Bogomolny's semiclassical transfer operator for rotationally invariant integrable systems

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Abstract. The transfer operator due to Bogomolny provides a convenient method for obtaining a semiclassical approximation to the energy eigenvalues of a quantum system, no matter what the nature of the analogous classical system. In this paper, the method is applied to integrable systems which are rotationally invariant, in two and three dimensions. In two dimensions, the transfer operator is expanded in a Fourier series in the angle variable, while in three dimensions it is expanded in spherical harmonics. In both cases, when the Fourier coefficients are evaluated using the stationary phase approximation, we arrive at the Einstein–Brillouin–Keller quantization conditions. The associated Maslov indices are shown to agree with the results calculated by well known simple rules. The theory is applied to several rotationally invariant systems, including the hydrogen atom and the isotropic harmonic oscillator in two and three dimensions, the circle billiard, a billiard inside a spherical cavity, and a harmonic potential with a singular magnetic flux line.

1. Introduction

In furthering our understanding of the relationship between classical mechanics and quantum mechanics, semiclassical approximations play an important role. Periodic orbit theory, developed by Gutzwiller, Balian and Bloch, Berry and others [1–3] employs the periodic orbits of the classical system to obtain a semiclassical approximation to the density of states or to individual energy eigenvalues of the analogous quantum system. Although formally elegant and satisfying, the theory is usually hard to apply in practice, because the periodic orbit sum is not absolutely convergent, and because it is difficult to find the periodic orbits in a systematic way. Alternative semiclassical approximations, which do not depend on knowing the periodic orbits, have been proposed by Bogomolny [4, 5] and by Doron and Smilansky [6, 7]. Exploiting the duality between the classical dynamics of a billiard inside a bounded region and the scattering of external particles by the system's boundary, Doron and Smilansky obtained semiclassical energy eigenvalues for the billiard system by constructing a semiclassical approximation to the scattering matrix for the exterior problem. In the theory proposed by Bogomolny, one chooses a Poincaré surface of section (PSS) which is frequently crossed during the motion of the system, and one constructs a semiclassical transfer operator from the classical trajectories which take the system from one position on the PSS to another. For billiard systems, the approaches based on the scattering matrix and on the transfer operator can be shown to yield the same determinantal equation for the energy eigenvalues of the interior system [4, 8].

This paper had its origin in trying to derive the correct quantum energy eigenvalues of the hydrogen atom (in three dimensions) by means of Bogomolny's semiclassical transfer

operator. By adding a small $1/r^2$ term to the Coulomb potential—a device which prevents the transfer operator from being singular—we achieved this goal. However, an essential part of the derivation was the use of the stationary phase approximation. Subsequently, we generalized our approach and showed that it led to the well known Einstein–Brillouin–Keller (EBK) quantization rules [9–12]. When viewed in this light, there is nothing special about our solution for the hydrogen atom. In fact, the main result of our paper can be summed up concisely: for rotationally invariant integrable systems, Bogomolny's transfer operator, plus the stationary phase approximation, yields EBK quantization. In a separate publication [13] we plan to show how the EBK quantization rules can also be obtained from Bogomolny's transfer operator formulated in terms of the angle-action variables.

The plan of the paper is as follows. After a brief description of the transfer operator in the next section, in section 3 we construct the transfer operator for a two-dimensional system having circular symmetry. By making a suitable Fourier expansion and evaluating the Fourier coefficients by means of the stationary phase approximation, we derive the EBK quantization conditions. This general formulation is applied in section 4 to the hydrogen atom (plus $1/r^2$ potential), the circular harmonic oscillator (plus $1/r^2$ potential), a harmonic potential plus a singular magnetic flux line, the circle billiard, and the annulus billiard. In section 5 a similar approach is described for three-dimensional systems having spherical symmetry. The resulting EBK quantization conditions are applied in section 6 to the hydrogen atom (plus $1/r^2$ potential), the isotropic harmonic oscillator (plus $1/r^2$ potential), and a billiard inside a spherical cavity. The paper concludes with a discussion of our results for the EBK energy eigenvalues in comparison with the exact quantum energies.

2. The transfer operator and the determinantal equation

We begin with a brief description of Bogomolny's semiclassical transfer operator. For a system with f freedoms, the PSS in configuration space is a surface or hypersurface of dimension $f - 1$, and the transfer operator in the coordinate representation is [4]

$$T(q'', q'; E) = \sum_{cl.tr.} \frac{1}{(2\pi i\hbar)^{(f-1)/2}} \left| \det \frac{\partial^2 S(q'', q'; E)}{\partial q'' \partial q'} \right|^{1/2} \exp[iS(q'', q'; E)/\hbar - i\mu\pi/2]$$

(2.1)

where q' and q'' denote $f - 1$ generalized coordinates for two points located on the PSS. The summation is over all classical trajectories which go from q' to q'', crossing the PSS at these points in the same sense and at no other points (in the same sense) in going from q' to q''. For each such trajectory one needs the action at energy E, denoted by $S(q'', q'; E)$, and the phase index μ, which is related to the occurrence of caustics—points on the trajectory at which the semiclassical approximation is not valid. The matrix of second derivatives of the action has dimension $f - 1$.

If $T(E)$ is the transfer operator and I is the unit operator, the corresponding semiclassical energy eigenvalues of the quantum system are determined from the condition [4]

$$\det[I - T(E)] = 0. \tag{2.2}$$

When properly formulated, the T-operator is unitary [4]. In the past few years there have been several applications of the transfer operator based on constructing an approximation to $T(E)$ in coordinate space [14–24]. However, when the system being treated has rotational symmetry, it is better to treat the transfer operator in the angular momentum representation, since it is then diagonal [17, 20]. In the next section we show how this may be carried out for two-dimensional systems with circular symmetry.

3. Two-dimensional systems with circular symmetry

Let us consider a particle of unit mass moving in two dimensions in a potential $V(r)$. The Hamiltonian is

$$H = \frac{p_r^2}{2} + \frac{p_\phi^2}{2r^2} + V(r) \tag{3.1}$$

where $p_r = \dot{r}$ and $p_\phi = r^2\dot{\phi}$ are the momenta conjugate to the polar coordinates r and ϕ describing the particle's position. Since the angular momentum p_ϕ is a constant of the motion, let us denote it as L. For given E and L, the turning points of the classical motion along the radial direction are determined by

$$\frac{L^2}{2r^2} + V(r) = E. \tag{3.2}$$

Clearly, the turning point radii, r_- and r_+, depend on L as well as E.

In setting up the transfer operator, we choose the PSS to be a circle of radius R. While in principle any radius between r_- and r_+ could be used, there is a natural choice for given energy E. At that energy there is a trajectory with maximal angular momentum $L_{\max}(E)$ which is a circle, corresponding to the radial kinetic energy being zero. We define R to be the radius of this circle. It can also be thought of as the circle for which the radial turning points coincide. Then, trajectories at energy E having $|L| < |L_{\max}(E)|$ have nonzero radial kinetic energy, and, therefore, must repeatedly cross this circle, making it a suitable choice for the PSS. (It is easy to show from equation (3.2) and the derivative of this equation that R is the solution of $2V(r) + rV'(r) = 2E$.)

The coordinate q on the PSS will be taken to be the polar coordinate ϕ. From equation (2.1) the transfer operator from ϕ to ϕ' (where $0 \leqslant \phi \leqslant 2\pi$ and $0 \leqslant \phi' \leqslant 2\pi$) on the PSS is

$$T(\phi', \phi; E) = \sum_j \frac{1}{(2\pi i\hbar)^{1/2}} \left| \frac{\partial^2 S_j(\phi', \phi; E)}{\partial\phi'\partial\phi} \right|^{1/2} \exp[iS_j(\phi', \phi; E)/\hbar - i\mu_j\pi/2] \tag{3.3}$$

where j labels different possible classical trajectories at energy E which go from ϕ to ϕ' without crossing the PSS (in the same sense) at any other point. Let us define the angle γ to be $\gamma = \phi' - \phi$ (modulo 2π) in order that $0 \leqslant \gamma \leqslant 2\pi$. The trajectories can be labelled in such a way that the angle traversed by the particle in going from ϕ to ϕ' is $\xi^{(j)} = \gamma + 2\pi j$, where $0 \leqslant \gamma \leqslant 2\pi$ and j is an integer (positive, negative or zero). The action along the jth trajectory can be written as $S(\xi^{(j)}; E)$. Also, we can write

$$\frac{\partial^2 S(\xi^{(j)}; E)}{\partial\phi\partial\phi'} = -\frac{\partial^2 S(\xi^{(j)}; E)}{\partial\gamma^2}. \tag{3.4}$$

