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Closed orbits and the regular bound spectrum

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The energy levels of systems whose classical motion is multiply periodic are accurately given by the quantum conditions of Einstein, Brillouin & Keller (E.B.K.). We transform the E.B.K. conditions into a representation of the spectrum in terms of a 'topological sum' involving only the closed classical orbits; the theory applies equally to separable and non-separable systems; stability parameters are not involved. Significant contributions come from complex closed orbits which however have real constants of the motion. Clustering of levels on different scales is demonstrated by smoothing the spectrum using the formal device, due to Balian & Bloch, of adding a variable imaginary part to the energy. The topological sum is shown to agree very well with exactly-computed spectra for circular and spherical potential wells with repulsive core.

1. INTRODUCTION

Einstein (1917) showed that the Bohr–Sommerfeld quantum conditions could be generalized in an invariant manner to include systems whose classical motion is not separable in the coordinates, provided the classical motion is multiply periodic. Brillouin (1926) explained how Einstein's conditions were a consequence of the single-valuedness of the quantum-mechanical wave function and Keller (1958) showed that caustics in the classical motion require a slight modification of Brillouin's argument and Einstein's conditions. Percival (1973) introduced the term 'regular' to describe the spectrum of energy levels given by this theory and distinguished it from the 'irregular' spectrum expected when the classical motion is not multiply periodic. In this paper we discuss only the regular spectrum.

In the Einstein–Brillouin–Keller (E.B.K.) theory each energy level of this spectrum arises from a set of values of the irreducible action integrals associated with the different periods of the motion, and thus corresponds not to a single classical orbit but to a *family* of orbits. Moreover, in the families selected by the quantum condition the fundamental frequencies need not be commensurable, so that the orbits in the family need not be closed. And yet Gutzwiller (1967, 1969, 1970, 1971) claims that it is precisely the closed orbits that give rise to the discrete energy levels. His approach has been criticized by Berry & Mount (1972, hereinafter called I) who point out that in some circumstances Gutzwiller's method predicts discrete states in the continuum and a continuous level distribution in a bound system and also by Miller (1975) who points out that the method often gives too few quantum numbers and fails in the limit of separability.

Some clarification of this confused situation has been achieved by Balian & Bloch (1972), who study in great detail the spectra of empty hard-walled enclosures of various shapes. Like Gutzwiller, they write the *density of states* $n(E)$ as a series over closed classical orbits, using a semiclassical representation of the Green function. By allowing the energy to be complex they define a partially smoothed density of states, and this shows very clearly how the simplest closed orbits give rise not to individual energy levels but to *clusters* of levels. As the degree of smoothing is diminished, more and more closed orbits contribute to $n(E)$ and at the same time the clusters are resolved into individual levels.

In this paper we give a general treatment of the regular spectrum. Rather than using the Green function as a starting point, we prefer to begin with the E.B.K. theory, which is summarized in § 2. This has a sound quantum-mechanical basis (Keller 1958) and moreover gives eigenvalues in close numerical agreement with exact calculations based on Schrödinger's equation (Noid & Marcus 1975; Percival & Pomphrey 1975). In § 3 we transform the E.B.K. formula for $n(E)$ into a series of contributions from closed classical orbits at the energy E, similar to the series obtained by Gutzwiller (1970) and Balian & Bloch (1972, 1974), but very different from that of Gutzwiller (1971). Our result, however, is expressed in terms of general action–angle variables, and shows that there are no essential differences between the separable and non-separable cases.

Nevertheless, the 'topological sum' has serious deficiencies, which our method of derivation enables us to surmount by introducing, in § 4, *complex periodic orbits* of a type unfamiliar in semiclassical theory. This results in a uniform approximation for $n(E)$, valid near or far from potential minima and independently of the degree of anharmonicity. In § 5, we employ a smoothing technique similar to that of Balian & Bloch (1972). In this more general case each periodic orbit is weighted by a decay factor whose exponent is proportional to the orbital period.

Finally, in § 6 we present numerical tests of our formulae for separable cases involving circular and spherical potentials. These show (1) that $n(E)$ starts as a smooth 'Thomas–Fermi' background density when only the first term is included in the topological sum, and that this background is gradually 'eaten away' as more terms are added, the final result being a series of δ-functions. (2) That the uniform approximation, based on complex orbits, is required to get improved numerical agreement between the smoothed $n(E)$ given by the topological sum and by exact quantum calculation, and (3) that circular and spherical potentials of the same form have very different spectra, not only because of the degeneracy factor but also because of the different caustic structure of the two families of orbits.

2. Quantization by tori

Consider a bound classical system with n degrees of freedom. If the motion is multiply periodic, it is possible to describe it using action-angle variables

$$(I_1, \ldots, I_n, \theta_1, \ldots, \theta_n) \equiv (\boldsymbol{I}, \boldsymbol{\theta}).$$

Here $\boldsymbol{I}$ is a vector whose components are $1/2\pi$ times the n independent action integrals (see Einstein 1917; Keller 1958), which can be employed as canonical momenta in a Hamiltonian description of the motion. They are constants of the motion, so that the n conjugate 'angle' coordinates $\boldsymbol{\theta}$ are ignorable, and the Hamiltonian function H depends only on $\boldsymbol{I}$, that is, the energy E of the system is

$$E = H(\boldsymbol{I}). \tag{1}$$

For a given set of constants $\boldsymbol{I}$, each of the multiple oscillations of the system is described by one component of $\boldsymbol{\theta}$ changing by 2π, the rates of change

$$\boldsymbol{\omega}(\boldsymbol{I}) \equiv \dot{\boldsymbol{\theta}} = \nabla_{\boldsymbol{I}} H \tag{2}$$

being equal to the n frequencies of the system. Because the n-fold periodicity of the coordinate motion for given $\boldsymbol{I}$ has the same topology as an n-dimensional torus, the regions in phase space corresponding to the given $\boldsymbol{I}$ are often called 'invariant tori'.

As was clearly understood by Einstein (1917), the E.B.K. theory depends on the possibility of writing the Hamiltonian in the form (1), that is on the existence of invariant tori. Tori obviously exist for all separable systems. For example, the n-dimensional harmonic oscillator has frequencies independent of $\boldsymbol{I}$, and Hamiltonian

$$H = \boldsymbol{\omega} \cdot \boldsymbol{I}. \tag{3}$$

The 'energy contours' $H(\boldsymbol{I}) = E$ are hyperplanes in the $\boldsymbol{I}$ space. Again, for particle motion in two-dimensional circular potentials $V(r)$ of the Lennard–Jones type (attractive at large distances and repulsive at short distances), the radial action $I_1 = S/\pi$ and the angular action $I_2 = L$, where L is the angular momentum of the particle, give the Hamiltonian $H = E$ implicitly by the equation

$$S = \int_{r_1}^{r_2} \sqrt{[2m(E - V(r) - L^2/2mr^2)]}\, \mathrm{d}r, \tag{4}$$

where r_1 and r_2 are the radial limits of the motion for given E and L.

For non-separable systems it was conjectured by Kolmogorov (1954, 1957) and proved by Arnol'd (1963) and Moser (1962) that invariant tori exist for systems that differ from separability by a small perturbation, although the distribution of these tori may be exceedingly complicated near closed orbits (Arnol'd & Avez 1968). Further, numerical experiments by Henon & Heiles (1964) strongly suggest that departures from separability can be quite strong before the tori cease to exist in the sense that some orbits become 'ergodic', that is they explore the whole $2n-1$ dimensional region in phase space defined by their energy instead of being confined to the n-dimensional tori.

We therefore expect a Hamiltonian of the form (1) to exist for a large class of motions; in these cases the determination of $H(\boldsymbol{I})$ from any given Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p})$ is a difficult problem in classical (rather than semiclassical) mechanics (see Percival & Pomphrey (1975), and Chapman, Garrett & Miller (1976)).

Given $H(\boldsymbol{I})$, E.B.K. quantization is quite simple: define a vector

$$\boldsymbol{m} = (m_1, m_2, \ldots, m_n),$$

where the m_i are positive integers or zero, and form the regular lattice

$$\boldsymbol{I} = (\boldsymbol{m} + \tfrac{1}{4}\boldsymbol{\alpha})\hbar \tag{5}$$

in $\boldsymbol{I}$ space, where $\boldsymbol{\alpha}$ is a vector to be defined presently. Then quantum energy levels occur at those energies for which the energy contour $H(\boldsymbol{I}) = E$ touches a lattice point. The levels are labelled with the set of quantum numbers $\boldsymbol{m}$ corresponding to the lattice point at which contact occurs. Explicitly, the level $E_{\boldsymbol{m}}$ is

$$E_{\boldsymbol{m}} \equiv E_{m_1,\ldots,m_n} = H((\boldsymbol{m} + \tfrac{1}{4}\boldsymbol{\alpha})\hbar) = H(I_1 = (m_1 + \tfrac{1}{4}\alpha_1)\hbar_1 \ldots, I_n = (m_n + \tfrac{1}{4}\alpha_n)\hbar)$$
$$(m_i = 0, 1, 2, \ldots). \tag{6}$$

All that remains is the specification of the vector $\boldsymbol{\alpha}$. Keller (1958) shows that the ith component α_i equals the number of caustics of the family of orbits $\boldsymbol{I}$ encountered by any one of the family during a cycle of the motion corresponding to the period ω_i (see also § 7.3 of *I*). For the oscillator (equation (3)) all coordinate cycles are librations (Born 1927) each with two turning points; these turning points are limits of the motion and hence lie on the envelope of the family of orbits, i.e. on the caustic. Thus all components α_i equal two for this case. For the circular attractive potential with repulsive core (equation (4)) the radial motion is a libration between r_1 and r_2, so that $\alpha_1 = 2$. The angular motion on the other hand is a pure rotation with no caustics, so $\alpha_2 = 0$ (the angular motion in the spherical case does have caustics, as we explain in § 6).

