $P(r,z)=\sqrt{r^2-z^2}$ is the x,y component of a vector $\mathbf{r}$ with z component z. $F(\lambda J_1 - \frac{1}{2},\ \lambda J_2, \lambda J_3)$ may be factorized in the following way:

$$F(\lambda J_1 - \tfrac{1}{2},\ \lambda J_2,\ \lambda J_3)$$
$$= [F(\lambda J_1 - 1,\ \lambda J_2,\ \lambda J_3) F(\lambda J_1,\ \lambda J_2,\ \lambda J_3)]^{1/2}$$
$$\times\left[\frac{F(J_1-(1/2\lambda),\ J_2,\ J_3)}{F(J_1-(1/\lambda),\ J_2,\ J_3)}\ \frac{F(J_1-(1/2\lambda),\ J_2,\ J_3)}{F(J_1,\ J_2,\ J_3)}\right]^{1/2}$$
$$= [1+0(\lambda^{-2})][F(\lambda J_1-1, \lambda J_2, \lambda J_3)F(\lambda J_1, \lambda J_2, \lambda J_3)]^{1/2}.$$

Performing this factorization also for $P(\lambda J_1 - \frac{1}{2},\ \lambda m_1)$ and $\lambda J_1 + \frac{1}{2}$ gives

$$(j_1+1)\,a(j_1) = [1+0(\lambda^{-2})]\,4[\lambda J_1(\lambda J_1+1)\,F(\lambda J_1-1, \lambda J_2, \lambda J_3)$$
$$\times F(\lambda J_1, \lambda J_2, \lambda J_3)\,P(\lambda J_1-1,\ \lambda m_1)P(\lambda J_1, \lambda m_1)]^{1/2}.$$

Substitution of the classical angular momenta λJ_i into (5c) yields

$$b(j_1) = 2\lambda^2 J_1^2 \lambda m_2 + (\lambda^2 J_1^2 + \lambda^2 J_2^2 - \lambda^2 J_3^2)\lambda m_1 - \tfrac{1}{2}\lambda m_2 - \tfrac{1}{4}\lambda m_1$$
$$= [1+O(\lambda^{-2})][2\lambda^2 J_1^2 \lambda m_2 + (\lambda^2 J_1^2 + \lambda^2 J_2^2 - \lambda^2 J_3^2)\lambda m_1].$$

Neglecting then terms of order $O(\lambda^{-2})$ allows us to write (5a) in the more symmetric form

$$\left(\frac{F(\lambda J_1-1, \lambda J_2, \lambda J_3)\,P(\lambda J_1-1, \lambda m_1)}{\lambda J_1 - 1}\right)^{1/2}\begin{pmatrix} \lambda j_1-1 & \lambda j_2 & \lambda j_3 \\ \lambda m_1 & \lambda m_2 & \lambda m_3\end{pmatrix}$$

$$-\,2\,\frac{2\lambda^2 J_1^2 \lambda m_2 + (\lambda^2 J_1^2 + \lambda^2 J_2^2 - \lambda^2 J_3^2)\lambda m_1}{4F(\lambda J_1, \lambda J_2, \lambda J_3)P(\lambda J_1, \lambda m_1)}$$

$$\times\left(\frac{F(\lambda J_1, \lambda J_2, \lambda J_3)\,P(\lambda J_1, \lambda m_1)}{\lambda J_1}\right)^{1/2}\begin{pmatrix} \lambda j_1 & \lambda j_2 & \lambda j_3 \\ \lambda m_1 & \lambda m_2 & \lambda m_3\end{pmatrix}$$

$$+\left(\frac{F(\lambda J_1+1, \lambda J_2, \lambda J_3)\,P(\lambda J_1+1, \lambda m_1)}{\lambda J_1 + 1}\right)^{1/2}$$

$$\times\begin{pmatrix} \lambda j_1+1 & \lambda j_2 & \lambda j_3 \\ \lambda m_1 & \lambda m_2 & \lambda m_3\end{pmatrix} \approx 0 \tag{7}$$

if one sets in addition $\lambda J_1/[(\lambda J_1 - 1)(\lambda J_1 + 1)]^{1/2} = 1 + O(\lambda^{-2}) \approx 1$.

Keeping the parameter λ explicitly in the following derivations would lead to a somewhat cumbersome notation. We will therefore omit the parameter λ in the remaining formulas and assume instead the quantum numbers $j_i(J_i)$ and m_i to be large.

The classical vector diagram (prism) in Fig. 1a is the geometrical counterpart of the $3j$-coefficients $\left(\begin{smallmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{smallmatrix}\right)$. Its triangular base $\Delta(J_1, J_2, J_3)$ contains the sides $j_1 + \frac{1}{2}$, $j_2 + \frac{1}{2}$, and $j_3 + \frac{1}{2}$, the parallel edges L_1, L_2, L_3 are connected with the magnetic quantum numbers through

$$m_1 = L_2 - L_3, \quad m_2 = L_3 - L_1, \quad m_3 = L_1 - L_2. \tag{8}$$

The second base in the x,y plane is the triangle $\Delta[P(j_1,m_1);\ P(j_2,m_2);\ P(j_3,m_3)]$. To emphasize the geometric interpretation of the $3j$-coefficients we define

$$\begin{bmatrix} J_1 & J_2 & J_3 \\ L_1 & L_2 & L_3\end{bmatrix} \equiv \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3\end{pmatrix}. \tag{9}$$

Since for nonvanishing $3j$-coefficients $m_1 + m_2 = 0$, the three magnetic quantum numbers represent only two independent variables for the $3j$-coefficient. This property is reflected upon the new variables L_1, L_2, and L_3 through

$$\begin{bmatrix} J_1 & J_2 & J_3 \\ L_1+L & L_2+L & L_3+L\end{bmatrix} = \begin{bmatrix} J_1 & J_2 & J_3 \\ L_1 & L_2 & L_3\end{bmatrix}$$

for any constant L. Addition of such a constant L is geometrically equivalent to a parallel displacement of the x,y plane in Figs. 1a and 2a along the z axis.

The coefficients in Eq. (7) are related algebraically to the classical vector diagram associated with $\left[\begin{smallmatrix} J_1 & J_2 & J_3 \\ L_1 & L_2 & L_3\end{smallmatrix}\right]$. The area A of $\Delta[P(j_1,m_1);\ P(j_2,m_2);\ P(j_3,m_3)]$ is

$$A=\frac{F(J_1,J_2,J_3)P(J_1,m_1)}{J_1}\ \sin\theta_1 \tag{10}$$

where θ_1, the dihedral angle of the prism adjacent to the side J_1, is determined algebraically through[1]

$$\cos\theta_1=[2J_1^2m_2+(J_1^2+J_2^2-J_3^2)m_1]/4F(J_1,J_2,J_3)P(J_1,m_1). \tag{11}$$

By virtue of Eqs. (10) and (11), Eq. (7) becomes

$$\left(\frac{A(J_1-1)}{\sin\theta_1(J_1-1)}\right)^{1/2}\begin{bmatrix}J_1-1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}+\left(\frac{A(J_1+1)}{\sin\theta_1(J_1+1)}\right)^{1/2}$$

$$\times\begin{bmatrix}J_1+1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}$$

$$+2\cos\theta_1(J_1)\left(\frac{A(J_1)}{\sin\theta_1(J_1)}\right)^{1/2}\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}\approx 0. \tag{12}$$

This equation, the asymptotic form of Eq. (5) for large quantum numbers, may be regarded as the semiclassical version of the recursion equation for the 3j-coefficients in Fig. 1c.

The asymptotic form of recursion equation (6) can also be derived by expansion in terms of the parameter λ introduced above. We will not follow this procedure explicitly, but point out that the approximation taken again neglects only terms of order $O(\lambda^{-2})$. Equations (6b) and (6c) are then approximately

$$c(m_2,m_3)\approx[P(J_2,m_2-1)P(J_2,m_2)P(J_3,m_3)P(J_3,m_3+1)]^{1/2},$$

$$d(m_2,m_3)\approx J_2^2+J_3^2-J_1^2+2m_2m_3,$$

so that (6a) takes the symmetric form

$$[P(J_2,m_2-1)P(J_3,m_3+1)]^{1/2}\begin{pmatrix}j_1 & j_2 & j_3\\ m_1 & m_2-1 & m_3+1\end{pmatrix}$$

$$+[P(J_2,m_2+1)P(J_3,m_3-1)]^{1/2}\begin{pmatrix}j_1 & j_2 & j_3\\ m_1 & m_2+1 & m_3-1\end{pmatrix}$$

$$+\frac{J_2^2+J_3^2-J_1^2+2m_2m_3}{P(J_2,m_2)P(j_3,m_3)}[P(J_2,m_2)P(J_3,m_3)]^{1/2}$$

$$\times\begin{pmatrix}j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix}\approx 0. \tag{13}$$

The coefficients in this equation can be related algebraically to the classical vector diagram in Fig. (2a). By means of the identities[1]

$$2A=P(J_2,m_2)P(J_3,m_3)\sin\eta_1 \tag{14}$$

and

$$\cos\eta_1=-\tfrac{1}{2}\frac{J_2^2+J_3^2-J_1^2+2m_2m_3}{P(J_2,m_2)P(J_3,m_3)} \tag{15}$$

where η_1 is the dihedral angle of the angular momentum prism adjacent to the side L_1, Eq. (13) becomes

$$\left(\frac{A(L_1-1)}{\sin\eta_1(L_1-1)}\right)^{1/2}\begin{bmatrix}J_1 & J_2 & J_3\\ L_1-1 & L_2 & L_3\end{bmatrix}+\left(\frac{A(L_1+1)}{\sin\eta_1(L_1+1)}\right)^{1/2}$$

$$\times\begin{bmatrix}J_1 & J_2 & J_3\\ L_1+1 & L_2 & L_3\end{bmatrix}-2\cos\eta_1(L_1)\left(\frac{A(L_1)}{\sin\eta_1(L_1)}\right)^{1/2}$$

$$\times\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}\approx 0. \tag{16}$$

Equations (12) and (16) may be formally written as second order difference equations. Defining

$$f(J_1)=(-1)^{j_1+j_2+j_3}\left(\frac{A(J_1)}{\sin\theta_1(J_1)}\right)^{1/2}\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}, \tag{17a}$$

$$g(L_1)=(-1)^{j_1+j_2+j_3}\left(\frac{A(L_1)}{\sin\eta_1(L_1)}\right)^{1/2}\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}, \tag{17b}$$

(12) and (16) are

$$[\Delta^2(J_1)+2-2\cos\theta_1(J_1)]f(J_1)\approx 0, \tag{18a}$$

$$[\Delta^2(L_1)+2-2\cos\eta_1(L_1)]g(L_1)\approx 0, \tag{18b}$$

where the second order difference operator is defined through $\Delta^2(x)h(x)=h(x+1)-2h(x)+h(x-1)$.

The complete *quantum* number domains of Eqs. (18a) and (18b) are confined by the selection rules for 3j-coefficients. Equation (18a) holds over the J_1-domain

$[j_{1\,\min}+\frac{1}{2},\ j_{1\,\max}+\frac{1}{2}]$ with $j_{1\,\min}=\max\{|m_1|,|j_2-j_3|\}$

and $j_{1\,\max}=j_2+j_3$.

Equation (18b) holds over the m_2-domain

$[m_{2\,\min},m_{2\,\max}]$ with $m_{2\,\min}=\max\{-j_2,-j_3-m_1\}$

and $m_{2\,\max}=\min\{j_2,j_3-m_1\}$.

The J_1- and m_2-values occurring in the manifolds of the *classical* vector diagrams in Figs. 1a and 2a, respectively, are further confined to the smaller domains $[J_{1\,\min},J_{1\,\max}],[M_{2\,\min},M_{2\,\max}]$. In Fig. 1a the smallest and largest J_1-values $J_{1\,\min}$ and $J_{1\,\max}$ are assumed in the limit that the triangle $\Delta(J_1,J_2,J_3)$ comes to lie perpendicular to the x,y plane (flat prism!). Hence, $J_{1\,\min}$ and $J_{1\,\max}$ are determined as solutions of

$$A^2(J_1)=0 \tag{19}$$

or, alternatively, as solutions of either of the equations

$$\cos\theta\,(J_1)=\pm 1,\quad \cos\eta_i(J_1)=\pm 1 \tag{20}$$

where θ_i and η_i are the dihedral angles of the prism $\left[\begin{smallmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{smallmatrix}\right]$ adjacent to the sides J_i and L_i, respectively. The algebraic expressions for θ_2, θ_3 and η_2, η_3 can be obtained from Eqs. (11) and (15) by circular permutation of the labels of J_1, J_2, J_3 and m_1, m_2, m_3. Clearly, in the limit of a flat prism the dihedral angles are either 0 or π.

