Bohr-Sommerfeld Quantization of Spin Hamiltonians

Anupam Garg
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208

Michael Stone
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801

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Abstract

The Bohr-Sommerfeld rule for a spin system is obtained, including the first quantum corrections. The rule applies to both integer and half-integer spin, and respects Kramers degeneracy for time-reversal invariant systems. It is tested for various models, in particular the Lipkin-Meshkov-Glick model, and found to agree very well with exact results.

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*e-mail address: agarg@northwestern.edu
The question in this Letter was investigated twentysome years ago by R. Shankar, in a paper in this journal with a nearly identical title \cite{1}. Many physical systems involve large-magnitude spin or pseudospin degrees of freedom. Examples include spinning molecules \cite{2, 3}, superdeformed rotating nuclei \cite{4}, magnetic molecular solids \cite{5}, and the Lipkin-Meshkov-Glick (LMG) model of certain collective excitations in nuclei \cite{6}. In all these cases, because the spin magnitude, \(j\), is large, a semiclassical approach is natural. In some cases, such an approach is effective even for \(j\) as small as \(1/2\), e.g., in studies of magnetic order \cite{7, 8, 9}.

It may therefore surprise some readers that so far we have lacked even the Bohr-Sommerfeld (BS) quantization rule for a single spin. All previous authors cited have used heuristic or ad hoc BS rules that vary in their treatment of the first quantum corrections \cite{10}. In this paper, we use the semiclassical propagator for spin, which has only recently been fully understood \cite{11}, to find the BS rule systematically. We shall first state the rule, then apply it to a few model problems, and finally prove it.

The general problem is as follows. We are given a quantum Hamiltonian

\[
\mathcal{H} = \mathcal{H}(J^\text{op}_x, J^\text{op}_y, J^\text{op}_z),
\]

where \(J^\text{op}_i (i = x, y, z)\) are components of the dimensionless spin operator, \(\mathbf{J}^\text{op}\), with the commutator \([J^\text{op}_i, J^\text{op}_j] = i\epsilon_{ijk}J^\text{op}_k\), and \(\mathcal{H}\) is a polynomial in \(J^\text{op}\) \cite{12}. Since \(\mathbf{J} \cdot \mathbf{J}\) is conserved, we can regard the motion as taking place on a sphere of radius \(j = |\mathbf{J}|\). All orbits on this sphere are closed and nonintersecting, so it may regarded as the phase space of the system. With polar coordinates \(\theta\) and \(\phi\), and the usual identification of \(J_z\) and \(\phi\) as canonically conjugate momentum and coordinate, we can expect the BS rule to quantize the action integral

\[
\oint \cos \theta d\phi = (2n + 1)\pi.
\]

The first step is to understand the classical limit. We expect \(\mathcal{H}\) to correspond to some classical Hamiltonian \(H_c(\mathbf{J})\) of a c-number angular momentum \(\mathbf{J}\), with dynamics defined by the Poisson brackets \(\{J_i, J_j\} = \epsilon_{ijk}J_k\). Since \(\mathbf{J} \cdot \mathbf{J}\) is conserved, we can regard the motion as taking place on a sphere of radius \(j = |\mathbf{J}|\). All orbits on this sphere are closed and nonintersecting, so it may regarded as the phase space of the system. With polar coordinates \(\theta\) and \(\phi\), and the usual identification of \(J_z\) and \(\phi\) as canonically conjugate momentum and coordinate, we can expect the BS rule to quantize the action integral \(\oint \cos \theta d\phi\). Robbins et al. \cite{3} set this integral to \((2n+1)\pi/(j+\frac{1}{2})\), Harter and Patterson \cite{2} set it to \(2n\pi/[j(j+1)]^{1/2}\), and Shankar \cite{1} equates \(jA^{\text{sc}}_c\) [see paragraph below Eq. (27)] to \(2n\pi\). Neither rule is formulated in a context that extends to half-integer \(j\). The rule we find is

\[
(j + \frac{1}{2})A^+_c(E) + \frac{1}{2j} \int_0^{T(E)} \mathbf{J} \cdot \nabla_j H_c dt = (2n + 1)\pi.
\]
Here, $n$ is an integer ranging from 0 to $2j$, and
\[ A_c^+(E) = \oint_{H_c=E} (1 - \cos \theta) d\phi \pmod{4\pi} \] (3)
is the area enclosed by an orbit of energy $E$. For future use, let us denote the two terms in Eq. (2) by $I_1$ and $I_2$, and also define
\[ \tilde{j} = j + \frac{1}{2}. \] (4)
The term $I_2$ is also evaluated along the orbit $H_c = E$, which is taken to have a period $T(E)$. This term, and the extra $\frac{1}{2}$ in the $j + \frac{1}{2}$ factor in $I_1$ represent the first quantum corrections.