3. The topological sum

We rewrite the E.B.K. quantization formula (6) in terms of the density of states function $n(E)$, using the fact that each state gives a unit δ-function contribution. This gives

$$n(E) = \sum_{\boldsymbol{m}} \delta(E - H((\boldsymbol{m} + \tfrac{1}{4}\boldsymbol{\alpha})\hbar)). \tag{7}$$

(In order to avoid complication we have omitted degeneracy factors of 2 for each non zero quantum number m_i that corresponds to rotation; these factors, to which we shall return in § 6, arise because for rotation, unlike libration, the two senses of motion are distinguishable.) There are several advantages in a formalism based on $n(E)$: the effect of the closed orbits can be elucidated, the clustering of levels can be understood, and many features of the theory should remain valid in the continuum (which, however, we shall not consider further here).

Next we transform (7) into a series of integrals over the positive 'quadrant' in $\boldsymbol{I}$ space, using the Poisson sum formula

$$n(E) = \frac{1}{\hbar^n} \sum_{\boldsymbol{M}} \mathrm{e}^{-\mathrm{i}\frac{1}{2}\pi\boldsymbol{\alpha}\cdot\boldsymbol{M}} \int_{\substack{+\mathrm{ve} \\ \text{'quadrant'}}} \mathrm{d}^n I \delta(E - H(\boldsymbol{I}))\, \mathrm{e}^{(2\pi\mathrm{i}/\hbar)\boldsymbol{M}\cdot\boldsymbol{I}}. \tag{8}$$

Here $\mathrm{d}^n I \equiv \mathrm{d}I_1, \mathrm{d}I_2, \ldots, \mathrm{d}I_n$, and $\boldsymbol{M} = (M_1, \ldots, M_n)$ where M_1 is an arbitrary integer. The points $\boldsymbol{M}$ form a lattice which for reasons that will emerge later we shall call the 'topological lattice'. The result (8) is precisely equivalent to (7). To retain only the term $\boldsymbol{M} = 0$ would correspond to the crude approximation of replacing the summations in (7) by integrations, and would give

$$\begin{aligned} n(E) \approx n_{TF}(E) &\equiv \frac{1}{\hbar^n}\int \mathrm{d}^n I \delta(E - H(\boldsymbol{I})) \\ &= \frac{1}{\hbar^n}\int \mathrm{d}^n I \int \frac{\mathrm{d}^n\theta}{(2\pi)^n}\delta(E - H(\boldsymbol{I})) \\ &= \frac{1}{h^n}\int\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\delta(E - H(\boldsymbol{q},\boldsymbol{p})). \end{aligned} \tag{9}$$

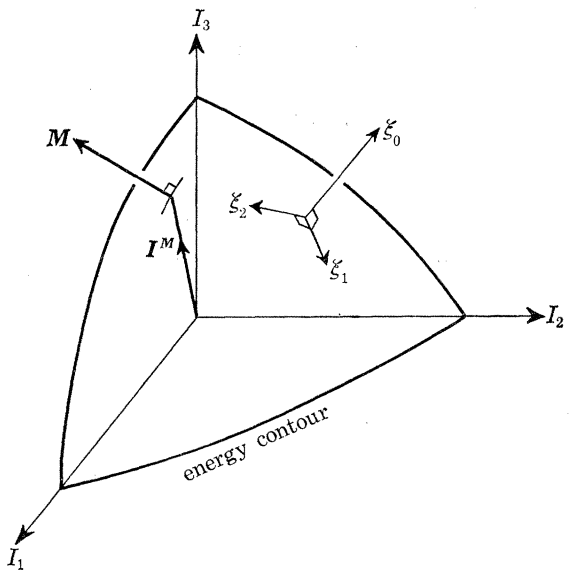

FIGURE 1. Coordinates ξ on the energy contour, and torus $\boldsymbol{I}^{\boldsymbol{M}}$ with topology $\boldsymbol{M}$.

This is the 'Thomas–Fermi' result (§ 7.4 of *I*), in which $n(E)$ is replaced by a smooth function calculated on the basis that each quantum state occupies a volume h^n in the phase space $(\boldsymbol{q},\boldsymbol{p})$ of the system.

The terms $\boldsymbol{M} \neq 0$ in (8) give oscillatory corrections to the featureless background $n_{TF}(E)$. To evaluate them we first define the oscillatory integrals $n_{\boldsymbol{M}}$ in (8) by

$$n_{\boldsymbol{M}} \equiv \int \mathrm{d}^n I \delta(E - H(\boldsymbol{I}))\, \mathrm{e}^{(2\pi\mathrm{i}/\hbar)\boldsymbol{M}\cdot\boldsymbol{I}}. \tag{10}$$

To remove the δ-function we introduce coordinates in I space as follows: the perpendicular distance of a point $\boldsymbol{I}$ from the energy contour $H(\boldsymbol{I}) = E$ is ξ_0 (figure 1)

and the position of points on the energy contour is labelled by the $n-1$ dimensional vector $\xi \equiv (\xi_1, \ldots, \xi_{n-1})$. Then n_M becomes

$$n_M = \int \mathrm{d}^{n-1}\xi \, \mathrm{e}^{(2\pi \mathrm{i}/\hbar)\boldsymbol{M}\cdot\boldsymbol{I}(\xi)} \int \mathrm{d}\xi_0 \frac{\delta(\xi_0)}{|\partial H/\partial \xi_0|}$$

$$= \int_{\text{energy contour}} \mathrm{d}^{n-1}\xi \frac{\mathrm{e}^{(2\pi \mathrm{i}/\hbar)\boldsymbol{M}\cdot\boldsymbol{I}(\xi)}}{|\boldsymbol{\omega}(\boldsymbol{I}(\xi))|}, \tag{11}$$

where we have used equation (2) for the denominator.

Because the factor $\mathrm{i}/\hbar$ in the exponent, the integrand in (11) is a rapidly oscillating function of position ξ on the energy contour, and the most important contributions will come from those points $\boldsymbol{M}$ in the topological lattice for which the phase $\boldsymbol{M}\cdot\boldsymbol{I}$ is stationary for some point $\xi^{\boldsymbol{M}}$. This gives the $n-1$ conditions

$$\boldsymbol{M}\cdot\frac{\partial \boldsymbol{I}}{\partial \xi_i} = 0 \quad \text{if} \quad \xi = \xi^{\boldsymbol{M}} \quad (i = 1, 2, \ldots, n-1). \tag{12}$$

Now the $\partial \boldsymbol{I}/\partial \xi_i$ are the $n-1$ tangent vectors on the energy contour (figure 1), so that (12) has the geometrical interpretation that the stationary point $\xi^{\boldsymbol{M}}$ occurs where the energy contour is perpendicular to the lattice vector $\boldsymbol{M}$.

The point $\xi^{\boldsymbol{M}}$ corresponds to the action vector $\boldsymbol{I}^{\boldsymbol{M}}$, that is, to a particular invariant torus of orbits that contributes to the $\boldsymbol{M}$th integral in the series (8) for $n(E)$. Now, if we differentiate $H(\boldsymbol{I})$ with respect to any ξ_i, we must obtain zero because of the definition of the ξ. Therefore

$$\frac{\partial H}{\partial \xi_i} = \nabla_{\boldsymbol{I}} H \cdot \frac{\partial \boldsymbol{I}}{\partial \xi_i} = \boldsymbol{\omega}\cdot\frac{\partial \boldsymbol{I}}{\partial \xi_i} = 0. \tag{13}$$

These are the same form as the stationary phase conditions (12), so that on the contributing torus $\boldsymbol{I} = \boldsymbol{I}^{\boldsymbol{M}}$ we have

$$\boldsymbol{\omega}(\boldsymbol{I}^{\boldsymbol{M}}) \propto \boldsymbol{M}, \quad \text{i.e.} \quad \omega_1 : \omega_2 : \ldots \omega_n = M_1 : M_2 : \ldots M_n. \tag{14}$$

But the M_i are integers, so that we have shown the ω_i to be *commensurable* and the orbits on the torus $\boldsymbol{I}^{\boldsymbol{M}}$ are all *closed*. Closure occurs after M_1 periods of the angle coordinate θ_1, M_2 periods of $\theta_2 \ldots M_n$ periods of θ_n. Therefore $\boldsymbol{M}$ defines the *topology* of the periodic orbit. That is why we called the set of all $\boldsymbol{M}$ the topological lattice, and why we shall call the series (8) the *topological sum*. The action round the closed orbit $\boldsymbol{I}^{\boldsymbol{M}}$ is

$$W(\boldsymbol{M}) = 2\pi M_1 I_1^{\boldsymbol{M}} + \ldots 2\pi M_2 I_2^{\boldsymbol{M}} = 2\pi \boldsymbol{M}\cdot\boldsymbol{I}^{\boldsymbol{M}}. \tag{15}$$

In figure 2 we sketch orbits in a two dimensional potential well with central repulsive core (equation (4)), for some simple topologies $\boldsymbol{M} = (M_S, M_L)$.

It is helpful to reduce $\boldsymbol{M}$ to its lowest terms by writing

$$\boldsymbol{M} = q\boldsymbol{\mu}, \tag{16}$$

where the components $\mu_1, \ldots, \mu_n$ of $\boldsymbol{\mu}$ are relatively prime, and q is a positive integer. Then equation (15) shows that the orbital action is

$$W(\boldsymbol{M}) = qW(\boldsymbol{\mu}). \tag{17}$$

Obviously all lattice points $\boldsymbol{M}$ with the same $\boldsymbol{\mu}$ will satisfy the same stationary phase equation (14), whatever the value of q. The value $q = 1$ corresponds to a single traversal of a closed orbit, while higher values correspond to multiple traversals. We say that lattice points $\boldsymbol{M}$ with the same $\boldsymbol{\mu}$ lie on a *ray* in the topological lattice.