In Fig. 2a the smallest and largest m_2-values $M_{2\,\min}$ and $M_{2\,\max}$ are also assumed in the limit that $\Delta(J_1,J_2J_3)$ is oriented perpendicular to the x,y plane; i.e., $M_{2\,\min}$ and $M_{2\,\max}$ are the solutions of

$$A^2(m_2)=0 \tag{19'}$$

or

$$\cos\theta_i(m_2)=\pm 1,\quad \cos\eta_i(m_2)=\pm 1. \tag{20'}$$

As an illustration we may consider the string of 3j-coefficients $\left(\begin{smallmatrix}j_1 & 100 & 60\\ -10 & 60 & -50\end{smallmatrix}\right)$ in Fig. 1, the solution of Eq. (18a). In this case, the full *quantum mechanical domain* is [40.5, 160.5], and is divided into the smaller *classical* *domain* [47.5, 114.5] and the two complementary *nonclassical domains* [40.5, 46.5] and [115.5, 160.5]. The division into a classical and two nonclassical domains is reflected by the functional behavior of the 3*j*-coefficients, as can be seen from Fig. 1c. While progressing along the j_1-domain, the 3*j*-coefficients oscillate rapidly in the classical region, but decay monotonically to zero in the outer nonclassical domains. This situation that the domain of Eq. (18a) can be divided into a middle classical region and two outer nonclassical regions applies in general, though in some instances a nonclassical domain may contain only one or no quantum number.

Figure 2b which presents the string of 3*j*-coefficients $\begin{pmatrix}120 & 60 & 70\\ -10 & m_2 & 10-m_2\end{pmatrix}$ demonstrates that the partitioning into a classical domain and two distinct nonclassical domains prevails also for the domain of Eq. (18b). For the example chosen, the classical m_2-domain [−21, 30] lies well within the quantum mechanical domain [−60, 60] separating the two nonclassical domains [−60, −22] and [31, 60]. Again, the values of the 3*j*-coefficients oscillate while progressing through the classical domain and monotonically decay to zero in the nonclassical domains.

How is the existence of classical and nonclassical domains reflected by the difference equations (18a) and (18b)? Over the classical domains the dihedral angles θ_1 and η_1 are real by definition through the geometric formulas (11) and (15). In the nonclassical domains the angles θ_1 and η_1 together with all remaining dihedral angles are complex. This can be verified directly from the expressions (11) and (15), which give absolute values <1 for classically allowed quantum numbers and absolute values >1 for nonclassical quantum numbers. One can also show from Eq. (4) that A^2 is positive in the classical region, zero at the boundaries of the classical domain $J_{1\,\min}$, $J_{1\,\max}$ or $M_{2\,\min}$, $M_{2\,\max}$ as postulated by Eqs. (19) and (19′), and negative in the nonclassical domains. Although the classical vector diagrams do not exist for 3*j*-coefficients in the nonclassical domains, the algebraic formulas originating from these diagrams, i.e., Eqs. (4), (10), (11), (14), and (15), remain valid beyond the domain of classically allowed quantum numbers. Of importance for the following, is the fact that the expressions for $\cos\theta_i$ and $\cos\eta_i$ are real in the nonclassical regions, so that the real parts of θ_i and η_i are constant in these regions, and equal to either 0 or π.

To solve Eqs. (18a) and (18b) we start from the observation that the dihedral angles θ_1 and η_1, in the limit of large quantum numbers, vary slowly with J_1 and L_1. To demonstrate this for $\theta_1(J_1)$ one may again employ an expansion in terms of the parameter λ introduced above. From (11)

$$\cos\theta_1(\lambda J_1 \pm 1) = -\frac{2J_1^2 m_2 + [J_1^2 + J_2^2 - J_3^2]m_1 \pm (4J_1 m_2 + 2J_1 m_1)\lambda^{-1} + (2m_2 + m_1)\lambda^{-2}}{4F(J_1, J_2, J_3)\,P(J_1, m_1)} = \cos\theta_1(\lambda J_1) \pm O(\lambda^{-1}) + O(\lambda^{-2}),$$

or

$$\cos\theta_1(\lambda J_1 + 1) - 2\cos\theta_1(\lambda J_1) + \cos\theta_1(\lambda J_1 - 1) = O(\lambda^{-2}). \qquad (21)$$

For slowly varying $\theta_1(J_1)$ and $\eta_1(L_1)$ the difference equations (18a) and (18b) can be solved by a discrete analog of the WKB approximation, commonly applied to the solution of the Schrödinger second order differential equation in the semiclassical limit. The "discrete WKB approximation" for *difference* equations is developed in the following section. It should be pointed out here that this approximation applied to Eqs. (18a), (18b) neglects again only terms of order $O(\lambda^{-2})$ and, thus, is consistent with the approximations so far employed.

III. WKB APPROXIMATION APPLIED TO SECOND ORDER DIFFERENCE EQUATIONS

We will now consider the approximate solution of the second order difference equations (18a) and (18b) which may be written

$$[\Delta^2 + 2 - 2\cos k(x)]\,f(x) = 0 \qquad (22)$$

where we assume $k(x)$ to be real and $0 \leq k(x) \leq \pi$. The case of imaginary $k(x)$ can be treated the same way as the case of real $k(x)$ and will be commented upon at the end of this section.

Equation (22) determines $f(x)$ over a discrete set of values x, $x\pm 1$, $x \pm 2$, $\cdots$. However, since x stands for some classical angular momentum variable, Eq. (22) can be assumed to hold over a continuous domain of real numbers x. In this instance the solution of (22) can be viewed as a function over a continuous domain, too, since one may take any x as a starting point for the recursion implied by Eq. (22). As a function of a continuous variable one would expect $f(x)$ to be determined as a solution of a differential equation, rather than a difference equation. Indeed, there exists a second order differential equation which is closely related to the difference equation (22) and which has $f(x)$ as a solution. This holds, however, only within the realm of the semiclassical approximation which had been employed when the difference Eqs. (18a) and (18b) were derived.

We will show now that the differential equation which, within the semiclassical approximation, determines the $f(x)$ in Eq. (22) is

$$\left(\frac{d^2}{dx^2} + k^2(x)\right)\left(\frac{\sin k(x)}{k(x)}\right)^{1/2} f(x) = 0. \qquad (23)$$

The semiclassical approximation implies that $k(x)$ is a slowly varying function of x, so that we may neglect in solving Eq. (23) all terms of order $O(k'^2)$ and smaller $[k' = (d/dx)k(x)]$ and also all derivatives of $k(x)$ of order 2 and higher. With $N = [\sin k(x)/k(x)]^{1/2}$ Eq. (23) can then be written

$$f^{(2)} \approx -k^2 f - 2\frac{N'}{N} f^{(1)} \qquad (24)$$

since $N''/N \approx 0$ within the approximation stated. We define here $f^{(n)} = (d^n/dx^n)f$. Equations (24) allows us to express all derivatives of $f(x)$ in terms of $f(x)$ itself and its first derivative. It is then readily checked that the third and fourth order derivatives are approximately

$$f^{(3)} \approx -k^2 f^{(1)} - 2kk'f - pk^2 f,$$
$$f^{(4)} \approx k^4 f - 4kk'f^{(1)} - 2pk^2 f^{(1)}$$

where $p = -2N'/N$. The even order derivatives are in general

$$f^{(2n)} \approx (-1)^n [k^{2n} f - 2(n-1)n\, k^{2n-3} k' f^{(1)} - n\, k^{2n-2}\, pf^{(1)}]. \tag{25}$$

This result permits the evaluation of the difference $\Delta^2 f = f(x+1) - 2f(x) + f(x-1)$ by a Taylor series expansion around x:

$$\Delta^2 f \approx 2 \sum_{n=0}^{\infty} (-1)^n \frac{k^{2n}}{(2n)!} f - 2f - \sum_{n=2}^{\infty} (-1)^n \frac{(2n-2)2n}{(2n)!} k^{2n-3} k' f^{(1)} - \sum_{n=1}^{\infty} (-1)^n \frac{2n}{(2n)!} k^{2n-2} p f^{(1)}$$
$$= [2\cos k(x) - 2] f(x) + \left[\left(\frac{d}{dx} \frac{\sin k(x)}{k(x)}\right) + \frac{\sin k(x)}{k(x)}\, p(x)\right] \times f^{(1)}(x).$$

The second term on the right-hand side of the last equation vanishes identically since

$$p(x) = -\frac{d}{dx} \ln \frac{\sin k(x)}{k(x)},$$

so that $f(x)$, the solution of the differential Eq. (23), also obeys the difference Equation (22). It may be noted that the derivation carried out here holds also if $k(x)$ is pure imaginary.

The approximation which had been invoked to derive the connection between the difference equation (22) and the differential equation (23) is also employed within the customary WKB approximation applied to these equations. Hence, it must be possible to demonstrate by means of the WKB approximation that (22) and (23) have identical solutions. The application of the WKB approximation to Eq. (23) is standard and we may just state that from it results

$$f(x) = \frac{C}{\sqrt{\sin k(x)}} \cos\left(\int_{x_0}^{x} k(x')\, dx' + \alpha\right) \quad (0 < k < \pi), \tag{26}$$

where α and C are constants to be chosen in accordance with possible boundary and normalization conditions.

The WKB approximation can also be applied to the difference equation (22). One sets

$$f(x) = A(x) \cos[\Omega(x) + \alpha] \tag{27}$$

where the functions $A(x)$ and $\Omega(x)$ to be determined are assumed to be slowly varying such that

$$|\Omega''| \ll 1 \quad \text{and} \quad |A'/A| \ll 1 \tag{28}$$

and all higher derivatives of $\Omega(x)$ and $A(x)$ can be neglected. One has

$$f(x \pm 1) \approx A\left(1 \pm \frac{A'}{A}\right) \cos(\Omega + \alpha \pm \Omega' + \Omega''/2)$$

where

$$\cos\left(\Omega + \alpha \pm \Omega' + \frac{\Omega''}{2}\right) \approx \left[1 - \frac{1}{2}\left(\frac{\Omega''}{2}\right)^2\right] \cos(\Omega + \alpha \pm \Omega') - \frac{\Omega''}{2} \sin(\Omega + \alpha \pm \Omega').$$

Neglecting the terms $(\Omega''/2)^2$ and $(A'/A)(\Omega''/2)$, one obtains

$$f(x \pm 1) \approx A\left(\cos\Omega' \mp \frac{\Omega''}{2} \sin\Omega' \pm \frac{A'}{A} \cos\Omega'\right) \cos(\Omega + \alpha) + A\left(\mp \sin\Omega' - \frac{\Omega''}{2} \cos\Omega' - \frac{A'}{A} \sin\Omega'\right) \sin(\Omega + \alpha),$$

which inserted into Eq. (22) leads to

$$A(2\cos\Omega' - 2\cos k)\cos(\Omega + \alpha), \quad -A\left(\Omega'' \cos\Omega' + 2\frac{A'}{A} \sin\Omega'\right) \sin(\Omega + \alpha) \approx 0,$$

or

$$\Omega' \approx k,$$
$$\frac{A'}{A} \approx -\frac{\Omega''}{2} \frac{\cos\Omega'}{\sin\Omega'}.$$

These last equations determine $\Omega(x)$ and $A(x)$ as

$$\Omega(x) = \int_{x_0}^{x} k(x')\, dx', \tag{29}$$
$$A(x) = C/\sqrt{\sin k(x)}, \tag{30}$$

which together with (27) shows that the WKB solutions of (22) and (23) are indeed identical. This finding holds, of course, only as long as the conditions (28) are met. The condition $|\Omega''| \ll 1$ is equivalent to $|k'| \ll 1$ which had also been assumed in deriving the equivalence of (22) and (23). The condition $|A'/A| \ll 1$ is more restrictive and does not hold for k close to either 0 or π.

