Phase operator and phase fluctuations of spins

1980 J. Phys. A: Math. Gen. 13 3479

(http://iopscience.iop.org/0305-4470/13/11/020)

J. Phys. A: Math. Gen. **13** (1980) 3479–3494. Printed in Great Britain

Phase operator and phase fluctuations of spins

I Goldhirsch

Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel

Received 23 January 1980

Abstract. It is shown that a Hermitian phase operator exists for quantum spins. Its spectrum is not continuous but has the values $[2\pi/(2S+1)]n$, $0 \leqslant n \leqslant 2S$ for spin S. The precession of a high-S spin in a magnetic field is shown to consist essentially of a set of jumps from one value of phase to the next one, at equal time intervals. At intermediate times the value of the phase is uncertain. By going to a larger Hilbert space than the spin space, a Hermitian phase operator whose eigenvalue spectrum covers the entire real line is defined, and its relation to the formerly defined operator is clarified. Possible applications to spin and other systems are outlined.

1. Introduction

The concepts of amplitude and phase play important roles in the description of quantum mechanical systems. The theories of superfluidity, superconductivity and coherent optics are examples where the phase is one of the central objects of investigation. On the other hand, phase operators have been shown not to exist in quantum mechanics (Carruthers and Nieto 1968 and references therein, Susskind and Glogower 1964, Zak 1969), or at least not to be defined on the entire physical Hilbert space (Alimov and Damaskinskii 1979, Garrison and Wong 1970). The question arises whether phase is a purely classical concept that has no exact meaning in the quantum world, or whether it does have a quantum counterpart, but the latter does not comply with the assumptions that stand behind the above statement of non-existence.

One of the basic assumptions made in the first three references cited is that the phase operator $\hat{q}$ must be conjugate to the spin operator S^z (or the number operator in the case of bosons) or in other words

$$S^z = -\mathrm{i}(\partial/\partial\hat{q}). \tag{1.1}$$

This assumption contains in it implicitly another assumption, namely that $\hat{q}$ has a continuum of eigenvalues, so that the derivative operator makes sense. This assumption can certainly not hold in the finite Hilbert space on which the spin operators act.

The aim of this paper is to show that by dropping these assumptions one can find an operator whose classical limit is the phase. This is done in § 2. The resulting phase operator has a discrete spectrum with eigenvalues $[(2\pi/(2S+1)]n$, where n is an integer. Section 3 deals with some properties of the phase operator and its eigenvectors. It turns out that the phase operator and S^z are still conjugate in some sense: $\exp\{-\mathrm{i}[2\pi/(2S+1)]S^z\}$ shifts the phase by one quantum and $\exp\{\mathrm{i}(2\pi/(2S+1)]\hat{q}\}$ shifts S^z by one quantum.

0305-4470/80/113479+16$01.50

Section 4 deals with the precession of a single spin in a magnetic field. It is shown that the state of the spin progresses through eigenvalues of $\hat{q}$ at times $[T/(2S+1)]n$, where T is the time of a complete period. After being at the value of phase $q = 2\pi n/(2S+1)$ at time $[T/(2S+1)]n$, high enough spins have a high probability of staying close to this value for additional time $T/2(2S+1)$; then the highest probability is to be in the state $[T/(2S+1)](n+1)$. Pictorially one could describe the precession as a set of jumps from one eigenvalue of the phase operator to the next one, the spin staying at one value of phase for a period of time $\Delta t = T/(2S+1)$. This uncertainty in the phase of the spin is discussed in a quantitative manner in § 5, where—loosely speaking—it is shown that the sum of the uncertainties in the phase and the uncertainty in S^z is bounded from below. The case of minimal uncertainty occurs in the high-S limit when the uncertainty in S^z is $S^{1/2}$ (thus $\Delta(S^z/S) \sim S^{-1/2}$) and the uncertainty in the phase is $2\pi S^{-1/2}$. Lieb (1979) and Simon (1979) have proven that the classical limit of quantum spin systems is essentially given by the $S \to \infty$ limit, provided the spin operators are normalised by S^{-1}. It seems reasonable that a S^{-1} expansion around the classical limit should exist. Indeed, such an expansion has been found in the high temperature limit (Harrigan and Jones 1973). In the second part of § 5 it is shown how a S^{-1} expansion around the classical limit model can be constructed.

Section 6 shows how a phase operator with a continuum of eigenvalues can be defined as a canonical operator. To do so one has to embed the spin Hilbert space in an infinite Hilbert space.

The reason is essentially the fact that a classical description contains more information than a quantum one, so in order to describe a quantum system in a classical language, one has to use redundant states. A famous example of such a description is the coherent state representation of bosons (Glauber 1968). In the enlarged Hilbert space the eigenvalues of $\hat{q}$ can take any real value between $-\infty$ and ∞. It is then shown that S^z can be taken as the conjugate of $\hat{q}$ only in the zeroth approximation is S^{-1}. This shows that the definitions of spin operators in terms of canonical operators in Villain (1974) and Bar'yakhtar and Yablonskii (1976) are correct only in the $S \to \infty$ or the classical limit. Section 7 summarises the results.

2. Derivation of the phase amplitude representation

A classical vector $\boldsymbol{V}$ of length V can be represented in cylindrical coordinates through the components $V^{\pm}$ and V^z where

$$V^{\pm} = \exp(\pm iq)[V^2 - (V^z)^2]^{1/2}. \tag{2.1}$$

q is the 'phase' of $\boldsymbol{V}$ in the x–y plane. The problem addressed in this work is to find a quantum expression for the quantum raising and lowering operators $S^{\pm}$ in the case of spin S such that it resembles equation (2.1) and goes over to it in the classical limit $S \to \infty$. In particular, q is a candidate for a (Hermitian) phase operator. The general form of S^+ we seek is:

$$S^+ = \exp(i\hat{q})R(S^z) \tag{2.2}$$

where $R(S^z)$ is a real function of the operator S^z and $\exp(i\hat{q})$ symbolises a unitary operator whose eigenvalues lie on the unit circle. $\exp(-i\hat{q})$ will denote the Hermitian

conjugate of $\exp(i\hat{q})$:

$$\exp(-i\hat{q})\exp(i\hat{q}) = \exp(i\hat{q})\exp(-i\hat{q}) = 1. \tag{2.3}$$

Representation (2.2) is henceforth referred to as the phase representation of spin operators. So far $\exp(i\hat{q})$, $\exp(-i\hat{q})$ should be treated as symbols since an operator $\hat{q}$ has not been proven to exist yet. Let m be an eigenket of S^z with eigenvalue m, $-S \leq m \leq S$. From equation (2.2):

$$S^+|m\rangle = R(m)\exp(i\hat{q})|m\rangle. \tag{2.4}$$

The number m has been substituted in $R(S^z)$ instead of the operator S^z. On the other hand, as is well known:

