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Quantum theory of rotation angles

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The formulation of the quantum description of the rotation angle of the plane rotator has been beset by many of the long-standing problems associated with harmonic-oscillator phases. We apply methods recently developed for oscillator phases to the problem of describing a rotation angle by a Hermitian operator. These methods involve use of a finite, but arbitrarily large, state space of dimension $2l+1$ that is used to calculate physically measurable quantum properties, such as expectation values, as a function l. Physical results are then recovered in the limit as l tends to infinity. This approach removes the indeterminacies caused by working directly with an infinite-dimensional state space. Our results show that the classical rotation angle observable does have a corresponding Hermitian operator with well-determined and reasonable properties. The existence of this operator provides deeper insight into the quantum-mechanical nature of rotating systems.

I. INTRODUCTION

Classical simple-harmonic motion may be described as the projection into one dimension of a two-dimensional uniform circular motion. The phase of the simple-harmonic motion is the rotation angle ϕ of the corresponding circular motion, and both of these quantities are multivalued classical observables. The phase and rotation angle often appear as the inverse trigonometric functions and are usually chosen to lie in a specified 2π range, that is, ϕ can take values from θ_0 up to, but not including, $\theta_0+2\pi$. The choice of θ_0 is arbitrary, but commonly used values are 0 and $-\pi$. If we take this restriction on the values of rotation angle (or phase) seriously, then the evolution of the rotation angle will not be smooth, but will jump by 2π when its value reached the edge of the allowed range. However, if we wish to avoid this discontinuity in the evolution, we can still choose an initial rotation angle and then allow it to evolve without a bound to its allowed values. Naturally, the physical properties of the system under investigation should be independent of the manner in which we deal with the multivalued nature of angle or phase. The quantum description of phase and angle is more complicated than its classical counterpart and has met with considerable difficulties since Dirac[1] first postulated the existence of an operator for the phase of an electromagnetic-field mode. These difficulties have received much theoretical interest and have been described by a number of authors.[2-5]

We have recently obtained the Hermitian operator corresponding to the phase of a single mode of the electromagnetic field.[6-8] A complete description of the field requires an infinite basis of number states, and thus an infinite limit must be involved in any theory. The crucial feature which distinguishes our procedure from previous approaches is the stage at which this limit is taken. We begin with a finite, but arbitrarily large, state space of $s+1$ dimensions and calculate measurable quantities, such as expectation values and variances, as a function of s. The limit as s tends to infinity is then taken only *after* these expectation values and variances are calculated and is thus simply the limit of a sequence of real numbers. This procedure avoids the indeterminacies associated with approaches in which the limit is taken at an earlier, intermediate stage, for example, by embedding the finite space in an infinite Hilbert space.

In this paper we extend our method to derive the form of the Hermitian rotation-angle operator (henceforth referred to as an angle operator). This operator corresponds to the angular position of a plane rotator, that is, a body in uniform circular motion—for example, a bead on a circular wire. The angle operator will be applicable to a wider range of problems than the bead on a wire, but we initially restrict our attention to this system because of its simplicity and because it has featured in earlier attempts to describe quantum angle variables.[2–4] Moreover, it is the natural analog of the oscillator with its associated phase. We note that finite state spaces have been used in some earlier discussions of phase and angle variables.[9,10] However, where a transition has been attempted to an infinite (unbounded) system, these approaches have involved limiting procedures that enforce a return to the original problems noted by Susskind and Glogower.[11] By delaying the taking of limits until the final stage of the calculation after physical results, that is, real numbers, are obtained, we circumvent these difficulties. As noted by Merzbecher,[12] by confining ourselves to a complex linear vector space of finite dimensions, we succeed in avoiding questions which concern the convergence of sums over infinitely many terms, the interchangeability of several such summations, and the legitimacy of certain limiting procedures.

One of the problems inherent in the oscillator phase problem was the existence of a cutoff in the spectrum of the number operator, which excludes the negative integers. For the plane rotator, however, the corresponding angular momentum operator has a spectrum that includes both positive and negative integers. This suggests that our approach, which delays taking the limit of the dimensions of the state space, may not be necessary for the derivation of the angle operator. We show, however, that direct use of an infinite state space can lead to problems and that these may be understood and overcome by using our limiting procedure. The infinite state space may only be used with extreme care.

II. CLASSICAL ROTATION ANGLES AND SIMPLE QUANTIZATION

We begin our discussion with a description of classical angles and their quantization by application of the correspondence principle. For simplicity and definiteness we restrict our investigation to a bead constrained to move on a circular wire whose axis is aligned in the z direction. The classical z component of angular momentum and the azimuthal rotation angle of the bead can be expressed in terms of the Cartesian coordinates and momenta as

$$L_z = xp_y - yp_x \; , \tag{2.1}$$

$$\phi = \arctan(y/x) \; . \tag{2.2}$$

The angle is defined as the inverse of a trigonometric function and may be defined to lie within a chosen 2π range or to be assigned an initial value and then evolve as a continuous and unbounded variable. If we treat ϕ as a continuous variable, then the Poisson bracket for the angular momentum and the angle has the form

$$\{\phi, L_z\} = 1 \; . \tag{2.3}$$

Direct application of the correspondence between Poisson brackets and commutators suggests that the angular momentum and angle operators obey a commutator of the form

