Bohr-Sommerfeld Quantization of Pseudospin Hamiltonians

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(Received 4 June 1980)

It is shown here how to map the problem with pseudospin J into an equivalent one in which $1/J$ plays the role of $\hbar$ and canonical variables exist at the classical level. Bohr-Sommerfeld quantization of the equivalent theory is found to produce a spectrum in very good agreement with the exact results for the Lipkin-Meshkov-Glick model at $J = 15$ and 25. The method readily extends to the SU(n) case.

PACS numbers: 03.65.Ca

Consider the eigenvalues of a Hamiltonian expressed in terms of the generators of SU(n) in the symmetrized N-fold tensor product of the fundamental representation. (Such a problem arises in describing a system of N identical particles, each of which may be in one of n states.) I develop here a Bohr-Sommerfeld quantization procedure in which $1/N$ plays the role of $\hbar$ and is thus complementary to numerical methods which are good for small N. To illustrate the idea, I will work with the Lipkin-Meshkov-Glick (LMG) Hamiltonian[1]

$$H = \epsilon[J_z + (r/2J)(J_x^2 - J_y^2)], \qquad (1)$$

where J_i are SU(2) generators of dimensionality $2J+1$, with $J = N/2$, N being the conserved particle number. Exact solution is possible if J is modest (by explicit matrix diagonalization[1]) or if $r=0$, when it becomes a trivial example of a class of models solvable by group-theoretic methods alone.[2] Here we are concerned with a reliable approximation scheme for J large, $r \neq 0$. Using the Bloch coherent states[3]

$$|\Omega\rangle = \exp[\tfrac{1}{2}\theta(J_- e^{i\Phi} - J_+ e^{-i\Phi})]\,|JJ\rangle, \qquad (2)$$

Lieb[4] showed that in general $Z_q = (2J+1)^{-1} \times \mathrm{Tr}\exp(-\beta H)$, the quantum partition function, can be bracketed by two classical partition functions:

$$\int \frac{d\Omega}{4\pi}\exp[-\beta H_Q(\Omega)] \le Z_q \le \int \frac{d\Omega}{4\pi}\exp[-\beta H_P(\Omega)], \qquad (3)$$

where $H_Q(\Omega) = \langle\Omega|H|\Omega\rangle$ and $H_P(\Omega)$ is defined by

$$H = [(2J+1)/4\pi]\int d\Omega\,|\Omega\rangle H_P(\Omega)\langle\Omega|. \qquad (4)$$

In our case we get, from Ref. 4,

$$H_P = \epsilon(J+1)[\cos\theta + \tfrac{1}{2}r(1+3/2J)\sin^2\theta\cos 2\Phi], \qquad (5a)$$

$$H_Q = \epsilon J[\cos\theta + \tfrac{1}{2}r(1-1/2J)\sin^2\theta\cos 2\Phi]. \qquad (5b)$$

The $\beta\to\infty$ limit of Eq. (3) brackets E_g, the ground-state energy:

$$\min_\Omega\{H_P\} \le E_g \le \min_\Omega\{H_Q\}. \qquad (6)$$

Fend and Gilmore[5] studied this inequality numerically and found that $\min\{H_Q\}$ is a very good approximation to E_g for large J. As $J\to\infty$, $H_P/J = \hat{H}_P$ and $H_Q/J = \hat{H}_Q$ approach a common limit $\hat{H}$ and

$$\lim_{J\to\infty}(E_g/J) = \min_\Omega\{\hat{H}(\Omega)\}. \qquad (7)$$

That the exact quantum ground state can be found by minimizing a classical $\hat{H}$ in the limit $1/J\to 0$ is reminiscent of the way any quantum problem becomes classical as $\hbar\to 0$. It is then natural to ask the following question: *Is there some equivalent quantum theory in which $1/J$ plays the role of $\hbar$?* Finding such a theory would help us move off the $J=\infty$ limit to a region of small but nonzero $1/J$. And if the equivalent theory were described by canonical variables at the classical level, Bohr-Sommerfeld (BS) quantization would give a good estimate for *all* the levels, not just the ground state. Here is how we find that theory.

We first write Z_q as a path integral:

$$Z_q = \frac{1}{2J+1}\mathrm{Tr}\,e^{-\beta H} = \int\frac{d\Omega}{4\pi}\langle\Omega|e^{-\beta H}|\Omega\rangle = \lim_{n\to\infty}(2J+1)^n\int\frac{d\Omega}{4\pi}\frac{d\Omega_1}{4\pi}\cdots\frac{d\Omega_n}{4\pi}\langle\Omega|(1-\epsilon H)|\Omega_n\rangle \times\langle\Omega_n|(1-\epsilon H)|\Omega_{n-1}\rangle\cdots\langle\Omega_1|(1-\epsilon H)|\Omega\rangle, \qquad (8)$$

where $\epsilon = \beta/(n+1)$ and the expansion of the identity I [Eq. (4), with H set equal to I] has been used n times. The multiple integral expresses the Euclidean transition amplitude $\langle\Omega|e^{-\beta H}|\Omega\rangle$ as a sum over discretized paths which leave Ω at Euclidean time $\tau=0$, pass Ω_i at τ_i, and return to Ω at time $\tau=\beta$.