The equivalence of Eqs. (22) and (23) within the semiclassical approximation allows a solution which holds uniformly over the entire domain $0 \le k \le \pi$. Such solution is obtained by means of the uniform WKB approximation applied to the differential equation (23) setting

$$\left(\frac{\sin k(x)}{k(x)}\right)^{1/2} f(x) = A(x)\, F(\Omega(x)), \tag{31}$$

where $F(\Omega)$ stands for the regular or the irregular Airy function,[8] the solutions of

$$F''(\Omega) - \Omega F(\Omega) = 0. \tag{32}$$

Inserting (31) into (23) gives by virtue of (32)

$$\left(\frac{A''}{A} + \Omega'^2\Omega + k^2\right) F(\Omega) + \left(2\frac{A'}{A} \Omega' + \Omega''\right) F'(\Omega) = 0.$$

Assuming now that A' is slowly varying such that $A''/A \approx 0$ leads to the equations

$$\Omega'^2 \Omega + k^2 \approx 0,$$
$$A'/A \approx -\tfrac{1}{2}(\Omega''/\Omega'),$$

the solutions of which are

$$\Omega(x) \approx -\left(\tfrac{3}{2} \left| \int_{x_0}^{x} k(x')\, dx' \right|\right)^{2/3}, \tag{33a}$$
$$A(x) \approx C\{|\Omega(x)|^{1/4}/[k(x)]^{1/2}\} \tag{33b}$$

Finally,

$$f(x)=C\,\frac{|\Omega|^{1/4}}{[\sin k(x)]^{1/2}}\,F(\Omega(x)). \tag{34}$$

The integration limit x_0 in (33a) must be either of the zeroes of $\sin k(x)$. In the x region distant from x_0 where $|\Omega(x)|$ is large, i.e., where the solution (26) holds, the expressions (34) and (26) can be identically matched. This follows from the asymptotic behavior of Airy functions[8]: For $|\Omega(x)|\gg 1$ and $\omega=\int_{x_0}^{x}k(x')\,dx'$

$$\sqrt{\pi}\,|\Omega|^{1/4}Ai(-\Omega)=\begin{cases}\cos(\omega-\pi/4) & \text{for } \omega>0\\ \cos(\omega+\pi/4) & \text{for } \omega<0\end{cases}, \tag{35a}$$

$$\sqrt{\pi}\,|\Omega|^{1/4}Bi(-\Omega)=\begin{cases}\cos(\omega+\pi/4) & \text{for } \omega>0\\ \cos(\omega-\pi/4) & \text{for } \omega<0\end{cases}. \tag{35b}$$

The derivation above for the equivalence of Eqs. (22) and (23) holds also in the case that $k(x)$ is purely imaginary. The uniform WKB approximation applied to Eq. (23) gives in this case

$$\Omega(x)\approx\left(\tfrac{3}{2}\int_{x_0}^{x}|k(x')|\,dx'\right)^{2/3}, \tag{36a}$$

$$A(x)\approx C\,|\Omega(x)|^{1/4}/|k(x)|^{1/2}, \tag{36b}$$

and hence

$$f(x)=\frac{|\Omega(x)|^{1/4}}{[\sinh k(x)]^{1/2}}\,F(|\Omega(x)|). \tag{37}$$

IV. SEMICLASSICAL SOLUTION FOR 3*j*-COEFFICIENTS

The semiclassical solutions for the difference equations (18a) and (18b) have been derived formally, and we will now evaluate explicit expressions for individual 3j-coefficients from these solutions. It is instructive to consider first solution (26) for the difference equations which holds only in the classical domain distant from the classical boundaries $J_{1\,\min}$, $J_{1\,\max}$, and $M_{2\,\min}$, $M_{2\,\max}$. For Eq. (18a) this is

$$\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}=(-1)^{j_1+j_2+j_3}\,\frac{C_1}{\sqrt{A}}\cos[\Omega(J_1)+\alpha] \tag{38}$$

where

$$\Omega(J_1)=\int_{J_{1\,\min}}^{J_1}\theta_1(J_1')\,dJ_1' \tag{39}$$

and for Eq. (18b)

$$\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}=(-1)^{j_1+j_2+j_3}\,\frac{C_2}{\sqrt{A}}\cos[\Phi(L_1)+\beta] \tag{40}$$

where

$$\Phi(L_1)=\int_{L_{1\,\min}}^{L_1}\eta_1(L_1')\,dL_1'. \tag{41}$$

Of course expressions (38) and (40) must be identical and to show this the phase functions $\Omega(J_1)$ and $\Phi(L_1)$ need to be evaluated explicitly. In doing so, we will closely follow Ref. 1.

We had pointed out above that the three variables L_1, L_2, and L_3 in $\left[\begin{smallmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{smallmatrix}\right]$ are only defined up to a constant which can be added to these variables without changing the value of the 3j-coefficient. Hence, one is free to let L_1, L_2, L_3 go to infinity keeping the differences $m_1=L_2-L_3$, $m_2=L_3-L_1$, $m_3=L_1-L_2$ constant. In this limit the angular momentum prism associated with $\left[\begin{smallmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{smallmatrix}\right]$ resembles a tetrahedron $T(J_1,J_2,J_3,L_1,L_2,L_3)$ with the triangular base $\Delta(J_1,J_2,J_3)$ and infinite edges L_1,L_2,L_3. In order to evaluate $\Omega(J_1)$ and $\Phi(L_1)$ one can, hence, take advantage of the identity

$$\sum_{i=1}^{3}(J_i\,d\theta_i+L_i\,d\eta_i)=0, \tag{42}$$

a special case of a theorem first derived by Schlaefli[9] which holds more generally for elliptic tetrahedra. From (42) follows

$$d\sum_{i=1}^{3}(J_i\theta_i+L_i\eta_i)=\sum_{i=1}^{3}\theta_i dJ_i+\eta_i dL_i$$

or

$$\begin{aligned}\frac{\partial}{\partial J_k}\sum_{i=1}^{3}(J_i\theta_i+L_i\eta_i)&=\theta_k,\\ \frac{\partial}{\partial L_k}\sum_{i=1}^{3}(J_i\theta_i+L_i\eta_i)&=\eta_k,\end{aligned} \tag{43}$$

and one can conclude immediately that $\sum_{i=1}^{3}(J_i\theta_i+L_i\eta_i)$ is the solution of both Eq. (39) and (41).

It should be demonstrated that with this solution (38) and (40) are indeed independent of the absolute lengths of L_1, L_2 and L_3. This follows from the geometrical relationship

$$\eta_1+\eta_2+\eta_3=2\pi,$$

since then

$$\sum_{i=1}^{3}L_i\eta_i=-\eta_1 m_2+\eta_2 m_1+2\pi L_3.$$

The constant term $2\pi L_3 \pmod{2\pi}$ can be added to the phase constants α and β in (38) and (40), so that we may set

$$\Omega(J_1)=\Phi(L_1)=\sum_{i=1}^{3}J_i\theta_i-\eta_1 m_2+\eta_2 m_1. \tag{44}$$

(38) and (40) are therefore identical if we set $C_1=C_2$ and $\alpha=\beta$.

The normalization constant C_1 and the phase constant α still need to be determined. We will derive here only C_1 and must leave the problem of choosing α correctly to a later discussion of the boundary conditions of the 3j-coefficients in the nonclassical domains. The 3j-coefficients represent the matrix elements of the unitary transformation T connecting the basis sets $|j_2m_2\rangle|j_3m_3\rangle$ and $|(j_2,j_3)j_1m_1\rangle$. One may exploit the unitary property of T in order to determine the normalization constant C_1:

$$\sum_{J_1}2J_1\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}\begin{bmatrix}J_1 & J_2 & J_3\\ L_1' & L_2 & L_3\end{bmatrix}=\delta_{L_1L_1'}. \tag{45}$$

In the limit of large quantum numbers this may be written for $L_1\approx L_1'$ with

$$\begin{bmatrix}J_1 & J_2 & J_3\\ L_1 & L_2 & L_3\end{bmatrix}\approx N(J_1,L_1)\cos[\Omega(J_1,L_1)+\alpha],$$

$$\int_{-\infty}^{+\infty} dJ_1\, 2J_1\, N(J_1, L_1)^2 \cos[\Omega(J_1, L_1)+\alpha]$$
$$\times \cos[\Omega(J_1, L_1')+\alpha] \approx \delta(L_1 - L_1').$$

The method of stationary phase can be applied to get

$$\int_{-\infty}^{+\infty} dJ_1\, J_1 N(J_1, L_1)^2 \cos\left((L_1' - L_1)\,\frac{\partial\Omega}{\partial L_1}\right) \approx \delta(L_1 - L_1')$$

which holds only if

$$N = \pm\left(\frac{1}{\pi J_1}\,\left|\frac{\partial^2\Omega}{\partial J_1 \partial L_1}\right|\right)^{1/2}. \qquad (46)$$

To evaluate $\partial^2\Omega/\partial J_1\partial L_1 = \partial\eta_1/\partial J_1$ we note that

$$\cos\eta_1 = -4\,\frac{\partial A^2/\partial J_1^2}{P(J_2, m_2)P(J_3, m_3)}$$

which can be derived from Eq. (4) and Eq. (15). Together with (14) this gives

$$\frac{\partial\eta_1}{\partial J_1} = -\frac{J_1}{2A} \qquad (47)$$

and, hence,

$$N = \pm\left(\frac{1}{2\pi A}\right)^{1/2}.$$

This result is in agreement with (38) and (40) for $C_1 = 1/\sqrt{2\pi}$. Evidently, this determination of the normalization constant also yields the correct functional dependence $1/\sqrt{A}$ for N. It is well known that the phase function of a semiclassical operator alone determines the normalization factor N. Our result supports therefore (38) as the correct semiclassical $3j$-coefficient. We have finally for the $3j$-coefficients in the classical domain

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\,\frac{1}{\sqrt{2\pi A}}$$
$$\times \cos(J_1\theta_1 + J_2\theta_2 + J_3\theta_3 - \eta_1 m_2 + \eta_2 m_1 + \alpha). \qquad (48)$$

This result, except for the phase constant α to be determined yet, is identical with the expression of Ponzano and Regge and that derived by Miller from the correspondence relationships of classical and quantum mechanics.

The expression for semiclassical $3j$-coefficients uniformly valid over the entire quantum number domain can be evaluated from the solutions (34) and (37) of the difference equation (22). These solutions are valid even near the classical turning points $J_{1\,\min}$ and $J_{1\,\max}$ ($M_{2\,\min}$ and $M_{2\,\max}$) provided that $k(J_{1\,\min})$, etc. vanish. However, in Eqs. (18a) and (18b) θ_1 and η_1 are either 0 or π at the turning points. In the latter case, a phase transformation has to be employed which induces the proper turning point behavior of the difference equation.

