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Relating the classical and quantal theories of angular momentum and spin

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Abstract. The classical and quantal theories of angular momentum and spin are related using the spherical top as a model. The quantum mechanical spectral operator kernel of the spherical top is evaluated and expressed exactly as a sum over classical paths of terms containing the classical action. A relation between corresponding values of the classical and quantal angular momentum is obtained which holds for all values of the angular momentum quantum number j.

1. Introduction

The properties of angular momentum and spin can be obtained from the commutation relations satisfied by the components of the angular momentum and the usual $J_{\pm}$ operators. The treatment of angular momentum in this elegant way unfortunately has little physical content.

The treatment of angular momentum in terms of rotational coordinates, although being more physical, is unsatisfactory in that the wavefunctions for half integer values of j are double valued.

Recently an alternative treatment of spin in terms of rotational coordinates has been given by Schulman (1968) who approaches the subject by path integration. The reasons given by Schulman for considering spin in this way were that, firstly, Feynman and Hibbs (1965) had commented on the existing inability to incorporate into nonrelativistic path integral theories the very important concept of spin; and secondly Schulman felt that spin was basically a property of rotations anyway that could be treated in terms of rotational or internal spin coordinates as opposed to the rather formal spinor wavefunctions.

Because of the relevance of Schulman's work to this present study we briefly outline the important features of his paper. His model for spin is a spherically symmetric top and by path integration Schulman obtains the quantum mechanical evolution operator kernel or propagator of this system. This propagator propagates all spins corresponding to $j = 0, \frac{1}{2}, 1, \ldots$ etc, and the recovery of the usual Pauli spinors can be achieved by projection to a specific spin subspace. Finally, the propagator, rather surprisingly, is expressible solely as a sum over *classical* paths.

Based as it is on a classical model this treatment certainly lends physical content to the theory of spin and indeed to angular momentum in general. Further, since only the classical paths occur in the theory, it would appear that here, through the propagator of the spherical top, was a direct way of relating the corresponding classical and quantum mechanical theories of angular momentum and spin. However, as a means of relating the two theories, this particular method is not as satisfactory as it might seem at first sight. The quantum mechanical propagator is a function of the time of propagation τ and in accordance with the uncertainty principle, if τ is known then all corresponding energies of propagation are likely. This is why Schulman's propagator propagates all spins and why we cannot simply deal with spin $\frac{1}{2}$ or some other single value.

In the classical theory, the time of propagation of each classical path is fixed and consequently the energy of rotation of the top is different along each trajectory (which varies in length). Thus the propagator, expressed as a sum over classical paths, involves not one particular value of the classical angular momentum, but infinitely many values. Instead of relating a particular value of the classical angular momentum to a given quantum mechanical value, the propagator relates a distribution of classical values to a distribution of discrete quantal values.

In the present paper we again propose to relate the two theories of total angular momentum using the spherical top as a model, but this time in such a way as to be able to relate directly corresponding values of the classical and quantal angular momentum. Our approach will be time independent and instead of evaluating the propagator we shall obtain its time independent analogue, which is the kernel of the spectral operator $\delta(E-H)$. This operator has been discussed in general terms by Norcliffe and Percival (1968a) and a time independent path integral approach to quantum mechanics through this operator has been given by Garrod (1966). We do not propose to obtain the spectral operator kernel by path integration since there are easier ways of doing this. We shall instead evaluate the kernel first by the standard technique of summing over the stationary states of the spherical top and then show that it is expressible exactly as a sum over classical paths, thus providing an identity between the classical and quantal theories. By way of this identity we shall then be able to relate the corresponding values of the classical and quantal angular momentum for all possible values of j.

The motivation for this particular study stems from the widely held view (eg Biedenharn and Van Dam 1965) that classical considerations are possibly deeper than is immediately evident in theories of spin and angular momentum. In several respects this has already been shown to be the case by Schulman; but we feel that a time independent approach is more appropriate.

Our results explain the success of Landé's empirical formula (eg Biedenharn and Van Dam 1965, p 2)

$$j^2_{\text{classical}} \Rightarrow j(j+1)_{\text{quantal}} \tag{1}$$

which he used to good effect prior to wave mechanics in studying the anomalous Zeeman effect, and also throw light on the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ in WKB theories (eg Kramers 1926, Langer 1937). Further, we show that spin ($j = \frac{1}{2}$) has its classical counterpart in a spherically symmetric top whose classical angular momentum is $\hbar$.