$$[\hat{\phi}, \hat{L}_z] = i\hbar \; . \tag{2.4}$$

If we represent an angular momentum operator as

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi} \tag{2.5}$$

and the angle operator as multiplication by ϕ, then the commutator (2.4) is satisfied. However, this representation of the angle operator causes problems:[13] if $u(\phi)$ is a periodic wave function, then $\phi u(\phi)$ will not be and is therefore outside the angular momentum state space. Judge and Lewis realized that the eigenvalues of a well-behaved angle operator would have to be restricted to a 2π interval. Their solution was to modify the angle operator so that it corresponded to multiplication by ϕ plus a series of step functions. These step functions sharply change the angle by 2π at appropriate points.[14] The resulting commutation relation between this operator and $\hat{L}_z$ has a δ-function term in addition to the $i\hbar$ term from the commutator (2.4). The Judge-Lewis commutator corresponds to the classical Poisson bracket of L_z and a single-valued angle variable.[15] Another approach is to avoid the problem of multivaluedness by not dealing with an Hermitian angle operator at all, but rather only periodic functions of the angle operator.[2–4] Naturally, this approach does not allow us to investigate the properties of the angle operator itself.

There is a further difficulty associated with the proposed commutator (2.4). This problem was originally discovered in association with Dirac's phase operator,[16] but is readily extended to the present situation. The difficulty arises when we take matrix elements of the proposed commutator (2.4) in the angular momentum basis

$$\langle m | [\hat{\phi}, \hat{L}_z] | m' \rangle = i\hbar \delta_{mm'} \; , \tag{2.6}$$

where the states $|m\rangle$ are eigenstates of $\hat{L}_z$ with eigenvalue m. This expression implies that the matrix elements of $\hat{\phi}$ are undefined in the angular momentum basis

$$(m' - m) \langle m | \hat{\phi} | m' \rangle = i\hbar \delta_{mm'} \; . \tag{2.7}$$

Consideration of the diagonal matrix elements in this equation clearly demonstrates the problem. A similar problem occurs if we use this commutator in an attempt to construct an angle-state representation of the angular momentum operator.

The above difficulties are only partially resolved by employing a single-valued operator obeying a commutation relation similar to that proposed by Judge and Lewis.[13] We shall see in Sec. V that such a commutator arises naturally if we work directly in an infinite angular momentum state space. The resulting matrix elements of the angle operator in the angular momentum basis states are well defined and correct. However, the angle-state matrix elements of the angular momentum operator are not. We shall show how these problems associated with the angle operator can be resolved by methods previously used for the treatment of optical phase.[6–8]

III. ANGLE STATES AND THE HERMITIAN ANGLE OPERATOR

By analogy with our phase operator approach, we work in a $(2l+1)$-dimensional state space Ψspanned by the $\hat{L}_z$ eigenvectors $|m\rangle$, with $m=-l,\ldots,-1,0,1,\ldots,l$. Later, and only *after* physical results such as expectation values are calculated, we shall let l tend to infinity.

A sensible rotation-angle state will have $\hat{L}_z$ as a generator, that is, it will obey

$$\exp(-i\eta\hat{L}_z/\hbar)|\phi\rangle=|\phi+\eta\rangle\ , \tag{3.1}$$

which can be achieved by defining

$$|\phi\rangle\equiv\exp(-i\phi\hat{L}_z/\hbar)|\alpha_0\rangle\ , \tag{3.2}$$

where $|\alpha_0\rangle$ is the zero angle state. If an Hermitian angle operator $\hat{\phi}$ exists in a conjugate relationship with $\hat{L}_z$, we would expect it to be the generator of an angular momentum shift,

$$\exp(in\hat{\phi})|m\rangle=|m+n\rangle \tag{3.3}$$

for all integers n. We can use these shift properties to obtain the form of the angle states by operating with $\exp(in\hat{\phi})$ on both sides of the expansion

$$|\alpha_0\rangle=\sum_m c_m|m\rangle\ . \tag{3.4}$$

If the zero angle state is an eigenstate of $\hat{\phi}$ with eigenvalue zero, we obtain

$$|\alpha_0\rangle=\sum_m c_m|m+n\rangle\ . \tag{3.5}$$

Comparison of (3.5) and (3.4) shows that the coefficients c_m should be independent of m.[17] The space Ψ has dimensional $2l+1$; thus we normalize the coefficients c_m to be $(2l+1)^{-1/2}$. Such a normalization cannot be achieved in an infinite state space. This analysis leads unambiguously to the form of the angle state $|\phi\rangle$,

$$|\phi\rangle=(2l+1)^{-1/2}\sum_{m=-l}^{l}\exp(-im\phi)|m\rangle\ . \tag{3.6}$$

The form of this state is similar to that of the optical phase states.[18]

We see from (3.6) that the angle states have a periodic structure: $|\phi+2\pi\rangle$ is the same state as $|\phi\rangle$. All distinct angle states can be specified by the points on the real line between some value θ_0 and up to, but not including, $\theta_0+2\pi$. These states, however, are overcomplete and are not all mutually orthogonal:

$$\begin{aligned}\langle\phi'|\phi\rangle&=(2l+1)^{-1}\sum_{m=-l}^{l}\exp[-im(\phi'-\phi)]\\&=(2l+1)^{-1}\frac{\sin[(2l+1(\phi-\phi')/2]}{\sin[(\phi-\phi')/2]}\ .\end{aligned} \tag{3.7}$$