For the following, it may be sufficient to consider Eq. (18a) only, since (18b) would lead to an identical solution. We define the phase function

$$\Omega_0 = J_1\theta_1^0 + J_2\theta_2^0 + J_3\theta_3^0 + m_1\eta_2^0 - m_2\eta_1^0 \qquad (49)$$

where

$$\theta_i^0 = \begin{cases} 0 & \text{if } 0 \le \mathrm{Re}\,\theta_i \le \pi/2 \\ \pi & \text{if } \pi/2 < \mathrm{Re}\,\theta_i \le \pi \end{cases}, \qquad (50a)$$

$$\eta_i^0 = \begin{cases} 0 & \text{if } 0 \le \mathrm{Re}\,\eta_i \le \pi/2 \\ \pi & \text{if } \pi/2 < \mathrm{Re}\,\eta_i \le \pi \end{cases}. \qquad (50b)$$

$\mathrm{Re}\,\theta_i$ ($\mathrm{Re}\,\eta_i$) stands here for the real part of $\theta_i(\eta_i)$. For all quantum mechanically allowed J_i and m_i, Ω_0 thus defined is either an integer or a half-integer multiple of π. A simple criterion can be found which distinguishes between these two possibilities if $J_1 \approx J_{1\,\min}$ or $J_1 \approx J_{1\,\max}$:

$$\Omega_0/\pi \text{ half integer (integer)} \iff \Omega - \Omega_0 \text{ positive (negative)}. \qquad (51)$$

To derive this rule one may express $\Omega - \Omega_0$ through $\int(\theta_1 - \theta_1^0)dJ_1$. For $J_1 \approx J_{1\,\min}$

$$\Omega - \Omega_0 = \int_{J_{1\,\min}}^{J_1} (\theta_1 - \theta_1^0)\, dJ_1$$

and since θ_1 is a monotonous function in the neighborhood of $J_{1\,\min}$ it follows from $\theta_1(J_{1\,\min}) = \theta_1^0$

$$\Omega - \Omega_0 = \begin{cases} >0 & \text{if } \theta_1^0 = 0 \\ <0 & \text{if } \theta_1^0 = \pi \end{cases}.$$

However, for $\theta_1^0(J_{1\,\min}) = 0$

$$\begin{bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{bmatrix} = \begin{bmatrix} 0 & \pi & 0 \\ \pi & 0 & \pi \end{bmatrix} \qquad (52a)$$

and Ω_0/π is half integer, and for $\theta_1^0(J_{1\,\min}) = \pi$

$$\begin{bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{bmatrix} = \begin{bmatrix} \pi & 0 & \pi \\ \pi & 0 & \pi \end{bmatrix} \qquad (52b)$$

and Ω_0/π is integer. Similarly, for $J_1 \approx J_{1\,\max}$

$$\Omega - \Omega_0 = -\int_{J_1}^{J_{1\,\max}} (\theta_1 - \theta_1^0)\, dJ_1$$

is negative for $\theta_1^0 = 0$ and positive for $\theta_1^0 = \pi$. But in this case one finds for $\theta_1^0(J_{1\,\max}) = 0$

$$\begin{bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{bmatrix} = \begin{bmatrix} 0 & \pi & \pi \\ 0 & \pi & \pi \end{bmatrix}, \qquad (52c)$$

i.e., Ω_0/π integer, and for $\theta_1^0(J_{1\,\max}) = \pi$

$$\begin{bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{bmatrix} = \begin{bmatrix} \pi & 0 & 0 \\ 0 & \pi & \pi \end{bmatrix}, \qquad (52d)$$

i.e., Ω_0/π half integer. Equations (52a)–(52d) are readily checked geometrically by drawing the corresponding angular momentum diagrams.

At the boundaries of the classical domain $J_{1\,\min}$, $J_{1\,\max}$ the dihedral angles θ_i and η_i are either 0 or π. Since the dihedral angles are slowly varying functions of the quantum numbers, the angles θ_i^0 and η_i^0 are constant near $J_{1\,\min}$ and $J_{1\,\max}$. One may then set for the solution f of Eq. (18a)

$$f = \cos\Omega_0 f_1 - \sin\Omega_0 f_2 \qquad (53)$$

and show that in the regions of constant $\theta_1^0 = 0$ or π the functions f_1 and f_2 must satisfy the modified difference equation.

$$[\Delta^2(J_1) + 2 - 2\cos(\theta_1 - \theta_1^0)]\, f_i(J_1) \approx 0. \qquad (54)$$

The new representation (53) for the $3j$-coefficients together with this new difference equation, has favorable behavior at the boundaries of the classical region, and will also facilitate the evaluation of the $3j$-coefficients in the nonclassical region.

In the classical domain distant from $J_{1\,\min}$ and $J_{1\,\max}$ $f(J_1)$ may be written according to Eqs. (17a) and (48)

$$f=[2\pi\sin\theta_1]^{-1/2}[\cos\Omega_0\cos(\Omega-\Omega_0+\alpha) - \sin\Omega_0\sin(\Omega-\Omega_0+\alpha)] \tag{55}$$

and f_1 and f_2 must be chosen such that (53) identically matches this expression for $J_{1\,\min} \ll J_1 \ll J_{1\,\max}$.

It had been shown in Sec. 3 that the solutions of (54) in the semiclassical limit must obey the differential equation

$$\left(\frac{d^2}{dJ_1^2}-(\theta_1-\theta_1^0)^2\right)\left(\frac{\sin(\theta_1-\theta_1^0)}{\theta_1-\theta_1^0}\right)^{1/2} f_i(J_1)=0 \tag{56}$$

where J_1 is now assumed to be a continuous variable. In this equation $(\theta_1-\theta_1^0)^2$ is positive in the classical domain, zero at $J_1=J_{1\,\min}$, $J_{1\,\max}$ and negative in the nonclassical domain. According to Eqs. (33a,b) and (34) the solutions of (56) are in the classical domain

$$\frac{Z^{1/4}}{(\sin\theta_1)^{1/2}}\ \mathrm{Ai}(-Z)\quad\text{and}\quad\frac{Z^{1/4}}{(\sin\theta_1)^{1/2}}\ \mathrm{Bi}(-Z)$$

where $Z=(\frac{3}{2}|\Omega-\Omega_0|)^{2/3}$. The solutions in the nonclassical domain obtained by analytical continuation are

$$\frac{Z^{1/4}}{(\sinh|\theta_1-\theta_1^0|)^{1/2}}\ \mathrm{Ai}(Z)\quad\text{and}\quad\frac{Z^{1/4}}{(\sinh|\theta_1-\theta_1^0|)^{1/2}}\ \mathrm{Bi}(Z).$$

To identify the functions f_1 and f_2 the boundary conditions to be imposed on the $3j$-coefficients have to be taken into consideration. Evidently, the $3j$-coefficients must decay monotonically to zero in the nonclassical domain so that the irregular Airy function $\mathrm{Bi}(J)$ which exhibit an exponential increase must be rejected in this domain. This boundary condition is satisfied if we set for $J_{1\,\min}\le J_1\le J_{1\,\max}$

$$f=\frac{Z^{1/4}}{(\sin\theta_1)^{1/2}}\times\begin{cases} a\cos\Omega_0\,\mathrm{Ai}(-Z)-b\sin\Omega_0\,\mathrm{Bi}(-Z), & \Omega-\Omega_0<0\\ a'\cos\Omega_0\,\mathrm{Bi}(-Z)-b'\sin\Omega_0\,\mathrm{Ai}(-Z), & \Omega-\Omega_0>0\end{cases} \tag{57}$$

which analytically continued into the nonclassical domain is

$$f=\frac{Z^{1/4}}{(\sinh|\theta_1-\theta_1^0|)^{1/2}}\times\begin{cases} a\cos\Omega_0\,\mathrm{Ai}(Z)-b\sin\Omega_0\,\mathrm{Bi}(Z), & \Omega-\Omega_0<0\\ a'\cos\Omega_0\,\mathrm{Bi}(Z)-b'\sin\Omega_0\,\mathrm{Ai}(Z), & \Omega-\Omega_0>0.\end{cases} \tag{58}$$

Over the discrete set of quantum mechanically allowed J_i and m_i (i.e., J_i, m_i either integer or half integer) the factors $\sin\Omega_0$ and $\cos\Omega_0$ multiplying the irregular Airy functions $\mathrm{Bi}(Z)$ vanish in the nonclassical domains as had been postulated. (57) becomes for $J_{1\,\min}\ll J_1\ll J_{1\,\max}$

$$f=\frac{1}{(\pi\sin\theta_1)^{1/2}}\times\begin{cases} a\cos\Omega_0\cos(\Omega-\Omega_0+\pi/4)-b\sin\Omega_0\sin(\Omega-\Omega_0+\pi/4), & \Omega-\Omega_0<0\\ a'\cos\Omega_0\cos(\Omega-\Omega_0+\pi/4)-b'\sin\Omega_0\sin(\Omega-\Omega_0+\pi/4), & \Omega-\Omega_0>0.\end{cases} \tag{59}$$

The condition that this expression must identically match (55) is met for $\alpha=\pi/4$ and $a=b=a'=b'=S/\sqrt{2}$ where $S=\pm1$, is an arbitrary phase factor. The $3j$-coefficients are then finally

$$\begin{pmatrix} j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix} = S(-1)^{j_1+j_2+j_3}\ \frac{Z^{1/4}}{\sqrt{2A}}\times\begin{cases}\cos\Omega_0\,\mathrm{Ai}(-Z)-\sin\Omega_0\,\mathrm{Bi}(-Z), & \Omega-\Omega_0<0\\ \cos\Omega_0\,\mathrm{Bi}(-Z)-\sin\Omega_0\,\mathrm{Ai}(-Z), & \Omega-\Omega_0>0\end{cases} \tag{60}$$

in the classical domain and

$$\begin{pmatrix} j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix} = S(-1)^{j_1+j_2+j_3}\ \frac{Z^{1/4}}{\sqrt{2|A|}}\times\begin{cases}\cos\Omega_0\,\mathrm{Ai}(Z)-\sin\Omega_0\,\mathrm{Bi}(Z), & \Omega-\Omega_0<0\\ \cos\Omega_0\,\mathrm{Bi}(Z)-\sin\Omega_0\,\mathrm{Ai}(Z), & \Omega-\Omega_0>0\end{cases} \tag{61}$$

in the nonclassical domain. The phase factor S may be defined according to the phase convention of Wigner

$$\mathrm{sgn}\left\{\begin{pmatrix} j_2+j_3 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix}\right\} = (-1)^{j_2-j_3-m_1}. \tag{62}$$

For $J_1=j_2+j_3+\frac{1}{2}$ in the nonclassical domain $\mathrm{Ai}(Z)>0$ and

$$\cos\Omega_0(\Omega-\Omega_0>0)=-\sin\Omega_0(\Omega-\Omega_0<0) = (-1)^{j_2+j_3+m_1+1},$$

so that

$$\mathrm{sgn}\left\{\begin{pmatrix} j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix}\right\} = S(-1)^{j_2+j_3+m_1+1}$$

and $S=(-1)^{-2j_3+1}$.

The $3j$-coefficients (60) and (61) had been derived as the semiclassical solutions of the recursion equations (5) and (6). These recursion equations can be derived from the following eigenvalue problems:

(5) : diagonalization of J_{2z} in the basis $|(j_2,j_3)j_1m_1\rangle$: eigenvalues $m_2=m_{2\,\min}+n$, $n=0,1,2,\cdots$,

(6) : diagonalization of $(\mathbf{J}_2+\mathbf{J}_3)^2$ in the basis $|j_2m_2\rangle\,|j_3m_3\rangle$: eigenvalues $j_1(j_1+1)$ where $j_1=j_{1\,\min}+n$, $n=0,1,2,\cdots$.

The eigenvectors i.e., the rows and columns of the unitary transformation matrix T defined in (1) and (2), are then determined except for overall constant factors by the recursion equations (5) and (6). In solving these recursion equations one may treat the eigenvalues m_2 and $j_1(j_1+1)$ as unknowns to be determined through the boundary conditions to be imposed on the solutions (60), (61). The boundary conditions that the $3j$-coefficients decay to zero in the nonclassical domains can only be satisfied if $J_i(j_i)$ and m_i are either integer or half-integer for otherwise the coefficients $\sin\Omega_0(\Omega-\Omega_0<0)$ and $\cos\Omega_0(\Omega-\Omega_0>0)$ in (61) multiplying the exponentially increasing irregular Airy functions $\mathrm{Bi}(Z)$ do not vanish. The semiclassical $3j$-coefficients exhibit, hence, a typical quantum character in the variables J_1 and $m_2(m_3)$. Since the semiclassical solution (60), (61) is independent of the recursion equation from which the derivation is started, this quantization property must hold for all the variables of the $3j$-coefficients. Furthermore, it is important to notice that the set of semiclassical quantum numbers J_i and m_i being thus defined as the allowed values J_i and m_i coincides with the set of quantum mechanical quantum numbers $j_i+\frac{1}{2}$, m_i.

V. SEMICLASSICAL 6j-COEFFICIENTS

The $6j$-coefficients $\left\{\begin{smallmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3\end{smallmatrix}\right\}$ define a unitary transformation T

$$T_{j_1 l_1}=[(2j_1+1)(2l_1+1)]^{1/2}\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3\end{Bmatrix} \tag{63}$$

between two total angular momentum states with the common internal angular momenta l_2, l_3, j_3 coupled in different ways to the same total angular momentum j_2.[7] One state is coupled according to the scheme $(j_3, (l_2, l_3)j_1; j_2)$, i.e., l_2 and l_3 are coupled to the *intermediate* j_1 which in turn is coupled with j_3 to give j_2. The other state is coupled according to the scheme $(l_3(l_2, j_3)l_1; j_2)$, i.e., l_2, j_3 are coupled to the *intermediate* l_1 which in turn is coupled with l_3 to give j_2. Classically this corresponds to two ways of addition of angular momentum vectors, namely $\mathbf{L}_2+\mathbf{L}_3=\mathbf{J}_1, \mathbf{J}_1+\mathbf{J}_3=\mathbf{J}_2$ and $\mathbf{L}_2+\mathbf{J}_3=\mathbf{L}_1$, $\mathbf{L}_1+\mathbf{L}_3=\mathbf{J}_2$. This angular momentum coupling situation is illustrated by the classical vector diagram in figure 3a where the classical angular momentum vectors are defined in the usual way, $J_i=j_i+\frac{1}{2}$ and $L_i=l_i+\frac{1}{2}$.