Thus, in accord with the invariance of the Hamiltonian under rotations about the origin, the transfer operator can be expressed in terms of the relative angle γ only. We can, therefore, expand (3.3) in a Fourier series:

$$T(\phi', \phi; E) = T(\gamma; E) = \sum_{m=-\infty}^{\infty} C_m(E) \exp(im\gamma) \tag{3.5}$$

where the expansion coefficients are

$$C_m(E) = \frac{1}{2\pi} \int_0^{2\pi} T(\gamma; E) \exp(-im\gamma) \, d\gamma. \tag{3.6}$$

We now construct a matrix representation of the transfer operator using the basis $\{(2\pi)^{-1/2}\exp(im\phi)\}$. Since $\gamma = \phi' - \phi$ (modulo 2π), a typical matrix element is

$$T_{m_1 m_2}(E) = \frac{1}{2\pi}\int_0^{2\pi}d\phi\int_0^{2\pi}d\phi'\,\exp(-im_1\phi')T(\gamma;E)\exp(im_2\phi) = 2\pi C_{m_1}(E)\delta_{m_1 m_2}.$$

(3.7)

Thus, the T-matrix is diagonal in this representation, and its eigenvalues (as a function of E) are just the diagonal elements. (Note that these T-matrix eigenvalues should not be confused with the semiclassical energy eigenvalues.) Denoting the mth eigenvalue curve as $\lambda_m(E)$, we obtain from equations (3.3)–(3.7),

$$\lambda_m(E) = \int_0^{2\pi}T(\gamma;E)\exp(-im\gamma)\,d\gamma = \frac{1}{(2\pi i\hbar)^{1/2}}\sum_j\exp(-i\mu_j\pi/2)$$

$$\times\int_0^{2\pi}d\gamma\left|\frac{\partial^2 S(\xi^{(j)};E)}{\partial\gamma^2}\right|^{1/2}\exp[iS(\xi^{(j)};E)/\hbar - im\gamma].$$

(3.8)

We remind the reader that $\xi^{(j)}$ depends on γ through the definition $\xi^{(j)} = \gamma + 2\pi j$.

Up to this point we have made no approximations other than the approximation involved in deriving Bogomolny's semiclassical transfer operator. We now evaluate the integrals in (3.8) using the stationary phase approximation. For the jth integral the point at which the phase is stationary is determined by the equation

$$\frac{\partial S(\xi^{(j)};E)}{\partial\gamma} = m\hbar.$$

(3.9)

The left-hand side of this relation is the classical angular momentum L for the jth trajectory. Thus, the stationary phase condition effectively quantizes the angular momentum of the particle. Because the possible trajectories from ϕ to ϕ' at energy E are uniquely specified by the angular momentum, it is clear that for each value of m (positive, negative or zero) there is *at most one trajectory* satisfying (3.9). (A solution exists if and only if $|L| \leqslant |L_{\max}(E)|$.) The value of j for this trajectory will be denoted j_m. Thus, for given m, we denote the solution of equation (3.9) (when it exists) as γ_m, and the corresponding angle traversed by the particle in going from ϕ to ϕ' as $\xi_m = \gamma_m + 2\pi j_m$.

When a solution γ_m of equation (3.9) exists for a particular value of j_m, we can evaluate the integral in the usual way, assuming that $\partial^2 S/\partial\gamma^2$ is a relatively slowly varying function of γ. Introducing the symbol ν_m through the definition

$$\begin{aligned}\nu_m &= 0 \qquad \text{if } \left(\frac{\partial^2 S}{\partial\gamma^2}\right)_{\gamma=\gamma_m} > 0\\[2mm]\nu_m &= 1 \qquad \text{if } \left(\frac{\partial^2 S}{\partial\gamma^2}\right)_{\gamma=\gamma_m} < 0\end{aligned}$$

(3.10)

and henceforth denoting μ_j for the trajectory j_m as μ_m, we obtain

$$\lambda_m(E) \approx \exp[iS(\xi_m;E)/\hbar - im\gamma_m - i(\mu_m + \nu_m)\pi/2].$$

(3.11)

The fact that these approximate eigenvalues of the T-matrix have unit modulus is consistent with the T-matrix being unitary [4]. Note that the symbols μ_m and ν_m have the same meaning as in the paper by Creagh *et al* [25].

It is useful to further simplify this expression by splitting the action for the trajectory j_m into radial and angular parts. The angular part, evaluated at γ_m, may be denoted by

$$S_{\text{ang}}(\xi_m;E) = \int p_\phi\,d\phi = m\hbar(\gamma_m + 2\pi j_m)$$

(3.12)

and the radial part, evaluated at the angular momentum $L = m\hbar$ determined by the stationary phase condition, is

$$S_{\text{rad}}(L = m\hbar; E) = \oint |p_r||\mathrm{d}r| = 2 \int_{r_-}^{r_+} |p_r|\mathrm{d}r. \tag{3.13}$$

Using the fact that $\exp(\mathrm{i}m2\pi j_m) = 1$, we arrive at the expression

$$\lambda_m(E) \approx \exp[\mathrm{i}S_{\text{rad}}(L = m\hbar; E)/\hbar - \mathrm{i}(\mu_m + \nu_m)\pi/2]. \tag{3.14}$$

The semiclassical energy eigenvalues of the quantum system are found from the determinantal equation (2.2), which is satisfied whenever an eigenvalue of the T-matrix is equal to unity. Thus, the condition for an energy eigenvalue is that $\lambda_m(E) = \exp(\mathrm{i}2\pi n_r)$. From equation (3.14) this yields

$$S_{\text{rad}}(L = m\hbar; E) = 2\pi\hbar(n_r + \sigma_m/4) \qquad n_r = 0, 1, 2, \ldots \tag{3.15}$$

where we define the Maslov index $\sigma_m = \mu_m + \nu_m$. This is associated with a complete cycle of the radial motion for a trajectory at energy E and angular momentum $L = m\hbar$. The allowed values of n_r in (3.15) are determined by the assumption that $S_{\text{rad}} \geqslant 0$.

In appendix A it is shown that, for smooth potentials, the combination $\sigma_m = \mu_m + \nu_m$ is always equal to 2. This is the result one would obtain for the Maslov index in EBK quantization [11, 12] using the simple rule of counting 1 for each of the soft turnarounds during a complete cycle of the radial motion. It is also shown in appendix A that if the particle is confined inside a circular disk with a hard wall (Dirichlet boundary condition on the wavefunction), the result for σ_m is 3. This agrees with the simple rule for computing the EBK Maslov index by counting 1 for the soft turnaround at the inner radial turning point and 2 for the collision with the disk boundary. Thus, for systems having circular symmetry in two dimensions, Bogomolny's transfer operator (modified using the stationary phase approximation) leads to EBK quantization, with the Maslov index for the radial motion computed by the well known simple rules. Note that σ_m is a canonical invariant, even though the transfer operator is not canonically invariant (since it depends on the choice of the PSS). In addition to (3.15), the other EBK quantization condition, $L = m\hbar$, was, of course, obtained from the stationary phase condition (3.9). It is worth noting that for systems that are invariant under time reversal, the energy eigenvalues with $m \neq 0$ are doubly degenerate.

4. Application to systems in two dimensions

4.1. The Coulomb plus $1/r^2$ potential

Let us now apply this general formulation to the hydrogen atom in two dimensions. In fact we shall treat a slightly more complicated potential, namely the Coulomb potential plus a term proportional to $1/r^2$. For the pure Coulomb potential, there is a one-parameter family of ellipses which start out from a given point on the PSS and return to the same point. Thus, this point is a focal point. By adding the $1/r^2$ term, we ensure that the trajectories are not ellipses, and thereby avoid difficulties associated with the initial point being a conjugate point.

Assuming that the nucleus is stationary at the origin, we take the potential to be

$$V(r) = -\frac{1}{r} \pm \frac{\alpha^2}{2r^2}. \tag{4.1}$$

For convenience we have taken the electronic charge e to be unity, and we have written the strength of the $1/r^2$ potential as $\alpha^2/2$, where α has the dimensions of angular momentum.