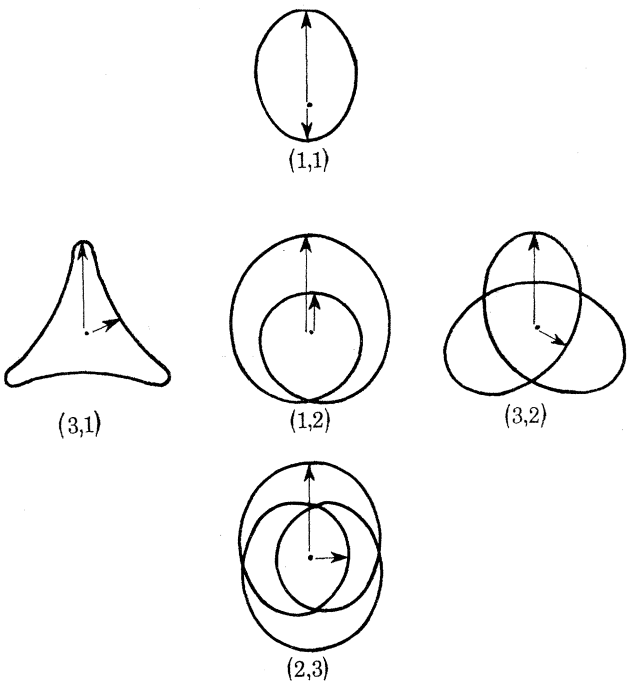

FIGURE 2. Some simple orbit topologies (M_S, M_L) in central potential well with repulsive core. Arrows indicate r_1 and r_2.

Returning to the stationary-phase evaluation of the integral (11), we need to evaluate the $(n-1)$ order determinant of second derivatives of the phase, namely

$$\det\left\|\frac{2\pi}{\hbar}\boldsymbol{M}\cdot\frac{\partial^2\boldsymbol{I}}{\partial\xi_i\partial\xi_j}\right\| = \left(\frac{2\pi q}{\hbar}\right)^{n-1}\det\left\|\boldsymbol{\mu}\cdot\frac{\partial^2\boldsymbol{I}}{\partial\xi_i\partial\xi_j}\right\|. \tag{18}$$

Now $\boldsymbol{\mu}\cdot(\partial^2\boldsymbol{I}/\partial\xi_i\partial\xi_j)$ is proportional to the component normal to the energy contour of the derivatives of the tangent vectors $\partial\boldsymbol{I}/\partial\xi_i$, i.e. proportional to the *normal curvatures* of the energy contour. Therefore

$$\det\left\|\boldsymbol{\mu}\cdot\frac{\partial^2\boldsymbol{I}}{\partial\xi_i\partial\xi_j}\right\| = |\boldsymbol{\mu}|^{n-1}K(\boldsymbol{I}), \tag{19}$$

where $K(\boldsymbol{I})$ is a *scalar curvature* of the energy contour (in a two dimensional system K is the curvature of a line, in a three dimensional system K is the Gaussian curvature of a surface).

Let $\beta(\boldsymbol{\mu})$ be the excess of positive over negative eigenvalues of the matrix $\boldsymbol{\mu}\cdot\partial^2\boldsymbol{I}/\partial\xi_i\,\partial\xi_j)$. Then the integral (11) becomes, in the stationary phase approximation

$$n_M = \left(\frac{\hbar}{q|\boldsymbol{\mu}|}\right)^{\frac{1}{2}(n-1)} \frac{\mathrm{e}^{\mathrm{i}q(W(\mu)/\hbar)+\mathrm{i}\frac{1}{4}\pi\beta(\mu)}}{|\omega(\boldsymbol{I}^\mu)|\sqrt{|K(\boldsymbol{I}^\mu)|}}. \tag{20}$$

This must now be inserted into the topological sum (8) over rays $\boldsymbol{\mu}$ and repetitions q. Only these rays satisfying (14) contribute, and because all ω_i are positive this means that all components μ_i of any ray $\boldsymbol{\mu}$ must have the same sign, so that only points in the first and third 'quadrants' of the topological lattice and points on the boundaries of these 'quadrants', will contribute to the sum. We thus obtain the *simple semi-classical formula* for the density of states:

$$n(E) = n_{TF}(E) + \frac{2}{\hbar^{\frac{1}{2}(n+1)}} \sum_{\substack{\boldsymbol{\mu} \\ \text{(1st 'quadrant' and boundary)}}} \frac{1}{|\boldsymbol{\mu}|^{\frac{1}{2}(n-1)}|\omega(\boldsymbol{I}^\mu)|\sqrt{|K(\boldsymbol{I}^\mu)|}} \sum_{q=1}^{\infty} \times \frac{\cos\left[q(W(\boldsymbol{\mu})/\hbar - \frac{1}{2}\pi\boldsymbol{\alpha}\cdot\boldsymbol{\mu}) + \frac{1}{4}\pi\beta(\boldsymbol{\mu})\right]}{q^{\frac{1}{2}(n-1)}}. \tag{21}$$

In practice the condition (14) often excludes many rays $\boldsymbol{\mu}$ – those which are normal to no part of the energy contour. In the case sketched in figure 1, for example, the energy contour deviates little from a plane and only rays lying within a fairly narrow cone in the topological lattice will contribute to $n(E)$.

Each term in (21) depends on properties of those tori $\boldsymbol{I}$ that lie on the energy contour E and whose orbits are closed because their frequencies $\boldsymbol{\omega}$ are commensurable. Because rational numbers constitute a subset of measure zero in the set of all real numbers, these contributing tori, although infinite in number, are infinitely sparsely distributed on the energy contour E. Therefore the formula (21), involving closed orbits, is a highly non-trivial representation of the E.B.K. condition (7).

The action W, curvature K and frequencies $\boldsymbol{\omega}$ corresponding to a given ray $\boldsymbol{\mu}$ all change with energy and thus contribute to the structure of the spectrum $n(E)$. It is tempting to evaluate each 'ray' sum over q analytically in (21), in terms of series of Riemann ζ-functions (Balian & Bloch 1972, p. 132). In the three dimensional case the series is particularly simple, being given by

$$\sum_{q=1}^{\infty} \frac{\mathrm{e}^{\mathrm{i}qA}}{q} = \ln(2\sin\tfrac{1}{2}A) + \mathrm{i}\tfrac{1}{2}(A-\pi) \quad (0 < A < 2\pi). \tag{22}$$

The real and imaginary parts of this periodic function of A give rise to a striking structure of 'scallops' and 'sawteeth'. However, it is a relatively rare occurrence for a single ray (that is, all the repetitions of a single closed orbit) to dominate the spectrum and the scallop and sawtooth structures from each ray are usually obscured in the superposition of several rays (Tabor 1976). In one dimension this does not occur; there is only one ray and the whole spectrum arises from repeated traversals of a single orbit (see § 7.4 of I).

The δ-functions (7) from which we started arise from divergences of the ray

summation in (21). These occur for rays in whose neighbourhood $W/\hbar - \frac{1}{2}\pi\boldsymbol{\alpha}.\boldsymbol{\mu}$ equals an integer, and in this way we can easily reclaim precisely the E.B.K. conditions (5). Gutzwiller (1970) gives a similar argument. In a later paper, however, Gutzwiller (1971) obtains a different quantum condition involving a single quantum number, by considering repeated traversals of one closed orbit. This quantum condition is intended to apply to non-separable systems and involves the stability parameters of the chosen orbit; these emerge from Gutzwiller's analysis after taking the trace of the Green function and employs the method of stationary phase on the assumption that the orbit is isolated. Later authors (Voros 1976; Miller 1975; Rajaraman 1975; Dashen Hasslacher & Neveu 1975) modify his method and obtain a quantum condition that still involves the stability parameters, but now contains a complete set of quantum numbers. We maintain that these quantum conditions certainly do not describe the regular spectrum because the summations employed in their derivation fail to include all the closed orbits that exist at a given energy. First, no account is taken of the fact that there are orbits with different topologies, whose lattice vectors $\boldsymbol{\mu}$ are, as we have seen, intimately related to the quantum numbers. Secondly, each closed orbit is assumed to be isolated, but if action-angle variables exist and the closed orbits form a continuous family filling the torus then stationary phase cannot be employed for taking the trace of the Green functions; the trace over the continuous family can however, be taken correctly by a trivial integration over angle variables $\boldsymbol{\theta}$, and in this way we have obtained precisely the result (21) starting from the Green function method. It is possible that the quantum conditions involving stability angles might apply to non-regular cases, but we point out that even here stable closed orbits will be surrounded by quasi periodic ones (Birkhoff 1927), and probably form complicated families.

4. Complex closed orbits

The topological sum (21), over all the closed orbits at the energy E, was derived by applying the method of stationary phase to the integrals (11). There are several ways in which this method can fail. Suppose for example that there are on the energy contour regions of dimension less than $n-1$ on which the curvature K is zero. These regions separate places where the normal to the energy contour can point in the same direction. Therefore there can be more than one family of orbits with a given topology $\boldsymbol{\mu}$, that is, more than one invariant torus $\boldsymbol{I}^{\mu}$ satisfying the stationary phase conditions (12). For rays $\boldsymbol{\mu}$ in the topological lattice whose directions approach those ($\boldsymbol{\mu}_c$) of the normals along the regions where K vanishes, the corresponding contributing tori, and hence the stationary points of the integrals (11) approach and coalesce. In these circumstances the result (21) is invalid and must be replaced by a uniform approximation whose form depends on the manner in which the coalescence occurs. Physically, the region $K = 0$ would give rise to a large peak in $n(E)$, a dense cluster of energy levels. The simplest region $K = 0$ is a point of inflexion on the energy contour for a two dimensional case, and the corresponding feature

in $n(E)$ could be called a 'bound state rainbow' (see I, § 6.3). More complicated coalescences would give rise to higher order 'catastrophes' (Thom 1975; Connor 1975; Duistermaat 1974). At present we know of no case involving smooth potentials where the energy contours have inflexions $K = 0$, and so we do not consider these coalescences any further here (Balian & Bloch (1972) study an enclosure in the shape of a waisted Greek vase whose modes show a rainbow).