Let us now assume as fixed the lengths of the classical angular momenta $\mathbf{J}_2, \mathbf{J}_3, \mathbf{L}_1, \mathbf{L}_2$ and $\mathbf{L}_3$ in Fig. 3a and, accordingly, the quantum numbers j_2, j_3, l_1, l_2, l_3 in $\left\{\begin{smallmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3\end{smallmatrix}\right\}$ and let us consider the $6j$-coefficients for all possible j_1 together with the corresponding classical vector diagrams. The manifold of all possible classical vector diagrams is generated by moving vertex 3 of the angular momentum vector tetrahedron in Fig. 3a along the circle indicated whereby the angle η_1 goes from 0 to π. J_1 assumes then all values which correspond to the varying distances between vertex 1 and 3. To complete the correspondence between $6j$-coefficients and classical vector diagrams it may be recalled that the matrix elements defined in (63) squared $T_{j_1 l_1}{}^2$ are to be interpreted as the quantum mechanical probability for l_2, l_3 to be coupled to give j_1, or, conversely, that $J_1-\frac{1}{2}\leq|\mathbf{L}_2+\mathbf{L}_3|\leq J_1+\frac{1}{2}$. On the basis of this interpretation Wigner[5] established an approximate functional relationship between $6j$-coefficients and the associated classical angular momentum tetrahedra. From the assumption that each angle η_1 in Fig. 3a is equally likely, he estimated for the probability $T_{j_1 l_1}{}^2$

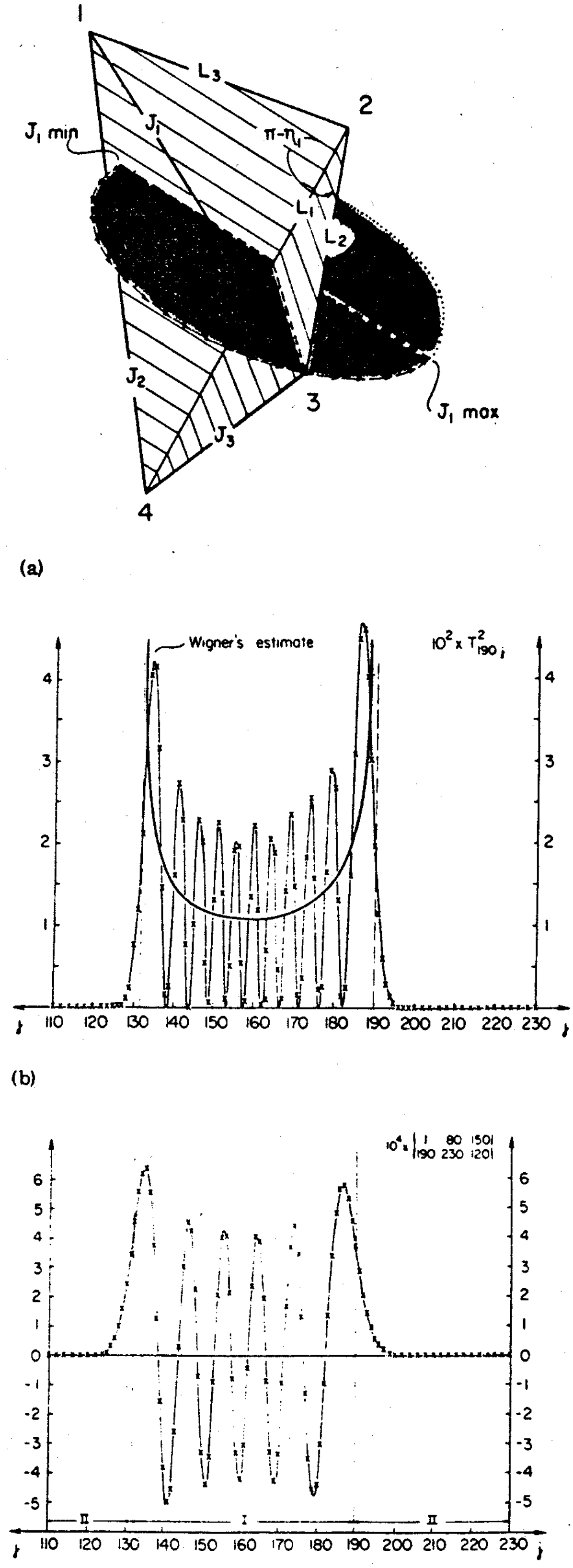

FIG. 3. The series of $6j$-coefficients $\left\{\begin{smallmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3\end{smallmatrix}\right\}$, $j_1\min\leq j_1\leq j_1\max$, in (c) and the corresponding manifold of classical angular momentum tetrahedra ($J_i=j_i+\frac{1}{2}$, $L_i=l_i+\frac{1}{2}$) generated by rotation of vertex 3 around the shaded circle. The quantum mechanical probability distribution $(2j_1+1)(2l_1+1)\left\{\begin{smallmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3\end{smallmatrix}\right\}^2$ for the occurrence of the classical vector diagram in (a) are compared with Wigner's semiclassical estimate $(2j_1+1)(2l_1+1)/24\pi V$.

$$T_{j_1 l_1}{}^2 = (2j_1+1)(2l_1+1)/24\pi V \tag{64}$$

where V is the volume of the angular momentum tetrahedron given by the Cayley determinant

$$V^2(J_1) = \frac{1}{288}\begin{vmatrix} 0 & L_1^2 & L_2^2 & L_3^2 & 1 \\ L_1^2 & 0 & J_3^2 & J_2^2 & 1 \\ L_2^2 & J_3^2 & 0 & J_1^2 & 1 \\ L_3^2 & J_2^2 & J_1^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix}. \tag{65}$$

Equation (64) provides only an estimate for the absolute magnitudes of the 6j-coefficients. Figure 3c which presents the series of 6j-coefficients $\begin{Bmatrix} j_1 & 80 & 150 \\ 190 & 236 & 120 \end{Bmatrix}$ illustrates that the 6j-coefficients oscillate rapidly while j_1 is progressing along the circle of classically allowed j_1-values in Fig. 3a. Figure 3b which compares the corresponding probabilities $T_{j_1 l_1}{}^2$ with Wigner's estimate (64) demonstrates that (*ii*) holds only as an average over several neighboring quantum numbers. The exact progression of the 6j-coefficients is, however, determined by the recursion equation[3]

$$j_1 g(j_1+1)\begin{Bmatrix} j_1+1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + h(j_1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + (j_1+1)g(j_1)\begin{Bmatrix} j_1-1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = 0 \tag{66a}$$

where

$$g(j_1) = \{[(j_2+j_3+1)^2 - j_1^2][j_1^2 - (j_2-j_3)^2][(l_2+l_3+1)^2 - j_1^2] \times [j_1^2 - (l_2-l_3)^2]\}^{1/2}, \tag{66b}$$

$$\begin{aligned} h(j_1) = (2j_1+1)\{ & j_1(j_1+1)[-j_1(j_1+1) + j_2(j_2+1) + j_3(j_3+1)] \\ & + l_2(l_2+1)[j_1(j_1+1) + j_2(j_2+1) - j_3(j_3+1)] \\ & + l_3(l_3+1)[j_1(j_1+1) - j_2(j_2+1) + j_3(j_3+1)] \\ & - 2j_1(j_1+1)\,l_1(l_1+1)\}. \end{aligned} \tag{66c}$$

We will show in the remainder of this section that for large angular momentum quantum numbers this recursion equation allows us to refine Wigner's result (64).

In the limit of large quantum numbers recursion equation (66) takes on a more symmetric form which allows a geometrical interpretation in terms of the classical vector diagram 3a. This asymptotic recursion equation is again derived through a dilation of the angular momentum quantum numbers (i.e., $j_i, l_i \to \lambda j_i, \lambda l_i$) and a consecutive expansion of (66) in terms of λ neglecting terms of order $O(\lambda^{-2})$ and smaller, assuming that λ is large. Thus (66b) and (66c) may be written

$$\begin{aligned} (\lambda j_1+1)\,g(\lambda j_1) = [1+O(\lambda^{-2})]\,16[&\lambda J_1(\lambda J_1+1)\,F(\lambda J_1, \lambda J_2, \lambda J_3) \\ &\times F(\lambda J_1, \lambda L_2, \lambda L_3)\,F(\lambda J_1 - 1, \lambda J_2, \lambda J_3) \\ &\times F(\lambda J_1 - 1, \lambda L_2, \lambda L_3)]^{1/2} \end{aligned}$$

and

$$\begin{aligned} h(\lambda j_1) &= -2\lambda J_1[1+O(\lambda^{-2})][2\lambda^2 J_1^2 \lambda^2 L_1^2 - \lambda^2 J_1^2(-\lambda^2 J_1^2 + \lambda^2 L_2^2 + \lambda^2 L_3^2) \\ &\quad - \lambda^2 J_2^2(\lambda^2 J_1^2 + \lambda^2 L_2^2 - \lambda^2 L_3^2) \\ &\quad - \lambda^2 J_3^2(\lambda^2 J_1^2 - \lambda^2 L_2^2 + \lambda^2 L_3^2)]. \end{aligned}$$

Neglecting terms of order $O(\lambda^{-2})$ allows us then to bring (66a) into the following symmetric form:

$$\begin{aligned} &\left(\frac{F(\lambda J_1 - 1, \lambda J_2, \lambda J_3)\,F(\lambda J_1 - 1, \lambda L_2, \lambda L_3)}{\lambda J_1 - 1}\right)^{1/2} \begin{Bmatrix} \lambda j_1 - 1 & \lambda j_2 & \lambda j_3 \\ \lambda l_1 & \lambda l_2 & \lambda l_3 \end{Bmatrix} \\ &+ \left(\frac{F(\lambda J_1 + 1, \lambda J_2, \lambda J_3)\,F(\lambda J_1 + 1, \lambda L_2, \lambda L_3)}{\lambda J_1 + 1}\right)^{1/2} \begin{Bmatrix} \lambda j_1 + 1 & \lambda j_2 & \lambda j_3 \\ \lambda l_1 & \lambda l_2 & \lambda l_3 \end{Bmatrix} \\ &- 2\,\frac{2J_1^2 L_1^2 - J_1^2(-J_1^2 + L_2^2 + L_3^2) - J_2^2(J_1^2 + L_2^2 - L_3^2) - J_3^2(J_1^2 - L_2^2 + L_3^2)}{16\,F(J_1, J_2, J_3)\,F(J_1, L_2, L_3)} \\ &\times \left(\frac{F(\lambda J_1, \lambda J_2, \lambda J_3)\,F(\lambda J_1, \lambda L_2, \lambda L_3)}{\lambda J_1}\right)^{1/2} \begin{Bmatrix} \lambda j_1 & \lambda j_2 & \lambda j_3 \\ \lambda l_1 & \lambda l_2 & \lambda l_3 \end{Bmatrix} \approx 0. \end{aligned} \tag{67}$$

We will omit the parameter λ in the following derivation to avoid a somewhat cumbersome notation. Doing so, we assume the quantum numbers j_i and l_i to be large. It is again pointed out that all the following approximations taken to solve Eq. (67) are consistent with the neglect of terms $O(\lambda^{-2})$.