2. The spherical top as a model for angular momentum

In this section we put forward the reasons for choosing the spherical top as a model for total angular momentum.

In classical mechanics if the angular momentum is a constant of the motion then the Hamiltonian of the system is symmetric with respect to rotations about the origin of coordinates. The spherical top Hamiltonian as we shall show is invariant with respect to rotations about any axis through its centre of mass and hence in classical mechanics the spherical top is a natural choice as a model for angular momentum.

The connection between total angular momentum and the rotation of rigid bodies in quantum mechanics is well known (eg Casimir 1931) and in terms of the Euler angles (see figure 1), which specify the rotation of a rigid body, the square of the total angular momentum operator $\boldsymbol{J}^2$ may be expressed as follows (eg Edmonds 1960, p 65, Brink and Satchler 1962, p 27)

$$\boldsymbol{J}^2 = \hbar^2\left\{-\frac{\partial^2}{\partial\beta^2} - \cot\beta\frac{\partial}{\partial\beta} - \frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\gamma^2} - 2\cos\beta\frac{\partial^2}{\partial\alpha\partial\gamma}\right)\right\}. \qquad (2)$$

From a quantum mechanical point of view, the spherical top is again an ideal model for angular momentum because apart from a multiplicative constant of $1/2I$, I being the moment of inertia of the top about any axis through its centre of mass, the Hamiltonian operator is the same as the expression for the $\boldsymbol{J}^2$ operator, and the eigenfunctions of the $\boldsymbol{J}^2$ operator are thus solutions of the spherical top wave equation.

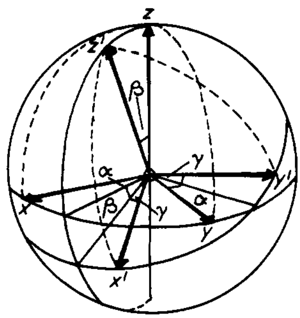

Figure 1. The Euler angles.

However the following points must be noted. The eigenfunctions of the $\boldsymbol{J}^2$ operator for half integer values of j (see for example Bopp and Haag 1950) are double valued and as corresponding wavefunctions of the top they are regarded as unphysical and tend to be discarded (eg Brink and Satchler 1962). This is why half integer states of angular momentum, out of context of any physical system, are represented by spinor wavefunctions. Fortunately in this paper we shall not have need to deal directly with double valued wavefunctions, and the problem will not arise. Before going on to evaluate the kernel of the spherical top spectral operator we first consider the classical mechanics of the top.

3. Classical mechanics of the spherical top

Since we will be concerned with definite values of the angular momentum the classical mechanics of the spherical top is best considered without any explicit reference to time. This may be done by formulating and solving the time independent Hamilton–Jacobi equation, the solution of which is, to within an additive constant, the time independent action function (Goldstein 1950). In this section we shall evaluate directly the classical action of the top as it rotates between two configurations A and B say.

We can simplify the problem by regarding the rotation as being about a particular axis $\hat{\boldsymbol{n}}$, through a given angle ω. This is possible in classical mechanics, but not of course in quantum mechanics. Because of spherical symmetry the angular momentum vector $\boldsymbol{\kappa}$ and the axis of rotation are in the same direction. In terms of ω and its derivative the classical Lagrangian function is given by

$$L(\omega, \dot{\omega}, t) = \tfrac{1}{2} I \dot{\omega}^2 \tag{3}$$

and the generalized momentum P_ω conjugate to ω is

$$P_\omega = \frac{\partial L}{\partial \dot{\omega}} = I\dot{\omega} = k \tag{4}$$

where $k = |\boldsymbol{\kappa}|$. In terms of P_ω and ω the Hamiltonian function is

$$H(P_\omega, \omega) = \frac{P_\omega^2}{2I} = \frac{k^2}{2I} \tag{5}$$

which is invariant under rotations and hence constant. The value of the time independent action (not to be confused with $\int L(\omega, \dot{\omega}, t)\, \mathrm{d}t$) is

$$S = \int_A^B P_\omega \,\mathrm{d}\omega = k \int_A^B \mathrm{d}\omega = k\Gamma \tag{6}$$

where Γ is the net angle of rotation (about $\hat{\boldsymbol{n}}$) between the two configurations $A(\alpha_0\beta_0\gamma_0)$ and $B(\alpha\beta\gamma)$.