(Recall $\tau = it$, and t is the Minkowski time). *Although these paths are generally nondifferentiable, let us write Z_q in a form that is appropriate to differentiable paths.* The reason will be clear in a moment. To order ϵ, we get

$$\langle \Omega_{i+1} | (1-\epsilon H) | \Omega_i \rangle = \langle \Omega_{i+1} | \Omega_i \rangle - \epsilon \langle \Omega_{i+1} | H | \Omega_i \rangle \quad (9a)$$

$$= 1 - i\epsilon J(1-\cos\theta)\dot{\Phi} - \epsilon H_Q(\Omega_i)$$

$$\cong \exp\{J[-i(1-\cos\theta)\dot{\Phi} - \hat{H}_Q(\Omega)]\epsilon\}, \quad (9b)$$

where $\langle \Omega_{i+1} | \Omega_i \rangle$ is calculated with use of

$$\langle \Omega' | \Omega \rangle = (\cos\tfrac{1}{2}\theta' \cos\tfrac{1}{2}\theta + e^{i(\Phi-\Phi')} \sin\tfrac{1}{2}\theta' \sin\tfrac{1}{2}\theta)^{2J}. \quad (10)$$

Upon dropping the $\dot{\Phi}$ term, because it is a total derivative and will be irrelevant in a classical Lagrangian, we get, in obvious notation,

$$Z_q = \int (d\Omega/4\pi) \int \mathfrak{D}\Omega \exp\{J\int_0^\beta [(i\cos\theta)\dot{\Phi} - \hat{H}_Q]\, d\tau\}. \quad (11)$$

It is clear from the path integral that the original theory has been transformed into one in which $1/J$ plays the role of $\hbar$ and for which the Minkowski-space Lagrangian is

$$L = (\cos\theta)\dot{\Phi} - \hat{H}_Q. \quad (12)$$

Knowing the effective Planck's constant $1/J$, and the action functional for continuous paths, we are ready to do Bohr-Sommerfeld quantization, which should be good when $1/J$ is small. This is why we wanted Z_q for continuous paths, and not because only continuous paths contribute to the integral. (In fact, such paths have zero measure. But they are all important for the classical limit as well as Bohr-Sommerfeld quantization.)

Proceeding along, we see that L has no kinetic term in θ. *In fact, Eq. (12) is just the Legendre transform from $\hat{H}_Q$ to L; Φ and $p \equiv \cos\theta$ are canonical variables obeying Hamilton's equations*

$$\dot{p} = -\partial\hat{H}_Q/\partial\Phi, \quad \dot{\Phi} = \partial\hat{H}_Q/\partial p. \quad (13)$$

The Bloch sphere is thus the *phase space* for this theory. Notice that it is *compact.* In this compact space, the BS condition is

$$\oint p\, d\Phi = 2\pi n/J, \quad n = 0, \pm 1, \pm 2, \ldots, \pm J, \quad (14)$$

where the upper bound on $|n|$ comes from the fact that $|p| \leq 1$. Notice also that in Eq. (11), $\int \mathfrak{D}\Omega = \int \mathfrak{D}p\, \mathfrak{D}\Phi$ is a sum over paths in *phase space.* This is in fact the form of the path integral in general. Only for the case where $H(p,q) = \frac{1}{2}p^2 + V(q)$ can one do the Gaussian functional integration over $\mathfrak{D}p$ explicitly and be left with the familiar Feynman sum over paths in configuration space, i.e., an integral over $\mathfrak{D}q$ with $(i/\hbar)\int dt \times L(q;\dot{q})$ in the exponential.

Here are the results of BS quantization of the LMG Hamiltonian [Eq. (5b)]. On a trajectory labeled by $\hat{H}_Q = \hat{E}_Q$,

$$p = \frac{\bar{r}^{-1} \pm [\bar{r}^{-2} + \cos 2\Phi(\cos 2\Phi - 2\hat{E}_Q/\epsilon\bar{r})]^{1/2}}{\cos 2\Phi}, \quad (15)$$

where

$$\bar{r} = r(1 - 1/2J). \quad (16)$$

Since $\hat{E}_Q \to -\hat{E}_Q$ under $p \to -p$ and $\Phi \to \Phi + \pi/2$, it is clear that the BS levels will have mirror symmetry about $\hat{E}_Q = 0$. Notice also that $\Phi \to \Phi + \pi$ does not change $\hat{E}_Q$.