The $1/r^2$ potential may be repulsive or attractive, and provided α^2 is not too large in the repulsive case, the electron will always be bound to the nucleus, implying that the energy E is negative. From equation (3.2), the classical turning points of the radial motion occur at radii r_- and r_+ given by

$$r_\pm = \frac{1 \pm \beta}{2|E|} \tag{4.2}$$

$$\beta = [1 - 2|E|(L^2 \pm \alpha^2)]^{1/2}. \tag{4.3}$$

The radius of the Poincaré circle defined in the previous section is $R = 1/(2|E|)$ (although we shall not make explicit use of this in what follows). For the repulsive $1/r^2$ potential, each trajectory traverses an angle less than 2π before returning to the PSS, while in the attractive case, the trajectories go through angles greater than 2π. This means that the possible trajectories are qualitatively different in the two cases, there being only two possibilities in the former case and many in the latter case. Note from (4.3) that, for given E, the maximum possible value of the classical angular momentum is given by

$$[L_{\max}(E)]^2 = \frac{1}{2|E|} \mp \alpha^2. \tag{4.4}$$

To obtain the semiclassical energy eigenvalues from equation (3.15), we must calculate the radial action integral with $L = m\hbar$, as in (3.13). Using equation (3.1) with $L = m\hbar$ to solve for $|p_r|$ as a function of r, we obtain

$$S_{\text{rad}}(L = m\hbar; E) = 2 \int_{r_-}^{r_+} |p_r| \, dr = \pi \left(\frac{2}{|E|}\right)^{1/2} - 2\pi (m^2\hbar^2 \pm \alpha^2)^{1/2}. \tag{4.5}$$

Here the first term on the right-hand side is the action of each member of the family of elliptical orbits at energy E of the pure Coulomb potential. To write down the EBK quantization condition from equation (3.15), we set $\sigma_m = 2$, corresponding to two soft turnarounds at the radial turning points (see appendix A). Hence,

$$\frac{\pi}{\hbar} \left(\frac{2}{|E|}\right)^{1/2} - 2\pi (m^2 \pm \alpha^2/\hbar^2)^{1/2} = (2n_r + 1)\pi \qquad n_r = 0, 1, 2, \dots. \tag{4.6}$$

Using the fact that E is negative for the bound state solutions we are considering, we obtain

$$E_{mn_r} = -\frac{1}{2\hbar^2[n_r + \frac{1}{2} + (m^2 \pm \alpha^2/\hbar^2)^{1/2}]^2} \tag{4.7}$$

$$m = 0, \pm 1, \pm 2, \dots \qquad n_r = 0, 1, 2, \dots.$$

This expression gives the approximate semiclassical energy eigenvalues for the Coulomb plus $1/r^2$ potential. Note that the energy is the same for positive and negative values of m, implying that the energy eigenvalues are doubly degenerate for $m \neq 0$ and nondegenerate for $m = 0$. The allowed values of m are constrained by the condition $|m|\hbar \leqslant |L_{\max}(E)|$, with $|L_{\max}(E)|$ given by equation (4.4).

The pure Coulomb potential is obtained by letting $\alpha \to 0$ in equation (4.7). Until now we have assumed that α is nonzero and sufficiently large (presumably, $\alpha \gg \hbar$) that the trajectories are not close to being ellipses, thereby avoiding the point ϕ' on the PSS being a focal point. At this stage, however, it is permissible to relax this requirement and let α become zero. Putting $n = |m| + n_r$, we obtain

$$E_n = -\frac{1}{2\hbar^2(n + \frac{1}{2})^2} \qquad n = 0, 1, 2, \dots. \tag{4.8}$$

(It is satisfying that the limit does not depend on the sign of the $\alpha^2/(2r^2)$ term in the potential, despite the fact that the two problems are quite different, as mentioned earlier.) This expression for the energy eigenvalues is exactly the same as the result found by solving the two-dimensional Schrödinger equation for the Coulomb potential. The eigenvalues do not depend explicitly on m, but it is clear from the definition of n that $|m| \leqslant n$. This condition, which also arises, for example, in solving the radial Schrödinger equation by the method of series expansion, or by using group-theoretical considerations, correctly determines the degeneracies of the energy levels given by (4.8).

In an earlier study of the hydrogen atom in two dimensions using Bogomolny's transfer operator [23], the PSS was chosen to be a radial line. The 'half-mapping' transfer operators introduced by Haggerty [19] were used to avoid the problem associated with the family of trajectories (ellipses) at energy E starting from a point on the PSS and returning to the same point on the PSS. The outcome of this work was similar to equation (4.8) but with $(n + \frac{1}{2})^2$ replaced by $(n + \frac{3}{4})^2$. We now realize that this peculiar result was due to an incorrect assignment of the phase indices associated with the elliptical trajectories. In figure 2 of [23], there is a caustic associated with the longer solid trajectory, but there is *no* caustic associated with the shorter solid trajectory. When this fact is properly taken into account, the energy levels turn out to be the same as equation (4.8). Thus, the energy levels of this system do not depend on the choice of the PSS, at least for the two choices considered.

4.2. The circular harmonic oscillator plus $1/r^2$ potential

A particle moving in two dimensions in a circular harmonic oscillator plus $1/r^2$ potential has been treated in an earlier paper [24] using a slightly different method based on Bogomolny's transfer operator. Here we show that our general formulation of section 3 leads quickly to the same results for the energy eigenvalues of this system.

We take the potential to be

$$V(r) = \tfrac{1}{2}\omega^2 r^2 \pm \frac{\alpha^2}{2r^2} \tag{4.9}$$

where, as in the last section, $\alpha^2/2$ is the strength of the $1/r^2$ potential, which may be attractive or repulsive. When the particle has energy E, equation (3.2) leads to the following expression for the classical turning-point radii:

$$r_\pm^2 = \frac{E \pm [E^2 - \omega^2(L^2 \pm \alpha^2)]^{1/2}}{\omega^2}. \tag{4.10}$$

Using this, and solving equation (3.1) to find $|p_r|$ as a function of r, one finds,

$$S_{\mathrm{rad}}(L; E) = 2 \int_{r_-}^{r_+} |p_r|\,\mathrm{d}r = \frac{\pi E}{\omega} - \pi(L^2 \pm \alpha^2)^{1/2}. \tag{4.11}$$

When this is substituted in equation (3.15), with L set equal to $m\hbar$ and σ_m set equal to 2 (corresponding to soft turnarounds at r_- and r_+), we obtain for the energy eigenvalues belonging to a given value of m

$$\begin{aligned} E_{mn_r} &= \hbar\omega[2n_r + (m^2 \pm \alpha^2/\hbar^2)^{1/2} + 1] \\ m &= 0, \pm 1, \pm 2, \ldots \qquad n_r = 0, 1, 2 \ldots. \end{aligned} \tag{4.12}$$

This expression agrees with the result obtained from an exact solution of the Schrödinger equation (see, for example, Flügge [26]). A plausible explanation of this agreement, despite the approximations inherent in our semiclassical approach, has been put forward earlier [24] and will be briefly discussed in the final section of the paper. Note that the energy eigenvalues are doubly degenerate when $m \neq 0$ and nondegenerate when $m = 0$.

4.3. Circular harmonic oscillator plus singular magnetic flux line

The development in the last section can be extended to include a singular magnetic flux line passing through the origin. This means that, in addition to the circular harmonic oscillator potential and the $1/r^2$ potential, the particle motion occurs in the presence of a magnetic field (perpendicular to the plane of the motion) having the form of a δ-function singularity at the origin. The magnetic field breaks the time-reversal symmetry and removes the degeneracy of the energy eigenvalues when $m \neq 0$.

It is convenient to paramatrize the strength of the flux line by the positive quantity $\delta = e\Phi/(hc)$, where e is the magnitude of the charge on the particle and Φ is the total magnetic flux through the singular point. In the presence of the flux line the Hamiltonian is (see Brack *et al* [27])

$$H = \frac{p_r^2}{2} + \frac{(p_\phi - \delta)^2}{2r^2} + V(r) \tag{4.13}$$

where p_ϕ, the momentum canonical to the coordinate ϕ, is a constant of the motion, and $V(r)$ is given by equation (4.9). Then, for the trajectory labelled by j in equation (3.8), the angular part of the action is

$$S_{\text{ang}}(\xi^{(j)}; E) = p_\phi \xi^{(j)} = p_\phi(\gamma + 2\pi j). \tag{4.14}$$

Thus, the stationary phase condition (3.9) becomes $p_\phi = m\hbar$. However, by comparing (4.13) with equation (3.1) we see that $(p_\phi - \delta)^2$ now plays the role that L^2 played in section 3. For given m the quantization condition (3.15) becomes

$$S_{\text{rad}}(L = |m\hbar - \delta|; E) = 2\pi\hbar(n_r + \sigma_m/4) \qquad n_r = 0, 1, 2, \ldots. \tag{4.15}$$

Making this replacement in (4.11) and setting $\sigma_m = 2$ (corresponding to soft turnarounds at r_- and r_+), we obtain the following expression for the energy eigenvalues:

$$E_{mn_r} = \hbar\omega\{2n_r + [(m - \delta/\hbar)^2 \pm \alpha^2/\hbar^2]^{1/2} + 1\}$$
$$m = 0, \pm 1, \pm 2, \ldots \qquad n_r = 0, 1, 2, \ldots. \tag{4.16}$$

For the case of a singular flux line at the centre of a circular harmonic oscillator potential, we can let $\alpha \to 0$ in (4.16). The resulting energy eigenvalues are

$$E_{mn_r} = \hbar\omega(2n_r + |m - \delta/\hbar| + 1)$$
$$m = 0, \pm 1, \pm 2, \ldots \qquad n_r = 0, 1, 2, \ldots \tag{4.17}$$

which clearly are different for positive and negative values of m. This result is the same as the exact analytical solution of the Schrödinger equation for this problem, which can be obtained from the exact harmonic oscillator solution by replacing $|m|\hbar$ by $|m\hbar - \delta|$ wherever it occurs [27].