When K never changes sign there can only be one torus $\boldsymbol{I}^{\mu}$ for each orbit topology $\boldsymbol{\mu}$. However, if this lies outside the range of integration in (11), that is if any action variable I_i^{μ} is negative, then the torus does not contribute to the sum (21). Now, as E changes, the torus $\boldsymbol{I}^{\mu}$ for fixed $\boldsymbol{\mu}$ moves along a smooth trajectory in $\boldsymbol{I}$ space and can cross the integration boundary into the region where all I_i are positive. Therefore contributions to the sum (21) can appear suddenly as E changes, giving rise to discontinuities in $n(E)$. In reality the contributions must appear gradually, and the method of stationary phase must be modified to cover cases where the stationary point can be close to the boundary of integration.

We shall see that it is necessary to include in the topological sum tori for which some components I_i are slightly negative. When the coordinate motion is a libration these tori correspond to *complex closed orbits* with the topology $\boldsymbol{\mu}$. For as I_i diminishes through zero the limits of the libration (e.g. r_1 and r_2 in equation (4)) approach, coalesce and separate as a pair of complex quantities (this is trivial to demonstrate explicitly for a harmonic oscillator.) These complex orbits giving 'periodic motion below the bottom of a well' have the interesting feature that all their constants of the motion are real, in contrast to, say, complex orbits beyond caustics (see § 7.3 of I) where some constants of the motion are complex (e.g. the angular momentum in rainbow scattering).

Before describing how to include complex orbits in the topological sum, we point out yet another deficiency of the simple semiclassical formula (21): it fails to give correctly the harmonic oscillator limit! In this limit the Hamiltonian is a linear function (3) of the actions, the curvature K of the energy contours vanishes everywhere, and the terms of (21) diverge. The harmonic limit arises for particles bound in potential wells with a single minimum as the energy tends to that of the bottom of the well or as the anharmonicity is switched off. The limit does not arise in circular potential wells with a repulsive core, because the well topology is that of a circular trough rather than a single minimum, and it turns out that even the low energy contours are curved (§ 6). Rather surprisingly, the same modification to (21) that gives the contribution of the complex orbits also ensures that $n(E)$ has the correct harmonic oscillator limit.

In discussing the modification of (21) we restrict ourselves to the two dimensional case, where (figure 3) the energy contour is a line parameterized by a single variable ξ, and the integration boundary consists simply of two end points ξ_1 and ξ_2 at which the actions, I_1 and I_2, correspond to one dimensionally periodic motions with topologies μ_1 and μ_2 (figure 3). For a given ray $\boldsymbol{\mu}$ there is a single stationary point, the torus $\boldsymbol{I}^{\mu}$, corresponding to a value ξ_{μ} that may or may not lie between ξ_1 and ξ_2.

To evaluate (11) we use a method of integration explained in the appendix, and the result is that instead of (20) the topological lattice vector $\boldsymbol{M}$ gives the following contribution:

$$n_{\boldsymbol{M}} \equiv \int_{\xi_1}^{\xi_2} \mathrm{d}\xi \frac{\mathrm{e}^{(2\pi\mathrm{i}/\hbar)\boldsymbol{M}\cdot\boldsymbol{I}(\xi)}}{|\boldsymbol{\omega}(\boldsymbol{I}(\xi))|} \tag{23}$$

$$= \left(\frac{\hbar}{2\pi q|\boldsymbol{\mu}|K_{\mu}}\right)^{\frac{1}{2}} \frac{\mathrm{e}^{\mathrm{i}q(W(\mu)/\hbar)}}{|\boldsymbol{\omega}_{\mu}|} \int_{\Lambda_1/\sqrt{\hbar}}^{\Lambda_2/\sqrt{\hbar}} \mathrm{d}X\, \mathrm{e}^{\mathrm{i}\frac{1}{2}\beta X^2} + \frac{\hbar}{2\pi\mathrm{i}q}\left(\frac{\mathrm{e}^{\mathrm{i}q(W_2/\hbar)}}{|\boldsymbol{\omega}_2|\boldsymbol{\mu}_2\cdot\boldsymbol{I}_2'|} - \frac{\mathrm{e}^{\mathrm{i}q(W_1/\hbar)}}{|\boldsymbol{\omega}_1|\boldsymbol{\mu}_1\cdot\boldsymbol{I}_1'|}\right)$$

$$-\left(\frac{1}{2\pi q|\boldsymbol{\mu}|K_{\mu}}\right)^{\frac{1}{2}} \frac{\hbar}{\beta|\boldsymbol{\omega}_{\mu}|}\left(\frac{\mathrm{e}^{\mathrm{i}q(W_2/\hbar)}}{\Lambda_2} - \frac{\mathrm{e}^{\mathrm{i}q(W_1/\hbar)}}{\Lambda_1}\right). \tag{24}$$

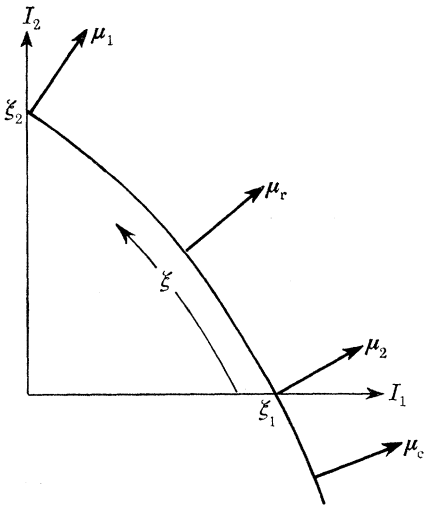

FIGURE 3. Real ($\boldsymbol{\mu}_r$), complex $\boldsymbol{\mu}_c$) and limiting ($\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$) rays contributing to $n(E)$.

Here the quantities Λ_1 and Λ_2 are defined by

$$\Lambda_{1,2} \equiv [(2q/\beta)(W_{1,2} - W(\boldsymbol{\mu}))]^{\frac{1}{2}} \quad (\Lambda_{1,2} \gtrless 0 \quad \text{if} \quad \xi_{1,2} \gtrless \xi_{\mu}), \tag{25}$$

the subscripts 1, 2, $\boldsymbol{\mu}$ denote quantities evaluated at $\boldsymbol{I}(\xi_1)$, $\boldsymbol{I}(\xi_2)$, $\boldsymbol{I}^{\mu}$, $\beta = \pm 1$ if the energy contour is concave/convex away from $\boldsymbol{I} = 0$, and primes denote $\partial/\partial\xi$.

The integral in (24) is of the Fresnel type (Abramowitz & Stegun 1964), tabulated or easily computed. To obtain $n(E)$ it is necessary to sum contributions (24) over topologies $\boldsymbol{M} = q\boldsymbol{\mu}$. The resulting formula, which supersedes (21), still involves only the *closed orbits at energy E*, even though each of the 'endpoint' tori $\boldsymbol{I}_1$ and $\boldsymbol{I}_2$ has incommensurable frequencies $\boldsymbol{\omega}$. The reason is that for $\boldsymbol{I}_1$ and $\boldsymbol{I}_2$ one of the two periods has zero amplitude of motion, so that its frequency is irrelevant and the orbit is one dimensional and closed.

There are four limiting cases; to study them, it is convenient to label terms in (24) as I, II and III. We simply state the results – the derivations are tedious but elementary.

Case a: real contributing torus. ξ_1 and ξ_2 are not close together, and ξ_μ lies between them. In term I of (24) Λ_1 and Λ_2 can be set equal to $\mp\infty$ respectively, and the integral then becomes $\sqrt{(2\pi)}\,\mathrm{e}^{\mathrm{i}\frac{1}{4}\pi\beta}$. Term I is then precisely equal to the stationary phase result (20) for this case, and is $O(\hbar^{\frac{1}{2}})$. Terms II and III are $O(\hbar)$, and therefore negligible by comparison.

Case b: complex contributing torus. ξ_1 and ξ_2 are not close together and ξ_μ does not lie between them. In term I, Λ_1 and Λ_2 both have the same sign and therefore the stationary point $X = 0$ is not included in the range. Therefore the integral can be evaluated asymptotically by integration by parts, whereupon terms I and III cancel. This leaves term II, which is precisely the result of evaluating the original formula (23) by partial integration. In this case n_M is $O(\hbar)$, so that as expected the complex tori give small contributions.

Case c: harmonic oscillator limit with incommensurable frequencies. The energy contour tends to a straight line that is not normal to any topological lattice vector $\boldsymbol{M}$, so that there are no stationary points between ξ_1 and ξ_2. We model this situation by writing the exponent in (23) as

$$\frac{2\pi\boldsymbol{M}\cdot\boldsymbol{I}(\xi)}{\hbar} = A + B\xi + \tfrac{1}{2}\epsilon\xi^2, \tag{26}$$

where we shall let the anharmonicity ϵ tend to zero. A and B are nonzero constants, positive without loss of generality, and $\beta = +1$ if ϵ is positive. The stationary point at ξ_c is

$$\xi_c = -B/\epsilon, \tag{27}$$

and recedes to infinity in the harmonic limit. The limits $\Lambda_{1,2}$ are

$$\Lambda_{1,2} = [2B\xi_{1,2} + \epsilon\xi_{1,2}^2 + B^2/\epsilon]^{\frac{1}{2}} \to B/\epsilon^{\frac{1}{2}}, \tag{28}$$

which also recede to infinity but slower than, and in the opposite direction to, ξ_c which therefore lies outside them. Therefore term I can be evaluated by partial integration, and it cancels with term III. Moreover these cancelling terms are finite, since $\Lambda_{1,2}$ is $O(\epsilon^{-\frac{1}{2}})$ and K_μ is $O(\epsilon)$. This leaves term II, which we evaluate by setting $|\boldsymbol{\omega}|$ equal to a constant, ω_0. The result is

$$n_M = 2\,\mathrm{e}^{\mathrm{i}(A+\frac{1}{2}B(\xi_2+\xi_1))}\sin\tfrac{1}{2}B(\xi_2-\xi_1)/B\omega_0, \tag{29}$$

which is the exact value of the original integral (23) when $\boldsymbol{I}(\xi)$ is given by (26).