$$S^+|m\rangle = [S(S+1) - m(m+1)]^{1/2}|m+1\rangle. \tag{2.5}$$

From equation (2.4) we conclude

$$\exp(i\hat{q})|m\rangle = f(m)|m+1\rangle \tag{2.6}$$

for $-S \leq m < S$, where $f(m)$ satisfies

$$R(m)f(m) = [S(S+1) - m(m+1)]^{1/2}. \tag{2.7}$$

From the conjugate of equation (2.6) it is easy to show that

$$\exp(-i\hat{q})|m\rangle = f^*(m-1)|m-1\rangle \tag{2.8}$$

for $-S < m \leq S$. Hence, using equations (2.6) and (2.8),

$$\exp(-i\hat{q})\exp(i\hat{q})|m\rangle = |f(m)|^2|m\rangle \tag{2.9}$$

for $m \neq S$ and, using equation (2.3):

$$|f(m)|^2 = 1, \qquad m \neq S. \tag{2.10}$$

Putting $f(m) = \exp[i\psi(m)]$, where $\psi(m)$ is a real number, we obtain from equation (2.7)

$$R(m) = [S(S+1) - m(m+1)]^{1/2}\exp[i\psi(m)] \qquad m \neq S. \tag{2.11}$$

The operator $R(S^z)$ is then defined:

$$R(S^z) = [S(S+1) - S^z(S^z+1)]^{1/2}\exp[i\psi(S^z)]. \tag{2.12}$$

Equation (2.12) is the most general form of R compatible with equation (2.2). Hence

$$S^+ = \exp(i\hat{q})[S(S+1) - S^z(S^z+1)]^{1/2}\exp[i\psi(S^z)]$$

$$\exp(i\hat{q})|m\rangle = \exp[i\psi(m)]|m+1\rangle \qquad \text{for } -S \leq m < S. \tag{2.13}$$

One should note that we have not defined $\exp(i\hat{q})|S\rangle$. Its definition is irrelevant for S^+ since the square root in equation (2.12) will always yield zero when acting on $|S\rangle$. On the other hand, a complete definition of the operator $\exp(i\hat{q})$ requires the knowledge of $\exp(i\hat{q})|S\rangle$ as well. This is done below, subject to the restrictions of unitarity (equation (2.3)). The most general form of $\exp(i\hat{q})|S\rangle$ is given by

$$\exp(i\hat{q})|S\rangle = \sum_{m=-S}^{S} a_m|m\rangle. \tag{2.14}$$

From equation (2.13):

$$\langle m|\exp(-i\hat{q}) = \langle m+1|\exp[-i\psi(m)] \qquad \text{for } -S \leq m < S. \tag{2.15}$$

Hence from equations (2.14) and (2.15):

$$\langle m|\exp(-\mathrm{i}\hat{q})\exp(\mathrm{i}\hat{q})|S\rangle = a_{m+1}\exp[-\mathrm{i}\psi(m)]. \tag{2.16}$$

Using the unitarity of $\exp(\mathrm{i}\hat{q})$ (equation (2.3)) we obtain from equation (2.16) that $a_{m+1}\exp[-\mathrm{i}\psi(m+1)]=0$ for $-S\leqslant m<S$, or

$$a_m = 0 \qquad \text{for } -S<m\leqslant S. \tag{2.17}$$

Hence $\exp(\mathrm{i}q)|S\rangle = a_S|-S\rangle$. Using unitarity again it follows that $|a_S|^2=1$. Hence we can write $a_S=\exp[\mathrm{i}\psi(S)]$ with $\psi(S)$ a real phase. This completes the definition of $\exp(\mathrm{i}\hat{q})$. For future reference we summarise:

$$\begin{aligned}&\exp(\mathrm{i}\hat{q})|m\rangle = \exp[\mathrm{i}\psi(m)]|m+1\rangle \qquad \text{for } m\neq S\\ &\exp(\mathrm{i}\hat{q})|S\rangle = \exp[\mathrm{i}\psi(S)]|-S\rangle.\end{aligned} \tag{2.18}$$

The above defined $\exp(\mathrm{i}\hat{q})$ is unitary by construction. We shall now proceed to find its spectrum and eigenvectors.

Let λ be an eigenvalue of $\exp(\mathrm{i}\hat{q})$ and $|\lambda\rangle$ the eigenvector associated with it. The most general form of $|\lambda\rangle$ can be written as

$$|\lambda\rangle = \sum_{m=-S}^{S} b_m|m\rangle. \tag{2.19}$$

Hence, using equation (2.18),

$$\lambda\sum_{m=-S}^{S} b_m|m\rangle = \sum_{m=-S+1}^{S} b_{m-1}\exp[\mathrm{i}\psi(m-1)]|m\rangle + b_S\exp[\mathrm{i}\psi(S)]|-S\rangle$$

or

$$\begin{aligned}&\lambda b_m = \exp[\mathrm{i}\psi(m-1)]b_{m-1} \qquad \text{for } m\neq -S\\ &\lambda b_{-S} = b_S\exp[\mathrm{i}\psi(S)].\end{aligned} \tag{2.20}$$

Hence

$$\lambda^{2S+1}\prod_{m=-S}^{S} b_m = \exp\Big(\mathrm{i}\sum_{m=-S}^{S}\psi(m)\Big)\prod_{m=-S}^{S} b_m. \tag{2.21}$$

None of the b_m's is zero, because if one of them is zero it follows from equation (2.20) that all are. Hence we obtain from equation (2.21)

$$\lambda^{2S+1} = \exp(\mathrm{i}\psi) \tag{2.22}$$

where $\psi = \Sigma_{m=-S}^{S}\psi(m)$. The eigenvalues of $\exp(\mathrm{i}\hat{q})$ are therefore

$$\lambda_n = \exp\{\mathrm{i}[\psi/(2S+1)+2\pi n/(2S+1)]\} \qquad 0\leqslant n\leqslant 2S. \tag{2.23}$$

Equation (2.23) teaches us that the phase of a quantum spin is quantised. In this sense a theory of quantum spin S resembles a $Z(2S+1)$ gauge theory ('t Hooft 1978). When $S\to\infty$ the possible values of phase cover the entire $[0, 2\pi]$ segment. It should be noted that up to a constant phase factor $[\psi/(2S+1)]$ the values of $\psi(m)$ have no influence on the eigenvalue spectrum.