To make Eq. (2) precise, we must also state the rule for associating $H_c$ with $H$. We do this by writing
\[ H(J^{\text{op}}) = \sum_{\ell=0}^{2j} \sum_{m=-j}^{j} c_{\ell m} Y_{\ell m}(J^{\text{op}}), \] (5)
where $Y_{\ell m}$ are the spherical harmonic tensor operators, and the coefficients $c_{\ell m}$ are uniquely determined since $\text{Tr}(Y_{\ell m}^* Y_{\ell' m'}) \propto \delta_{\ell \ell'} \delta_{m m'}$. Then,
\[ H_c(J) = \sum_{\ell m} c_{\ell m} Y_{\ell m}(J) \] (6)
with the same $c_{\ell m}$’s, and the $Y_{\ell m}$’s are solid harmonics. Along with the $Y_{\ell m}$’s, they may be defined by the generating function
\[ \left[ (a \cdot J)^\ell \right] = \sqrt{\frac{4\pi}{2\ell + 1}} \sum_{m=-\ell}^{\ell} a_{\ell m} \lambda^m \left[ Y_{\ell m}(J) \right], \] (7)
where, $a_{\ell m} = \ell!/[((\ell + m)!(\ell - m)!)]^{1/2}$, and
\[ a = \hat{z} - \frac{\lambda}{2}(\hat{x} + i\hat{y}) + \frac{1}{2\lambda}(\hat{x} - i\hat{y}) \] (8)
is a complex vector with $a \cdot a = 0$. Note that given $H$, $H_c$ is completely determined. To get $H_c$ from $H$, we also need to give the value of $j$. Hence, the $H \leftrightarrow H_c$ correspondence is one-to-one. Note also that the trinomial expansion of $(a \cdot J^{\text{op}})^\ell$ is analogous to the expansion of $(aq + bp)^n$ that gives Weyl ordering.

Let us now apply Eq. (2) to a few models. Our first example is $H = \omega J_x^{\text{op}}$, and $H_c = \omega J_z$. The orbits are given by $\cos \theta = E/\omega j = \text{const}$, and $\dot{\phi} = \omega$. Hence, $I_1 = 2j\pi(1 - E/j\omega)$, and $I_2 = \pi E/j\omega$, so the quantization condition is $E_n = \omega(j - n)\pi$, with $n = 0, 1, 2, \ldots, 2j$. In this simple case, the rule is exact.
Our next example is somewhat less trivial, $\mathcal{H} = \nu (J_z^{\text{op}})^2$, $H_c = \nu J_z^2$. Again $\cos \theta = \text{const}$, $E = \nu j^2 \cos^2 \theta$, and $\dot{\phi} = 2\nu j \cos \theta$. The rule again yields $j \cos \theta = (j - n)$, i.e., $E_n = \nu (j - n)^2$. This is also exact, but more importantly, it is in accord with Kramers’ theorem. It is not hard to see that this is true for any time-reversal invariant $\mathcal{H}$, for which $H_c(-J) = H_c(J)$.

As our third example, we consider the LMG model, just as done by Shankar. The Hamiltonian now is

$$\mathcal{H} = J_z^{\text{op}} + \frac{r}{2j} [(J_x^{\text{op}})^2 - (J_y^{\text{op}})^2],$$

and $H_c$ is obtained by simply deleting the ‘op’ suffixes. On the orbit with energy $E$,

$$\cos \theta = \frac{1 + [1 + r \cos 2\phi (r \cos 2\phi - 2E/j)]^{1/2}}{r \cos 2\phi}.$$  

(10)

Now, $H_c \to -H_c$ under a 180° rotation about $\hat{x} \pm \hat{y}$, i.e., $\theta \to \pi - \theta$, $\phi \to \phi + \pi/2$. This symmetry forces states to occur in pairs, $E$ and $-E$, plus a nondegenerate state at $E = 0$ for integer $j$. For orbits related by this symmetry, we have $I_1 \to 4\pi j - I_1$, and $I_2 \to -I_2$, so the BS spectrum is also symmetric about $E = 0$. For the orbit at $E = 0$, $I_1 = (2j + 1)\pi$, and $I_2 = 0$, so $E = 0$ is an allowed energy for integer $j$ only. From now on, we consider only $E \geq 0$.