If we were to ignore the factor $(2l+1)^{-1}$ and take the limit of the second factor as l tends to infinity, we would obtain a sum of δ functions with peaks separated by 2π. However, it makes little sense to take the limit of the second term without including the normalization factor. We see from (3.7) that two angles states $|\phi\rangle$ and $|\phi'\rangle$ are orthogonal if $\phi-\phi'$ is a nonzero multiple of $2\pi/(2l+1)$. We can thus form a complete orthonormal basis of $(2l+1)$ angle states $|\theta_n\rangle$ be selecting values of θ_n as

$$\theta_n=\theta_0+\frac{2\pi n}{2l+1}\quad(n=0,1,\ldots,2l)\ . \tag{3.8}$$

The choice of θ_0 is arbitrary and determines the particular basis set. Choosing the basis beginning with θ_0 to span the space Ψ corresponds to the classical procedure of choosing a particular 2π window in which to express the value of $\arctan(y/x)$. We have already noted a similar correspondence in our analysis of the optical phase operator.[7]

Angle states in different basis sets will not be orthogonal and will be eigenstates of *different noncommuting* angle operators. It is therefore necessary to attach a label to the angle operator in order to specify which basis set forms its eigenstates. We label the angle operator $\hat{\phi}_\theta$ to indicate that its eigenvalues are θ_n as given in (3.8):

$$\hat{\phi}_\theta\equiv\sum_{n=0}^{2l}\theta_n|\theta_n\rangle\langle\theta_n| \tag{3.9}$$

$$=\theta_0+\sum_{n=0}^{2l}\frac{2\pi n}{2l+1}|\theta_n\rangle\langle\theta_n|\ . \tag{3.10}$$

The matrix elements of $\hat{\phi}_\theta$ in the angular momentum basis $|m\rangle$ are

$$\begin{aligned}\langle m'|\hat{\phi}_\theta|m\rangle&=\sum_{n=0}^{2l}\theta_n\langle m'|\theta_n\rangle\langle\theta_n|m\rangle\\&=(2l+1)^{-1}\sum_{n=0}^{2l}\theta_n\exp[i(m-m')\theta_n]\ ,\end{aligned} \tag{3.11}$$

which gives

$$\langle m|\hat{\phi}_\theta|m\rangle=\theta_0+\frac{2\pi l}{2l+1} \tag{3.12}$$

and

$$\langle m'|\hat{\phi}_\theta|m\rangle=\frac{2\pi\exp[i(m-m')\theta_0]}{(2l+1)\{\exp[i(m-m')2\pi/(2l+1)]-1\}} \tag{3.13}$$

for the diagonal and off-diagonal elements, respectively. These allow us to express the angle operator in the angular momentum basis as

$$\hat{\phi}_\theta=\theta_0+\frac{2\pi l}{2l+1}+\frac{2\pi}{2l+1}\sum_{\substack{m,m'\\m\neq m'}}\frac{\exp[i(m-m')\theta_0]|m'\rangle\langle m|}{\exp[i(m-m')2\pi/(2l+1)]-1}\ . \tag{3.14}$$

Of particular interest are the physical states for which all the moments of $\hat{L}_z$ are finite.[19] The states may be approximated to any desired accuracy by an expansion

$\sum_m b_m|m\rangle$, where all b_m are zero for $|m|>M$, with the bound M being as large as necessary, but always less than l. If we restrict the domain of $\hat{\phi}_\theta$ to these physical states, we can employ a "physical" angle operator obtained from (3.14) in the limit of large l:

$$(\hat{\phi}_\theta)_p=\theta_0+\pi-i\sum_{\substack{m,m'\\m\neq m'}}\frac{\exp[i(m-m')\theta_0]}{m-m'}|m'\rangle\langle m| \ . \tag{3.15}$$

Here the label p is a reminder that this simplified form can only replace $\hat{\phi}_\theta$ when operating on physical states. Nonphysical states include the angle states themselves, for which the exact form (3.14) must be used.

From (3.14) we obtain the commutator

$$[\hat{\phi}_\theta,\hat{L}_z]=\frac{2\pi\hbar}{2l+1}\times\sum_{\substack{m,m'\\m\neq m'}}\frac{(m-m')\exp[i(m-m')\theta_0]|m'\rangle\langle m|}{\exp[i(m-m')2\pi(2l+1)]-1} \ . \tag{3.16}$$

In the special case $\theta_0=0$, this reduces to the finite-space commutator obtained by Sunthanam.[10]

We can use the expansion

$$|m\rangle=\sum_{n=0}^{2l}|\theta_n\rangle\langle\theta_n|m\rangle=(2l+1)^{-1/2}\sum_{n=0}^{2l}\exp(im\theta_n)|\theta_n\rangle \tag{3.17}$$

to express $\hat{L}_z$ in the angle-state basis

$$\hat{L}_z=-i\frac{\hbar}{2}\sum_{\substack{n,n'\\n\neq n'}}\frac{(-1)^{n-n'}|\theta_{n'}\rangle\langle\theta_n|}{\sin[(n-n')\pi/(2l+1)]} \ . \tag{3.18}$$

It is now straightforward to express the angle–angular-momentum commutator in the angle-state basis

$$[\hat{\phi}_\theta,\hat{L}_z]=i\frac{\hbar\pi}{2l+1}\times\sum_{\substack{n,n'\\n\neq n'}}\frac{(n-n')(-1)^{n-n'}|\theta_{n'}\rangle\langle\theta_n|}{\sin[(n-n')\pi/(2l+1)]} \ . \tag{3.19}$$

The commutator clearly has well-defined matrix elements. In particular, the diagonal elements are

$$\langle m|[\hat{\phi}_\theta,\hat{L}_z]|m\rangle=0 \ , \tag{3.20}$$

$$\langle\theta_n|[\hat{\phi}_\theta,\hat{L}_z]|\theta_n\rangle=0 \ . \tag{3.21}$$

The commutator does not suffer from the difficulties discussed earlier in Sec. II.