The solution of the recursion relations (equation (2.20)) is

$$\begin{aligned}&b_m^{(n)} = \lambda_n^{-S-m-1}\exp\Big(\mathrm{i}\sum_{m'=-S}^{m-1}\psi(m')+\psi(S)\Big)b_S^{(n)} \qquad m\neq -S\\ &b_{-S}^{(n)} = \lambda_n^{-1}\exp[\mathrm{i}\psi(S)]b_S^{(n)}.\end{aligned} \tag{2.24}$$

The superscript (n) indicates that one deals with the state $|\lambda_n\rangle$. The absolute value of b_S is $(2S+1)^{-1/2}$ for $|\lambda_n\rangle$ to be normalised to unity. Its phase is irrelevant since it merely fixes the overall phase of $|\lambda_n\rangle$. However, for reasons which will become clear in § 3.1 we choose

$$b_S^{(n)} = \lambda_n^{S+1} \exp[-i\psi(S)]. \tag{2.25a}$$

Hence

$$\begin{aligned} b_m^{(n)} &= \lambda_n^{-m} \exp\Big(i \sum_{m'=-S}^{m-1} \psi(m')\Big) \qquad m \neq -S \\ b_{-S}^{(n)} &= \lambda_n^{S}. \end{aligned} \tag{2.25b}$$

If $\Sigma_{-S}^{-S-1} \psi(m')$ is taken to be zero then the first line of equation (2.25b) is valid for $m = -S$ too.

The $(2S+1)$ states $|\lambda_n\rangle$ constitute a complete orthonormal basis of the spin Hilbert space for *any* choice of the values of the $\psi(m)$'s. This enables one to define a phase operator $\hat{q}$, such that the previously defined symbol $\exp(i\hat{q})$ is *really* the exponent of i times the operator $\hat{q}$:

$$\hat{q}|\lambda_n\rangle_\psi \equiv \frac{2\pi n + \psi}{2S+1} |\lambda_n\rangle_\psi. \tag{2.25c}$$

The subscript ψ indicates that $|\lambda_n\rangle_\psi$ depends on the $\psi(m)$'s. Equation (2.25c) completes the definition of the phase operator we set out to find. All operators in equation (2.12) are now well defined.

The case $\psi(m) = 0$, $-S \leqslant m \leqslant S$ is of special importance as is shown in the next section. In this case we attach no subscript to the phase eigenstates:

$$|\lambda_n\rangle = \frac{1}{(2S+1)^{1/2}} \sum_{m=-S}^{S} \exp[-i2\pi nm/(2S+1)]|m\rangle. \tag{2.26}$$

3. Some properties of the phase operator and its eigenstates

3.1. Conjugacy

Although the pair $(\hat{q}, -S^z)$ is not a pair of conjugate operators, it shares an important property of conjugate pairs of canonical operators. As has been shown in § 2, equation (2.18), $\exp(i\hat{q})$ shifts the eigenstates of S^z, except for $|S\rangle$, by one unit. The effect of the operator $\exp[-i2\pi S^z/(2S+1)]$ when acting on an eigenstate of phase $|\lambda_n\rangle$ is

$$\begin{aligned} &\exp[-i2\pi S^z/(2S+1)]|\lambda_n\rangle = |\lambda_{n+1}\rangle \qquad 0 \leqslant n < 2S \\ &\exp[-i2\pi S^z/(2S+1)]|\lambda_{2S}\rangle = |\lambda_0\rangle \end{aligned} \tag{3.1}$$

as can be easily checked using equation (2.26).

3.2. Connection with coherent spin states

The coherent spin states (CSS) or the Wigner states have been used by Wigner (1959) to investigate the classical limit of Clebsch–Gordan coefficients. Let $\hat{n}$ be a unit vector specified by the spherical angle (θ, ϕ). The corresponding CSS $|\hat{n}\rangle$ is given by

$$\boldsymbol{S} \cdot \hat{n}|\hat{n}\rangle = S|\hat{n}\rangle \tag{3.2}$$

i.e. it has the maximal projection in the direction specified by $\hat{n}$. Using a classical language one can call it a spin that points in the $\hat{n}$ direction. Using equation (3.2) it can be shown that

$$\langle \hat{n}|\boldsymbol{S}|\hat{n}\rangle = S\hat{n}. \tag{3.3}$$

Intuitively one would expect an eigenstate $|\lambda_n\rangle$ of the phase operator to be close in some sense to a CSS whose corresponding (θ, ϕ) is $(\pi/2, 2\pi n/(2S+1))$. This is indeed the case. To illustrate this connection the CSS whose (θ, ϕ) is $(\pi/2, 0)$ is expressed in terms of the phase eigenstates. The CSS is (Messiah 1965)

$$\left|\hat{n}\left(\theta=\frac{\pi}{2}, \phi=0\right)\right\rangle = |S^x = S\rangle = \exp\left(-\mathrm{i}\frac{\pi S^y}{2}\right)|m=S\rangle$$

$$= \frac{1}{2S}\sum_{m=-S}^{S}\left(\frac{(2S)!}{(S+m)!(S-m)!}\right)^{1/2}|m\rangle. \tag{3.4}$$

Hence

$$\left|\left\langle \lambda_n\middle|\hat{n}\left(\theta=\frac{\pi}{2}, \phi=0\right)\right\rangle\right|^2$$

$$= \frac{1}{2^{2S}(2S+1)}\left|\sum_{m=-S}^{S}\left(\frac{(2S)!}{(S+m)!(S-m)!}\right)^{1/2}\exp\left(-\mathrm{i}\frac{2\pi n}{2S+1}m\right)\right|^2. \tag{3.5}$$

Figure 1 shows the above matrix elements for different values of the spin S. In all cases the $|\hat{n}(\theta=\pi/2, \phi=0)\rangle$ is strongly concentrated around the $n=0$ phase (note that the $n=2S$ phase is close to the $n=0$ phase). The CSS cannot be phase eigenstates in

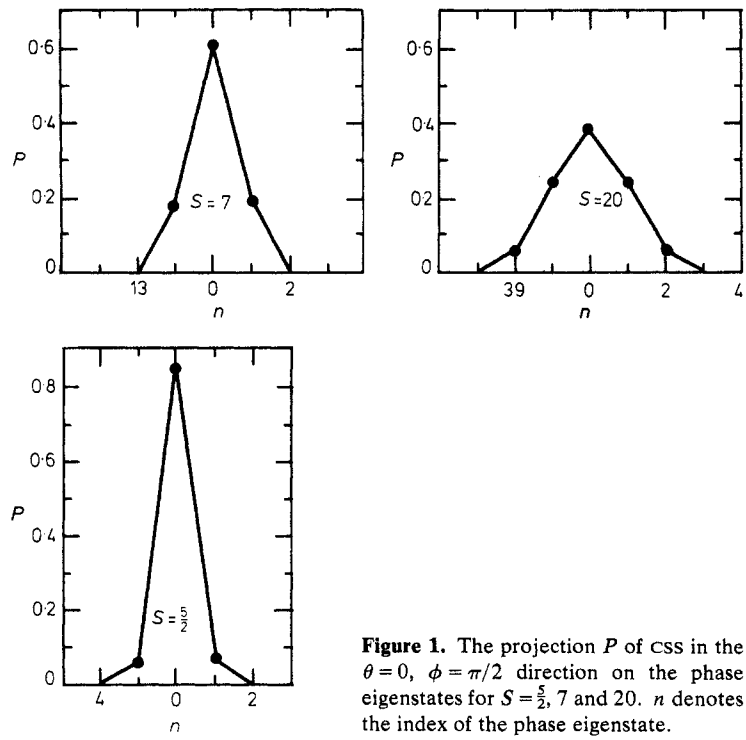

Figure 1. The projection P of CSS in the $\theta=0$, $\phi=\pi/2$ direction on the phase eigenstates for $S=\frac{5}{2}$, 7 and 20. n denotes the index of the phase eigenstate.