The energy landscape for this model looks like this. If $r \leq 1$, $H_c$ has a maximum at $\theta = 0$ ($H_c = j$) and a minimum at $\theta = \pi$. If $r > 1$, these points turn into saddle points, and $H_c$ develops two degenerate maxima [with $H_c = \frac{j}{2}[(r + r^{-1})]$] along the $\phi = 0$ and $\phi = \pi$ meridians. Orbits at slightly lower energies circle these maxima, and are separated by a separatrix at $E = j$ passing through the north pole. (See Fig. 1 in Ref. 1.) Hence for $r > 1$, we expect to have pairs of levels split by tunneling for $E$ above or around $j$, and single levels below. In this paper, due to limited space, we will not incorporate tunneling effects into our BS calculations. In principle this may be done by allowing the orbits to become complex \[3\]. We have discussed how to find ground pair splittings from the propagator elsewhere \[15\]. For the orbits with $E > j$, both signs in Eq. (10) are valid, but for $E < j$ (and any $r$) only the minus sign is meaningful.

The evaluation of the two action terms in Eq. (2) requires simple one-dimensional numerical integration. The resulting BS spectrum is compared with the exact one (from numerical diagonalization of $\mathcal{H}$) in Table II. The values of $j$ and $r$ are the same as those used by Shankar, and it is evident that our BS analysis improves on his. Indeed, it is rather good almost uniformly, but a few aspects call for comment. For $r < 1$, the highest energy exceeds
TABLE I: Positive part of energy spectrum of the LMG model from the BS rule (2) and numerical diagonalization for $j = 15$.

|       | $r = 0.6$ |       | $r = 1.0$ |       | $r = 5.0$ |
|-------|-----------|-------|-----------|-------|-----------|
| BS    | exact     | BS    | exact     | BS    | exact     |
| 15.10 | 15.09     | 15.33 | 15.31     | 37.98 | 38.05     |
| 14.26 | 14.26     | 14.77 | 14.80     | 37.98 | 38.05     |
| 13.38 | 13.38     | 14.12 | 14.09     | 31.37 | 31.44     |
| 12.46 | 12.46     | 13.28 | 13.27     | 31.37 | 31.44     |
| 11.52 | 11.51     | 12.38 | 12.37     | 25.35 | 25.42     |
| 10.54 | 10.54     | 11.41 | 11.41     | 25.35 | 25.42     |
| 9.55  | 9.54      | 10.40 | 10.39     | 20.02 | 20.14     |
| 8.53  | 8.53      | 9.34  | 9.33      | 20.02 | 20.05     |
| 7.50  | 7.50      | 8.24  | 8.24      | 15.66 | 16.13     |
| 6.45  | 6.45      | 7.12  | 7.11      | 15.01 | 15.24     |
| 5.39  | 5.39      | 5.97  | 5.96      | 12.82 | 12.63     |
| 4.33  | 4.33      | 4.80  | 4.79      | 10.46 | 10.47     |
| 3.25  | 3.25      | 3.61  | 3.61      | 7.96  | 7.93      |
| 2.17  | 2.17      | 2.41  | 2.41      | 5.36  | 5.35      |
| 1.09  | 1.09      | 1.21  | 1.21      | 2.69  | 2.69      |
| 0.00  | 0.00      | 0.00  | 0.00      | 0.00  | 0.00      |