When operating on physical state, the commutator (3.16) can be replaced by

$$[\hat{\phi}_\theta,\hat{L}_z]_p=-i\hbar\sum_{\substack{m,m'\\m\neq m'}}\exp[i(m-m')\theta_0]|m'\rangle\langle m| \ , \tag{3.22}$$

which is obtained by taking the large-l limit. However, we stress that it is not in general possible to take the limit before expectation values are calculated. If there is any doubt as to the validity of this procedure, the full expressions involving l should be used. The physical commutator has matrix elements given by

$$\langle m'|[\hat{\phi}_\theta,\hat{L}_z]_p|m\rangle=-i\hbar(1-\delta_{mm'})\exp[i(m-m')\theta_0] \ . \tag{3.23}$$

We note that we cannot make a similar approximation when using the angle-state basis (3.19), as values of $n-n'$ up to $2l+1$ are allowed for physical states such as an angular momentum eigenstate. The definition of the angle states allows us to express the physical commutator in the form

$$[\hat{\phi}_\theta,\hat{L}_z]_p=i\hbar[1-(2l+1)|\theta_0\rangle\langle\theta_0|] \ . \tag{3.24}$$

For any physical state $|p\rangle$, the expectation value of the commutator will be

$$\langle p|[\hat{\phi}_\theta,\hat{L}_z]|p\rangle=i\hbar[1-(2l+1)|\langle p|\theta_0\rangle|^2] \ . \tag{3.25}$$

The second term can be written as $2\pi P(\theta_0)$, where $P(\theta_0)\delta\theta$, with $\delta\theta=2\pi/(2l+1)$, is the probability that the system will be found within $\delta\theta$ of the value θ_0. In the limit as $2l+1$ tends to infinity, $P(\theta)$ will be the normalized probability density

$$\int_{\theta_0}^{\theta_0+2\pi}P(\theta)d\theta=1 \ . \tag{3.26}$$

The expectation value of the commutator (3.25) corresponds precisely to the classical Poisson bracket for a single-valued angle variable.[20] The effect of the second term is to step the angle by 2π at $\theta_0+2\pi$. If $P(\theta)$ is a δ-function distribution $\delta(\theta-\theta')$, corresponding to a physical state of quite well-defined angle θ', then (3.25) becomes

$$\langle p|[\hat{\phi}_\theta,\hat{L}_z]|p\rangle=i\hbar 1-2\pi\delta(\theta_0-\theta')] \ , \tag{3.27}$$

which clearly displays the 2π jump at $\theta'=\theta_0$. This is precisely the behavior anticipated by Judge and Lewis[13] and Susskind and Glogower[2] for a well-behaved single-valued operator. However, the expressions (3.25) and (3.27), which may be used for physical state of quite well-defined angle, are *not* applicable to state of precisely defined angle, that is, the angle states. For these we must resort to the exact expressions. It is clear that the expectation value of the physical commutator (3.24) for a system in state $|\theta_n\rangle$ is $i\hbar[1-(2l+1)\delta_{n0}]$, which is nonzero for all values of n. Clearly, (3.24) cannot be used in place of the exact commutator $[\hat{\phi}_\theta,\hat{L}_z]$ if the angle states are to be used because the commutator must have zero expectation value for angle eigenstates.

IV. PERIODIC ANGLE OPERATORS

In line with our earlier approach to phase, we construct unitary angle operators from the Hermitian angle operator:[21]

$$\exp(\pm i\hat{\phi}_\theta)=\exp\left[\pm i\sum_{n=0}^{2l}\theta_n|\theta_n\rangle\langle\theta_n|\right] . \quad (4.1)$$

The unitarity of these operators follows directly from the Hermiticity of the angle operator. The unitary operators act as angular momentum raising or lowering operators:

$$\exp(\pm i\hat{\phi}_\theta)|m\rangle=\exp\left[\pm i\sum_{n=0}^{2l}\theta_n|\theta_n\rangle\langle\theta_n|\right]\times\sum_{n'}\frac{\exp(im\theta_{n'})}{\sqrt{(2l+1)}}|\theta_{n'}\rangle$$
$$=(2l+1)^{-1/2}\sum_n\exp[i(m\pm1)\theta_n|\theta_n\rangle \quad (4.2)$$
$$=|m\pm1\rangle . \quad (4.3)$$

Here the states are labeled modulo $2l+1$, so that, for example,

$$|\pm(l\pm1)\rangle\equiv\exp[\pm i(2l+1)\theta_0]|\pm(-l)\rangle . \quad (4.4)$$

The cyclic nature of $\exp(i\hat{\phi}_\theta)$ is made clear by writing the unitary operator in the angular momentum basis

$$\exp(i\hat{\phi}_\theta)=|-l+1\rangle\langle-l|+\cdots+|m+1\rangle\langle m|+\cdots+|l\rangle\langle l-1|+\exp[i(2l+1)\theta_0]|-l\rangle\langle l| . \quad (4.5)$$

The lowering operator is given by the Hermitian conjugate of this operator. These unitary operators are functions of a common angle operator and must therefore commute. The sine and cosine angle operators have well-behaved properties. In general, we find

$$[\cos\hat{\phi}_\theta,\sin\hat{\phi}_\theta]=0 , \quad (4.6)$$

$$\cos^2\hat{\phi}_\theta+\sin^2\hat{\phi}_\theta=1 , \quad (4.7)$$

$$\langle m|\cos^2\hat{\phi}_\theta|m\rangle=\langle m|\sin^2\hat{\phi}_\theta|m\rangle=\tfrac{1}{2} , \quad (4.8)$$

$$\langle m|\cos\hat{\phi}_\theta|m\rangle=\langle m|\sin\hat{\phi}_\theta|m\rangle=0 . \quad (4.9)$$

The last two of those are consistent with a state of precise angular momentum having a random orientation.