general, because the absolute value of each of the expansion coefficients of the latter in terms of the $|S^z = m\rangle$ states are $(2S+1)^{-1/2}$ (see equation (2.24)), whereas equation (3.4) shows that this is not the case for CSS. There is however one exception, namely, the case $S = \frac{1}{2}$. Its CSS in any direction ϕ is given by

$$|\hat{n}(\theta = \pi/2, \phi)\rangle = 2^{-1/2} \exp[-i(\phi/2)]|-\tfrac{1}{2}\rangle + 2^{-1/2} \exp[i(\phi/2)]|\tfrac{1}{2}\rangle. \tag{3.6}$$

The $|\lambda_0\rangle$ and $|\lambda_1\rangle$ states are, from equations (2.23) and (2.24),

$$\begin{aligned} |\lambda_0\rangle &= 2^{-1/2} \exp[i(\psi(\tfrac{1}{2}) + \psi(-\tfrac{1}{2}))/4]|-\tfrac{1}{2}\rangle + 2^{-1/2} \exp[i(3\psi(-\tfrac{1}{2}) - \psi(\tfrac{1}{2}))/4]|\tfrac{1}{2}\rangle \\ |\lambda_1\rangle &= 2^{-1/2} \exp[i(\psi(\tfrac{1}{2}) + \psi(-\tfrac{1}{2}) + 2\pi)/4]|-\tfrac{1}{2}\rangle + 2^{-1/2} \exp[i(3\psi(-\tfrac{1}{2}) - \psi(\tfrac{1}{2}))/4]|\tfrac{1}{2}\rangle. \end{aligned} \tag{3.7}$$

By choosing $\psi(\frac{1}{2}) = -2\phi$, $\psi(-\frac{1}{2}) = 0$, $|\lambda_0\rangle$ equals $|\hat{n}(\theta = \pi/2, \phi)\rangle$. The choice $\psi(-\frac{1}{2}) = 0$, $\psi(\frac{1}{2}) = -2\phi - 2\pi$ makes $|\lambda_{0,1}\rangle$ equal to the corresponding CSS. There is, however, one important difference between the CSS and the phase eigenstates, which holds even in the $S = \frac{1}{2}$ case. The $(2S+1)$ phase eigenstates are eigenstates of the same operator $\hat{q}$, whereas the CSS in any two different directions $\hat{n}$, $\hat{n}'$ are eigenstates of two different operators $\boldsymbol{S} \cdot \hat{n}$, $\boldsymbol{S} \cdot \hat{n}'$. As a consequence the phase eigenstates are a complete orthogonal basis of the spin Hilbert space whereas the CSS are an overcomplete basis. This fact is important in applications.

4. Precession of a single spin in a magnetic field: the phase fluctuations

In this section the precession of a single spin in a magnetic field in the z direction is analysed. The Hamiltonian is

$$H = \omega S^z. \tag{4.1}$$

The change in time of $\exp(i\hat{q})$ is found from

$$i(d/dt) \exp(i\hat{q}) = [\exp(i\hat{q}), \omega S^z] \tag{4.2}$$

which can be rewritten as

$$i(d/dt) \exp(i\hat{q}) = \omega \exp(i\hat{q})[S^z - \exp(-i\hat{q}) S^z \exp(i\hat{q})]. \tag{4.3}$$

Using equation (2.18) with $\psi = 0$:

$$\begin{aligned} &\exp(-i\hat{q}) S^z \exp(i\hat{q})|m\rangle = (m+1)|m\rangle \qquad \text{for } m \neq S \\ &\exp(-i\hat{q}) S^z \exp(i\hat{q})|S\rangle = -S|S\rangle. \end{aligned} \tag{4.4}$$

Hence

$$\begin{aligned} &(S^z - \exp(-i\hat{q}) S^z \exp(i\hat{q}))|m\rangle = -|m\rangle \qquad \text{for } m \neq S \\ &(S^z - \exp(-i\hat{q}) S^z \exp(i\hat{q}))|S\rangle = 2S|S\rangle. \end{aligned} \tag{4.5}$$

Let P_S be a projection operator on $|S\rangle$:

$$P_S|m\rangle = \delta_{m,S}|m\rangle \qquad \text{or } P_S = |S\rangle\langle S|. \tag{4.6}$$

Then, using equation (4.5) we obtain

$$S^z - \exp(-i\hat{q}) S^z \exp(i\hat{q}) = -(1 - P_S) + 2SP_S = -1 + (2S+1)P_S. \tag{4.7}$$

Substitution of equation (4.7) in equation (4.3) yields

$$i\frac{d\exp(i\hat{q})}{dt} = \omega \exp(i\hat{q})[-1+(2S+1)P_S]. \tag{4.8}$$

P_S clearly commutes with S^z:

$$dP_S/dt = 0. \tag{4.9}$$

Hence, the solution of equation (4.8) is

$$\exp[i\hat{q}(t)] = \exp[i\hat{q}(0)]\exp\{-i\omega[-1+(2S+1)P_S)t] \tag{4.10}$$

since P_S is a projection operator, that is

$$P_S^2 = P_S. \tag{4.11}$$

One can rewrite equation (3.10) as

$$\exp[i\hat{q}(t)] = \exp[i\hat{q}(0)]\exp(i\omega t)(1+\{\exp[-i\omega(2S+1)t]-1\}P_S). \tag{4.12}$$

Hence the expectation value of $\exp(i\hat{q})$ in a state that was at $q=0$ at $t=0$, namely $|\lambda_0\rangle$, is

$$\langle\lambda_0|\exp[iq(t)]|\lambda_0\rangle = \exp(i\omega t)(1+\{\exp[-i\omega(2S+1)t]-1\}/(2S+1)). \tag{4.13}$$

A similar result is obtained for any other state. When $S\to\infty$ there is only the classical precession. For finite S there is a 'fast' correction of order S^{-1}. Further understanding of the nature of this precession and its fast component is furnished by the computation of the time development of the state $|\lambda_n\rangle$:

$$|\lambda_n(t)\rangle = \exp(-i\omega S^z t)|\lambda_n(0)\rangle$$

or using the definition of $|\lambda_n\rangle$, equation (2.26):

$$|\lambda_n(t)\rangle = (2S+1)^{-1/2}\sum_{m=-S}^{S}\lambda_n^{-m}\exp(-i\omega mt)|m\rangle. \tag{4.14}$$