Relating Γ to the Euler angles is easily achieved. Suppose the rotation $(\alpha\beta\gamma)$ is represented by a matrix R, and $(\alpha_0\beta_0\gamma_0)$ by R_0. Then the net rotation Γ is produced by the rotation RR_0^{-1} and it is well known (eg Plumpton and Chirgwin 1966, p 6) that

$$1 + 2\cos\Gamma = \mathrm{Tr}(RR_0^{-1}) \tag{7}$$

which results in the relation

$$\begin{aligned}\cos\tfrac{1}{2}\Gamma = {} & \cos\tfrac{1}{2}(\beta - \beta_0)\cos\tfrac{1}{2}(\gamma - \gamma_0)\cos\tfrac{1}{2}(\alpha - \alpha_0) \\ & - \cos\tfrac{1}{2}(\beta + \beta_0)\sin\tfrac{1}{2}(\gamma - \gamma_0)\sin\tfrac{1}{2}(\alpha - \alpha_0).\end{aligned} \tag{8}$$

The value of the action given by equation (6) is that for the most direct (shortest) path from A to B and clearly another possible path from A to B is one where the top returns to B after c complete revolutions. The angle turned through in this case is $\Gamma + 2\pi c$, and the corresponding value of the action is $k(\Gamma + 2\pi c)$. The next shortest path from A to B (see figure 2) is that where the top turns through an angle $2\pi - \Gamma$ radians about $\hat{\boldsymbol{n}}$, and rotations through an angle of $2\pi c - \Gamma$ also bring the top back to B. The action for these paths is then $k(2\pi c - \Gamma)$. Thus if c is an integer ranging from $-\infty$ to ∞ it can be used to label all the possible paths between A and B, and the values of the classical action $S_c(k, \Gamma)$ along these paths are then given by

$$S_c(k, \Gamma) = k|2\pi c + \Gamma| \qquad c = 0, \pm 1, \pm 2, \ldots . \tag{9}$$

It should be noted that along each of the paths the angular momentum of the top is the same. This is not the case in the time dependent theory given for example by Schulman.

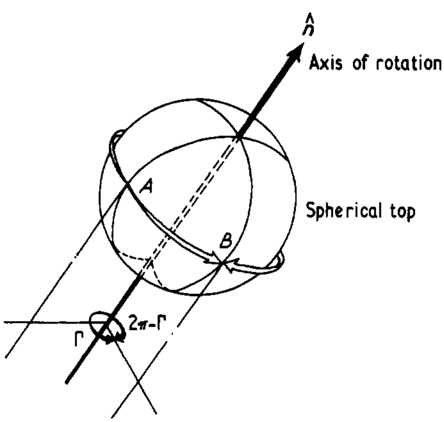

Figure 2. Diagram illustrating two possible classical paths between the positions A and B of the spherical top.

4. Quantum mechanical theory and the spectral operator

Expressed as a sum over quantum mechanical states (Norcliffe and Percival 1968a) the spectral operator for a discrete spectrum is given by

$$I_E = \delta(E-H) = \sum_\nu \delta(E-E_\nu)P_\nu \tag{10}$$

where P_ν are the projection operators onto the levels ν which may be degenerate. The completeness relation of the states is expressed by the requirement

$$\sum_\nu P_\nu = I. \tag{11}$$

The kernel of the spectral operator is a function of the energy E and unless E is equal to one of the values E_ν the value of the kernel is thus zero.

The wavefunctions of the top that correspond to integer values of the total angular momentum are single valued and any single valued function of the Euler angles can be expressed as a sum over these states. Because they are complete we may construct an operator I_E^+, say, which is nonzero only for values of E equal to $j(j+1)\hbar^2/2I$ where j is an integer. We shall refer to this operator as the spectral operator for integer spins, and we shall obtain the kernel of this operator to begin with. The spectral operator kernel for half integer spins will then be obtained directly from I_E^+ without summing over half integer values of j.