4.4. The circle billiard

In this section we apply the general formulation based on the transfer operator to a particle moving in a constant potential (which we take to be zero) inside a circle of radius R. We show that this leads to well known results for the EBK energy eigenvalues.

At energy E and angular momentum L, the radial motion has an inner turning point at the radius r_- given by $|L| = r_-(2E)^{1/2}$. Choosing the radius of the Poincaré circle to be R (or just slightly less than R so that the PSS is crossed just after the particle has made a collision with the boundary) ensures that all trajectories cross the PSS.

At fixed values of E and L, the radial part of the action integral is

$$S_{\text{rad}}(L; E) = 2 \int_{r_-}^{R} |p_r| \, \mathrm{d}r = 2 \int_{r_-}^{R} (2E - L^2/r^2)^{1/2} \, \mathrm{d}r$$
$$= 2(2ER^2 - L^2)^{1/2} - 2|L| \cos^{-1}[|L|/(2E)^{1/2}R]. \tag{4.18}$$

Writing $E = \hbar^2 k^2/2$ and setting $L = m\hbar$, with the values of m restricted by the condition $|m|\hbar \leqslant |L_{\max}(E)| = (2E)^{1/2}R$, we obtain from equation (3.15) the following condition for an approximate energy eigenvalue of the quantum system:

$$(k^2 R^2 - m^2)^{1/2} - |m| \cos^{-1}[|m|/(kR)] = \pi(n_r + \tfrac{3}{4})$$
$$m = 0, \pm 1, \pm 2, \ldots \qquad n_r = 0, 1, 2, \ldots. \tag{4.19}$$

Here we have put $\sigma_m = 3$, corresponding to a soft turnaround at the inner turning point and a hard-wall collision at the circle boundary. (See the discussion in appendix A.) Equation (4.19) can be solved numerically to determine the EBK energy eigenvalues. (This is equivalent to finding the zeros of the Bessel function $J_m(kR)$ when it is approximated by the leading term of the Debye asymptotic expansion. See [3, p 336].) Results for the lowest energy eigenvalues have been tabulated by Keller and Rubinow [12] and by Brack and Bhaduri (see [3, p 88]). The fractional difference between the EBK eigenvalues and the exact energy eigenvalues (determined from the zeros of the Bessel function $J_m(kR)$) was found to decrease fairly rapidly with increasing energy.

4.5. The annulus billiard

The annulus billiard consists of a particle moving in a constant potential (which we take to be zero) in the region between two concentric circles of radii R and a. (We assume $R > a$.) In this section we show how equation (3.15) may be used to obtain the EBK energy eigenvalues for this system.

As in the case of the circle billiard, we choose the Poincaré circle to have radius R. At energy E and angular momentum L the radial motion may have an inner turning point at the radius r_- given by $|L| = r_-(2E)^{1/2}$. Provided $a < r_-$, the minimum value of r during the radial motion will be r_-. However, if $a > r_-$, the radial motion is reversed by a hard-wall collision at $r = a$. In the former case with a soft turnaround at r_-, the Maslov index is $\sigma_m = 3$, as for the circle billiard. In the latter case, there are two hard-wall collisions, and the Maslov index is $\sigma_m = 4$.

The radial part of the action involves the same integral as in equation (4.18), but is now evaluated at the limits $r_{\min}$ and R, where $r_{\min}$ is r_- or a, whichever is larger. Putting $E = \hbar^2 k^2/2$ and setting $L = m\hbar$, with the values of m restricted by the condition $|m|\hbar \leqslant |L_{\max}(E)| = (2E)^{1/2}R$, we obtain the following condition for an approximate energy eigenvalue of the quantum system, similar to equation (4.19):

$$(k^2 r^2 - m^2)^{1/2}\big|_{r_{\min}}^{R} - |m| \cos^{-1}[|m|/(kr)]\big|_{r_{\min}}^{R} = \pi(n_r + \sigma_m/4)$$
$$m = 0, \pm 1, \pm 2, \ldots \qquad n_r = 0, 1, 2, \ldots. \tag{4.20}$$

Here, $\sigma_m = 3$ if $r_{\min} = r_-$, and $\sigma_m = 4$ if $r_{\min} = a$. The solution of this equation gives the EBK energy eigenvalue E_{mn_r}. Numerical values for the lowest 30 distinct EBK energy eigenvalues are tabulated in [29] for three cases: $a = 0.1R$, $a = 0.3R$, and $a = 0.5R$. Also tabulated in [29] are the energy eigenvalues computed from Bogomolny's transfer operator without making use of the stationary phase approximation or any other approximation. The results differ appreciably from the EBK energy eigenvalues. This draws attention to the fact that the stationary phase approximation used to derive equation (3.15)

constitutes an approximation *in addition to* the main semiclassical approximation contained in Bogomolny's transfer operator. It is clear that Bogomolny's approach and EBK quantization are generally equivalent only to leading order in $\hbar$.

5. Three-dimensional systems with spherical symmetry

A theory of the transfer operator for three-dimensional systems with spherical symmetry is only slightly more complicated than in two dimensions. For a particle of unit mass moving in a potential $V(r)$, the Hamiltonian is

$$H = \frac{p_r^2}{2} + \frac{p_\theta^2}{2r^2} + \frac{p_\phi^2}{2r^2 \sin^2 \theta} + V(r) \tag{5.1}$$

where $p_r = \dot{r}$, $p_\theta = r^2\dot{\theta}$ and $p_\phi = r^2 \sin^2 \theta \dot{\phi}$ are the momenta conjugate to the spherical polar coordinates (r, θ, ϕ) describing the particle's position. Because the component of the angular momentum about the polar axis, p_ϕ, is a constant of the motion, let us denote it as L_z. In addition, the square of the total angular momentum, $L^2 = p_\theta^2 + L_z^2/\sin^2 \theta$, is a constant of the motion. Therefore, the Hamiltonian may be written as

$$H = \frac{p_r^2}{2} + \frac{L^2}{2r^2} + V(r). \tag{5.2}$$

For given E and L, the turning points of the radial motion are determined by

$$\frac{L^2}{2r^2} + V(r) = E. \tag{5.3}$$

Thus, as in two dimensions, the turning point radii, r_- and r_+, depend on L^2 as well as E.

In constructing the transfer operator, we choose the PSS to be a sphere of radius R. The argument following equation (3.2) applies equally well to the three-dimensional situation. Therefore, we choose R to be equal to the radius of the circular trajectory at energy E for which the angular momentum has its maximum possible value. Then, for any angular momentum $|L| \leqslant L_{\max}(E)$, the trajectories of the system will repeatedly cross this surface.

The generalized coordinates q for the transfer operator are the polar angles (θ, ϕ) on the Poincaré sphere, which we denote collectively as Ω. Then, from equation (2.1) with $f = 3$, the transfer operator from Ω to Ω' is

$$T(\Omega', \Omega; E) = \sum_{cl.tr.} \frac{1}{2\pi i\hbar} \left| \det \frac{\partial^2 S}{\partial\Omega\partial\Omega'} \right|^{1/2} \exp[iS(\Omega', \Omega; E)/\hbar - i\mu\pi/2]. \tag{5.4}$$

Here the sum is over all possible classical trajectories at energy E which go from Ω to Ω' without crossing the PSS (in the same sense) at any other point. Let γ be the angle subtended at the origin by these points, with $0 \leqslant \gamma \leqslant \pi$. All possible trajectories from Ω to Ω' lie in the plane defined by these points and the origin, and each such trajectory can be uniquely identified by the total angle traversed as the particle moves along the trajectory. The trajectories fall into two classes, which we treat separately. In the first class, the angles traversed are $\xi_+^{(j)} = 2\pi j + \gamma$, $j = 0, 1, 2, \ldots$, while in the second class, the angles traversed are $\xi_-^{(j)} = 2\pi j - \gamma$, $j = 1, 2, \ldots$. The sum in (5.4) is over the trajectories of both classes.