The coefficients in Eq. (67) are related algebraically to the classical vector diagrams in Fig. 3(a). This can be recognized by virtue of the relations

$$\tfrac{3}{2} V J_1 = F(J_1, J_2, J_3)\,F(J_1, L_2, L_3)\sin\theta_1 \tag{68}$$

and[1]

$$\cos\theta_1 = \frac{2J_1^2 L_1^2 - J_1^2(-J_1^2 + L_2^2 + L_3^2) - J_2^2(J_1^2 + L_2^2 - L_3^2) - J_3^2(J_1^2 - L_2^2 + L_3^2)}{16\,F(J_1, J_2, J_3)\,F(J_1, L_2, L_3)}. \tag{69}$$

(67) may then be formally written as a second order difference equation

$$[\Delta^2(J_1)+2-2\cos\theta_1]f(j_1)\approx 0 \tag{70}$$

where

$$f(J_1)=\left(\frac{V}{\sin\theta_1}\right)^{1/2}\begin{Bmatrix} j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{Bmatrix}. \tag{71}$$

This difference equation is valid over the domain $[j_{1\,\min}, j_{1\,\max}]$ of the j_1-manifold of $6j$-coefficients $\{\begin{smallmatrix} j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{smallmatrix}\}$. $j_{1\,\min}$ and $j_{1\,\max}$ are determined as the smallest and largest j_1-values satisfying the triangular conditions for $\{\begin{smallmatrix} j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{smallmatrix}\}$, i.e., $j_{1\,\min}=\max\{|j_2-j_3|, |l_2-l_3|\}$ and $j_{1\,\max}=\min\{j_2+j_3, l_2+l_3\}$. Obviously, the J_1-values occuring in the manifold of the classical vector diagrams in Fig. 3a also lie within a finite interval $[J_{1\,\min}, J_{1\,\max}]$. The smallest and largest classically allowed J_1-values, $J_{1\,\min}$ and $J_{1\,\max}$, are those for which all angular momentum vectors in Fig. 3a happen to lie within a single plane (flat tetrahedron). Hence, $J_{1\,\min}$ and $J_{1\,\max}$ are determined as solutions of either of the equations

$$\cos\theta_i(J_1)=\pm 1,\quad \cos\eta_i(J_1)=\pm 1 \tag{72a}$$

where θ_i and η_i are the dihedral angles of the angular momentum tetrahedron adjacent to the edges J_i and L_i, respectively. The algebraic expressions for $\theta_2, \theta_3, \eta_1, \eta_2, \eta_3$ can be obtained from (69) by permutation of the labels of J_i and L_i and by permutation of J and L. Clearly, in the limit of a flat tetrahedron the dihedral angles are all either 0 or π. Alternatively, $J_{1\,\min}$ and $J_{1\,\max}$ may be determined as solutions of

$$V^2(J_1)=0. \tag{72b}$$

To compare the quantum mechanical domain $[j_{1\,\min}, j_{1\,\max}]$ and the classical domain $[J_{1\,\min}, J_{1\,\max}]$ we turn to Fig. 3c which presents the whole string of $6j$-coefficients $\{\begin{smallmatrix} j_1 & 80 & 150\\ 190 & 230 & 120\end{smallmatrix}\}$. The classical j_1-domain is for this case [131, 190] and lies well within the domain [110, 230] of all quantum mechanically allowed j_1-values. Hence, the quantum mechanical domain [110, 230] is divided into a classical domain [131, 190] and two nonclassical domains [110, 130] and [191, 230]. This situation that the quantum mechanical j_1-domain of a series of $6j$-coefficients can be divided into a middle classical domain and two outer nonclassical domains applies in general, though in some instances the nonclassical domains may contain only a few or no j_1-quantum numbers. The division into classical and nonclassical domains has an important meaning which is reflected by the functional behavior of the $6j$-coefficients, as can be seen from Fig. 3c. The $6j$-coefficients as one progresses along the j_1-domain oscillate rapidly in the classical domain and decay to zero in the nonclassical domains.

The existence of classical and nonclassical domains is also reflected by the difference equation (70). Over the classical domain $[J_{1\,\min}, J_{1\,\max}]$ the dihedral angle $\theta_1(J_1)$ is real by virtue of its geometrical meaning, but in the nonclassical domains the angle $\theta_1(J_1)$ together with the remaining dihedral angles is complex. This can be verified directly from the algebraic expression for $\cos\theta_1$ given in Eq. (69) which gives values between -1 and $+1$ for classical J_1 and values exceeding -1 and $+1$ for nonclassical J_1. Equation (65) reveals that $V^2(J_1)$ is positive in the classical domain, zero at the classical limits $J_{1\,\min}$ and $J_{1\,\max}$, and negative in the nonclassical domains. Hence, to a $6j$-coefficient in the non-classical domain corresponds an angular momentum vector diagram with complex dihedral angles and imaginary volume.

To solve the difference equation (70) we start as before in the case of the $3j$-coefficients from the observation that for large quantum numbers $\theta_1(J_1)$ is a slowly varying function of J_1, since again

$$\cos\theta_1(\lambda J_1+1, \lambda J_2, \cdots)=\cos\theta_1(J_1+1/\lambda, J_2, \cdots),$$

as can be readily checked from Eq. (69). Hence, the "discrete" WKB approximation derived in Sec. 3 may be employed to solve Eq. (70).

In the classical domain $J_{1\,\min}\ll J_1\ll J_{1\,\max}$ the solution as given by (26) is

$$\begin{Bmatrix} j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{Bmatrix}=\frac{C}{\sqrt{V}}\cos[\Omega(J_1)+\alpha] \tag{73}$$

where

$$\Omega(J_1)=\int_{J_{1\,\min}}^{J_1}\theta_1(J_1')\,dJ_1'. \tag{74}$$

$\Omega(J_1)$ is again readily evaluated by means of Eq. (43) which holds also for the angular momentum tetrahedron in Fig. 3a:

$$\Omega(J_1)=\sum_{i=1}^{3}(J_i\theta_i+L_i\eta_i). \tag{75}$$

To determine the normalization constant C in (73) the unitary property of $6j$-coefficients

$$\sum_{j_1} T_{j_1l_1}T_{j_1l_1'}=\delta_{l_1l_1'} \tag{76}$$

can be employed. With

$$\begin{Bmatrix} j_1 & j_2 & j_3\\ l_1 & l_2 & l_3\end{Bmatrix}=N(J_1,L_1)\cos[\Omega(J_1,L_1)+\alpha] \tag{77}$$

for $L_1\approx L_1'$, we have for large quantum numbers

$$\int dJ_1\,4J_1L_1N^2(J_1,L_1)\cos[\Omega(J_1,L_1)+\alpha]$$
$$\times\cos[\Omega(J_1,L_1')+\alpha]\approx\delta(L_1-L_1').$$

The method of stationary phase applied to this integral gives

$$\int dJ_1\,2J_1L_1\,N^2(J_1,L_1)\cos\left((L_1'-L_1)\frac{\partial\Omega}{\partial L_1}\right)\approx\delta(L_1-L_1'),$$

which holds only if

$$N=\left(\frac{1}{2J_1L_1\pi}\left|\frac{\partial\Omega}{\partial J_1\partial L_1}\right|\right)^{1/2}.$$

However, by virtue of Eq. (43) and $\partial\eta_1/\partial J_1=J_1L_1/6V$ this is

$$N=1/\sqrt{12\pi V}, \tag{78}$$

so that $C=1/\sqrt{12\pi}$ is the correct normalization constant.

The validity of solution (73) is subject to the condition $N^{-1}|\partial N/\partial J_1|\ll 1$. This condition cannot be satisfied for small V in the neighborhood of $J_{1\,\min}$ and $J_{1\,\max}$. An expression for the semiclassical $6j$-coefficients which is also valid in these regions is found by performing first a suitable phase transformation of the solution $f(J_1)$ of the difference equation (70). We define for this purpose the phase function

$$\Omega_0 = \sum_{i=1}^{3} (J_i \theta_i^0 + L_i \eta_i^0) \tag{79}$$

where

$$\theta_i^0 = \begin{cases} 0 & \text{if } 0 \le \theta_i \le \pi/2 \\ \pi & \text{if } \pi/2 < \theta_i \le \pi \end{cases}, \tag{80a}$$

$$\eta_i^0 = \begin{cases} 0 & \text{if } 0 \le \eta_i \le \pi/2 \\ \pi & \text{if } \pi/2 < \eta_i \le \pi \end{cases}, \tag{80b}$$

Ω_0 is either an integer or a half-integer multiple of π. It can be shown as for the phase function (49) defined for $3j$-coefficients that

$$\Omega_0/\pi \text{ half-integer (integer)} \Longleftrightarrow \Omega - \Omega_0 \text{ positive (negative)}. \tag{81}$$

We then set for the solution of (70)

$$f(J_1) = \cos\Omega_0 \, f_1 - \sin\Omega_0 f_2 \tag{82}$$

and it is readily checked that $f_1(J_1)$ and $f_2(J_1)$ thus defined must satisfy the modified difference equation

$$[\Delta^2(J_1) + 2 - 2\cos(\theta_1 - \theta_1^0)] f_i(J_1) \approx 0 \tag{83}$$

in the region of constant θ_1^0. For $J_{1\,\min} \ll J_1 \ll J_{1\,\max}$, $f(J_1)$ determined through (73) and (78) is

$$f(J_1) = (12\pi \sin\theta_1)^{-1/2} [\cos\Omega_0 \cos(\Omega - \Omega_0 + \alpha) - \sin\Omega_0 \sin(\Omega - \Omega_0 + \alpha)]. \tag{84}$$

Hence, $f_1(J_1)$ and $f_2(J_1)$ should be determined as to satisfy Eq. (83) in the neighborhood of $J_{1\,\min}$, $J_{1\,\max}$ and to match identically through Eq. (82) this expression for $J_{1\,\min} \ll J_1 \ll J_{1\,\max}$.

From the result of Sec. 3 one can infer that the solutions of the difference equation (83) in the semiclassical limit must obey the differential equation

$$\left(\frac{d^2}{dJ_1^2} - (\theta_1 - \theta_1^0)^2\right) \left(\frac{\sin(\theta_1 - \theta_1^0)}{\theta_1 - \theta_1^0}\right)^{1/2} f_i(J_1) = 0 \tag{85}$$

where J_1 is assumed to be a continuous variable. As was the case in Eq. (56), $(\theta_1 - \theta_1^0)^2$ is positive in the classical domain, zero at $J_{1\,\min}$, $J_{1\,\max}$ and negative in the nonclassical domain. The solutions of (85) and (56) are therefore formally identical, only the explicit algebraic form of the variables involved being different. Furthermore, the boundary conditions to be imposed on the solutions of the $6j$-coefficients (82) are identical to the boundary conditions postulated for the $3j$-coefficients, i.e., the $6j$-coefficients must decay to zero in the nonclassical domain as is illustrated by the example given in Fig. 3c. We have therefore for $J_{1\,\min} \le J_1 \le J_{1\,\max}$

$$f = \frac{Z^{1/4}}{(\sin\theta_1)^{1/2}} \times \begin{cases} a\cos\Omega_0 \operatorname{Ai}(-Z) - b\sin\Omega_0 \operatorname{Bi}(-Z), & \Omega - \Omega_0 < 0 \\ a'\cos\Omega_0 \operatorname{Bi}(-Z) - b'\sin\Omega_0 \operatorname{Ai}(-Z), & \Omega - \Omega_0 > 0 \end{cases} \tag{86}$$

and for $J_1 \le J_{1\,\min}$, $J_1 \ge J_{1\,\max}$

$$f = \frac{|Z|^{1/4}}{[\sinh|\theta_1 - \theta_1^0|]^{1/2}} \times \begin{cases} a\cos\Omega_0 \operatorname{Ai}(Z) - b\sin\Omega_0 \operatorname{Bi}(Z) & \text{for } \Omega - \Omega_0 < 0 \\ a'\cos\Omega_0 \operatorname{Bi}(Z) - b'\sin\Omega_0 \operatorname{Ai}(Z) & \text{for } \Omega - \Omega_0 > 0 \end{cases} \tag{87}$$

where

$$Z = (\tfrac{3}{2}|\Omega - \Omega_0|)^{2/3}. \tag{88}$$

Over the discrete set of quantum mechanically allowed J_i and L_i, the factor $\sin\Omega_0$ $(\Omega - \Omega_0 < 0)$ and $\cos\Omega_0$ $(\Omega - \Omega_0 > 0)$ of the irregular Airy functions $\operatorname{Bi}(Z)$ vanish in (87), so that (86) in the classical domain together with its analytical continuation (87) in the nonclassical domains indeed represent a possible solution. This solution matches identically with (84) if one chooses $a = b = a' = b' = S/\sqrt{12}$ in (86) and (87) and $\alpha = \pi/4$ in (84), S being an arbitrary phase factor. The $6j$-coefficients are then finally