For times t that satisfy

$$\omega t = \frac{2\pi}{2S+1}r \tag{4.15}$$

with r any integer

$$|\lambda_n(t)\rangle = \frac{1}{(2S+1)^{1/2}}\sum_{m=-S}^{S}\exp(-i[2\pi(n+r)/(2S+1)]m)|m\rangle = |\lambda_{n+r}\rangle. \tag{4.16}$$

In equation (4.16), $(n+r)$ in $|\lambda_{n+r}\rangle$ should be understood modulo $(2S+1)$. Thus, after an integer number of time intervals of length $T/(2S+1)$, where $T=2\pi/\omega$ is the classical period of precession, the spin is in a phase eigenstate. Another interesting question is what happens at intermediate times. To discover the answer we use equation (4.14) to calculate $|\langle\lambda_{n'}|\lambda_n(t)\rangle|^2$ for those times:

$$|\langle\lambda_{n'}|\lambda_n(t)\rangle|^2 = \frac{1}{(2S+1)^2}\frac{\sin^2\omega t(S+1/2)}{\sin^2\{[\pi/(2S+1)](n'-n)-\omega t/2\}}. \tag{4.17}$$

It can readily be seen that this matrix element is of order S^{-2} unless the denominator becomes of order S^{-2} too. This happens whenever $\omega t \sim 2\pi(n'-n)/(2S+1)$, i.e. when

the value of n' is as one would expect from a classical precession calculation. Figure 2 shows the matrix element of equation (4.17) for $n = 0$ and different values of n. Note the maxima at the quantised time. At intermediate times, the state is a superposition of several $|\lambda_n\rangle$ states. This is explicitly shown in figure 3. Figure 4 is a plot of the average of the phase operator q as time progresses. One can see that (for high enough spin) the system spends most time near the quantised values of the phase, and moves very quickly from the neighbourhood of one phase state to the next one. This process has been described in the Introduction as phase jumps. The phase has well-defined values only at the quantised times, and is uncertain at the intermediate times. This fact may have interesting physical consequences for physical quantities (as in superconductors and Josephson devices) that are coupled to a phase, namely that they might have a natural width that is due to the quantum fluctuations of the phase. Such possibilities are now being investigated.

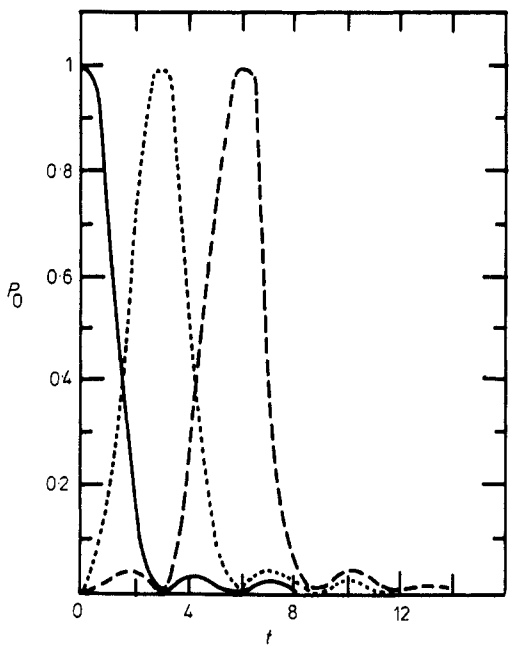

Figure 2. The probability P_0 for a spin in a magnetic field whose state at time $t = 0$ is a phase eigenstate $|\lambda_0\rangle$ to be at state $n = 0, 1, 2$ at later times t. The full curve corresponds to $n = 0$, the dotted curve to $n = 1$ and the dashed curve to $n = 2$. The time scale is in units of $2\pi/(2S+1)$ and $S = 20$.

5. Properties of high-S spins

5.1. Uncertainty relations and minimal uncertainty states in the high-S limit

The phase operator $\hat{q}$ and the operator S^z do not commute. Consequently one can find, as is common in quantum mechanics, a lower bound to the sum or product of their uncertainties. However, since we deal here with a finite Hilbert space, in which the states can be normalised to unity, the lower bound on the product of uncertainties is zero. This is so because in an eigenstate of $\hat{q}$, for example, the uncertainty of $\hat{q}$ is zero. In

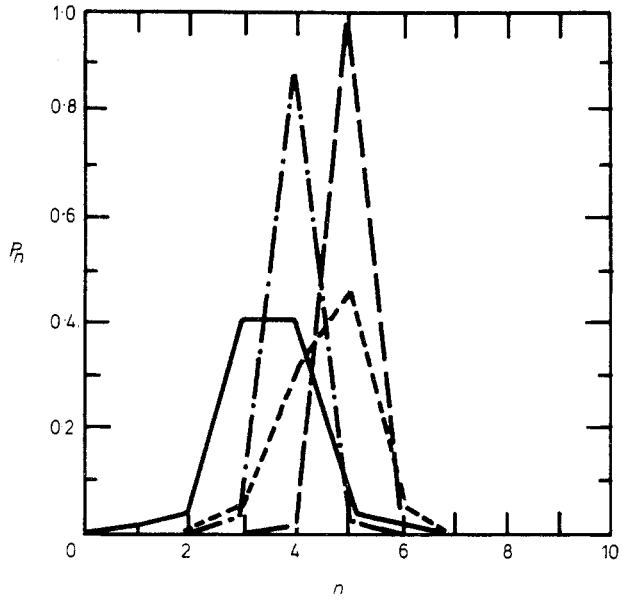

Figure 3. The probability distribution P_n for a spin in a magnetic field whose state at time $t = 0$ is a phase eigenstate. Each graph represents different time: the full curve $\omega t = 1{\cdot}05$, the chain curve $\omega t = 1{\cdot}125$, the small dashed curve 1·13 and the dashed curve $\omega t = 1{\cdot}47$. The lines are drawn only to guide the eye. n is the index of the phase eigenstate and $S = 20$.

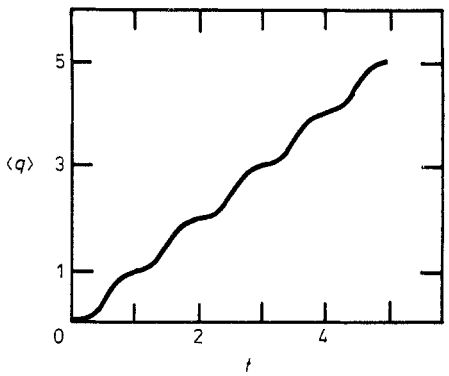

Figure 4. The average phase $\langle q \rangle$ as a function of time in units of $2\pi/(2S+1)$ for $S = 20$. Note that at the 'quantised' values of time the value of the phase changes very slowly.

the same state the uncertainty of S^z is finite (at most of order S), so the product of uncertainties is zero and it teaches us nothing interesting. The sum of uncertainties has, however, a non-trivial lower bound, which we set out to find. First one has to define the uncertainties quantitatively. The uncertainty in S^z, ΔS^z, is defined:

$$(\Delta S^z)^2 = \langle (S^z - \langle S^z \rangle)^2 \rangle = \langle S^z \rangle^2 - \langle S^z \rangle^2 \tag{5.1}$$

where the angular brackets mean, as usual, the expectation value in a normalised state belonging to the (spin) Hilbert space.