Case d: harmonic oscillator limit with commensurable frequencies. The energy contour tends to a straight line that is normal to a ray $\boldsymbol{\mu}$ of the topological lattice, so that there is a stationary point between ξ_1 and ξ_2. If we take $\xi_1 < 0$ and $\xi_2 > 0$, this situation can be modelled by (26) with B set identically zero, so that (equation (27)) $\xi_c = 0$ for all ϵ. Terms II and III are now both $O(\epsilon^{-1})$ but they cancel identically. This leaves term I. From (28) the range of integration has width

$$\frac{\Lambda_2}{\sqrt{\hbar}} - \frac{\Lambda_1}{\sqrt{\hbar}} = \sqrt{\left(\frac{\epsilon}{\hbar}\right)}\,(\xi_2-\xi_1), \tag{30}$$

which vanishes as $\epsilon \to 0$, so that the integral is trivially evaluated by setting its integrand equal to unity. The result is that (24) becomes

$$m_M = \mathrm{e}^{\mathrm{i}A}/\omega_0. \tag{31}$$

But this is just (29) with $B = 0$, and so our approximation again gives the exact value for n_M.

In view of these limiting cases we are confident that (24) is a uniform approximation to n_M that gives correctly the contributions of the closed orbits in all cases where the energy contours have no inflections. The density of states $n(E)$ can then be obtained from equations (8–11).

5. Smoothing and level clustering

When all the energy levels are resolved it is not easy to perceive the different scales on which clustering occurs. Therefore we follow Balian & Bloch (1972) and introduce the *smoothed density of states* $n_\gamma(E)$ which results when E is given an imaginary part $\mathrm{i}\gamma$. If E_m are the exact energy levels corresponding to quantum numbers $\boldsymbol{m} = (\mathrm{m}_1, \ldots, m_n)$ (cf. the E.B.K. approximation (6)), this procedure gives

$$n_\gamma(E) = \frac{\mathrm{Im}}{\pi} \sum_{\boldsymbol{m}} \frac{1}{E_m - E - \mathrm{i}\gamma} = \sum_{\boldsymbol{m}} \frac{\gamma/\pi}{(E-E_m)^2 + \gamma^2}, \tag{32}$$

so that each δ-function level is smoothed in a Lorentzian manner.

The effect of smoothing on the semiclassical formulae is simple only when $\gamma \ll E$, and we confine ourselves to this case. The effect of γ will be strongest in the phases of the orbit contributions in (20) and (24), since these are magnified by the factor $\hbar^{-1}$. Therefore we expand the orbital action to the first order in γ:

$$W(E+\mathrm{i}\gamma) - W(E) \approx \mathrm{i}\gamma \frac{\partial W}{\partial E} = 2\pi\mathrm{i}\gamma \boldsymbol{M} \cdot \frac{\partial \boldsymbol{I}}{\partial E}. \tag{33}$$

But

$$\frac{\partial H}{\partial E} = \nabla_I H \cdot \frac{\partial \boldsymbol{I}}{\partial E} = \boldsymbol{\omega} \cdot \frac{\partial \boldsymbol{I}}{\partial E} = 1, \tag{34}$$

so that in view of (14) we can write (33) as

$$2\pi\mathrm{i}\gamma \boldsymbol{M} \cdot \frac{\partial \boldsymbol{I}}{\partial E} = \mathrm{i}\gamma M_i \frac{2\pi}{\omega_i}, \tag{35}$$

where I_i refers to any of the motion's multiple periods. Now, $2\pi/\omega_i$ is the time taken for the ith cycle, and the orbit closes after M_i such cycles. Therefore $M_i 2\pi/\omega_i$ is simply the *period* $T(\boldsymbol{M})$ of the orbit with topology $\boldsymbol{M}$. For q traversals we have

$$T(\boldsymbol{M}) = qT(\boldsymbol{\mu}), \tag{36}$$

where $T(\boldsymbol{\mu})$ is the period of a single traversal. Thus, finally, the action phase factors in the smoothed density of states are

$$\mathrm{e}^{\mathrm{i}W(M)/\hbar} \to \mathrm{e}^{\mathrm{i}W(M)/\hbar}\, \mathrm{e}^{-\gamma T(M)/\hbar}. \tag{37}$$

To obtain semiclassical formulae for $n_\gamma(E)$, it is necessary only to insert decay factors $\exp(-\gamma T(\boldsymbol{M})/\hbar)$ before each cosine term in (21), and to replace all actions W in the uniform approximation (24) – even those corresponding to complex orbits or one dimensional motions – by $W+\mathrm{i}\gamma T$. The decay factor ensures the convergence of the topological sum, because orbits with large $|\boldsymbol{M}|$ will have long periods irrespective of whether they consist of many traversals of a simple orbit (large q along a low-order ray $\boldsymbol{\mu}$) or a single traversal of a complicated orbit ($q = 1$ and fundamental integers $\boldsymbol{\mu}$ large).

For large γ, all closed orbits are damped out of $n(E)$, which is then well approximated by the Thomas–Fermi expression (9), corresponding to $\boldsymbol{M} = 0$. As γ decreases, orbits with longer and longer periods (larger and larger values of $|\boldsymbol{M}|$) contribute to $n(E)$, giving level-clustering structure on ever finer scales until the individual levels are resolved.

6. Examples: circular and spherical potentials

Our numerical calculations of $n(E)$ are all for the separable case of a particle moving in a central potential $V(r)$ of the Morse type, namely

$$V(r) = V_0[\mathrm{e}^{-2\delta(r-r_0)} - 2\,\mathrm{e}^{-\delta(r-r_0)}], \tag{38}$$

which has a well of depth V_0 whose minimum is at $r = r_0$. In two dimensions the energy contours are given by equation (4) and have an approximately parabolic form. These contours are convex away from $\boldsymbol{I} = 0$ and this implies that the index β in equation (21) is always -1. As explained at the end of § 2 the 'caustic' indices $\boldsymbol{\alpha}$ are $\alpha_1 = 2$ (radial libration) and $\alpha_2 = 0$ (angular rotation).

It is convenient to use the action L as the coordinate ξ along the energy contour. Then we can express $|\omega|$ in (21) in terms of the 'arc time' $\tau(L, E)$ between apogee and perigee (half a libration), namely

$$\tau(L, E) \equiv \frac{\partial S}{\partial E}(L, E), \tag{39}$$

where $S(L, E)$ is defined by equation (4). Further, we can define the 'arc angle' $\Theta(L, E)$ swept out between apogee and perigee by

$$\Theta(L, E) \equiv -\frac{\partial S}{\partial L}(L, E); \tag{40}$$

then the curvature K can be expressed in terms of $\partial\Theta/\partial L$. For a given orbit topology $\boldsymbol{M} = (M_S, M_L)$, closure occurs after $2M_S$ arcs, and a total rotation angle of $2\pi \times M_L$. Therefore the arc angle must be

$$\Theta(L_M) = \pi\frac{M_L}{M_S}, \tag{41}$$

and this defines the angular momentum L_M of the contributing torus of orbits with topology $\boldsymbol{M}$. As L increases along the energy contour from 0 to its maximum

classically allowed value, $\Theta(L)$ increases from 0 to a value $\Theta_{\max}$, so that in the topological lattice a sector of points contributes, shown shaded in figure 4. $\Theta_{\max}$ increases with E, so that the sector opens up and more and more topologies contribute to $n(E)$.

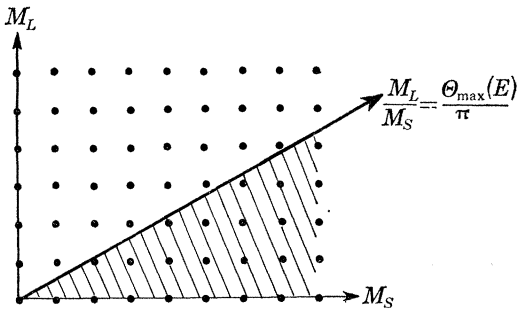

FIGURE 4. Sector (shaded) of contributing topologies for circular potential well with repulsive core.

In terms of the quantities just introduced, the simple semiclassical formula (21) becomes, with the smoothing described in § 5,

$$n_\gamma(E) = n_{TF}(E) + \frac{2}{\hbar^2\sqrt{\pi}} \sum_{M_S} \sum_{M_L} \frac{\epsilon(\boldsymbol{M})\,\tau(L_M, E)}{\sqrt{M_S(\partial\Theta(L_M)/\partial L)}} e^{-\gamma T(M)/\hbar} \cos\left[\frac{W(\boldsymbol{M})}{\hbar} - (M_S + \tfrac{1}{4})\pi\right], \tag{42}$$

where the summations include all topological lattice points in the 'allowed' sector (figure 4) in the positive quadrant, except $\boldsymbol{M} = 0$, and where $\epsilon(\boldsymbol{M})$ is a degeneracy factor equal to two if $M_L \neq 0$ (distinguishable rotations) and unity if $M_L = 0$ (pure libration between r_1 and r_2).

To calculate $n_\gamma(E)$ we use the following parameters:

$$\left.\begin{aligned} V_0 &= 0.2\,\text{eV}, \\ r_0 &= 0.25\,\text{nm}, \\ \delta &= 10\,\text{nm}^{-1}, \\ m &= 1 \text{ proton mass} \end{aligned}\right\} \tag{43}$$

(m is the reduced mass of the bound system). There are 166 bound states (not including degeneracy), whose positions were computed by integrating the radial Schrödinger equation by the Numerov–Cooley method.