The determinant of the second derivatives of $S(\xi_\pm^{(j)}; E)$ is evaluated in appendix B, where it is found that

$$\left| \det \frac{\partial^2 S}{\partial\Omega\partial\Omega'} \right| = \frac{1}{\sin\gamma} \left| \frac{\partial S}{\partial\gamma} \right| \left| \frac{\partial^2 S}{\partial\gamma^2} \right|. \tag{5.5}$$

Substituting in equation (5.4), we obtain

$$T(\Omega', \Omega; E) = \sum_{cl.tr.} \frac{1}{2\pi i\hbar} \frac{1}{(\sin\gamma)^{1/2}} \left|\frac{\partial S}{\partial\gamma}\right|^{1/2} \left|\frac{\partial^2 S}{\partial\gamma^2}\right|^{1/2} \exp[iS(\xi_\pm^{(j)}; E)/\hbar - i\mu_\pm^{(j)}\pi/2]. \quad (5.6)$$

The spherical symmetry of the system implies that $T(\Omega', \Omega; E)$ depends only on the angle γ subtended at the origin by the points Ω and Ω' on the Poincaré sphere. Therefore, we can expand the transfer operator in a Legendre series:

$$T(\Omega', \Omega; E) = T(\gamma; E) = \sum_{l=0}^{\infty} C_l(E) P_l(\cos\gamma) \quad (5.7)$$

where the expansion coefficients are

$$C_l(E) = \frac{2l+1}{2} \int_0^\pi T(\gamma; E) P_l(\cos\gamma) \sin\gamma \, d\gamma. \quad (5.8)$$

The spherical harmonic addition theorem

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\Omega) Y_{lm}^*(\Omega') \quad (5.9)$$

allows us to write

$$T(\Omega', \Omega; E) = T(\gamma; E) = \sum_{l=0}^{\infty} C_l(E) \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\Omega) Y_{lm}^*(\Omega') \quad (5.10)$$

where $Y_{lm}(\Omega)$ is a spherical harmonic function. We can now calculate matrix elements of the T-operator in the angular momentum representation. From the orthonormality of the spherical harmonics, a general matrix element is found to be

$$T_{l_1 m_1, l_2 m_2}(E) = \int d\Omega \int d\Omega' Y_{l_1 m_1}^*(\Omega) T(\Omega', \Omega; E) Y_{l_2 m_2}(\Omega')$$

$$= \left(\frac{4\pi}{2l_1+1}\right) C_{l_1}(E) \delta_{l_1 l_2} \delta_{m_1 m_2}. \quad (5.11)$$

Thus, the T-matrix is diagonal in this representation, and its eigenvalues (as a function of E) are just the diagonal elements. Denoting the lm-eigenvalue curve, which is $(2l+1)$-fold degenerate, as $\lambda_{lm}(E)$, we obtain from equations (5.6), (5.8) and (5.11),

$$\lambda_{lm}(E) = \frac{1}{i\hbar} \sum_{cl.tr.} \int_0^\pi d\gamma \left|\frac{\partial S}{\partial\gamma}\right|^{1/2} \left|\frac{\partial^2 S}{\partial\gamma^2}\right|^{1/2} \exp[iS(\xi_\pm^{(j)}; E)/\hbar - i\mu_\pm^{(j)}\pi/2]$$

$$\times P_l(\cos\gamma)(\sin\gamma)^{1/2}. \quad (5.12)$$

So far we have made no approximations beyond those used to derive Bogomolny's semiclassical transfer operator. For a given system, one can calculate the action $S(\xi_\pm^{(j)}; E)$ for each possible trajectory, as well as the derivatives with respect to γ, and hence evaluate the integrals. However, to proceed in a manner analogous to our treatment of two-dimensional systems, we make use of the following asymptotic expansion for $P_l(\cos\gamma)$, valid for large values of l (see [28, equations 8.10.7 and 6.1.46]):

$$P_l(\cos\gamma) \approx \frac{1}{(l+\frac{1}{2})^{1/2}} \left(\frac{1}{2\pi\sin\gamma}\right)^{1/2} \{\exp[i(l+\tfrac{1}{2})\gamma - i\pi/4] + \exp[-i(l+\tfrac{1}{2})\gamma + i\pi/4]\}$$

$$(5.13)$$

where terms of higher order in $1/l$ have been neglected. The same approximation has been used in the problem of scattering of waves by a sphere to show how the limit of geometrical optics can be obtained from physical optics [30]. After inserting (5.13) in equation (5.12), we can evaluate the resulting integrals using the stationary phase approximation.

The two terms in (5.13) yield the stationary phase conditions

$$\frac{\partial S(\xi_\pm^{(j)}; E)}{\partial \gamma} \pm (l + \tfrac{1}{2})\hbar = 0 \qquad (5.14)$$

where the $\pm$ between the terms refers to the two terms in the asymptotic expansion (5.13). At this point we find it convenient to treat separately the trajectories that traverse angles $\xi_+^{(j)} = 2\pi j + \gamma$, $j = 0, 1, 2, \ldots$ and those that traverse angles $\xi_-^{(j)} = 2\pi j - \gamma$, $j = 1, 2, \ldots$, where in both cases $0 \leqslant \gamma \leqslant \pi$. We shall show that both classes of trajectory lead to the same stationary phase condition, but that for a given value of l, the corresponding trajectory is either in one class or the other.

Let us suppose for the moment that the trajectory under consideration belongs to the first class. Because the action increases with the traversed angle $\xi_+^{(j)}$, we have $\partial S/\partial \gamma = \partial S/\partial \xi_+^{(j)} > 0$. Then equation (5.14) can be satisfied by taking the second term in (5.13). Since $\partial S/\partial \gamma$ is the magnitude of the total angular momentum, the stationary phase condition (5.14) effectively quantizes the total angular momentum:

$$L = |\mathbf{L}| = (l + \tfrac{1}{2})\hbar \qquad l = 0, 1, 2, \ldots. \qquad (5.15)$$

Furthermore, specifying the total angular momentum (with $L \leqslant L_{\max}(E)$; see below equation (5.3)) completely determines the trajectory at energy E in the plane containing Ω, Ω' and the origin. Thus, for a given value of l in (5.15), there is *at most one trajectory*, labelled by $j_l \geqslant 0$, which contributes to the sum in equation (5.12). For this trajectory (which, by assumption, belongs to the first class), we denote the angle traversed by the particle as $\xi_l = \gamma_l + 2\pi j_l$, where γ_l (in the range between 0 and π) is the stationary point determined by equation (5.14). We also denote the corresponding action by S_l and the phase index by μ_l. When slowly varying quantities are taken outside the integral (to be evaluated at $\gamma = \gamma_l$), the T-matrix eigenvalue curve (5.12) becomes

$$\lambda_{lm}(E) = \frac{1}{(2\pi)^{1/2} i\hbar} \frac{1}{(l + \tfrac{1}{2})^{1/2}} \left| \frac{\partial S}{\partial \gamma} \right|_{\gamma=\gamma_l}^{1/2} \left| \frac{\partial^2 S}{\partial \gamma^2} \right|_{\gamma=\gamma_l}^{1/2}$$
$$\times \int_0^\pi d\gamma \, \exp[iS_l(\gamma; E)/\hbar - i(l + \tfrac{1}{2})\gamma - i\mu_l \pi/2 + i\pi/4]. \qquad (5.16)$$

The integral is now evaluated in the usual way. Introducing the phase index ν_l as in equation (3.10), we obtain

$$\lambda_{lm}(E) \approx \exp[iS_l(\xi_l; E)/\hbar - i(l + \tfrac{1}{2})\gamma_l - i(\mu_l + \nu_l)\pi/2]. \qquad (5.17)$$

As in the two-dimensional case, these approximate T-matrix eigenvalue curves have unit modulus, consistent with the T-matrix being unitary.