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = S\frac{Z^{1/4}}{\sqrt{12V}} \times \begin{cases} \cos\Omega_0 \operatorname{Ai}(-Z) - \sin\Omega_0 \operatorname{Bi}(-Z), & \Omega - \Omega_0 < 0 \\ \cos\Omega_0 \operatorname{Bi}(-Z) - \sin\Omega_0 \operatorname{Ai}(-Z), & \Omega - \Omega_0 > 0 \end{cases} \tag{89}$$

in the classical domain and

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = S\frac{Z^{1/4}}{\sqrt{12|V|}} \times \begin{cases} \cos\Omega_0 \operatorname{Ai}(Z) - \sin\Omega_0 \operatorname{Bi}(Z), & \Omega - \Omega_0 < 0 \\ \cos\Omega_0 \operatorname{Bi}(Z) - \sin\Omega_0 \operatorname{Ai}(Z), & \Omega - \Omega_0 > 0 \end{cases} \tag{90}$$

in the nonclassical domain. The phase factor S may be determined according to the phase convention

$$\operatorname{sgn}\left(\begin{Bmatrix} j_{1\,\max} & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\right) = (-1)^{j_2+j_3+l_2+l_3}. \tag{91}$$

For $\Omega - \Omega_0 < 0$ one finds at $J_1 = J_{1\,\max}$

$$\begin{Bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{Bmatrix} = \begin{Bmatrix} 0 & \pi & \pi \\ 0 & \pi & \pi \end{Bmatrix},$$

i.e., $\cos\Omega_0 = (-1)^{j_2+j_3+l_2+l_3}$. For $\Omega - \Omega_0 > 0$ there are two possibilities:

(a) $j_2 + j_3 > l_2 + l_3$:

$$\begin{Bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{Bmatrix} = \begin{Bmatrix} \pi & \pi & \pi \\ 0 & 0 & 0 \end{Bmatrix}$$

(b) $j_2 + j_3 < l_2 + l_3$:

$$\begin{Bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{Bmatrix} = \begin{Bmatrix} \pi & 0 & 0 \\ 0 & \pi & \pi \end{Bmatrix},$$

i.e., $-\sin\Omega_0 = (-1)^{j_1+j_2+j_3}$ or $-\sin\Omega_0 = (-1)^{j_1+l_2+l_3}$. But

$$\begin{Bmatrix} \theta_1^0 & \theta_2^0 & \theta_3^0 \\ \eta_1^0 & \eta_2^0 & \eta_3^0 \end{Bmatrix}$$

is constant throughout the nonclassical domains, hence for (a) $j_{1\,\max} = l_2 + l_3$, i.e., $-\sin\Omega_0 = (-1)^{j_2+j_3+l_2+l_3}$ and for (b) $j_{1\,\max} = j_2 + j_3$; i.e. $-\sin\Omega_0 = (-1)^{j_2+j_3+l_2+l_3}$. Since in the nonclassical domain at $j_1 = j_{1\,max}$ Ai(Z) and Bi(Z) are both positive, the sign of (90) is

$$(-1)^{j_2+j_3+l_2+l_3},$$

so that the sign convention (91) is met for $S=1$.

Let us finally compare our result (89) and (90) with the semiclassical expressions for the $6j$-coefficients stated by Ponzano and Regge. These authors give three formulas, one valid for $J_{1\,min} \ll J_1 \ll J_{1\,max}$, one for $J_1 \ll J_{1\,min}$, $J_1 \gg J_{1\,max}$ and one for $J_1 \approx J_{1\,min}$, $J_{1\,max}$. In the classical domain distant from $J_{1\,min}$, $J_{1\,max}$, we have

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \approx \frac{1}{\sqrt{12\pi V}} \cos\left(\Omega + \frac{\pi}{4}\right) \tag{92}$$

which is identical with the expression of Ponzano and Regge in this region. In the nonclassical domain distant from $J_{1\,min}$, $J_{1\,max}$ (90) becomes for J_i and L_i either integer or half-integer

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = (-1)^{j_2+j_3+l_2+l_3} \frac{1}{2\sqrt{12\pi|V|}} \exp(-|\Omega-\Omega_0|) \tag{93}$$

in agreement with the result of Ponzano and Regge.

To describe the $6j$-coefficients in the neighborhood of $J_{1\,min}$, $J_{1\,max}$ Ponzano and Regge introduced the variable

$$\frac{9}{2}\,\frac{V^3}{F_4} \approx |\Omega - \Omega_0| \tag{94}$$

where $F_4 = F(J_1, J_2, J_3)\,F(J_1, L_2, L_3)\,F(L_1, L_2, J_3)\,F(L_1, J_2, L_3)$ and the variable

$$\Phi = \begin{cases} \Omega_0 - 2\pi & \text{for } \Omega - \Omega_0 < 0 \\ \Omega_0 - \frac{3}{2}\pi & \text{for } \Omega - \Omega_0 > 0 \end{cases}.$$

Inserting these variables into (89) and (90) yields for $\Omega - \Omega_0 \gtrless 0$

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = 2^{-4/3} F_4^{-1/6}[\cos\Phi\ \mathrm{Ai}(-Z) \pm \sin\Phi\ \mathrm{Bi}(-Z)] \tag{89$'$}$$

and

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = 2^{-4/3} F_4^{1/6}[\cos\Phi\ \mathrm{Ai}(Z) - \sin\Phi\ \mathrm{Bi}(Z)] \tag{90$'$}$$

where $Z = (3V)^2/(4F_4)^{2/3}$. For physical values of J_i and L_i, Φ is an integer multiple of π and (89′) and (90′) are then identical with the expressions of Ponzano and Regge.

Thus we have demonstrated that the semiclassical expressions for $6j$-coefficients first stated by Ponzano and Regge on the basis of only heuristic arguments can be derived systematically from the recursion relationship (66). It is admirable that Ponzano and Regge succeeded in obtaining their results without the guideline of a step-by-step derivation.

Equation (94) holds only in a small neighborhood of $J_{1\,min}$, $J_{1\,max}$. For this reason the expressions of Ponzano and Regge (89′) and (90′), though identical with our results (89) and (90) near $J_{1\,min}$, $J_{1\,max}$, do not match the functions (92) and (93) which hold distant from the classical boundaries. But our results (89) and (90) hold uniformly over the entire domain of quantum numbers and represent therefore an improvement over the approximations of Ponzano and Regge.

The recursion equation (66) of the $6j$-coefficients can be derived as the secular equation of a certain eigenvalue problem in which $l_1(l_1+1)$ represents the eigenvalues and $\nu_{l_1}(j_1) = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$ $(j_{1\,min} \le j_1 \le j_{1\,max})$ the eigenvectors.[3] We may have regarded $L_1^2 \approx l_1(l_1+1)$ in Eqs. (66c) and (67), (69) as unknown, carried through the derivation to be finally determined by the boundary conditions, i.e., $\nu_{l_1}(j_1) \to 0$ for $j_1 \gg J_{1\,max}$ and $j_1 \ll J_{1\,min}$. The semiclassical expressions (89) and (90) reveal then, that these boundary conditions are met only for L_1 being either integer or half-integer, for otherwise the coefficients $\sin\Omega_0(\Omega - \Omega_0 < 0)$ and $\cos\Omega_0(\Omega - \Omega_0 > 0)$ in (90) multiplying the irregular Airy functions do not vanish. The semiclassical solution of the $6j$-coefficient recursion (eigenvalue) equation exhibit thus the expected quantum character for L_1. More interestingly, it predicts the *exact* discrete set of quantum numbers (integer and half-integer). Since the solution (89) and (90) is independent of the recursion equation used as a starting point for the derivation (there are 6 different recursion equations), this remark holds as well for all variables in the $6j$-coefficients which must all be quantized according to Eq. (90). It is a remarkable fact that the semiclassical quantum numbers coincide with the set of exact quantum numbers for such a coincidence is only found in few situations (for example, for the Coulomb potential and harmonic oscillator eigenvalue problem) which possess special underlying symmetries. It may be speculated that it is the puzzling Regge-symmetry of $6j$-coefficients[10] (and $3j$-coefficients) which is responsible for this remarkable coincidence.

VI. COMPARISON OF EXACT AND SEMICLASSICAL WIGNER COEFFICIENTS

A comparison of exact and semiclassical $6j$-coefficients had already been carried out by Ponzano and Regge. Since earlier algorithms (and tables) for $6j$-coefficients were restricted to the domain of only moderate quantum numbers, these authors were not in a position to demonstrate directly the accuracy of semiclassical $6j$-coefficients (and $3j$-coefficients by the same token) involving large quantum numbers. Because of the surprisingly good agreement between exact and semiclassical $6j$-coefficients at small and moderate quantum numbers Ponzano and Regge expected that the semiclassical expressions should give very satisfactory values for large quantum number $6j$-coefficients.

Recently, we have developed an algorithm for the evaluation of $3j$- and $6j$-coefficients on the basis of the same recursion equations (5), (6), and (66) from which the semiclassical $3j$- and $6j$-coefficients had been derived as asymptotic solutions.[3] This algorithm was found numerically stable even for large quantum numbers-in fact, it served to evaluate the $3j$- and $6j$-coefficients in Figs. 1—3. Hence, it is now possible to examine directly the accuracy of large quantum number semiclassical Wigner coefficients. In Tables I—III are given some sample values of the Wigner coefficients

TABLE I. Accuracy of semiclassical 3j-coefficients $\begin{pmatrix} j_1 & 100 & 60 \\ -10 & 60 & -50 \end{pmatrix}$.

j_1	Exact quantum mechanical[a]	Uniform semiclassical[b]
40	0.4999 (−04)	0.4833 (−04)
46	0.0848 (−01)	0.0847 (−01)
48	0.1563 (−01)	0.1562 (−01)
50	0.1857 (−01)	0.1858 (−01)
52	0.1139 (−01)	0.1141 (−01)
54	−0.0352 (−01)	−0.0349 (−01)
56	−0.1385 (−01)	−0.1385 (−01)
58	−0.0927 (−01)	−0.0929 (−01)
60	0.0519 (−01)	0.0517 (−01)
70	0.0119 (−01)	−0.0115 (−01)
80	−0.0213 (−01)	−0.0214 (−01)
90	−0.0808 (−01)	−0.0807 (−01)
100	−0.0926 (−01)	−0.0927 (−01)
106	0.0320 (−01)	0.0322 (−01)
108	0.1051 (−01)	0.1052 (−01)
110	0.1372 (−01)	0.1372 (−01)
112	0.1300 (−01)	0.1300 (−01)
114	0.1006 (−01)	0.1005 (−01)
116	0.0665 (−01)	0.0664 (−01)
118	0.0385 (−01)	0.0384 (−01)
120	0.0197 (−02)	0.0197 (−01)
130	0.1407 (−04)	0.1404 (−04)
140	0.7206 (−08)	0.7191 (−08)
150	0.1438 (−12)	0.1433 (−12)
160	0.3811 (−20)	0.3672 (−20)

[a]Evaluated by recursion, Ref. 3.
[b]Evaluated from Eqs. (60), (61).

TABLE II. Accuracy of semiclassical 3j-coefficients $\begin{pmatrix} 120 & 60 & 70 \\ -10 & m & 10-m \end{pmatrix}$.

m	Exact quantum mechanical[a]	Uniform semiclassical[b]
−60	0.1749 (−30)	0.1626 (−30)
−50	0.7794 (−17)	0.7760 (−17)
−40	0.5450 (−09)	0.5436 (−09)
−30	0.4795 (−04)	0.4788 (−04)
−24	0.0286 (−01)	0.0286 (−01)
−22	0.0682 (−01)	0.0682 (−01)
−20	0.1207 (−01)	0.1207 (−01)
−18	0.1445 (−01)	0.1446 (−01)
−16	0.0841 (−01)	0.0842 (−01)
−14	−0.0462 (−01)	−0.0461 (−01)
−12	−0.1163 (−01)	−0.1163 (−01)
−10	−0.0255 (−01)	−0.0257 (−01)
0	0.0863 (−01)	0.0862 (−01)
10	0.0357 (−01)	0.0354 (−01)
20	−0.0810 (−01)	−0.0812 (−01)
22	−0.1043 (−01)	−0.1042 (−01)
24	0.0120 (−01)	0.0122 (−01)
26	0.1229 (−01)	0.1230 (−01)
28	0.1418 (−01)	0.1418 (−01)
30	0.0974 (−01)	0.0974 (−01)
32	0.0474 (−02)	0.0474 (−02)
34	0.0174 (−02)	0.0174 (−02)
40	0.1951 (−04)	0.1948 (−04)
50	0.8202 (−10)	0.8177 (−10)
60	0.3218 (−19)	0.3099 (−19)

[a]Evaluated by recursion, Ref. 3.
[b]Evaluated from Eqs. (60), (61).

presented in Figs. 1–3 together with the corresponding semiclassical values. The relative errors between the exact and the semiclassically evaluated 3j- and 6j-coefficients are found to be in general small (less than 1%). Exceptions are only the terminal 3j- and 6j-coefficients $\begin{pmatrix} j_{1\,\max} & 100 & 60 \\ -10 & 60 & -50 \end{pmatrix}$, etc. for which the error is of the order 1%.