The energy levels of the spherical top are degenerate with respect to m and m' which label the eigenvalues of the operators J_z and $J_{z'}$ ($J_{z'}$ plays the role of J_z in the body-fixed frame), and the normalized single valued wavefunctions are (Schulman 1968)

$$\psi_{jmm'}(\alpha\beta\gamma) = \left(\frac{2j+1}{8\pi^2}\right)^{1/2} \mathscr{D}^{j*}_{m'm}(\alpha\beta\gamma) \qquad j = 0, 1, 2\dots \tag{12}$$

The $\mathscr{D}$ are the representation matrices of the rotation group. The kernel of the projection operator P_j onto the level j is thus

$$\begin{aligned} P_j(\alpha\beta\gamma,\alpha_0\beta_0\gamma_0) &= \sum_{mm'} \psi_{jmm'}(\alpha\beta\gamma)\psi^*_{jmm'}(\alpha_0\beta_0\gamma_0) \\ &= \frac{2j+1}{8\pi^2}\sum_{mm'} \mathscr{D}^{j*}_{m'm}(\alpha\beta\gamma)\mathscr{D}^{j}_{m'm}(\alpha_0\beta_0\gamma_0) \\ &= \frac{2j+1}{8\pi^2}\frac{\sin(j+\frac{1}{2})\Gamma}{\sin\Gamma/2} \end{aligned} \tag{13}$$

where Γ is the angle defined by equation (8).

The spectral operator kernel $I^+_E(\Gamma)$ for integer values of j is thus given by

$$I^+_E(\Gamma) = \sum_{j=0,1,\ldots} \delta\left(E - \frac{j(j+1)\hbar^2}{2I}\right)\frac{2j+1}{8\pi^2}\frac{\sin(j+\frac{1}{2})\Gamma}{\sin\Gamma/2}. \tag{14}$$

We express the energy E as $(k^2-\hbar^2/4)/2I$, where k is a continuous variable greater than or equal to $\hbar/2$ (later to be identified with the magnitude of the classical angular momentum) and write

$$I^+_k(\Gamma) = \sum_j \delta\left(\frac{k^2-\hbar^2/4}{2I} - \frac{j(j+1)\hbar^2}{2I}\right)\frac{2j+1}{8\pi^2}\frac{\sin(j+\frac{1}{2})\Gamma}{\sin\Gamma/2}. \tag{15}$$

Using the properties of the Dirac delta function (Dirac 1958, p 60) and noting that k is positive, we have

$$\begin{aligned} I^+_k(\Gamma) &= \sum_j \frac{I}{4\pi^2\hbar^2}\delta\left(\frac{k}{\hbar} - (j+\tfrac{1}{2})\right)\frac{\sin(j+\frac{1}{2})\Gamma}{\sin\Gamma/2} \\ &= \frac{I}{4\pi^2\hbar^2}\frac{\sin k\Gamma/\hbar}{\sin\Gamma/2}\sum_j \delta\left(\frac{k}{\hbar} - (j+\tfrac{1}{2})\right). \end{aligned} \tag{16}$$

Using now the identity in Lighthill (1960, p 68) we may re-express this infinite sum in an alternative way to give

$$\begin{aligned} I^+_k(\Gamma) &= \sum_{c=-\infty}^{\infty} \frac{\epsilon(k)I\sin k\Gamma/\hbar}{4\pi^2\hbar^2\sin\Gamma/2}\cos 2\pi\left(\frac{k}{\hbar}-\frac{1}{2}\right)c \\ &= \sum_c \frac{\epsilon(k)I}{4\pi^2\hbar^2\sin\Gamma/2}\frac{(-1)^c|c|}{c}\sin\frac{k}{\hbar}|\Gamma+2\pi c| \end{aligned} \tag{17}$$

where $\epsilon(k) = 0$ if $k < 0$ and 1 otherwise.

This expression for $I^+_k(\Gamma)$ is now in the form of a classical path sum and by equation (9) may be written as

$$I^+_k(\Gamma) = \sum_c |D(\Gamma)|^{1/2} d^+(c)\sin\frac{S_c(k,\Gamma)}{\hbar} \tag{18}$$

where

$$D(\Gamma) = \frac{I^2}{16\pi^4\hbar^4\sin^2\Gamma/2} \tag{19}$$

and $d^+(c)$, the phase associated with each path, is given by

$$d^+(c) = \frac{(-1)^c|c|}{c}. \tag{20}$$

To obtain $I_k^-(\Gamma)$, the spectral operator kernel for half integer values of j, we simply add together the classical path contributions with different phases given by

$$d^-(c) = \frac{|c|}{c} \tag{21}$$

so that

$$I_k^-(\Gamma) = \sum_c |D(\Gamma)|^{1/2} d^-(c) \sin \frac{S_c(k,\Gamma)}{\hbar}. \tag{22}$$