We now split the action $S(\xi_l; E)$ into radial and angular parts. From the stationary phase condition, equation (5.14), the magnitude of the angular momentum along the trajectory is $(l + \tfrac{1}{2})\hbar$. Thus, since the particle traverses the angle $\xi_l = \gamma_l + 2\pi j_l$ when it moves along this trajectory, we obtain for the angular part of the action

$$S_{\text{ang}}(\xi_l; E)/\hbar = (l + \tfrac{1}{2})(\gamma_l + 2\pi j_l). \qquad (5.18)$$

The radial part of the action, evaluated for $L^2 = (l + \frac{1}{2})^2 \hbar^2$, is denoted as

$$S_{\mathrm{rad}}(L^2 = (l + \tfrac{1}{2})^2 \hbar^2; E) = \oint |p_r||\mathrm{d}r| = 2 \int_{r_-}^{r_+} |p_r| \, \mathrm{d}r. \qquad (5.19)$$

Hence, equation (5.17) becomes

$$\lambda_{lm}(E) \approx \exp[\mathrm{i} S_{\mathrm{rad}}(L^2 = (l + \tfrac{1}{2})^2 \hbar^2; E)/\hbar - \mathrm{i}(\mu_l + \nu_l - 2 j_l)\pi/2]. \qquad (5.20)$$

Next we suppose that the trajectory corresponding to a given value of l belongs to the second class, in which case the angle traversed by the particle has the form $\xi_-^{(j)} = 2\pi j - \gamma$, $j = 1, 2, \dots$. Here too the action must increase with the traversed angle $\xi_-^{(j)}$, implying that $\partial S/\partial \gamma = -\partial S/\partial \xi_-^{(j)} < 0$. Then the stationary phase condition, equation (5.14), can be satisfied by taking the first term in the asymptotic expansion (5.13). One obtains in this case the same condition, equation (5.15), for the magnitude of the angular momentum. However, the T-matrix eigenvalue curve corresponding to equation (5.17) becomes in this case

$$\lambda_{lm}(E) \approx \exp[\mathrm{i} S_l(\xi_l; E)/\hbar + \mathrm{i}(l + \tfrac{1}{2})\gamma_l - \mathrm{i}(\mu_l + \nu_l + 1)\pi/2] \qquad (5.21)$$

where $\xi_l = 2\pi j_l - \gamma_l$ and $j_l \geqslant 1$. The angular part of the action in this case is

$$S_{\mathrm{ang}}(\xi_l; E)/\hbar = (l + \tfrac{1}{2})(2\pi j_l - \gamma_l) \qquad (5.22)$$

which yields the T-matrix eigenvalue curve

$$\lambda_{lm}(E) \approx \exp[\mathrm{i} S_{\mathrm{rad}}(L^2 = (l + \tfrac{1}{2})^2 \hbar^2; E)/\hbar - \mathrm{i}(\mu_l + \nu_l - 2 j_l + 1)\pi/2]. \qquad (5.23)$$

The semiclassical energy eigenvalues of the quantum system are found from the determinantal equation (2.2), which is satisfied whenever an eigenvalue of the T-matrix is equal to unity. Thus, the condition for an energy eigenvalue is that $\lambda_{lm}(E) = \exp(\mathrm{i} 2\pi n_r)$. From equations (5.20) and (5.23) this yields the following condition for an energy eigenvalue:

$$S_{\mathrm{rad}}(L^2 = (l + \tfrac{1}{2})^2 \hbar^2; E) = 2\pi \hbar (n_r + \sigma_l/4) \qquad n_r = 0, 1, 2, \dots \qquad (5.24)$$

where the Maslov index σ_l associated with a complete cycle of the radial motion at energy E and $L^2 = (l + 1/2)^2 \hbar^2$ is defined to be

$$
\begin{aligned}
\sigma_l &= \mu_l + \nu_l - 2 j_l &\quad &\text{for trajectories in class } \xi_l = 2\pi j_l + \gamma_l &\quad &j_l = 0, 1, \dots \\
\sigma_l &= \mu_l + \nu_l - 2 j_l + 1 &\quad &\text{for trajectories in class } \xi_l = 2\pi j_l - \gamma_l &\quad &j_l = 1, 2, \dots
\end{aligned}
\qquad (5.25)
$$

As in the two-dimensional case, the values of n_r in (5.24) are determined by the assumption that $S_{\mathrm{rad}} \geqslant 0$.

It is shown in appendix A that this definition always leads to the result $\sigma_l = 2$ for soft potentials, and to $\sigma_l = 3$ for a particle inside a spherical cavity, making a hard-wall collision with the boundary in each cycle of the radial motion. These results are consistent with computing σ_l by the simple EBK rules of counting 1 for each soft turnaround of the radial motion and 2 for each hard-wall collision. Thus, equations (5.24) and (5.25) give the EBK quantization condition for the radial part of the action in three dimensions. The other EBK quantization conditions are $L^2 = (l + \frac{1}{2})^2 \hbar^2$ and $L_z = m\hbar$ with $-l \leqslant m \leqslant l$. The first of these was obtained earlier from the stationary phase condition. The second is a natural interpretation of the quantum number m introduced through the expansion of the T-operator in spherical harmonics. Because of the spherical symmetry, the energy eigenvalues corresponding to a particular value of l are $(2l + 1)$-fold degenerate.

6. Application to systems with spherical symmetry

6.1. The Coulomb plus $1/r^2$ potential in three dimensions

As in the two-dimensional case, the pure Coulomb potential has the special property that all classical trajectories (ellipses) starting from a given point on the PSS will return to the same point, which is, therefore, a focal point. To avoid this singular behaviour we shall again add a small $1/r^2$ term to the potential, which may be attractive or repulsive. Thus, we take the Hamiltonian corresponding to equation (5.2) to be

$$H = \frac{p_r^2}{2} - \frac{1}{r} + \frac{L^2 \pm \alpha^2}{2r^2} \tag{6.1}$$

where, as in the two-dimensional case, $\alpha^2/2$ is the strength of the $1/r^2$ potential. The turning-point radii, determined from equation (5.3), are given by equations (4.2) and (4.3) with L^2 being the square of the angular momentum of the particle. As in the two-dimensional case, we choose the radius of the Poincaré sphere to be $R = 1/(2|E|)$.

   The calculation of the radial contribution to the action proceeds exactly as in two dimensions. The result, similar to equation (4.5), is

$$S_{\text{rad}}(L^2 = (l + \tfrac{1}{2})^2 \hbar^2; E) = \pi \left(\frac{2}{|E|} \right)^{1/2} - 2\pi [(l + \tfrac{1}{2})^2 \hbar^2 \pm \alpha^2]^{1/2}. \tag{6.2}$$

Setting the Maslov index σ_l equal to 2, corresponding to two soft turnarounds in the radial motion (see appendix A), we obtain from equation (5.24) the following condition for an energy eigenvalue for given l and m:

$$\pi \left(\frac{2}{|E|} \right)^{1/2} - 2\pi [(l + \tfrac{1}{2})^2 \hbar^2 \pm \alpha^2]^{1/2} = 2\pi \hbar (n_r + \tfrac{1}{2}) \qquad n_r = 0, 1, 2, \ldots. \tag{6.3}$$

Since E is negative for the bound-state solutions we are considering, the energy eigenvalues for given l and m ($-l \leqslant m \leqslant l$) are found to be

$$E_{lmn_r} = -\frac{1}{2\hbar^2 \{n_r + \tfrac{1}{2} + [(l + \tfrac{1}{2})^2 \pm \alpha^2/\hbar^2]^{1/2}\}^2} \qquad n_r = 0, 1, 2, \ldots. \tag{6.4}$$

This expression gives the approximate semiclassical energy eigenvalues for the Coulomb plus $1/r^2$ potential. As expected, they are $(2l+1)$-fold degenerate because of the spherical symmetry of the system. It should also be observed that the allowed values of l are constrained by the condition that $(l + \tfrac{1}{2})\hbar \leqslant L_{\max}(E)$, with $[L_{\max}(E)]^2 = 1/(2|E|) \mp \alpha^2$, as in the two-dimensional case.

   The result for the pure Coulomb potential is found by letting $\alpha \to 0$ in equation (6.4). Putting $n = l + n_r + 1$ we obtain,

$$E_n = -\frac{1}{2\hbar^2 n^2} \qquad n = 1, 2, \ldots \tag{6.5}$$

independent of the sign of the α^2 term, as in two dimensions. This is the same as the familiar result found by solving the three-dimensional Schrödinger equation for the Coulomb potential. It is clear from the definition of n that $l < n$. This condition, which also arises in solving the Schrödinger equation, leads to the degeneracy of the nth energy level being n^2.

   It is remarkable that we have obtained the same result as the exact energy levels of the hydrogen atom, despite having made three approximations: (i) the semiclassical approximation embodied in Bogomolny's transfer operator; (ii) the asymptotic expansion

(5.13) for $P_l(\cos\gamma)$; and (iii) the evaluation of the integral in (5.12) using the stationary phase approximation. A plausible explanation for this agreement will be given in the discussion at the end of the paper.

6.2. The spherical harmonic oscillator plus $1/r^2$ potential

In this section we treat the isotropic harmonic oscillator plus a small $1/r^2$ potential. We take the Hamiltonian corresponding to equation (5.2) to be

$$H = \frac{p_r^2}{2} + \frac{1}{2}\omega^2 r^2 + \frac{L^2 \pm \alpha^2}{2r^2} \tag{6.6}$$

where, as in the two-dimensional case, ω^2 describes the steepness of the harmonic oscillator potential, and $\alpha^2/2$ is the strength of the $1/r^2$ potential, which may be attractive or repulsive. The radial turning points, determined from equation (5.3) for fixed E and L^2, are given by equation (4.10), as in two dimensions. When L^2 has its maximum possible value, determined by

$$[L_{\max}(E)]^2 = \frac{E^2}{\omega^2} \mp \alpha^2 \tag{6.7}$$

the radial kinetic energy is zero and the particle trajectory is confined to the sphere of radius $R = E^{1/2}/\omega$. We take the Poincaré sphere to have this radius since all trajectories having $L \leqslant L_{\max}(E)$ must repeatedly cross this surface.