We discussed above the connection between Eqs. (89), (90) and the semiclassical expressions (92), (93), (89′), (90′) stated by Ponzano and Regge. While (89), (90) provide a uniform approximation to the 6j-coefficients over the entire domain of allowed quantum numbers, the expressions of Ponzano and Regge hold only over mu-

TABLE III. Accuracy of semiclassical 6j-coefficients $\begin{Bmatrix} j_1 & 80 & 150 \\ 190 & 230 & 120 \end{Bmatrix}$.

j_1	Exact quantum mechanical[a]	Uniform semiclassical[b]	Ponzano and Regge semiclassical
110	0.3865 (−13)	0.3725 (−13)	0.3737 (−13)
120	0.2191 (−06)	0.2186 (−06)	0.2206 (−06)
126	0.0307 (−03)	0.0307 (−03)	0.0315 (−03)
128	0.0973 (−03)	0.0972 (−03)	0.1018 (−03)
130	0.2405 (−03)	0.2402 (−03)	0.2362 (−03)
132	0.4552 (−03)	0.4550 (−03)	0.4541 (−03)
134	0.6285 (−03)	0.6284 (−03)	0.6154 (−03)
136	0.5503 (−03)	0.5507 (−03)	0.5466 (−03)
138	0.1216 (−03)	0.1224 (−03)	0.1069 (−03)
140	−0.3852 (−03)	−0.3847 (−03)	−0.3931 (−03)
150	−0.3367 (−03)	−0.3359 (−03)	−0.3381 (−03)
160	−0.4230 (−03)	−0.4231 (−03)	−0.4231 (−03)
170	−0.3378 (−03)	−0.3372 (−03)	−0.3392 (−03)
180	−0.4400 (−03)	−0.4398 (−03)	−0.4491 (−03)
182	−0.0969 (−03)	−0.0963 (−03)	−0.1090 (−03)
184	0.3378 (−03)	0.3383 (−03)	0.3265 (−03)
186	0.5611 (−03)	0.5612 (−03)	0.5606 (−03)
188	0.5289 (−03)	0.5288 (−03)	0.5202 (−03)
190	0.3666 (−03)	0.3664 (−03)	0.3665 (−03)
192	0.2021 (−03)	0.2019 (−03)	0.1983 (−03)
194	0.0919 (−04)	0.0918 (−04)	0.0964 (−04)
200	0.3194 (−05)	0.3190 (−05)	0.3239 (−05)
210	0.5648 (−09)	0.5637 (−09)	0.5667 (−09)
220	0.1537 (−14)	0.1533 (−14)	0.1537 (−14)
230	0.2427 (−23	0.2339 (−23)	0.2342 (−23)

[a]Evaluated by recursion, Ref. 3.
[b]Evaluated from Eqs. (89), (90).

TABLE IV. Convergence of semiclassical 3j-coefficients $\begin{pmatrix} j_1\lambda & 4.5\lambda & 3.5\lambda \\ \lambda & -3.5\lambda & 2.5\lambda \end{pmatrix}$.

j_1	$\lambda=1$	$\lambda=2$	$\lambda=4$	$\lambda=8$	$\lambda=16$	$\lambda=32$	
1	0.2789 (00)	0.1769 (00)	0.9692 (−01)	0.4032 (−01)	0.0977 (−01)	0.0806 (−02)	QM[a]
	0.3043 (00)	0.1959 (00)	0.9520 (−01)	0.3878 (−01)	0.0926 (−01)	0.0758 (−02)	SC
2	−0.9535 (−01)	−0.8063 (−01)	0.0457 (−01)	−0.3174 (−01)	0.1288 (−01)	0.0297 (−02)	QM
	−0.9303 (−01)	−0.8294 (−01)	0.0523 (−01)	−0.3172 (−01)	0.1285 (−01)	0.0285 (−02)	SC
3	−0.6742 (−01)	−0.6995 (−01)	−0.0141 (−01)	−0.2728 (−01)	0.1378 (−01)	0.6773 (−02)	QM
	−0.6975 (−01)	−0.7031 (−01)	−0.0143 (−01)	−0.2730 (−01)	0.1378 (−01)	0.6773 (−02)	SC
4	0.1533 (00)	0.5646 (−01)	−0.2083 (−01)	−0.1316 (−01)	−0.0825 (−01)	−0.0275 (−02)	QM
	0.1558 (00)	0.5571 (−01)	−0.2158 (−01)	−0.1325 (−01)	−0.0823 (−01)	−0.0281 (−02)	SC
5	−0.1564 (00)	0.9203 (−01)	0.5313 (−01)	0.2863 (−01)	0.1021 (−01)	−0.4379 (−02)	QM
	−0.1566 (00)	0.9204 (−01)	0.5315 (−01)	0.2865 (−01)	0.1023 (−01)	−0.4376 (−02)	SC
6	0.1099 (00)	0.4867 (−01)	0.1711 (−01)	0.0397 (−01)	0.4149 (−03)	0.8876 (−05)	QM
	0.1090 (00)	0.4835 (−01)	0.1704 (−01)	0.0397 (−01)	0.4145 (−03)	0.8870 (−05)	SC
7	−0.5536 (−01)	0.1177 (−01)	0.9524 (−03)	0.1178 (−04)	0.3496 (−08)	0.6071 (−15)	QM
	−0.5441 (−01)	0.1162 (−01)	0.9452 (−03)	0.1173 (−04)	0.3488 (−08)	0.6064 (−15)	SC
8	0.1800 (−01)	0.9460 (−03)	0.4072 (−05)	0.1220 (−09)	0.1804 (−18)	0.6568 (−36)	QM
	0.1727 (−01)	0.9079 (−03)	0.3915 (−05)	0.1174 (−09)	0.1738 (−18)	0.6332 (−36)	SC

[a]QM = quantum mechanical values; SC = semiclassical values.

tually exclusive regions of the quantum number domain and do not connect smoothly with each other near the classical boundaries $J_{i\,\min}$, $J_{i\,\max}$ ($M_{i\,\min}$, $M_{i\,\max}$) In Tables I—III the 3j- and 6j-coefficient quantum mechanical and semiclassical values are presented for several consecutive values near the classical boundaries to demonstrate the uniformity of the semiclassical formulas (60), (61) and (89), (90). As can be seen from the quoted numerical values, the uniform expressions are very accurate and furnish thereby an improvement over the expressions of Ponzano and Regge.

The derivation of the semiclassical Wigner coefficients as the asymptotic solutions to the recursion equations (5), (6) and (66) had been based on the expansion of

$$\begin{pmatrix} \lambda j_1 & \lambda j_2 & \lambda j_3 \\ \lambda m_1 & \lambda m_2 & \lambda m_3 \end{pmatrix} \quad \text{and} \quad \begin{Bmatrix} \lambda j_1 & \lambda j_2 & \lambda j_3 \\ \lambda l_1 & \lambda l_2 & \lambda l_3 \end{Bmatrix}$$

in terms of powers of λ, such that all terms up to order $O(\lambda^{-1})$ had been kept. This suggests that the semiclassical Wigner coefficients should converge to the quantum mechanical values with increasing λ. This conjecture is examined in Tables IV and V, for 3j- and 6j-coefficients. In Table IV the series of 3j-coefficients $\begin{pmatrix} j_1\lambda & 4.5\lambda & 3.5\lambda \\ \lambda & -3.5\lambda & 2.5\lambda \end{pmatrix}$ are evaluated for $\lambda=1,2,4,8,16,32$ by means of recursion of Eq. (5) and by its asymptotic semiclassical solution (60), (61). As can be inferred from the tabulated values the relative error of the semiclassical 3j-coefficients does decrease with increasing λ. Similarly, one can observe from Table V which presents the values of the 6j-coefficients $\begin{Bmatrix} j_1\lambda & 8\lambda & 7\lambda \\ 6.5\lambda & 7.5\lambda & 7.5\lambda \end{Bmatrix}$ for $\lambda=1,2,4,8,16$ that the semiclassical 6j-coefficients converge to the exact 6j-coefficients with increasing λ.

Finally, the question may be raised if for very large quantum numbers a semiclassical evaluation of the

TABLE V. Convergence of semiclassical 6j-coefficients $\begin{Bmatrix} j_1\lambda & 8\lambda & 7\lambda \\ 6.5\lambda & 7.5\lambda & 7.5\lambda \end{Bmatrix}$.

j_1	$\lambda=1$	$\lambda=2$	$\lambda=4$	$\lambda=8$	$\lambda=16$	
1	0.3491 (−01)	0.1218 (−01)	0.3226 (−02)	0.0513 (−02)	0.0302 (−03)	QM[a]
	0.3482 (−01)	0.1201 (−01)	0.3155 (−02)	0.0499 (−02)	0.0292 (−03)	SC
3	0.1891 (−01)	−0.7077 (−02)	0.0185 (−02)	−0.1458 (−02)	0.2156 (−03)	QM
	0.1905 (−01)	−0.7068 (−02)	0.0180 (−02)	−0.1458 (−02)	0.2157 (−03)	SC
5	−0.2359 (−01)	0.8663 (−02)	0.2973 (−02)	0.0887 (−02)	0.1358 (−03)	QM
	−0.2382 (−01)	0.8706 (−02)	0.2982 (−02)	0.0889 (−02)	0.1362 (−03)	SC
7	0.0129 (−01)	−0.7728 (−02)	0.1603 (−02)	−0.0698 (−02)	0.0315 (−03)	QM
	0.0152 (−01)	−0.7717 (−02)	0.1596 (−02)	−0.0699 (−02)	0.0318 (−03)	SC
9	0.1677 (−01)	0.0231 (−02)	−0.2800 (−02)	0.0854 (−02)	0.0697 (−03)	QM
	0.1671 (−01)	0.0198 (−02)	−0.2800 (−02)	0.0854 (−02)	0.0696 (−03)	SC
11	−0.2135 (−01)	0.7795 (−02)	0.2264 (−02)	−0.0020 (−02)	−0.3562 (−03)	QM
	−0.2147 (−01)	0.7793 (−02)	0.2259 (−02)	−0.0022 (−02)	−0.3561 (−03)	SC
13	0.2521 (−01)	0.9407 (−02)	0.1724 (−02)	−0.1184 (−02)	0.4040 (−03)	QM
	0.2527 (−01)	0.9429 (−02)	0.1731 (−02)	−0.1183 (−02)	0.4039 (−03)	SC
15	0.0271 (−01)	0.7636 (−04)	0.1171 (−06)	0.5415 (−12)	0.2293 (−22)	QM
	0.0257 (−01)	0.7175 (−04)	0.1095 (−06)	0.5051 (−12)	0.2136 (−22)	SC

[a]QM = quantum mechanical values; SC = semiclassical values.

Wigner coefficients should be favored over a recursive evaluation. The recursive evaluation of the Wigner coefficients generates simultaneously whole strings of $3j$- and $6j$-coefficients like

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \text{ and } \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \text{ for all allowed } j_1,$$

whereas the semiclassical formulas need to evaluate each $3j$- and $6j$-coefficient individually. In cases for which such whole arrays of coefficients are needed, the recursive method involves less numerical effort than the semiclassical method, and also provides more accurate numerical values. In cases where only individual coupling coefficients are needed a semiclassical evaluation may nevertheless be quite useful. In addition to numerical evaluation, our systematic derivation of the semiclassical Wigner coefficients should contribute to a better physical understanding of the quantum mechanical theory of angular momentum coupling.

*Supported by the National Science Foundation.
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