If the zero angle state is an eigenstate of ϕ_θ, then θ_0 must be an integer multiple of $2\pi/(2l+1)$ and the exponential factor on the right side of (4.5) is unity. In this case the action of $\exp(i\hat{\phi}_\theta)$ on $|l\rangle$ gives $|-l\rangle$. Use of the operator identity

$$\exp(in\hat{\phi}_\theta)\equiv[\exp(i\hat{\phi}_\theta)]^n \quad (4.10)$$

justifies our remarks concerning the consistency of the representation of the zero angle state in the $(2l+1)$ dimensional space.[17]

For completeness, we give here the commutation relations between the unitary angle operators and $\hat{L}_z$:

$$[\exp(\pm i\hat{\phi}_\theta),\hat{L}_z]=\pm\hbar\{-\exp(\pm i\hat{\phi}_\theta)+(2l+1)\exp[\pm i(2l+1)\theta_0]|\pm(-l)\rangle\langle\pm l|\} . \quad (4.11)$$

These commutators have been obtained previously in a finite space.[9]

V. IMPROPER VECTORS IN INFINITE STATE SPACE

The symmetry between the Hermitian rotation angle operator $\hat{\phi}_\theta$ and $\hat{L}_z$ is evident throughout our work so far. In the limit as l tends to infinity, both have a countable infinity of eigenstates related to each other by (3.6) and (3.17). The angular momentum and angle eignestates are equal in number and from alternative bases for the same state space. If the eigenvalues of $\hat{\phi}_\theta$ are mapped as points on a line from θ_0 up to but not including $\theta_0+2\pi$, then, in the limit of large l, they correspond to θ_0 plus all the rational fractions of 2π. That is, the eigenvalue spectrum of the angle operator is dense.

The angular momentum operator has both positive and negative eigenvalues. This is not true for the photon number operator and therefore we might hope that it is possible to construct an angle operator directly in an infinite state space without the necessity of employing our limiting procedure. We show, however, that there are inherent difficulties associated with using an infinite state space directly.

In an infinite state space we cannot normalize an angle state vector, but begin instead with the improper, unnormalizable state vector given by the linear superposition[22]

$$|\Theta\rangle\equiv(2\pi)^{-1/2}\sum_{m=-\infty}^{\infty}\exp(-im\Theta)|m\rangle , \quad (5.1)$$

where we use Θ to distinguish these from our previous proper state vectors labeled by θ_n. We note from (5.1) that the states form an uncountably infinite set. The scalar product of two of these angle states involves a factor $(2\pi)^{-1}$ in place of the factor $(2l+1)^{-1}$ and (3.7). Thus we have a δ-function normalization of these states:

$$\langle\Theta'|\Theta\rangle=\delta(\Theta'-\Theta)\quad\text{for }|\Theta'-\Theta|<2\pi . \quad (5.2)$$

We can obtain a resolution of the identity by integration over the angle states

$$\int_{\Theta_0}^{\Theta_0+2\pi}|\Theta\rangle\langle\Theta|d\Theta=1 . \quad (5.3)$$

If we define an infinite space angle operator as

$$\hat{\Phi}_\theta \equiv \int_{\Theta_0}^{\Theta_0+2\pi} \Theta|\Theta\rangle\langle\Theta| d\Theta \;, \tag{5.4}$$

then we see from (5.2) the *all* the angle states are angle eigenstates:

$$\hat{\Phi}_\Theta|\Theta'\rangle = \Theta'|\Theta'\rangle \;. \tag{5.5}$$

Substituting the expansion (5.1) into our expression for the angle operator (5.4) we find

$$\hat{\Phi}_\Theta = (2\pi)^{-1}\int_{\Theta_0}^{\Theta_0+2\pi} \Theta \times \sum_{m,m'} \exp[i(m-m')\Theta] \times |m'\rangle\langle m| d\Theta \;. \tag{5.6}$$

If we allow ourselves to interchange the order of the infinite summation and the integral, then we obtain the expression

$$\hat{\Phi}_\Theta = \Theta_0 + \pi - i \sum_{\substack{m,m' \\ m\neq m'}} \frac{\exp[i(m-m')\Theta_0]}{m-m'} |m'\rangle\langle m| \;. \tag{5.7}$$

This form of the angle operator implies that the angle–angular-momentum commutator is

$$[\hat{\Phi}_\Theta, \hat{L}_z] = i\hbar(1 - 2\pi|\Theta_0\rangle\langle\Theta_0|) \;. \tag{5.8}$$