To check that this is the desired operator kernel we note that

$$I_k^-(\Gamma) = \sum_c \frac{\epsilon(k)I}{4\pi^2\hbar^2 \sin \Gamma/2} \frac{|c|}{c} \sin \frac{k}{\hbar}|\Gamma + 2\pi c| \tag{23a}$$

$$= \sum_c \frac{\epsilon(k)I}{4\pi^2\hbar^2 \sin \Gamma/2} \sin \frac{k\Gamma}{\hbar} \cos \frac{2\pi c k}{\hbar} \tag{23b}$$

$$= \frac{I \sin k\Gamma/\hbar}{4\pi^2\hbar^2 \sin \Gamma/2} \sum_{j=1/2,3/2,\ldots} \delta\left(\frac{k}{\hbar} - (j+\tfrac{1}{2})\right) \tag{23c}$$

$$= \sum_{j=1/2,3/2,\ldots} \delta\left(\frac{k^2 - \hbar^2/4}{2I} - \frac{j(j+1)\hbar^2}{2I}\right) \frac{2j+1}{8\pi^2} \frac{\sin(j+\frac{1}{2})\Gamma}{\sin \Gamma/2} \tag{23d}$$

as required. $I_k(\Gamma)$, the spectral operator kernel for all values of j, is the sum of $I_k^+(\Gamma)$ and $I_k^-(\Gamma)$ and is thus expressible solely as a sum over classical paths

$$I_k(\Gamma) = \sum_c |D(\Gamma)|^{1/2} (d^+(c) + d^-(c)) \sin \frac{S_c(k,\Gamma)}{\hbar}. \tag{24}$$

This equation, expressing as it does the spectral operator kernel of the spherical top exactly as a sum over classical paths, thus relates directly the corresponding classical and quantal theories of angular momentum and spin.

5. Relating corresponding values of the angular momentum

If follows from equations (16) and (23c) together with the properties of the Dirac delta function that $I_k(\Gamma)$, as given in equation (24), is nonzero only for those values of k given by

$$k = (j+\tfrac{1}{2})\hbar \qquad j = 0, \tfrac{1}{2}, 1, \ldots. \tag{25}$$

k however is just the magnitude of the classical angular momentum vector $\boldsymbol{\kappa}$ and equation (25) thus specifies the correct quantization of classical angular momentum consistent with the quantum mechanics. Equation (25) holds for all values of j and is a correspondence identity for angular momentum (see also Norcliffe and Percival 1968b, Norcliffe *et al* 1969a, 1969b and 1971 for a discussion of the correspondence identities associated with the Coulomb potential).

The quantization of classical angular momentum is due to the interference of the classical path contributions in equation (24). For values of k given by equation (25) the contributions add constructively, whilst for other values they add destructively. The interference is illustrated in figure 3 where a partial classical path sum over nine paths of each of $I_k^{\pm}(\Gamma)$ and $I_k(\Gamma)$ is plotted for $\Gamma = 0$.

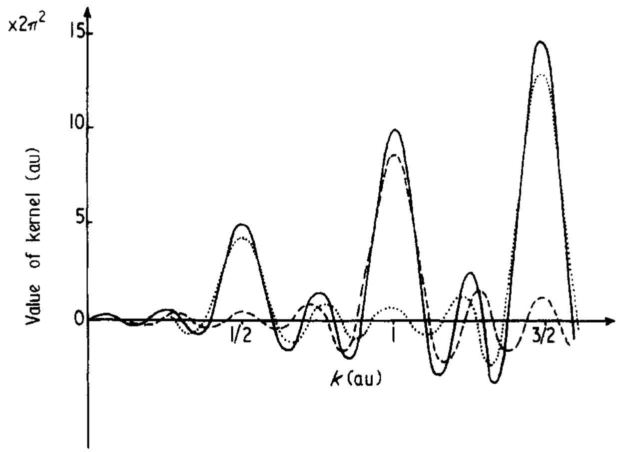

Figure 3. Partial sum over nine paths of $I_k^{\pm}(0)$, $I_k(0)$ against k. The full curve is $I_k(0)$; the dotted curve represents $I_k^{+}(0)$ and the broken curve is the curve representing $I_k^{-}(0)$.