For given E and L^2 the radial part of the action can be calculated as in the two-dimensional case. The result is the same as equation (4.11). Furthermore, from the analysis in appendix A, the Maslov index is $\sigma_l = 2$. Thus, from equation (5.24), the condition for an energy eigenvalue is

$$\frac{\pi E}{\omega} - \pi\hbar[(l + \tfrac{1}{2})^2 \pm \alpha^2/\hbar^2]^{1/2} = 2\pi\hbar(n_r + \tfrac{1}{2}) \qquad n_r = 0, 1, 2 \ldots. \tag{6.8}$$

Hence, the energy eigenvalue specified by l, m and n_r is

$$E_{lmn_r} = \hbar\omega\{2n_r + [(l + \tfrac{1}{2})^2 \pm \alpha^2/\hbar^2]^{1/2} + 1\} \qquad n_r = 0, 1, 2, \ldots. \tag{6.9}$$

These eigenvalues are clearly $(2l + 1)$-fold degenerate. Note that the permissible values of l are determined by the condition that $(l + \tfrac{1}{2})\hbar \leqslant L_{\max}(E)$, with $L_{\max}(E)$ given by equation (6.7).

The energies of the pure isotropic harmonic oscillator in three dimensions are found by letting $\alpha \to 0$. Defining $n = 2n_r + l$, we obtain (independent of the sign of the α^2 term)

$$E_n = \hbar\omega(n + \tfrac{3}{2}) \qquad n = 0, 1, 2, \ldots. \tag{6.10}$$

The ground state energy is the zero-point energy associated with three freedoms. The multiplicities of the levels are determined by the $(2l + 1)$-fold degeneracy associated with m and by the number of distinct ways of obtaining a given value of n from the integer values of l and n_r. The energy levels given by (6.10) and their degeneracies are the same as those obtained in the solution of the three-dimensional Schrödinger equation for the spherical oscillator (see, for example, [26, pp 166–8]).

6.3. Billiard in a spherical cavity

A particle moving in zero potential inside a spherical cavity of radius R is the three-dimensional analogue of the circle billiard. As in the two-dimensional system, for given values of the energy E and the square of the total angular momentum L^2, the inner turning

point radius r_- is given by $|L| = (2E)^{1/2}r_-$. We choose the PSS to be the sphere of radius R (or just slightly less than R, in order that the trajectories cross the PSS immediately after colliding with the spherical boundary).

To obtain the EBK eigenvalues from equation (5.24) we can use equation (4.18) for the radial part of the action integral, which is the same for the two- and three-dimensional systems. Furthermore, it was shown in appendix A that the Maslov index is $\sigma_l = 3$ for this system. Thus, from equations (5.24) and (4.18), the condition for an energy eigenvalue of the billiard in a spherical cavity is

$$[k^2R^2 - (l + \tfrac{1}{2})^2]^{1/2} - (l + \tfrac{1}{2})\cos^{-1}[(l + \tfrac{1}{2})/(kR)] = \pi(n_r + \tfrac{3}{4})$$
$$l = 0, 1, 2\ldots \qquad n_r = 0, 1, 2, \ldots. \tag{6.11}$$

Here the allowed values of l at energy E are restricted by the condition $(l + \tfrac{1}{2}) \leqslant kR$, where $k = (2E)^{1/2}/\hbar$. Equation (6.11) could be solved numerically in a manner similar to equation (4.19) to obtain the EBK energy eigenvalues. (This would be equivalent to finding approximate values for the zeros of the spherical Bessel function $j_m(kR)$ when it is approximated by the leading term of the Debye asymptotic expansion.)

7. Discussion

We have shown how, with the help of the stationary phase approximation, Bogomolny's transfer operator leads to the EBK quantization rules for the energy eigenvalues of integrable systems having rotational symmetry, in both two and three dimensions. An important aspect of the theory was showing that the Maslov indices are correctly given by the simple rules of counting 1 for each soft turnaround and 2 for each hard-wall collision occurring during one complete cycle of the radial motion.

In discussing the annulus billiard in section 4.5 we drew attention to the fact that the EBK energy eigenvalues are appreciably different from those obtained using Bogomolny's transfer operator unmodified by making the stationary phase approximation or any other approximation. It is noteworthy, however, that among the eight different rotationally invariant systems to which the theory was applied, in five cases the EBK energy eigenvalues turned out to be the same as those obtained from an exact solution of the Schrödinger equation. While EBK quantization is known to be exact for certain special systems (such as the Coulomb and harmonic oscillator potentials), we are not aware of a general theory which explains why this happens. Bogomolny's transfer operator, in its exact [31] and semiclassical forms, may be helpful in this regard.

For the hydrogen atom in three dimensions (section 6.1), it was pointed out that the correct energy levels were obtained despite having made three significant approximations in the theoretical development. A similar situation arose in a recent paper [24] concerning the application of Bogomolny's T-operator to a circular harmonic oscillator plus $1/r^2$ potential. For that system it was possible to write down an exact transfer operator, which led to the exact energy eigenvalues without making any approximations. It was then shown, with the help of the Poisson summation formula, that the exact transfer operator could be written as an infinite sum of certain integrals, and that the leading term in this sum was the same as Bogomolny's transfer operator. Further, it was shown that improving the stationary phase approximation leads to corrections to the energy eigenvalues that involve higher powers of $\hbar$ than the leading term. In short, the semiclassical result agreed with the exact quantum result simply because corrections to the semiclassical approximation (which are nonzero) and to the stationary phase approximation (which are also nonzero) were not evaluated.

Presumably, if corrections to all the approximations were evaluated systematically, they would cancel each other in all orders of $\hbar$.

It seems likely that we are dealing with a similar situation for the hydrogen atom in two and three dimensions, and for the harmonic oscillator with a singular magnetic flux line. For these systems we have not yet written down an exact transfer operator, which would make feasible an analysis similar to that of [24]. Nevertheless, if the EBK energy eigenvalue is regarded as the leading term of a semiclassical expansion in increasing powers of $\hbar$, it is perhaps not so surprising that, in some cases, it agrees with the exact quantum result.

Acknowledgments

Appendix A. Equivalence of σ with the Maslov index in EBK quantization

In this appendix we consider the index $\sigma_m = \mu_m + \nu_m$ introduced following equation (3.15) for a particle in two dimensions, and the index $\sigma_l = \mu_l + \nu_l$ defined in equation (5.25) for a particle in three dimensions. In both cases we consider a particle confined inside a finite region either by a smooth potential or a hard-wall boundary. From the definitions of the μ and ν indices we show that σ_m and σ_l have the values one would compute from the simple rules for obtaining the Maslov index in EBK quantization.

For two-dimensional systems, consider a particle moving in a smooth potential $V(r)$. Figure A1 shows typical trajectories along with trajectories having slightly larger and slightly smaller angular momenta than the main trajectory. The trajectory with smaller angular momentum approaches more closely to the origin, but on the outward leg also ventures farther away from the origin. In the course of doing so, it must necessarily intersect the trajectory with larger angular momentum. Thus, there is a focal point and μ_m is thereby incremented by 1. There are then two possibilities. Before returning to the Poincaré circle, the two orbits may intersect yet again, leading to $\mu_m = 2$, as shown in figure A1(a). If this happens one observes that the angle traversed is greater for the larger angular momentum, so that $\partial^2 S/\partial \gamma^2 > 0$ and $\nu_m = 0$. On the other hand, there may be no further intersection so that $\mu_m = 1$, as illustrated in figure A1(b). In this case one observes that $\partial^2 S/\partial \gamma^2 < 0$ so that $\nu_m = 1$. In either event we have $\sigma_m = 2$, which is the same as the value for the Maslov index in EBK quantization obtained by counting 1 for each of the turning points of the radial motion.

We have performed numerical studies for two-dimensional systems having potentials of the form $V(r) \sim \pm r^k$, where the plus sign is assumed for $k > 0$ and the minus sign for $k < 0$ (so that the potential is attractive). Our calculations show that for $-1 < k < 2$ one finds $\mu_m = 2$ and $\nu_m = 0$, while for $-2 < k < -1$ and $2 < k < \infty$ one finds $\mu_m = 1$ and $\nu_m = 1$. The cases $k = -1$ and $k = 2$, which are self-focusing, are marginal for the present analysis.