This commutation relation is equivalent to that postulated by Judge and Lewis.[13] We seem therefore to have arrived at the result (3.24), which we have seen is only applicable for physical states and not, for example, when operating on the angle states themselves. However, use of this commutator leads to inconsistencies. In the Appendix we reveal one of these inconsistencies by using the angle-state matrix elements of this commutator to rederive the form of $\hat{L}_z$. The source of these difficulties is the apparently innocent procedure of interchanging the order of infinite summations and integrations in the derivation of $\hat{\Phi}_\Theta$. From the definition of integration, we have

$$\int_{\Theta_0}^{\Theta_0+2\pi} \Theta \exp(ik\Theta) d\Theta \equiv \lim(\delta\to 0) \sum_{n=0}^{N} \exp[ik(\Theta_0+n\delta)](\Theta_0+n\delta) \;, \tag{5.9}$$

where $\delta = 2\pi/(N+1)$ and k is a nonzero integer. If we follow the usual rules of integration, the left-hand side becomes

$$\int_{\Theta_0}^{\Theta_0+2\pi} \Theta \exp(ik\Theta) d\Theta = \frac{2\pi}{ik}\exp(ik\Theta_0) \;. \tag{5.10}$$

However, the right-hand side can be summed exactly to give

$$\sum_{n=0}^{N} \exp[ik(\Theta_0+n\delta)](\Theta_0+n\delta) = -\frac{\delta^2(N+1)\exp(ik\delta\Theta_0)}{1-\exp(ik\delta)} \;. \tag{5.11}$$

Now *if and only if* $k\delta$ approaches zero as δ tends to zero does the limit of (5.11) become equal to (5.10). In our case $k = m - m'$ and therefore

$$k\delta = \frac{2\pi(m-m')}{N+1} \;. \tag{5.12}$$

Clearly, $k\delta$ approaches zero as N tends to infinity only if $m - m'$ is finite, as, for example, in the case of physical states. In general, however, the summation must be over all m and m', including $m - m'$ tending to infinity, and it is not permissible to exchange the order of summation and integration, unless we restrict the domain of operation to physical states.

In summary, we are not allowed in general to interchange the orders of limits associated with infinite summations and the integration. Such problems, which are associated with the direct use of an infinite state space, do not occur in our approach where we delay allowing the dimensionality of the space to approach infinity until after physical quantities such as expectation values are calculated, in which case the limits are those of sequences of real numbers. The problems described above emphasize the value of our approach.

VI. OTHER ANGULAR MOMENTUM OPERATORS

In this paper we have been concerned primarily with the quantum mechanics of a bead on a circular wire. This system has only one degree of freedom, the azimuthal angle, and one component of angular momentum. In this section we discuss breifly how the angle operator may be applied to more general problems in which all three components of angular momentum may be present. We examine a system with fixed total angular momentum—for example, a spinning top.

The eigenstates of this system are fixed by two quantum numbers and are labeled $|j,m\rangle$, where j is the total angular momentum quantum number which, bearing in mind that we shall eventually let l tend to infinity, is very much less than l. We begin by defining angular momentum raising and lowering operators in the space Ψ in terms of the angle operator $\hat{\phi}_\theta$.

$$\hat{J}_+ \equiv \exp(i\hat{\phi}_\theta)\hat{S}_j \;, \tag{6.1a}$$

$$\hat{J}_- \equiv \hat{S}_j \exp(-i\hat{\phi}_\theta) \;, \tag{6.1b}$$

where $\hat{S}_j$ is the amplitude operator

$$\hat{S}_j \equiv \hbar[j(j+1) - \hat{L}_z(\hat{L}_z+1)]^{1/2} \;. \tag{6.2}$$

We note that a different operator will be required for each value of j and that this amplitude operator will be Hermitian only when acting on states with $|m| \leq j$. The z component of angular momentum is as defined earlier:

$$\hat{L}_z = \sum_{m=-l}^{l} \hbar m |j,m\rangle\langle j,m| \;. \tag{6.3}$$

The action of the angular momentum raising and lowering operators on states for which $|m| \leq j$ is as expected:

$$\hat{J}_\pm |j,m\rangle = \hbar\{j(j+1) \pm [-m(m+1)]\}^{-1/2}|j,m\pm 1\rangle \;. \tag{6.4}$$

We note that these operators will also act on states $|m\rangle$ for which $|m|>j$. However, these states are not physically accessible, because the action of $\hat{J}_+$ or $\hat{J}_-$, which will occur in an interaction Hamiltonian, cannot couple states with $|m|\leq j$ to those with $|m|>j$:

$$\hat{J}_{\pm}|j,\pm(-j)\rangle=0 , \tag{6.5a}$$

$$\hat{J}_{\pm}|j,\pm(-j-1)\rangle=0 . \tag{6.5b}$$

Thus the physical region of the state space and the unphysical region are uncoupled, and a system which initially is in a superposition of states of the physical region must always remain in some superposition of these states.

We can use the definitions of $\hat{L}_z$, $\hat{J}_+$, and $\hat{J}_-$ to obtain the angular momentum commutation relations. From the definitions of $\hat{J}_+$ and $\hat{J}_-$ and the commutators we find eventually that

$$[\hat{J}_+,\hat{J}_-]=2\hbar\hat{L}_z , \tag{6.6}$$

$$[\hat{J}_{\pm},\hat{L}_z]=\pm\hbar\{-\hat{J}_{\pm}+(2l+1)\exp[\pm i(2l+1)\theta_0][j(j+1)-l(l+1)^{1/2}|\pm(-l)\rangle\langle\pm l|\} . \tag{6.7}$$

The first term in (6.7) is familiar. The second term will have no effect because l is greater than j, and therefore it gives zero when acting on states within the physical realm, for which $|m|\leq j$. Within the physical subspace we have the conventional commutation relations.