6. Discussion

The aim of this paper has been to relate in as direct a way as possible the classical and quantal theories of total angular momentum, and by expressing the kernel of the spherical top spectral operator exactly as a sum over classical paths we feel that we have achieved this. Our results together with Schulman's classical path expression for the propagator support the view that classical considerations are indeed deeper than is immediately evident in the quantum mechanical theory of angular momentum and spin.

We have not given a path integral method of evaluating the spectral operator kernel, but our results show that if such a method were adopted then only the classical paths would contribute. The reasons for not using the method of path integration arise out of the difficulty of formulating such a method in any coordinate system other than rectangular cartesians (eg Edwards and Gulyaev 1964, Peak and Inomata 1969 in the case of polar coordinates and Arthurs 1970 for general curvilinear coordinates). Schulman assumed correctly that only the classical paths would be important in evaluating the propagator and used the phase integral approximation as given by De Witt (1957), taking into account the curvature of the Euler angle space. To modify existing time independent phase integral approximation methods (eg Gutzwiller 1967) to take care of curvature did not seem worthwhile since there is no *a priori* reason to suppose that they should give the correct form for the spectral operator kernel.

The curvature of the Euler angle space is responsible for the corresponding classical and quantum mechanical energies of rotation of the spherical top being different. It is the classical energy $k^2/2I = (j+\frac{1}{2})^2\hbar^2/2I$ which corresponds to the quantal energy $E_j = j(j+1)\hbar^2/2I$. This correspondence between energies holds for all values of j by virtue of equation (25) and the success of Landé's formula is due directly to this fact. In the light of the present results a better relationship would appear to be

$$(j+\tfrac{1}{2})^2_{\text{classical}} \Rightarrow j(j+1)_{\text{quantal}} \tag{26}$$

but even though Landé's formula does not contain the term of $\frac{1}{2}$ it is of no consequence because although the possible quantized values of the classical angular momentum (see figure 3) are $\hbar/2$, $\hbar$, $3\hbar/2$, ... etc, Landé assumed them to be 0, $\hbar/2$, $\hbar$, ..., thus accounting, unknowingly for the $\frac{1}{2}$ term. It is important to remember that Landé's expression for the g factor, which utilizes equation (1) was only to be confirmed later by quantum mechanics.

Equation (26) with j replaced by l the orbital angular momentum quantum number, is not unfamiliar and is well known in WKB theories of radial motion (eg Kramers 1926, Langer 1937, Fröman and Fröman 1965 etc). The present work unfortunately cannot be used to prove the validity of such a formula for all values of l since the model for orbital angular momentum is not the spherical top but the two-particle rigid rotor (eg Buckingham 1961, p 97). The replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ is used even for low quantum numbers in WKB theories, but its success seems to depend largely on the type of potential in question and Engelke and Beckel (1970) have shown that this correction is by no means unique. Nevertheless for total angular momentum equation (26) is exact for all values of j and in particular for $j = \frac{1}{2}$ we have the important result that spin, a strictly quantum mechanical effect, can be discussed in terms of a classical spherically symmetric top of angular momentum $\hbar$.

Finally we comment briefly on the treatment of spin and angular momentum in terms of sums over classical paths. The problem of dealing with angular momentum by means of rotational coordinates has always been the unphysical nature of the boundary condition, namely double-valuedness, that must be imposed on the angular momentum wavefunctions to produce the half integer values of j. The usual boundary condition of single-valuedness gives only integer values. In the present work the role of boundary conditions is played by the phase factors $d^{\pm}(c)$ that occur in the classical path expansions of $I_k^{\pm}(\Gamma)$. With $d^{+}(c)$ the sum over paths yields integer values of j, and with $d^{-}(c)$ we get the half integer values. Phase factors are an accepted feature of path integral theories (eg Gutzwiller 1967, Schulman 1968 and Dowker 1970) and there is no reason to suppose that the phases $d^{-}(c)$ should be less acceptable than $d^{+}(c)$. In other words, by means of sums over classical paths, both integer and half integer values of j arise naturally out of the theory.

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