We begin with a case of no smoothing ($\gamma = 0$). Figures 5*a–d*, computed for a narrow range of the spectrum ($-0.1\,\text{eV} < E < -0.085\,\text{eV}$) show the effect of including increasing numbers of closed orbits in the simple semiclassical formula (42). In each case $n_{TF}(E)$ is shown as a dashed line, and on figure 5*d*, the exact positions of the levels are marked with arrows. We include all orbits in the allowed sector for which $M_s < 4$ (figure 5*a*), 10 (5*b*), 30 (5*c*), 50 (5*d*). It is quite clear how the Thomas–Fermi background is progressively eaten away and replaced by discrete levels. The use of the uniform approximation in this case gives no significant improvement.

Next (figure 6) we introduce a smoothing width $\gamma = 0.001\,\text{eV}$, and plot a wider

energy range ($-0.1\,\mathrm{eV} < E < -0.06\,\mathrm{eV}$). The full line is the exactly calculated $n_\gamma(E)$, the dotted line is the simple semiclassical approximation and the dashed line is the uniform approximation based on equation (24). Clearly the complex closed orbits now considerably improve the accuracy of the topological sum.

Figure 7 is similar to figure 6 but the smoothing, $\gamma = 0.0025\,\mathrm{eV}$, is greater and the spectrum shows less structure. Again the uniform approximation gives a significant increase in accuracy.

Finally, in figure 8 we present the complete spectrum $n_\gamma(E)$ with smoothing $\gamma = 0.0025\,\mathrm{eV}$, comparing exact calculations (full line) with the uniform approximation (dotted line). Again the agreement is good.

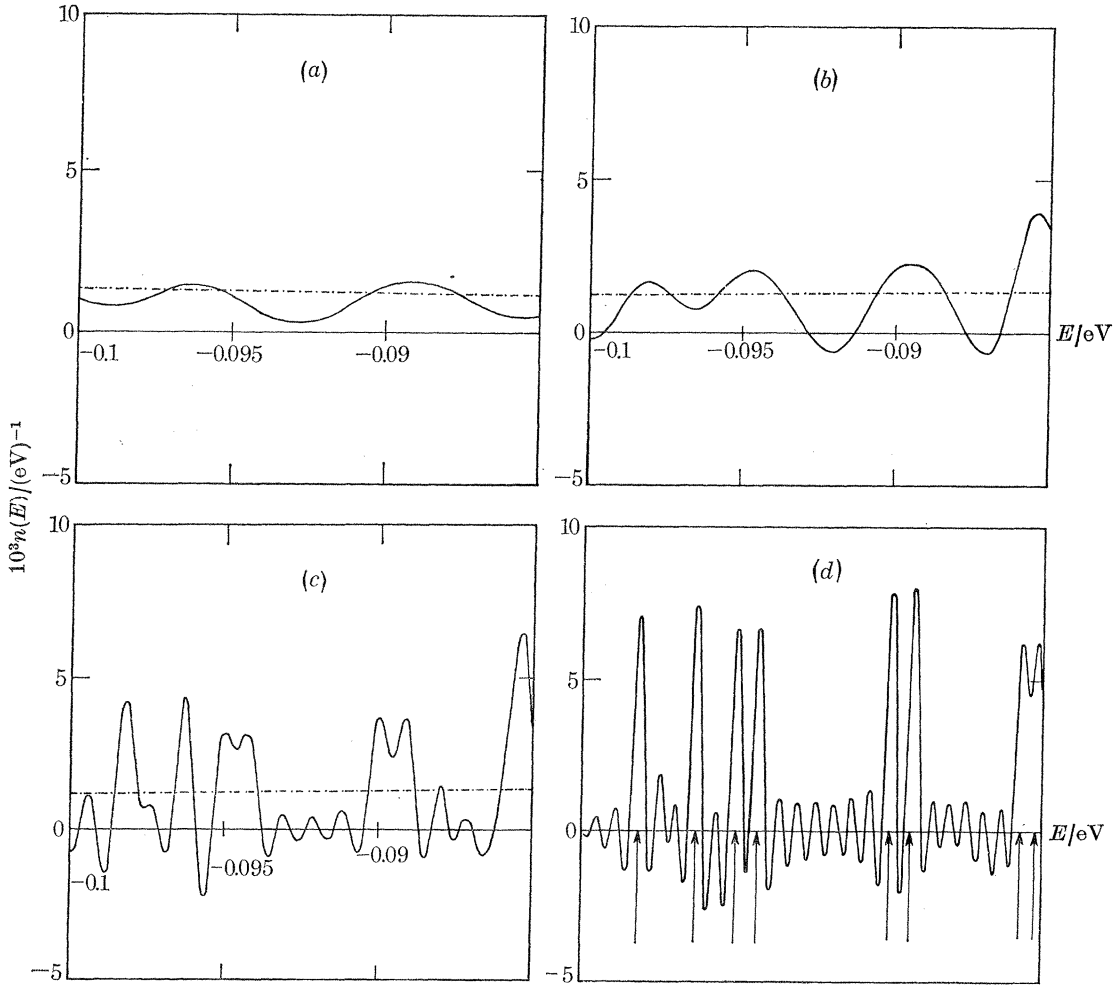

FIGURE 5. Density of states for a circular Morse potential, calculated from the simple semiclassical formula (42), without smoothing and including all topologies for which M_S does not exceed (*a*) 4, (*b*) 10, (*c*) 30, (*d*) 50. The chain curves are n_{TF} and the arrows on (*d*) mark exact quantum levels.

Now we turn to the *three dimensional* case where $V(r)$ represents a spherical rather than a circular potential. There are 159 bound states, because the centrifugal potential $l(l+1)/r^2$ is slightly more repulsive than $(l^2-\frac{1}{4})/r^2$. The structure of the spectrum differs considerably from the two dimensional case as a result of three seemingly innocent modifications of the simple semiclassical formula (42). The first is a change in the degeneracy factor $\epsilon(\boldsymbol{M})$, which now becomes

$$\epsilon(\boldsymbol{M}) = \frac{2L_M}{\hbar} (= 2l+1). \tag{44}$$

This eliminates the tori corresponding to pure librations ($M_L = 0$). The degeneracy arises, of course, from the different values of the z-component L_z of the angular momentum. The second modification arises from the same source: the rotational motion, as well as the radial motion, now has caustics. To see this we project onto the unit r-sphere all those orbits with fixed S, L and L_z. They form a family enveloped by parallels on the sphere, and these caustics lead to an extra term $-M_L\pi$ in the cosine factor of (42). The third modification is an obvious change in $n_{TF}(E)$

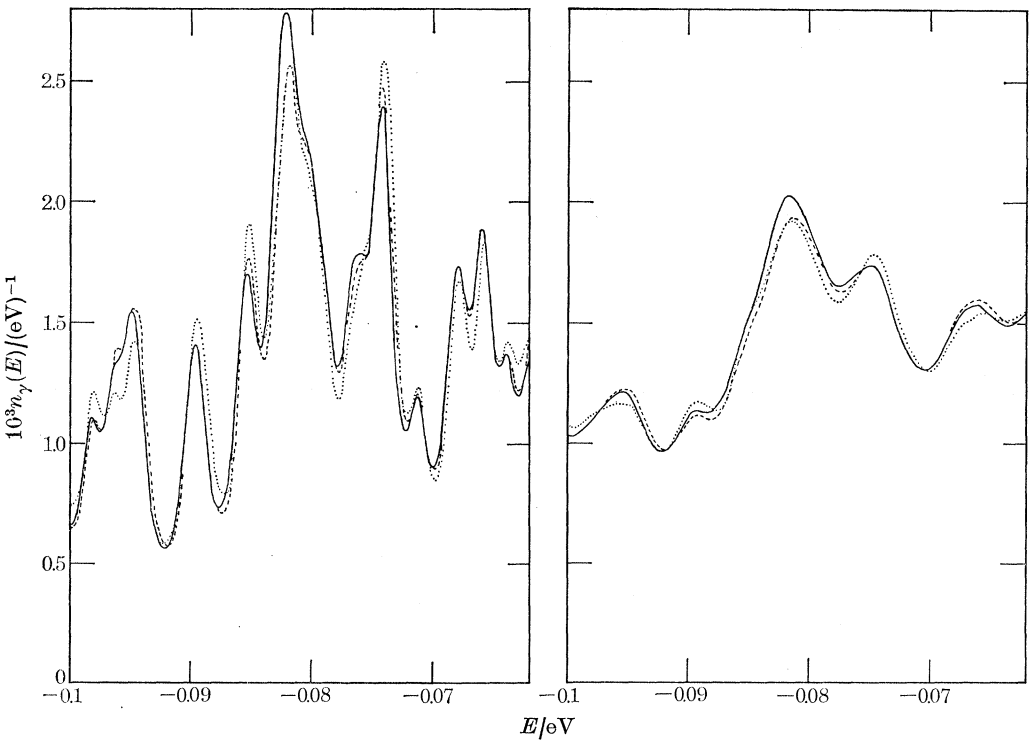

FIGURE 6 FIGURE 7

FIGURES 6 and 7. Density of states in a circular Morse potential, with smoothing width $\gamma = 0.001$ eV (figure 6) and $\gamma = 0.0025$ eV (figure 7). ——, Exact quantum calculation; • • •, simple semiclassical formula; - - - -, uniform approximation.

(equation 9). For $\gamma = 0$ the resulting simple semiclassical approximation can be shown to be identical with equation (44) of Gutzwiller (1970).