In defining the uncertainty of the angle, some care must be taken. This is so because the angle $[(2\pi)(2S)/(2S+1)]$ is close to the angle $[(2\pi)0/(2S+1)]$, whereas their corresponding values of phase are far apart. To overcome this difficulty we define

$$(\Delta q)^2 = \langle(\exp(\mathrm{i}\hat{q}) - \langle\exp(\mathrm{i}\hat{q})\rangle)(\exp(\mathrm{i}\hat{q}) - \langle\exp(\mathrm{i}\hat{q})\rangle)^+. \tag{5.2}$$

This definition is easy to understand if one notes that, loosely speaking, $\Delta\exp(\mathrm{i}q) \sim \exp(\mathrm{i}q)\mathrm{i}\,\Delta q$, hence $\Delta\exp(\mathrm{i}q)\,\Delta\exp(-\mathrm{i}q) \simeq (\Delta q)^2$. Since $(\exp(\mathrm{i}\hat{q}))^+ = \exp(-\mathrm{i}\hat{q})$ and $\langle\exp(\mathrm{i}q)\rangle^* = \langle\exp(-\mathrm{i}q)\rangle$, we can rewrite equation (5.2) as

$$(\Delta q)^2 = 1 - |\langle\exp(\mathrm{i}\hat{q})\rangle|^2. \tag{5.3}$$

Let $|X\rangle$ be a normalised state in the spin Hilbert space:

$$|X\rangle = \sum_{m=-S}^{S} a_m|m\rangle, \qquad \sum_{m=-S}^{S} |a_m|^2 = 1. \tag{5.4a, b}$$

Using definitions (5.1) and (5.3) the respective uncertainties in the state $|X\rangle$ are

$$(\Delta S^z)^2 = \sum_{m=-S}^{S} m^2|a_m|^2 - \Big(\sum_{m=-S}^{S} m|a_m|^2\Big)^2 \tag{5.5a}$$

$$(\Delta q)^2 = 1 - \Big|\sum_{m=-S+1}^{S} a_m^* a_{m-1} + a_{-S}^* a_S\Big|^2. \tag{5.5b}$$

If one replaces all a_m's in equation (5.5a) by their corresponding absolute values $|a_m|$, the uncertainty ΔS^z as well as the normalisation (equation (5.4b)) remain unchanged but Δq becomes smaller (or does not change). Hence without loss of generality one may assume all a_m's to be real non-negative numbers.

The scale of the eigenvalues of $\hat{q}$ is unity whereas the scale of the eigenvalues of $\hat{S}^z$ is S. To work with similar scales and having in mind the classical limit we shall work with the uncertainty of S^z/S, $\Delta(S^z/S)$, which is defined simply as

$$\Delta(S^z/S) = \Delta S^z/S. \tag{5.5c}$$

The object we wish to minimise is $(\Delta(S^z/S))^2 + (\Delta q)^2$. Using equations (5.5) and the normalisation condition (equation (5.4b)) we see that the functional to extremise is

$$F = \sum_{m=-S}^{S} \frac{m^2}{S^2} a_m^2 - \Big(\sum_{m=-S}^{S} \frac{m}{S} a_m^2\Big)^2 + 1 - \Big(\sum_{m=-S+1}^{S} a_m a_{m-1} + a_{-S}a_S\Big)^2 - \lambda \sum_{m=-S}^{S} a_m^2. \tag{5.6}$$

The a_m's are assumed to be real and λ is a Lagrange multiplier which ensures the normalisation constraint. Varying F with respect to the a_m's yields

$$(m^2/S^2 - 2Um/S - \lambda)a_m = v(a_{m+1} + a_{m-1}) \tag{5.7}$$

where

$$U = \sum_{m=-S}^{S} \frac{m}{S} a_m^2 \tag{5.8}$$

$$v = \sum_{m=-S+1}^{S} a_m a_{m-1} + a_{-S}a_S = \sum_{m=-S}^{S} a_m a_{m-1} \tag{5.9}$$

and a_{S+1}, a_{-S-1} are to be understood as a_{-S}, a_S respectively.

Using the reality of the a_m's and the above convention for the a_m's, we can rewrite $(\Delta q)^2$ as follows:

$$(\Delta q)^2 = 1 - \left(\frac{1}{2}\sum_{m=-S}^{S}[a_m^2 + a_{m-1}^2 - (a_m - a_{m-1})^2]\right)^2. \tag{5.10}$$

Then using equation (5.4*b*):

$$(\Delta q)^2 = 1 - \left(1 - \frac{1}{2}\sum_{m=-S}^{S}(a_m - a_{m-1})^2\right)^2. \tag{5.11}$$

Δq is minimal when $\Sigma_{m=-S}^{S}(a_m - a_{m-1})^2$ is minimal; hence in the high-S limit we can treat the a_m's as forming a quasi-continuous function of m. Defining

$$X = m/S, \qquad a_m = a(X)/S^{1/2} \tag{5.12a}$$

one can rewrite equation (5.7) to zeroth order in S^{-1}:

$$(X^2 - 2UX - \lambda - 2v)a(X) = S^{-2}va''(X). \tag{5.12b}$$

In equation (5.12*a*) we have used

$$a_{m+1} + a_{m-1} = 2a_m + (a_{m+1} - a_m) - (a_m - a_{m-1}) \simeq 2a_m + S^{-2}a''(X)/S^{1/2}.$$

Equation (5.12*b*) can be rewritten as

$$\tfrac{1}{2}((X - U)^2 - U^2 - \lambda - 2v)a(X) = \tfrac{1}{2}S^{-2}va''(x). \tag{5.13}$$