*By extrapolation

*By mapping to $q$, $p$ variables

$j$, and can be found by extrapolating the BS action. This amounts to allowing for complex orbits. For $r = 1$, the energy is not quadratic in deviations about the maximum at $\theta = 0$. In terms of the stationary phase approximation on which Eq. (2) is premised (see below), this corresponds to an exceptional case where we must include fluctuations higher than second order (Gaussian) about the stationary phase point. The two highest energies in Table I were obtained via the mapping $J_x^{\text{op}} \approx q$, $J_y^{\text{op}} \approx jp$, with $[q, p] = i$, and textbook BS quantization for a particle in one dimension. The same limitation on Eq. (2) is present for $r > 1$ close
to the tunneling barrier, i.e., \( E \simeq j \). Now, one may have a pair of tunnel split levels such that one level is below the barrier and the other above. Literal use of Eq. (2) then yields two degenerate levels just below the barrier, with large errors. We have chosen to find the unbound partner by extrapolating the action for \( E < j \). A proper semiclassical approach would require including complex orbits, and non-Gaussian fluctuations. These aspects are not unique to spin, and also occur with one-dimensional double well potentials.

In the rest of the paper, we show how we derive the BS rule (2). Let \( |\hat{n}\rangle \) be a spin coherent state with maximal spin projection along the direction \( \hat{n} \) with polar coordinates \( (\theta, \phi) \), i.e., \( J^{op} \cdot \hat{n} |\hat{n}\rangle = j |\hat{n}\rangle \). In terms of stereographic coordinates

\[
z = \tan \frac{1}{2} \theta e^{i\phi}, \quad \bar{z} = \tan \frac{1}{2} \theta e^{-i\phi},
\]

the state may also be written as \( |z\rangle = \exp(z J^{op} - \bar{z}) |\hat{z}\rangle \). Note that \( |z\rangle \) is not normalized, and \( \langle z | z \rangle = (1 + \bar{z} z) \). We shall write \( |\hat{n}\rangle, |z\rangle \), or \( |\theta, \phi\rangle \) interchangeably as needed. Secondly, we shall need to discuss points on the complex unit sphere, for which \( \theta \) and \( \phi \) are not real, or equivalently, \( \bar{z} \) and \( z \) are not true complex conjugates. Such points are specified by the pair \( (\bar{z}, z) \).

Our starting point is the semiclassical approximation [11] to the propagator \( K = \langle z_i | e^{-iHT} | z_f \rangle \):

\[
K_{sc}(\bar{z}_f, z_i; T) = \sqrt{\frac{N}{2j}} \left( \frac{\partial^2 S}{\partial \bar{z}_f \partial z_i} \right)^{1/2} \exp \left( S + \frac{i}{2} \int_0^T A dt \right). \tag{12}
\]

with,

\[
S = j \ln N + \int_0^T \left[ j \frac{\bar{z} \dot{z} - \bar{z} \dot{\bar{z}}}{1 + \bar{z} z} - iH_{sc}(\bar{z}, z) \right] dt, \tag{13}
\]

\[
A = \frac{\partial}{\partial \bar{z}} \left( \frac{1 + \bar{z} z}{4j} \frac{\partial H_{sc}}{\partial z} + z \leftrightarrow \bar{z} \right), \tag{14}
\]

\[
N = (1 + \bar{z}_f z(T))(1 + \bar{z}(0) z_i). \tag{15}
\]

Here, \( S \) is the action along the least action trajectory from the point \( (\bar{z}(0), z_i) \) to \( (\bar{z}_f, z(T)) \); as noted in Ref. [11], to find such a trajectory, i.e., a solution of the Euler-Lagrange equations,

\[
\dot{z} = \frac{i}{2j}(1 + \bar{z} z)^2 \frac{\partial H_{sc}}{\partial z}, \quad \dot{\bar{z}} = -\frac{i}{2j}(1 + \bar{z} z)^2 \frac{\partial H_{sc}}{\partial \bar{z}}, \tag{16}
\]

we must allow \( \bar{z}(0) \neq \bar{z}_i \) and \( z_f \neq z(T) \). The integral in \( S \) must be evaluated along this trajectory. So must \( \int A dt \), the Solari-Kochetov correction, which is \( O(1/j) \) relative to \( S \), and
key to getting a propagator that is self-consistently replicating under composition. Further,

$$H_{sc}(\bar{z}, z) = \langle z|\mathcal{H}|z\rangle,$$  \hspace{1cm} (17)

which we shall call the semiclassical Hamiltonian. Finally, we must sum the the right hand side in Eq. (12) over all solutions of the equations of motion if there is more than one.