We show in figures 9–12 spectra corresponding exactly to the two-dimensional figures 5–8. The density of states is much more complicated, and the overall agreement is not quite so good, but it is still clear that the topological sum gives a rather

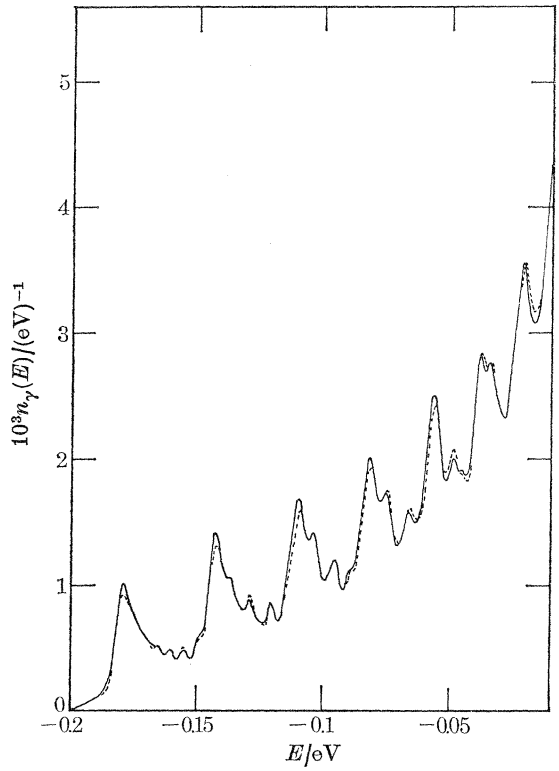

FIGURE 8. Complete spectrum for circular Morse potential with smoothing width $\gamma = 0.0025$ eV. ——, Exact quantum calculation; - - -, uniform approximation.

accurate description. On figure 9 the δ-functions now appear with different strengths, and it is satisfying that these are approximately proportional to $2l+1$ (the values of l, and also the principal quantum number n, are marked on figure 9*d*). Finally on figure 11 the simple semiclassical curve has a small discontinuity at $E = -0.0875$ eV, because of the sudden appearance of the low order ray $\boldsymbol{\mu}$ of tori with $M_S = 3M_L$. The uniform approximation removes this discontinuity.

7. Conclusions

By transforming the generalized quantum conditions of Einstein, Brillouin & Keller, we are able to describe the spectrum of bound energy levels entirely in terms of the closed classical orbits. By employing action-angle variables we arrive

at a formalism that applies in any number of dimensions and to separable and non-separable systems alike, the only condition for its validity being that the classical motion must be multiply periodic rather than ergodic. The analysis does not involve parameters of orbital stability as employed by, for example, Gutzwiller (1971).

The advantages of starting from the quantum conditions and deriving a topological sum, rather than proceeding in the reverse direction, are that the manner in which the full complement of quantum numbers arises, and the manner in which the complex closed orbits contribute, are clearly exhibited.

Numerically, the topological sum (with complex orbits) gives a rather accurate

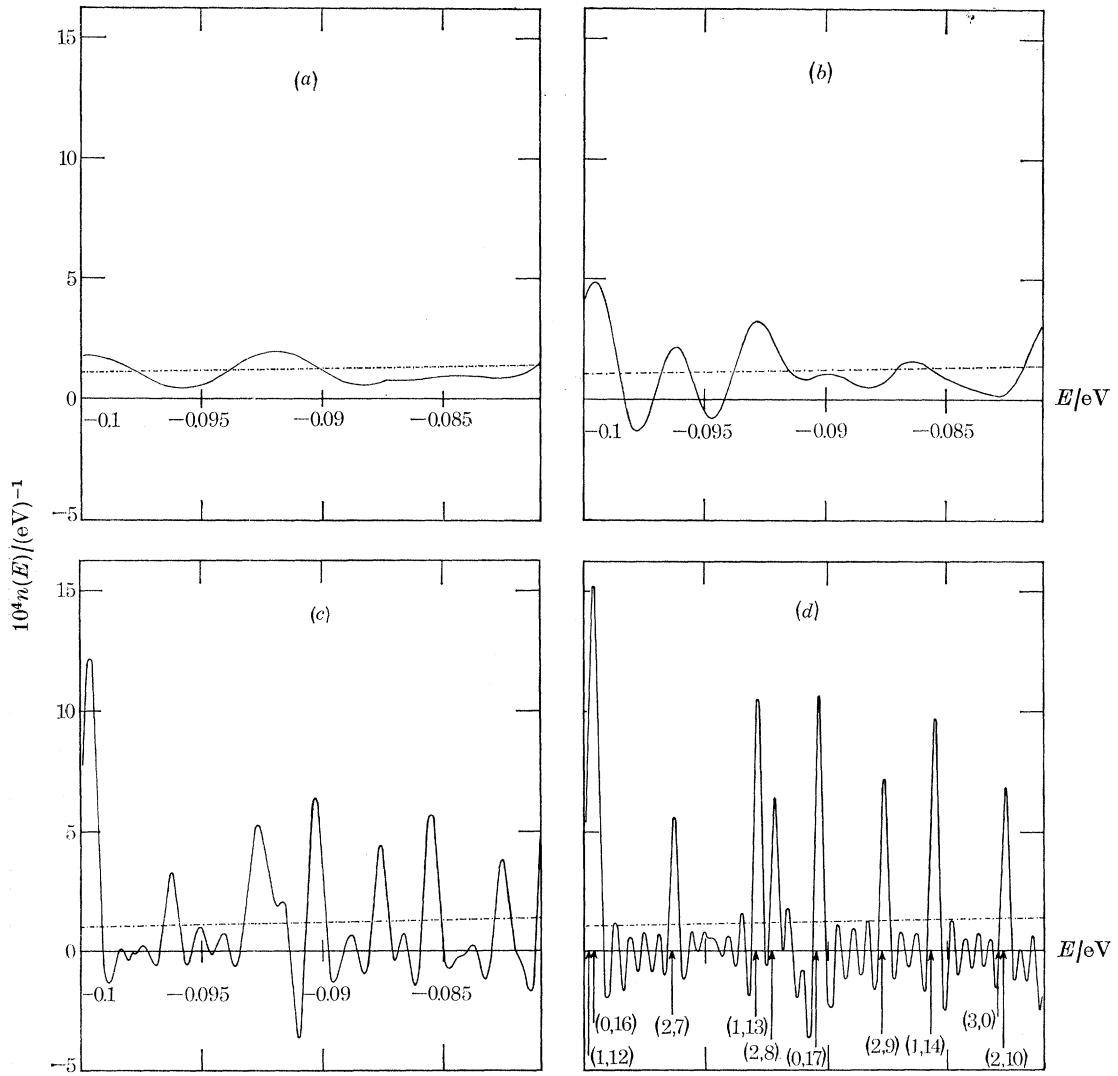

FIGURE 9. Three dimensional (spherical) case corresponding to figure 5. On 9*d* the quantum numbers (n, l) are marked on each level.

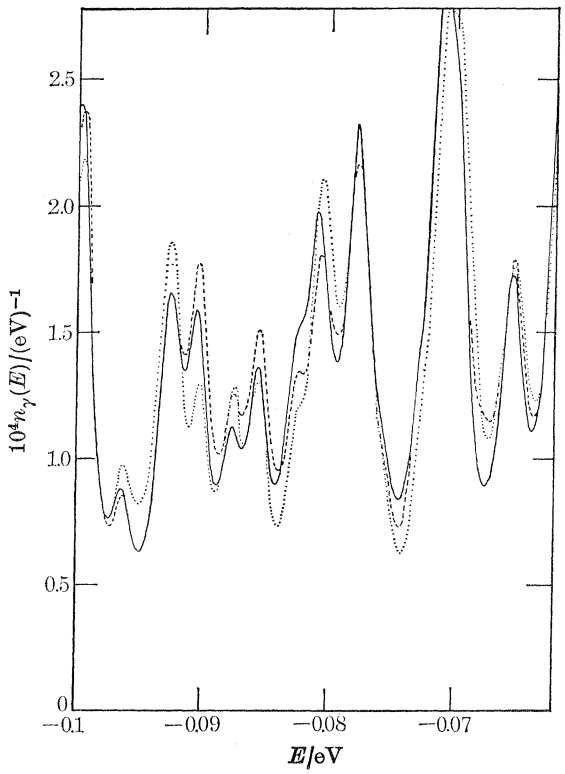

FIGURE 10. Three dimensional (spherical) case corresponding to figure 6.

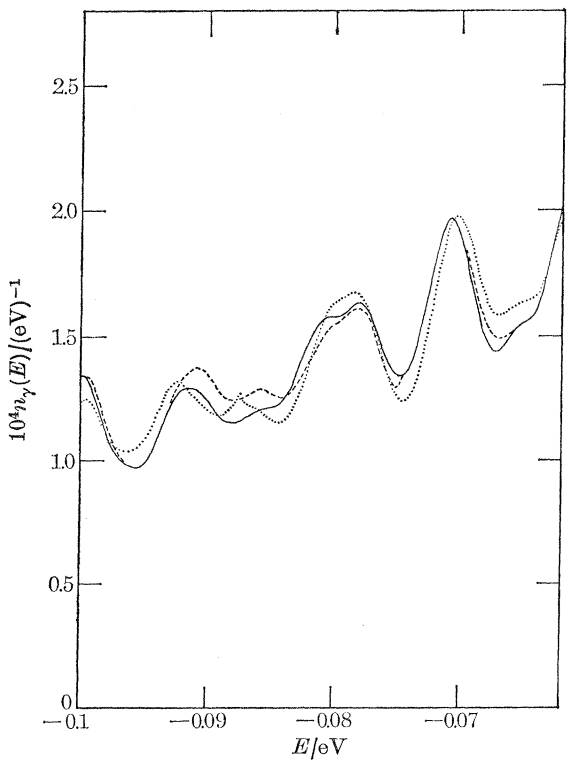

FIGURE 11. Three dimensional (spherical) case corresponding to figure 7.