In the trivial case $r = \bar{r} = 0$, it is easy to see that

$$\hat{E}_Q = n\epsilon/J, \quad n = 0, \pm 1, \pm 2, \ldots, \pm J, \quad (17)$$

which agrees with exact values of E/J. The BS orbits in this case are $2J+1$ equally spaced (in $p = \cos\theta$) latitudes on the Bloch sphere, with $\hat{E}_Q = \pm\epsilon$ being represented by $p = \pm 1$ (the poles). We shall call these *global* orbits because they go around the north pole or, equivalently, because Φ grows monotonically. For $0 < \bar{r} \leq 1$, only the minus sign in Eq. (15) satisfies $|p| \leq 1$. The orbits are again global. But now $p(\Phi)$ oscillates with maxima at $\Phi = \pm\pi/2$ and minima at $\Phi = 0$ and π, except for the $\hat{E}_Q = \pm\epsilon$ orbits which stay at the poles. For $\bar{r} > 1$, these too begin to oscillate. Four extra sets of orbits are formed in the void so created (Fig. 1). Their entry at $\bar{r} = 1$ signifies the phase transition noted by Feng and Gilmore.[5] There are two degenerate families in the upper hemisphere which circulate around the points ($p = 1/r$, $\Phi = 0$ or π) and have $\epsilon < \hat{E}_Q \leq \frac{1}{2}\epsilon(\bar{r} + 1/\bar{r})$ and two other degenerate families in the southern hemisphere which circulate around ($p = -1/\bar{r}$, $\Phi = \pm\pi/2$) with $-\frac{1}{2}\epsilon(r + 1/r) \leq \hat{E}_Q < -\epsilon$. Such *local* orbits are possible in this case because both

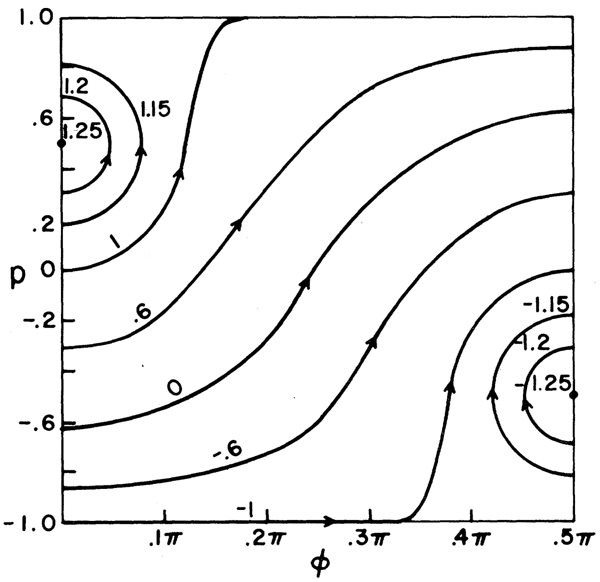

FIG. 1. A few orbits for $\bar{r}=2$, $J=25$ labeled by $\hat{E}=E/J\epsilon$. At $|\hat{E}|=1$, global orbits stop and local orbits begin. Only the region $0\leqslant\Phi\leqslant\pi/2$ is shown. Reflection on the line $\Phi=\pi/2$ gives the curves for $\pi/2\leqslant\Phi\leqslant\pi$, while invariance under $\Phi\to-\Phi$ gives curves for $-\pi\leqslant\Phi\leqslant 0$.

TABLE I. Positive energy eigenvalues (in units of ϵ) of the LMG Hamiltonian for $r=0.6$, 1, and 5 and $J=15$, compared with results of BS quantization.

$r=0.6$		$r=1$		$r=5$	
BS	LMG	BS	LMG	BS	LMG
15	15.1	15	15.3	37.8	38.0
14.2	14.3	14.5	14.8	37.8	38.0
13.3	13.4	13.8	14.1	31.3	31.4
12.4	12.5	13.0	13.3	31.3	31.4
11.4	11.5	12.1	12.4	25.3	25.4
10.5	10.5	11.2	11.4	25.3	25.4
9.5	9.5	10.2	10.4	20.0	20.1
8.5	8.5	9.1	9.3	20.0	20.0
7.5	7.5	8.1	8.3	16.1[a]	16.1
6.4	6.5	6.9	7.1	14.3	15.2
5.4	5.4	5.8	6.0	12.2	12.6
4.3	4.3	4.7	4.8	10.0	10.4
3.2	3.3	3.5	3.6	7.6	7.9
2.2	2.2	2.3	2.4	5.2	5.3
1.1	1.1	1.2	1.2	2.6	2.7
0.0	0.0	0.0	0.0	0.0	0.0

[a]Degenerate partner missing, presumed to be unbound by tunneling.

signs are allowed in Eq. (15). (The distinction between local and global orbits is not absolute and depends on our coordinate system.) Figure 1 shows some of the orbits for the case $J=25$, $\bar{r}=2$. (The Bloch sphere has been opened into a rectangle.)