Our goal is to find the Green function, and then the energy spectrum by looking for its poles. In step 1, we evaluate the Laplace transform

$$F_{sc}(\bar{z}_f, z_i; E) = \int_0^T K_{sc}(\bar{z}_f, z_i; T)e^{iET}dT$$  \hspace{1cm} (18)

by the stationary phase method. This naturally leads to the action at fixed energy $W(E) = S(T) + iET$, where $E$ and $T$ are related by

$$T(E) = -i\frac{\partial W(E)}{\partial E}, \quad E(T) = i\frac{\partial S(T)}{\partial T}.$$  \hspace{1cm} (19)

Then, using known methods [16], we can show that

$$F_{sc} = e^{i\gamma} \sqrt{\frac{N}{2j}} \left(\frac{2\pi}{z_i\bar{z}_f}\right)^{1/2} \exp \left(W + i\frac{1}{2} \int Adt\right)\bigg|_{T=T(E)}.$$  \hspace{1cm} (20)

Here we have included a Maslov-like phase $e^{i\gamma}$, which arises because the mapping from $T$ to $E$ is many to one. This is best seen by considering the case $z_f = z_i$, which we shall shortly encounter when we take the trace. Now, for the same energy $E$, there is more than one trajectory corresponding to multiple traverses of the same fundamental orbit. So, $T$ is an integer multiple of the basic period $T_0$, the different branches of $W$ differ by additive integer multiples of $iET_0$, and the phase $e^{i\gamma}$ is $(-1)^n$ for $n$ traverses.

In step 2, we again use stationary phase to perform the trace that gives the semiclassical Green function:

$$G_{sc}(E) = \frac{2j + 1}{\pi} \int \frac{dzd\bar{z}}{(1 + \bar{z}z)^{2j+2}} F_{sc}(\bar{z}, z; E).$$  \hspace{1cm} (21)

The stationary phase condition yields $z(T) = z$, and $\bar{z}(0) = \bar{z}$, so now we are only considering closed classical orbits with energy $E$, with momenta that match smoothly at the end points. Next, we must integrate over small fluctuations $\eta$ and $\bar{\eta}$ in $z$ and $\bar{z}$. For the fundamental orbit at energy $E$, we can write

$$G_{sc} = -\frac{j}{\pi} \int \frac{d\eta d\bar{\eta}}{(1 + \bar{z}z)} \frac{1}{|\bar{z}|} \exp(Z_{sc}) \exp(-\frac{1}{2}Q)$$  \hspace{1cm} (22)
using known classical mechanical identities. Here,
\begin{equation}
Z_{sc} = \int_0^T \left[ \frac{j \dot{\bar{z}} \hat{z} \bar{z} - (1 + \bar{z}) \partial^2 \bar{z}}{1 + \bar{z}} + i \frac{(1 + \bar{z})^2}{4j} \partial \hat{z} \partial \bar{z} \right] dt,
\end{equation}
\begin{equation}
Q = \frac{2j + 1}{(1 + \bar{z})^2} \left( 2\bar{\eta} \eta - \frac{\dot{\bar{z}}}{\bar{z}} \eta^2 - \frac{\dot{\bar{z}}}{\bar{z}} \eta^2 \right).
\end{equation}

The quadratic form $Q$ has a zero eigenvalue, corresponding to a fluctuation $(\bar{\eta}, \eta)$ that moves us along the orbit. If we parametrize this direction by the time $t$, and the orthogonal direction by a variable $r$, then,
\begin{equation}
\begin{pmatrix} \eta \\ \bar{\eta} \end{pmatrix} = \begin{pmatrix} \dot{\bar{z}} \\ \frac{\dot{\bar{z}}}{\bar{z}} \end{pmatrix} t + \begin{pmatrix} \dot{\bar{z}} \\ \frac{\dot{\bar{z}}}{\bar{z}} \end{pmatrix} r,
\end{equation}
and $Q = 4r^2 |\dot{\bar{z}}|^2$. The integration over all points along the orbit turns into an integral over $t$ from 0 to $T$, and with the jacobian $\partial(\eta, \bar{\eta})/\partial(t, r) = -2|\dot{\bar{z}}|^2$, the $r$ integral may also be done. The result is that for one traverse of the orbit we get $-iT \exp(Z_{sc})$. For $n$ traverses, we multiply by $(-1)^n$ and let $Z_{sc} \to nZ_{sc}$. Summing over all $n$, we get
\begin{equation}
G_{sc}(E) = iT(E) \frac{1}{1 + \exp(-Z_{sc}(E))}.
\end{equation}