The case of a hard wall may be approximated by taking the limit $k \to \infty$. However, when considering both large k and infinitesimally close trajectories, one must be careful about the order in which the limits are taken. For any fixed k, no matter how large, we can take the two nearby angular momenta close enough to the main trajectory that we obtain
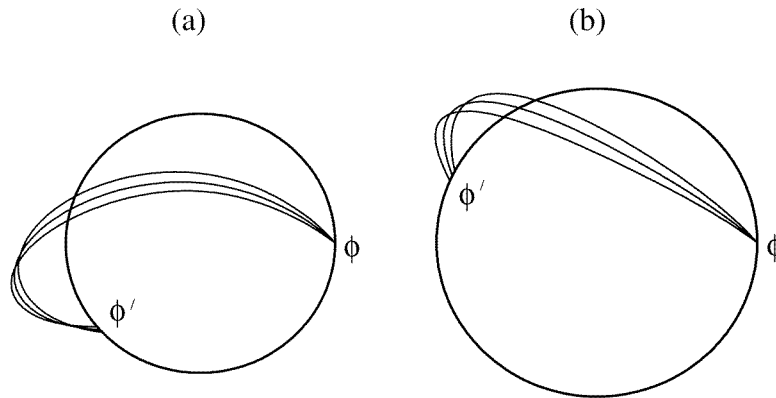
Figure A1. Examples of trajectories in two dimensions which start from an arbitrary point ϕ on the Poincaré circle and return (in the same sense) to the Poincaré circle at the point ϕ'. In each case there is a main trajectory together with trajectories having slightly larger and slightly smaller angular momenta. Figure A1(a) was computed for the potential $V(r) \sim r^k$ with $k = 0.5$. Figure A1(b) was computed for $V(r) \sim r^k$ with $k = 3.5$.

$\sigma_m = 2$, in conformity with the previous discussion. On the other hand, if we consider two fixed angular momenta, no matter how close, we can make k large enough that the two trajectories no longer intersect on the outer loop. This is the appropriate analysis for a disk with infinitely hard walls. In this case $\mu_m = 2$ from the collision with the hard wall (Dirichlet boundary conditions), while $\nu_m = 1$, giving the result $\sigma_m = 3$. This agrees with the result for the EBK Maslov index obtained by counting 1 for the soft turnaround at the inner turning point and 2 for the hard turnaround at the disk boundary. The same analysis applies even if the motion is not force-free within the disk. For example, one could include a uniform magnetic field, or a flux line, or a harmonic potential out to the disk radius. As long as the trajectory bounces off the disk boundary, $\sigma_m = 3$, but if the particle avoids colliding with the boundary, the discussion in the previous paragraph will apply and $\sigma_m = 2$.

Turning now to three-dimensional systems with a smooth potential, we recall that the Maslov index σ_l was defined in equation (5.25) for the two different classes of trajectories. We now show that, for soft potentials, this leads to the result $\sigma_l = 2$ in all cases.

For given points Ω and Ω' on the Poincaré sphere, a trajectory from Ω to Ω' lies in the plane containing these points and the origin. Focal points arising from variations within the plane of this trajectory yield the result $\mu_l + \nu_l = 2$ from the preceding analysis. In three dimensions, however, there may exist an additional focal point lying on the straight line from the point Ω to the origin. One can see that, provided the particle traverses an angle between π and 2π in moving along the trajectory for specified E and L^2, it will intersect this line at a point on the opposite side of the origin from Ω. Similar trajectories in all planes containing Ω and the origin will intersect at this point, which is, therefore, a focal point. In this case, μ_l must be incremented by 1, giving $\mu_l + \nu_l = 3$. But the angle traversed by the particle in this case is $\xi_l = 2\pi - \gamma_l$, which means the trajectory belongs to the class $\xi_l = 2\pi j_l - \gamma_l$ with $j_l = 1$. Hence, from equation (5.25), the Maslov index is $\sigma_l = 2$. Note that if the particle makes an additional circuit around the origin (corresponding to $\xi_l = 2\pi j_l - \gamma_l$ with $j_l = 2$) there will be two additional focal points on the line joining Ω to the origin (on both sides of the origin), but from (5.25) the Maslov index will still

be $\sigma_l = 2$. Clearly this generalizes to any number of complete circuits around the origin within the time of one cycle of the radial motion.

If the angle traversed by the particle in moving along the trajectory specified by E and L^2 lies between 0 and π, there is no focal point of the type described in the preceding paragraph. The angle traversed is $\xi_l = \gamma_l + 2\pi j_l$ with $j_l = 0$, and equation (5.25) gives $\sigma_l = 2$. If there are additional circuits around the origin corresponding to $\xi_l = \gamma_l + 2\pi j_l$, with $j_l = 1, 2, \ldots$, one can easily see that μ_l must be incremented by 2 for each circuit, but from equation (5.25), the Maslov index remains $\sigma_l = 2$. Thus, we have shown that $\sigma_l = 2$ for all possible trajectories in a soft potential. This result is the same as would be obtained from the simple EBK rule of counting 1 for each radial turning point of the effective potential $V(r) + L^2/(2r^2)$.

If the outer radial turning point is replaced by a hard-wall collision with the boundary (Dirichlet boundary condition on the wavefunction), the above analysis still holds up to the point of colliding with the boundary. As for the two-dimensional systems, the hard-wall collision requires incrementing μ_l by 1, giving the result $\sigma_l = 3$. This is the EBK result from the simple rule of counting 1 for the soft turnaround at the inner radial turning point plus 2 for the collision with the boundary.

Appendix B. The determinant of second derivatives of S

In this appendix we evaluate the determinant of second derivatives of the action, which constitutes the amplitude of the three-dimensional transfer operator:

$$\det \frac{\partial^2 S}{\partial \Omega \partial \Omega'} = \begin{vmatrix} \frac{\partial^2 S}{\partial \theta \partial \theta'} & \frac{\partial^2 S}{\partial \theta \partial \phi'} \\ \frac{\partial^2 S}{\partial \phi \partial \theta'} & \frac{\partial^2 S}{\partial \phi \partial \phi'} \end{vmatrix}. \tag{B.1}$$

Here $S = S(\xi_\pm^{(j)}; E)$, which, through $\xi_\pm^{(j)}$, depends on the angle γ introduced just after equation (5.4). Since γ is the angle subtended at the origin by the points Ω and Ω' on the Poincaré sphere, we have

$$\cos \gamma = \sin \theta \sin \theta' \cos(\phi - \phi') + \cos \theta \cos \theta' \qquad 0 \leqslant \gamma \leqslant \pi. \tag{B.2}$$

Our objective is to express the determinant in terms of γ.

First, let us write

$$\begin{aligned} \frac{\partial S}{\partial \theta} &= \frac{\partial S}{\partial \gamma} \frac{\partial \gamma}{\partial \theta} \\ \frac{\partial^2 S}{\partial \theta \partial \theta'} &= \frac{\partial^2 S}{\partial \gamma^2} \frac{\partial \gamma}{\partial \theta} \frac{\partial \gamma}{\partial \theta'} + \frac{\partial S}{\partial \gamma} \frac{\partial^2 \gamma}{\partial \theta \partial \theta'}. \end{aligned} \tag{B.3}$$

It will greatly simplify the calculation to evaluate the second derivatives assuming that $\theta = \theta' = \pi/2$. This means that the polar axis of the spherical polar coordinate system is chosen to be perpendicular to the plane containing the origin and the arbitrarily chosen points (R, Ω) and (R, Ω') on the PSS. Because of the spherical symmetry, the result obtained will be valid for any orientation of the axes of the spherical polar coordinate system. When $\theta = \theta' = \pi/2$, one finds that $\partial \gamma/\partial \theta = \partial \gamma/\partial \theta' = 0$ and $\partial^2 \gamma/(\partial \theta \partial \theta') = -1/\sin \gamma$. Hence,

$$\left(\frac{\partial^2 S}{\partial \theta \partial \theta'} \right)_{\theta = \theta' = \pi/2} = -\frac{1}{\sin \gamma} \frac{\partial S}{\partial \gamma}. \tag{B.4}$$

The other second derivatives can be evaluated in the same way. We obtain

$$
\left(\frac{\partial^2 S}{\partial\theta\,\partial\phi'}\right)_{\theta=\theta'=\pi/2} = \left(\frac{\partial^2 S}{\partial\phi\,\partial\theta'}\right)_{\theta=\theta'=\pi/2} = 0
$$
$$
\left(\frac{\partial^2 S}{\partial\phi\,\partial\phi'}\right)_{\theta=\theta'=\pi/2} = -\frac{\partial^2 S}{\partial\gamma^2}.
$$

(B.5)

Hence, the determinant in (B.1) has the value given in equation (5.5).

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