Equation (5.13) is essentially the Schrödinger equation of an harmonic oscillator, where $\hbar^2$ has been replaced by S^{-2}, $1/m$ by v and the 'energy' is represented by $U^2 + \lambda + 2v$. The minimal uncertainty in $\Delta S^z/S$ is the minimal uncertainty in the coordinate ΔX, and, as can be easily seen, the minimal uncertainty in the phase Δq corresponds to the minimal uncertainty in the momentum conjugate to X. The state of minimum uncertainty in their sum is the ground state of the harmonic oscillator (Glauber 1968). Its wavefunction does not usually satisfy the condition $a_{S+1} = a_{-S}$ or $a(1) = a(-1)$ but this can be achieved by changes of order $\exp(-S)$ of the a_m's as is seen below. Thus the minimal uncertainty wave packet is (neglecting $O(S^{-2})$)

$$a(X) = \Pi^{-1/4}\exp[-\tfrac{1}{2}(S/v^{1/2})(X - U)^2]. \tag{5.14}$$

v is obviously close to 1 (up to order S^{-1}). Taking a state with $U = \langle S^z\rangle = 0$ as a prototype one obtains

$$a_m \simeq (S^2\Pi)^{-1/4}\exp[-(1/2)m^2/S]. \tag{5.15}$$

In this state, to lowest order

$$\left(\Delta\frac{S^z}{S}\right)^2 \simeq (2S+1)^{-1}, \qquad (\Delta q)^2 \simeq (2S+1)^{-1},$$

$$\left(\Delta\frac{S^z}{S}\right)^2 + (\Delta q)^2 \simeq (S + 1/2)^{-1}. \tag{5.16a, b, c}$$

Equation (5.16) shows again the similarity between the pair $(S^z, \hat{q})$ and the usual canonical variables.

5.2. A remark on the 1/S expansion

A widely used approximation in quantum mechanics is the semiclassical approximation. It is essentially an expansion in powers of $\hbar$. However, it is not a perturbation expansion in the usual sense. One cannot divide a Hamiltonian into its classical and quantum parts, the latter being a perturbation of order $\hbar$. The reason is that in the classical limit all dynamical variables commute and it is impossible to divide a dynamical variable into a commuting and a non-commuting part or classical and quantum parts. Naturally, the same problems appear when one tries to expand the free energy (or any other property) of a quantum spin system around its classical limit. In the high-temperature limit such an expansion has been constructed by Harrigan and Jones (1973). However their method is inapplicable in the low-temperature regime.

The phase representation can offer a different way for performing a $1/S$ expansion. This expansion seems to be well suited for XY-like models (Domb and Green 1974). To demonstrate the basic idea let us choose the XY model of spin S on a d-dimensional lattice

$$H = -\sum_{ij} J_{ij} S_i^+ S_j^- \tag{5.17}$$

where i, j denote lattice sites and J_{ij} is a short-range interaction. The classical limit of H is given by

$$H^{\mathrm{Cl}} = -\sum_{ij} J_{ij} S^2 \cos(q_i - q_j) \tag{5.18}$$

where q_i and q_j are the corresponding phases. Let us write

$$H = -\sum_{i,j} J_{ij} S^2 \cos(\hat{q}_i - \hat{q}_j) + \Big(H + \sum_{i,j} J_{ij} S^2 \cos(\hat{q}_i - \hat{q}_j) \Big). \tag{5.19}$$

The difference between the first part of (5.19) and (5.18) is the fact that in the former the q_i are classical phases with a continuous spectrum in the $(0, 2\pi)$ segment, whereas in the latter $\hat{q}_i$ are quantum operators with a discrete spectrum. We shall denote the first term in (5.19) by $\hat{H}^{\mathrm{Cl}}$ and the second by H'. $\hat{H}^{\mathrm{Cl}}$ and H^{Cl} differ to order (S^{-1}). However, they can be both considered to be classical Hamiltonians in the sense that they do not contain non-commuting objects. As a result objects like $\mathrm{Tr}\exp(-\beta\hat{H}^{\mathrm{Cl}})$, where β is the inverse temperature (in energy units), can be easily calculated as power series in (S^{-1}). The S^{-1} low-temperature series for $\exp(-\beta H)$ will be constructed from

$$\exp(-\beta H) = \exp(-\beta\hat{H}^{\mathrm{Cl}}) - \int_0^\beta \mathrm{d}\beta' \exp[-(\beta - \beta')\hat{H}^{\mathrm{Cl}}] H' \exp(-\beta H). \tag{5.20}$$

To lowest order, H in the exponent in the RHS of (5.20) is substituted by $\hat{H}^{\mathrm{Cl}}$. The actual calculations for the XY and other models will be presented elsewhere. The form of the division into $\hat{H}^{\mathrm{Cl}}$ and $\hat{H} - \hat{H}^{\mathrm{Cl}}$ may differ from (5.19) in practical cases.

6. A continuous phase operator

As explained in the Introduction a definition of a continuous phase operator is possible only if the original, finite size, spin Hilbert space is embedded in an infinite Hilbert space.

Let $\hat{q}$, $\hat{p}$ be a pair of conjugate canonical operators $[\hat{q}, \hat{p}] = i$ ($\hbar$ is taken to be equal to unity). We shall embed the spin space in the Hilbert space corresponding to the canonical operators defined above. The way this is done is similar to the block construction when the spin space is embedded in a Bose space (Goldhirsch 1980, Goldhirsch *et al* 1979).

Let S be an integer or semi-integer. Any real number p can be uniquely written as

$$p = (2S+1)n + m + \Delta \tag{6.1}$$

where n, m are integers, $-S \leqslant m \leqslant S$ and $0 \leqslant \Delta < 1$. Let a state $|p\rangle$ denote an eigenstate of p with eigenvalue p. We shall define S^z through

$$S^z|p\rangle \equiv m|p\rangle. \tag{6.2}$$

Formally one can write

$$S^z|p\rangle = ((2S+1)\{[p+S]/(2S+1)\} - S)|p\rangle \tag{6.3}$$

where $[X]$ means 'the integer part of X' and $\{X\}$ denotes 'the fractional part of X'. Thus S^z can be directly defined as

$$S^z = (2S+1)\{[\hat{p}+S]/(2S+1)\} - S. \tag{6.4}$$

Using (6.1) we can denote any state $|p\rangle$ as $|m, (n, \Delta)\rangle$. In the language of Goldhirsch (1980), (n, Δ) is the index of a 'block' (this time not a discrete index). The way S^+ should be defined is clear:

$$S^+|m, (n, \Delta)\rangle = [S(S+1) - m(m+1)]^{1/2}|m+1, (n, \Delta)\rangle. \tag{6.5}$$

S^- is defined as the conjugate of S^+. According to their definitions S^+, S^- and S^z connect only states inside a given block (n, Δ) and their action there is completely isomorphic to the action of the usual spin operators in the spin Hilbert space, provided we make the correspondence $|m(n, \Delta)\rangle \Leftrightarrow |m\rangle$, $|m\rangle$ being an eigenstate of S^z with eigenvalue m. Since $\exp(i\hat{q})|p\rangle = |p+1\rangle$ we can define formally

$$S^+ \equiv \exp(i\hat{q})[S(S+1) - S^z(S^z+1)]^{1/2}. \tag{6.6}$$

Definition (6.6) is equivalent to (6.5). Hence

$$S^- \equiv [S(S+1) - S^z(S^z+1)]^{1/2} \exp(-i\hat{q}). \tag{6.7}$$

$\hat{q}$ is clearly identified as the phase operator.