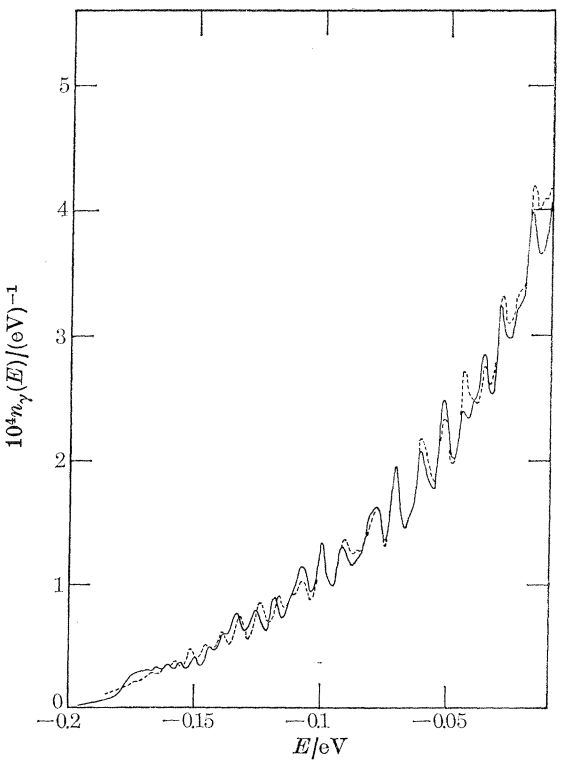

FIGURE 12. Three dimensional (circular) case corresponding to figure 8.

description of the spectrum, especially when smoothed by the prescription of Balian & Bloch (1972, 1974).

We have emphasized that the E.B.K. conditions and our transformations of them give the semiclassical limit of the quantum spectrum only when the classical orbits are confined to invariant tori. Almost nothing is known about the spectrum in cases where the classical motion is ergodic. Percival (1973) conjectures that the spectrum is 'irregular', meaning that in some sense the levels are randomly distributed. This suggests that for ergodic classical motion the semi-classical limit does not exist: reducing $\hbar$ (in comparison with classical quantics having the dimensions of action) simply uncovers an increasing complexity of classical path structure, rather than a smooth manifold of trajectories which could form the basis of a regular distribution of energy levels.

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References

Abramowitz, M. & Stegun, I. 1964 *Handbook of mathematical functions* National Bureau of Standards.
Arnol'd, V. I. 1963 *Russian Mathematical Surveys*, **18**, no 5, 13–40. **18**, no. 6, 85–192.
Arnol'd, V. I. & Avez, A. 1968 *Ergodic problems of classical mechanics*, New York: W. A. Benjamin, Inc.
Balian, R. & Bloch, C. 1972 *Ann. Phys.* **69**, 76–160.
Balian, R. & Bloch, C. 1974 *Ann. Phys.* **85**, 514–45.
Berry, M. V. & Mount, K. E. 1972 *Rep. Prog. Phys.* **35**, 315–397.
Birkhoff, G. D. 1927 *Dynamical systems*. New York: American Mathematical Society.
Born, M. 1927 *The mechanics of the atom*. London: G. Bell & Sons, Ltd.
Brillouin, L. 1926 *J. Phys. Radium* **7**, 353–368.
Chapman, S , Garrett, B. C. & Miller, W. H. 1976 To be published in *J. Chem. Phys.*
Connor, J. N. L. 1975 To be published in *Molec. Phys.*
Dashen, R. F., Hasslacher, B. & Neveu, A. 1975 To be published in *Phys. Rev.* D.
Duistermaat, J. J. 1974 *Comm. Pure appl. Maths.* **27**, 207–281.
Einstein, A. 1917 *Verhandl. Deut. Phys. Ges.* **19**, 82–92.
Gutzwiller, M. C. 1967 *J. Math. Phys.* **8**, 1979–2000.
Gutzwiller, M. C. 1969 *J. Math. Phys.* **10**, 1004–1020.
Gutzwiller, M. C. 1970 *J. Math. Phys.* **11**, 1791–1806.
Gutzwiller, M. C. 1971 *J. Math. Phys.* **12**, 343–358.
Henon, M. & Heiles, C. 1964 *Astron. J.* **69**, 73–79.
Keller, J. B. 1958. *Ann Phys.* **4**, 180–188.
Kolmogorov, A. N. 1954 *Doklady Akad. Nauk.* **98**, 527–530.
Kolmogorov, A. N. 1957 *Proceedings of the International Congress of Mathematicians*, Ser. II, 7th Congr.
Miller, W. H. 1975 *J. chem. Phys.* **63**, 996–999.
Moser, J. 1962 *Nachrichten Akad. Wiss. Göttingen*, no. **1**, 1–20.
Noid, D. W. & Marcus, R. A. 1975 *J. chem. Phys.* **62**, 2119–2124.
Percival, I. C. 1973 *J. Phys.* B **6**, L229–232.
Percival, I. C. & Pomphrey, N. 1975 To be published in *Molec. Phys.*
Rajaraman, R. 1975 *Phys. Rep.* **21**, no. 5, 227–313.
Tabor, M. 1976 Ph.D. Dissertation, University of Bristol.
Thom, R. 1975 *Structural stability and morphogenesis*. Massachusetts: W. A. Benjamin, Inc.
Voros, A. 1976 To be published in *Ann. Phys.*

Appendix

We seek a uniform asymptotic approximation to the integral (23), valid for small $\hbar$. The integral is of the form $I(\xi_2)-I(\xi_1)$, where

$$I(\bar{\xi}) \equiv \int_{-\infty}^{\bar{\xi}} \mathrm{d}\xi\, g(\xi)\, \mathrm{e}^{\mathrm{i}f(\xi)/\hbar}. \tag{A 1}$$

The phase is stationary, that is $f'(\xi)$ vanishes, at $\xi = \xi_c$, which may lie anywhere in relation to $\bar{\xi}$. To derive the approximation we express $I(\bar{\xi})$ in terms of the simplest 'comparison' integral with the same qualitative behaviour, namely interaction of stationary point with end point.

Define

$$J(A) \equiv \int_{-\infty}^{A/\sqrt{\hbar}} \mathrm{d}X\, \mathrm{e}^{\mathrm{i}\frac{1}{2}\beta X^2}, \tag{A 2}$$

where $\beta = \pm 1$ if $f(\xi)$ has a minimum/maximum at ξ_c, and let ξ be related to X by the mapping

$$\frac{f(\xi)}{\hbar} = A + \tfrac{1}{2}\beta X^2. \tag{A 3}$$

For a one-to-one mapping the stationary points $X = 0$ and $\xi = \xi_c$ must correspond; therefore

$$A = f(\xi_c)/\hbar. \tag{A 4}$$

For (A 2) to represent (A 1) the endpoints $X = \Lambda/\sqrt{\hbar}$ and $\xi = \bar{\xi}$ must correspond; this gives

$$A = \left[\frac{2}{\beta}(f(\bar{\xi}) - f(\xi_c))\right]^{\frac{1}{2}}, \tag{A 5}$$

where we choose $A \gtrless 0$ if $\bar{\xi} \gtrless \xi_c$. The factor β ensures that A is real.

The original integral $I(\bar{\xi})$ now becomes

$$I(\bar{\xi}) = \mathrm{e}^{\mathrm{i}f(\xi_c)/\hbar} \int_{-\infty}^{A/\sqrt{\hbar}} \mathrm{d}X\, g(\xi) \frac{\mathrm{d}\xi}{\mathrm{d}X} \mathrm{e}^{\mathrm{i}\frac{1}{2}\beta X^2}. \tag{A 6}$$

The important points X are the stationary point $X = 0$ and the end point $X = \Lambda$. Therefore we expand the non-exponential factor $g\,\mathrm{d}\xi/\mathrm{d}X$ in the form

$$g(\xi)\frac{\mathrm{d}\xi}{\mathrm{d}X} = C + DX + X(X - \Lambda/\sqrt{\hbar})\, G(X), \tag{A 7}$$

and henceforth neglect the term involving G since it vanishes at the stationary and end points. For C and D we obtain

$$\left.\begin{aligned} C &= \frac{\mathrm{d}\xi}{\mathrm{d}X}(\xi_c)\, g(\xi_c), \\ D &= \sqrt{\hbar}\left(\frac{\mathrm{d}\xi}{\mathrm{d}X}(\bar{\xi})\, g(\bar{\xi}) - \frac{\mathrm{d}\xi}{\mathrm{d}X}(\xi_c)\, g(\xi_c)\right)\Big/ A. \end{aligned}\right\} \tag{A 8}$$

Clearly we need the derivatives $\mathrm{d}\xi/\mathrm{d}X$. Differentiating the mapping relation (A 3) gives

$$\frac{\mathrm{d}\xi}{\mathrm{d}X}\frac{f'(\xi)}{\hbar} = \beta X, \quad \text{i.e.} \frac{\mathrm{d}\xi}{\mathrm{d}X}(\bar{\xi}) = \beta\frac{\Lambda\hbar}{f'(\bar{\xi})}. \tag{A 9}$$

Differentiating again gives

$$\left(\frac{\mathrm{d}\xi}{\mathrm{d}X}\right)^2\frac{f''(\xi)}{\hbar} + \frac{\mathrm{d}^2\xi}{\mathrm{d}X^2}\frac{f'(\xi)}{\hbar} = \beta, \quad \text{i.e.} \frac{\mathrm{d}\xi}{\mathrm{d}X}(\xi_c) = \sqrt{\left(\frac{\beta\hbar}{f''(\xi_c)}\right)} = \sqrt{\left(\frac{\hbar}{|f''(\xi_c)|}\right)}, \tag{A 10}$$

since $f'(\xi_c) = 0$. To obtain the uniform approximation we substitute (A 7) (without the term in $G(X)$) into (A 6), using (A 8)–(A 10) for C and D. The final result is

$$I(\bar{\xi}) = g(\xi_c)\sqrt{\left(\frac{\hbar}{|f''(\xi_c)|}\right)}\mathrm{e}^{\mathrm{i}f(\xi_c)/\hbar}J(\Lambda) + \left(\frac{g(\bar{\xi})}{f'(\bar{\xi})} - \frac{g(\xi_c)}{\beta\Lambda\sqrt{|f''(\xi_c)|}}\right)\frac{\hbar}{\mathrm{i}}\mathrm{e}^{\mathrm{i}f(\bar{\xi})/\hbar}, \tag{A 11}$$

and this leads directly to equation (24) of § 4. Retention of the term in $G(X)$ in (A 7) would lead to an asymptotic series for $I(\bar{\xi})$ in ascending powers of $\hbar$.