It may seem strange that our angle operator $\hat{\phi}_\theta$ acts on the whole $(2l+1)$-dimensional space, that is, it acts both outside as well as inside the physically accessible subspace. However, the accurate localization of the angle must involve states of extremely high angular momentum. An inability to access those states places fundamental limitations on the accuracy of angle measurements.

VII. ORIENTATION OF ROTATING SYSTEMS

The quantum properties of a rotating system are usually expressed in terms of its angular momentum. However, we can also use the angle states and angle operator to investigate the orientation, or more specifically the azimuthal coordinate, of the system.

A. States of random orientation

The angle-state expansion of the angular momentum eigenstates indicates that they are states of random orientation. This can be verified by calculating the expectation value and variance of the angle operator for these states. Remembering that, after these are calculated as a function of l, our procedure is then to allow l to tend to infinity, we obtain in the limit

$$\langle m|\hat{\phi}_\theta|m\rangle=\theta_0+\pi , \tag{7.1}$$

$$\Delta\phi_\theta^2=\frac{\pi^2}{3} . \tag{7.2}$$

These results are precisely the same as those obtained for the phase of a photon number state[7] and are characteristic of a state of random orientation. Any state that may be represented by a density matrix that is diagonal in the angular momentum basis will also be a state of random orientation.

B. Coherent angular momentum states

An interesting class of states are those states with partially, but not precisely, determined orientation. We note that, as with the optical phase operator, the interpretation of expectation values and variances is made more complicated by the arbitrary nature of the value of θ_0. However, a sensible choice of θ_0 will usually allow us to interpret these expectation values and variances simply. Perhaps the most important of these are the angular momentum spin, or atomic coherent states.[23,24] For a given total quantum number j these states are defined as[25]

$$|\zeta\rangle\equiv\exp(\zeta\hat{J}_+-\zeta^*\hat{J}_-)|-j\rangle$$
$$=(1+|\tau|^2)^{-j}\exp(\tau\hat{J}_+)|-j\rangle , \tag{7.3}$$

where $\tau=(\tan|\zeta|)\exp(i\arg\zeta)$. It is straightforward to obtain an angular momentum state expansion of this state:

$$|\zeta\rangle=\sum_{m=-j}^{j}\frac{\tau^{j+m}}{(1+|\tau|^2)^j}\left[\frac{(2j)!}{(j+m)!(j-m)!}\right]^{1/2}|m\rangle . \tag{7.4}$$

The angular momentum coherent state has a binomial distribution of angular momentum values m. The angle-states probability amplitudes for this state may be obtained by using the expansion of angle states in terms of the angular momentum basis (3.6):

$$\langle\theta_n|\zeta\rangle=(2l+1)^{-1/2}\times\sum_{m=-j}^{j}\exp(im\theta_n)\frac{\tau^{j+m}}{(1+|\tau|^2)^j}\times\left[\frac{(2j)!}{(j+m)!(j-m)!}\right]^{1/2} . \tag{7.5}$$

In general, evaluation of these amplitudes requires numerical summations. However, in cases where j is large (but still, of course very much less than l, which will ultimately tend to infinity) with[26]

$$(2j)^{-1}\ll|\tau|^2\ll 2j , \tag{7.6}$$

the binomial distribution of angular momentum states may be approximated by a normal or Gaussian distribution[27]

$$P(m)\approx\frac{(1+|\tau|^2)}{(4\pi j|\tau|^2)^{1/2}}\exp\left[-\left[j+m-\frac{2j|\tau|^2}{(1+|\tau|^2)}\right]^2\times\frac{(1+|\tau|^2)^2}{4j|\tau|^2}\right] . \tag{7.7}$$

This distribution is normalized so that

$$\lim_{l\to\infty} \int_{-l}^{l} P(m)dm = 1 \ . \tag{7.8}$$

There is no suggestion of a continuous spectrum of m values; the continuum approximation is simply a convenient mathematical maneuver. We can obtain the angle-state probability amplitudes by performing the Fourier transform of $P^{1/2}(m)$. The resulting approximate angle probability distribution is

$$P(\theta)=\frac{2\pi}{2l+1}\left[\frac{8j|\tau|^2}{2\pi(1+|\tau|^2)}\right]^{1/2} \times\exp\left[-\frac{4j|\tau|^2}{(1+|\tau|^2)^2}(\theta-\arg\zeta)^2\right] \ . \tag{7.9}$$

If we choose the reference angle θ_0 so that $P(\theta_0)$ is small, then the expectation value and variance of the angle operator are

$$\langle\zeta|\hat{\phi}_\theta|\zeta\rangle=\arg\zeta \ , \tag{7.10}$$

$$\Delta\phi_\theta^2=\frac{(1+|\tau|^2)^2}{8j|\tau|^2} \ . \tag{7.11}$$

This variance may be very small if j is large. In the region where the Gaussian approximation is good, the expectation value and variance of $\hat{L}_z$ are

$$\langle\zeta|\hat{L}_z|\zeta\rangle=\hbar\left[-j+\frac{2j|\tau|^2}{(1+|\tau|^2)}\right] \ , \tag{7.12}$$

$$\Delta L_z^2=\frac{2\hbar^2 j|\tau|^2}{(1+|\tau|^2)^2} \ . \tag{7.13}$$

We see that, to a good approximation, these states are angle–angular-momentum minimum uncertainty states with an uncertainty product given by