This has poles (each with unit residue) whenever
\begin{equation}
Z_{sc}(E) = (2n + 1)i\pi.
\end{equation}

Equation (27) is our quantization condition. The first term in Eq. (23) is $-i\bar{j}$ times the area $A_{sc}$. Unlike $A_{c}$, $A_{sc}$ is computed on the orbit $H_{sc} = E$, not $H_{c} = E$, since it is $H_{sc}$ that appears in Eq. (16). In the second term, we note that
\begin{equation}
(1 + \bar{z})^2 \partial^2 \frac{H_{sc}}{\partial \bar{z} \partial z} = \nabla^2_{\Omega} H_{sc},
\end{equation}
where $\nabla^2_{\Omega}$ is the angular part of the Laplacian.

A true BS rule must be in terms of the classical Hamiltonian, $H_c$, not $H_{sc}$. To cast Eq. (27) into the form (2), we must relate $H_c$ and $H_{sc}$. Using Eq. (7), we can show that
\begin{equation}
\langle \hat{n}|Y_{\ell m}(J^\ominus)|\hat{n}\rangle = \left[ 1 - \frac{\ell(\ell - 1)}{4j} + O(j^{-2}) \right] Y_{\ell m}(J),
\end{equation}
with $J = j\hat{n}$. Since, $\nabla^2_{\Omega} Y_{\ell m}(J) = -\ell(\ell + 1) Y_{\ell m}(J)$, and $J \cdot \nabla_{\ell} Y_{\ell m}(J) = \ell Y_{\ell m}(J)$, it follows that $H_{sc} = H_c + H_1$, where
\begin{equation}
H_1 = \frac{1}{4j} \nabla^2_{\Omega} H_c + \frac{1}{2j} J \cdot \nabla_{\ell} H_c.
\end{equation}
We have written $H_c$ instead of $H_{sc}$ on the right since the corrections are of $O(j^{-2})$.

The difference between $\mathcal{A}_{sc}^+$ and $\mathcal{A}_c^+$ is now easy to find. Let us denote the solutions of Eq. (10) ($\tilde{z}_{sc}, \tilde{z}_{sc}$) and those with $H_c$ instead of $H_{sc}$ by ($\tilde{z}_c, \tilde{z}_c$). If we regard $\tilde{z}_{sc}$ and $\tilde{z}_c$ as functions of $E$ and $z$, then

\begin{equation}
H_c(\tilde{z}_{sc}(E, z), z) = E - H_1, \quad (31)
\end{equation}
\begin{equation}
H_c(\tilde{z}_c(E, z), z) = E. \quad (32)
\end{equation}

Writing $\tilde{z}_{sc} = \tilde{z}_c + \tilde{z}_1$, $\tilde{z}_{sc} = \tilde{z}_c + z_1$, and using the equations of motion, we find

\begin{equation}
\tilde{z}_1 = i \frac{(1 + \tilde{z}z)^2 H_1}{2j \ddot{z}}, \quad z_1 = -i \frac{(1 + \tilde{z}z)^2 H_1}{2j \ddot{z}}. \quad (33)
\end{equation}

In this way we find

\begin{equation}
\tilde{\mathcal{J}} \mathcal{A}_{sc}^+ = \tilde{\mathcal{J}} \mathcal{A}_c^+ + \int_0^T H_1 dt. \quad (34)
\end{equation}

Substituting this in Eq. (23), and making use of Eqs. (28) and (30), we see that Eqs. (27) and (2) are equivalent.

We mention in closing that we can also use coherent states to find a BS rule for one dimensional potential problems. The result is akin to Eq. (27). To show its equivalence to the textbook rule, we use Weyl ordering and the Wigner-Moyal formalism to relate $\mathcal{H}$, $H_c$, and $H_{sc}$. In the spin case, the problems of ordering, and of relating $H_c$ to $H_{sc}$, are neatly solved by the generating formula (17).

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[12] The degree of this polynomial can be no greater than \(2j\), but in physical situations it is usually much smaller.

[13] Since every closed curve divides the sphere into two parts, we fix the orientation (indicated by the suffix +) on the sphere such that \(A_+\) is the area inside the orbit traversed in the counterclockwise sense.

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