Table I compares the positive energy eigenvalues from the BS calculation with the exact results from LMG[1] for $E=J\hat{E}_Q$ at $J=15$ and $r=0.6$, 1 and 5. In the first two cases the agreement is uniformly good. Notice that states with small quantum numbers are not any worse predicted. This is because small n does not mean a small global orbit. In the third case there are the following problems in the transition region ($\hat{E}_Q\simeq\epsilon$) between local and global orbits: (i) The level at $E/\epsilon=20.0$ is not exactly degenerate, (ii) a few global orbits below the transition point seem to be raised upwards in the exact answer, and, more seriously, (iii) the degenerate partner of the BS level at $E/\epsilon=16.1$ is missing in the exact answer. All these problems are presumably due to tunneling and mixing of orbits in this energy region.

The calculations were repeated at $J=25$. Not surprisingly, the same general features prevailed, with uniformly smaller errors. (Analysis at $J=25$, $\bar{r}=2$ showed that the BS analysis gives one state *less* unless I accept a BS orbit with $n=18.8$ instead of 19. Some improvisation seems inevitable in the transition region.)

This would be the end of the present discussions were it not for the fact that *there exists another continuum theory that follows from the same Z_q, which differs only in that $\hat{H}_Q\to\hat{H}_P$ in Eq. (11).* To show this, we must, instead of inserting the identity between the factors $(1-\epsilon H)$, write each one as

$$1-\epsilon H =[(2J+1)/4\pi]\int d\Omega_i|\Omega_i\rangle[1-\epsilon H_P(\Omega_i)]\langle\Omega_i| \quad (18)$$

and work to order ϵ. That we have two continuum representations for the same theory is not a contradiction, since continuum formulas like Eq. (11) are merely formal and need to be defined by a discretization procedure. This procedure will differ in the two cases in such a way as to lead back to the same Z_q. On the other hand, with respect to BS quantization, which is not exact, $\hat{H}_P$ and $\hat{H}_Q$ offer two inequivalent possibilities. What would happen if the above analysis were repeated with $\hat{H}_P$? As for the ground state, which will be given by a pointlike BS orbit at the minimum on the Bloch sphere, we have from Lieb, Eq. (6),

$$\hat{E}_g^{\,P}\leqslant E_g/J\leqslant\hat{E}_g^{\,Q}. \quad (19)$$

As for the highest state, we have, either from mirror symmetry in this problem, or in general, from the $\beta\to-\infty$ limit of Eq. (3) (which exists for a system with an upper bound on the energy),

$$\hat{E}_h^{\,Q} \leq E_h/J \leq \hat{E}_h^{\,P}. \tag{20}$$

Mirror symmetry, plus the fact that $2J+1$ is odd implies that there is a level at $E/J=0$ in all three cases. Given the above, I conjecture that every exact level is bracketed by the two BS levels, with $\hat{H}_P$ generating the lower bound for negative energies and $\hat{H}_Q$ generating the lower bound for positive energies. Explicit computation shows that such is the case. I also find that $\hat{H}_Q$ generates values much closer to the exact ones (a feature noted by Feng and Gilmore[5] for the ground state) which is why these values are listed in Table I. (From the derivation, it must be clear that $\hat{H}_P$ and $\hat{H}_Q$ do not exhaust the possible classical Hamiltonians; that they merely bracket the continuum of possibilities.)

Since completing this work, I have learned of several pieces of interesting and related work, which will not be discussed here because of lack of space: that of Jevicki and Papanicolaou[6] on path integrals for spin, that of Levit, Negels, and Paltiel[7] on a BS calculation with use of mean-field variables, that of Kuratsuji and Mizobuchi[8] on the semiclassical treatment of spin path integrals, and the pioneering work of Klauder[9] on coherent-state path integrals. Professor F. Iachello informs me that Gilmore[10] has found the classical Lagrangian that governs the evolution of the coherent states in the time-dependent Hartree-Fock approximation for SU(2) and other groups. His L coincides with mine, as it should. Of special significance is his finding that in all cases $L=\sum_i p_i\dot{q}_i-\hat{H}_Q$, which means that the Block sphere is a classical phase space. However, BS quantization in the cases with more degrees of freedom will be harder.[11] Lastly, there is the work of Kan *et al.*,[12] which reaches many similar conclusions from the time-dependent Hartree-Fock approach and also clarified the revision between the two approaches.

I am grateful to Itzhak Bars for useful conversations, to Chia Tze for telling me about Ref. 8, and to Francesco Iachello, whose seminar stimulated this work, and whose continued enthusiasm was indispensable. This work was supported in part by the U. S. Department of Energy under Contract No. EY-76-C-02-3075.

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