$$\Delta\phi_\theta\Delta L_z=\frac{\hbar}{2} \ . \tag{7.14}$$

VIII. CONCLUSION

It is well known that the premature replacement of a mathematical variable in a calculation by infinity can lead to an indeterminant form. This problem can sometimes be circumvented by performing the calculation first and then taking the limit. This latter approach is essentially that used in this paper and is closely related to our earlier work on the problem of optical phase. Instead of using an infinite-dimensional state space directly, we calcualte physical results, such as expectation values, in a space of $2l+1$ dimensions and *then* find the limit as l tends to infinity. By this method we obtain a well-behaved Hermitian rotation-angle operator, with a countable infinity of proper state vectors as its eigenstates. These eigenstates of the angle operator can be used as an alternative basis for the angular momentum state space. The properties of the angle operator are well determined and physically reasonable. They automatically resolve the problem of periodicity and the inconsistencies associated with the earlier expressions for the angle–angular–momentum commutator. In particular, these earlier expressions cannot be used consistently with the angle states themselves. The infinite state space may be used only with caution and may *not* be used in calculations involving the angle states.

We have shown that the angle operator fits in with the general properties of rotating systems and may be applied to more complicated problems than the simple bead on a wire. It can also be applied to investigate the orientation of a rotating system.

Finally, it is intriguing to note than an approach based on a finite but arbitrarily large state space, the dimensionality of which is only allowed to tend to infinity after the final calculations, can incorporate operators and states which the infinite state space is *too small* to accommodate. In particular, our approach has allowed us to introduce Hermitian operators for both optical phase and rotation angle.

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APPENDIX

In this appendix we highlight the dangers associated with the use of the infinite state space. The angle-state matrix elements of the commutator (5.8) are

$$\langle\Theta|[\hat{\Phi}_\Theta,\hat{L}_z]|\Theta'\rangle=i\hbar[\delta(\Theta-\Theta') -2\pi\delta(\Theta-\Theta_0)\delta(\Theta'-\Theta_0)] \ , \tag{A1}$$

which imply that

$$\langle\Theta|\hat{L}_z|\Theta'\rangle=i\hbar\frac{\delta(\Theta-\Theta')}{\Theta-\Theta'}[1-2\pi\delta(\Theta_0-(\Theta+\Theta')/2)] \ , \tag{A2}$$

where we have used an integral representation of the δ function to factorize the product of δ functions.[28] A δ function divided by its argument is simply minus the derivative of the δ function,[29] so we can write

$$\langle\Theta|\hat{L}_z|\Theta'\rangle=-i\hbar\delta'(\Theta-\Theta') \times[1-2\pi\delta(\Theta_0-(\Theta+\Theta')/2)] \ , \tag{A3}$$

where

$$\delta'(x)\equiv\frac{d\delta(x)}{dx} \ . \tag{A4}$$

We can use these elements together with the angle-state resolution of the identity to obtain the angular momentum matrix elements of $\hat{L}_z$:

$$\langle m|\hat{L}_z|m'=\int_{\Theta_0}^{\Theta_0+2\pi}d\Theta\int_{\Theta_0}^{\Theta_0+2\pi}d\Theta'\langle m|\Theta\rangle\langle\Theta|\hat{L}_z|\Theta'\rangle\langle\Theta'|m'\rangle$$
$$=-\frac{i\hbar}{2\pi}\int_{\Theta_0}^{\Theta_0+2\pi}d\Theta\int_{\Theta_0}^{\Theta_0+2\pi}d\Theta'\exp(-im\Theta)\exp(im'\Theta')\delta'(\Theta-\Theta')[1-2\pi\delta(\Theta_0-(\Theta+\Theta')/2)]\ . \quad \text{(A5)}$$

Introducing a change of variables

$$\Theta_-=\Theta-\Theta'\ , \quad \text{(A6a)}$$

$$\Theta_+=\frac{\Theta+\Theta'}{2}\ , \quad \text{(A6b)}$$

we find that

$$\langle m|\hat{L}_z|m'\rangle=-\frac{i\hbar}{2\pi}\int_{\Theta_0}^{\Theta_0+2\pi}d\Theta_+\int_{-Y}^{Y}d\Theta_-\exp[i\Theta_+(m'-m)]\exp[-i\Theta_-(m+m')/2]\delta'(\Theta_-)[1-2\pi\delta(\Theta_0-\Theta_+)]\ , \quad \text{(A7)}$$

where $Y=2(\Theta_+-\Theta_0)$ for $\Theta_+<\Theta_0+\pi$ and is $2(\Theta_0+2\pi-\Theta_+)$ for $\Theta_+\geq\Theta_0+\pi$. We integrate first with respect to Θ_-, dealing with the derivative of the δ function by integration by parts:

$$\int f(x)\delta'(x)dx=-f'(0)\ , \quad \text{(A8)}$$

provided the range of integration includes $x=0$. Subsequent integration with respect to Θ_+ then yields

$$\langle m|\hat{L}_z|m'\rangle=\hbar m\,\delta_{mm'}-\frac{\hbar(m+m')}{2}\exp[i\Theta_0(m'-m)]\ . \quad \text{(A9)}$$

The presence of the second term makes this clearly inconsistent with our starting point that $|m\rangle$ is an eigenstate of $\hat{L}_z$:

$$\langle m|\hat{L}_z|m'\rangle=\hbar m\,\delta_{mm'}\ .$$

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