Figure 5 shows S^z, or rather its eigenvalue, as a function of p in the case $S = 2$.

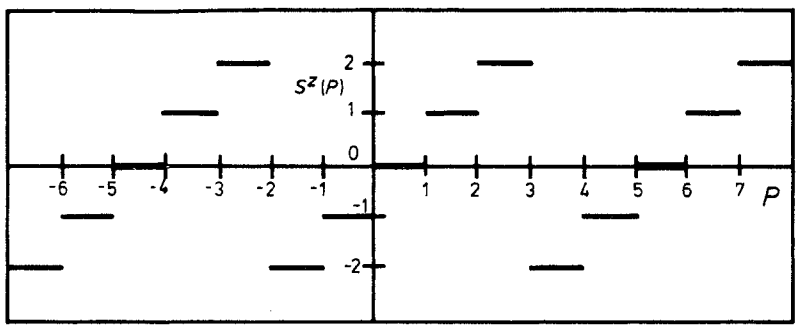

Figure 5. $S^z(p)$ as a function of p (see text) for $S = 2$.

In a given block (n, Δ), n and Δ are unchanged by the spin operators. They can be considered as block invariants (Goldhirsch 1980) and may be of use in writing partition functions of spin systems in the 'phase representation'. The definitions of the corresponding operators are

$$\hat{n} \equiv [(\hat{p}+S)/(2S+1)], \qquad \hat{\Delta} = \{\hat{p}+S\}. \tag{6.8), (6.9}$$

It is interesting to note that although the spin operator in the continuous phase representation satisfies the correct spin commutation relations, as is obvious from equations (6.2)–(6.4), their matrix elements contain δ functions:

$$\langle m'(n', \Delta')|S^z|m(n, \Delta)\rangle = \delta_{mm'}\delta_{n,n'}(\Delta - \Delta') \tag{6.10}$$

or

$$\langle p'|S^z|p\rangle = S^z(p)\delta(p-p') \tag{6.11}$$

where $S^z(p)$ is the corresponding eigenvalue. This fact creates no problem in the use of this representation, since the δ function is usually integrated over (for instance in calculating partition functions) and yields the same result as if one had used the original representation. Another possibility is to use only one n (e.g. $n = 0$) and define

$$|m\rangle \equiv \frac{1}{\epsilon^{1/2}} \int_0^{\epsilon} d\Delta |m, (0, \Delta)\rangle \tag{6.12a}$$

where $0 \leqslant \epsilon < 1$. In this case no δ functions appear. The price is the necessity to define and work with a projection into this subspace.

In the high-S limits $S^z \simeq \hat{p} + O(1)$ for $n = 0$. This is the form used in Villain (1974) and Bar'yakhtar and Yablonskii (1976). As is clear from the above discussion these references are correct only to zeroth order in S^{-1}, and additional corrections will arise in the next order. Moreover, it seems that the use of the discrete phase representation is more adequate for the construction of a S^{-1} expansion, in some cases.

Finally we would like to clarify the connection between the continuous phase representation and the discrete phase representation. Let q be an eigenstate of q with eigenvalue q. Then

$$\langle q'|S^+|q\rangle = \int_{-\infty}^{\infty} dp\, dp' \langle q'|p\rangle\langle p|S^+|p'\rangle\langle p'|q\rangle. \tag{6.12b}$$

Using the definition of S^+, equation (6.6), it follows that

$$\langle p|S^+|p'\rangle = \delta(p-p'-1)f(p) \tag{6.13}$$

where $f(p)$ is a periodic function of p, whose period length is $(2S+1)$. Hence

$$\langle q'|S^+|q\rangle = \exp(iq) \int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp[ip(q'-q)]f(p). \tag{6.14}$$

Using the periodicity of $f(p)$ we can write:

$$f(p) = \sum_{n=-\infty}^{\infty} \exp[i2\pi pn/(2S+1)]C_n \tag{6.15}$$

where C_n are a set of Fourier coefficients. Hence

$$\langle q'|S^+|q\rangle = \exp(iq) \sum_n C_n \delta\left(q - q' + \frac{2\pi n}{2S+1}\right). \tag{6.16}$$

Equation (6.16) means that S^+ does not connect eigenstates of phase unless they differ by an integer number times the phase quantum $2\pi/(2S+1)$. The same clearly holds for S^- and S^z. Consequently any subspace $\{|q\rangle;\ q = q_0 + 2\pi n/(2S+1),\ n = \text{all integers}\}$ of the Hilbert space with arbitrary real q_0 is closed under the spin operators. Thus the 'phase quantisation' holds even when one tries to construct a continuous phase representation. From this point on, one can rederive the results of the previous sections using the continuous phase representation.

7. Summary

This work shows how a Hermitian phase operator for spins can be constructed and presents some of its properties. It turns out that the phase operator is not conjugate to S^z as one might expect, yet its exponent acts as a shifting operator for eigenstates of S^z. The precession of spins in a magnetic field shows phase fluctuations, which might be observable in physical systems in which the phase can be probed. The phase representation can be used for developing S^{-1} expansions for quantum spin systems, a subject that is under current investigation.

Acknowledgment

An illuminating discussion with Professor B Simon of the Departments of Mathematics and Physics of Princeton University is gratefully acknowledged.

References

Alimov A L and Damaskinskii E V 1979 *Teor. Mat. Fiz.* **38** 58
Bar'yakhtar V G and Yablonskii D A 1976 *Theor. Math. Phys.* **24/25** 1109
Carruthers P and Nieto M 1968 *Rev. Mod. Phys.* **40** 411
Phase Transitions and Critical Phenomena 1974 vol III ed C Domb and M S Green (New York: Academic Press)
Garrison I C and Wong J 1970 *J. Math. Phys.* **11** 2243
Glauber R 1968 *Fundamental Problems in Statistical Mechanics II* ed E G D Cohen (Amsterdam: North-Holland)
Goldhirsch I 1980 *J. Phys. A: Math. Gen.* **13** 453
Goldhirsch I, Levich E and Yakhot V 1979 *Phys. Rev.* B **19** 4780
Harrigan M E and Jones G L 1973 *Phys. Rev.* **137** 4897
't Hooft G 1978 *Nucl. Phys.* B **138** 1
Lieb E 1979 *Commun. Math. Phys.* **31** 327
Messiah A 1965 *Quantum Mechanics* (Amsterdam: North-Holland)
Simon B 1979 *Commun. Math. Phys.* submitted for publication
Susskind L and Glogower R 1964 *Physics* **1** 49
Villain J 1974 *J. Physique* **35** 27
Wigner E P 1959 *Group Theory and its Applications to the Quantum Mechanics of Atomic Spectra* (New York: Academic)
Zak J 1969 *Phys. Rev.* **187** 1803