Calculating the bound spectrum by path summation in action-angle variables

1977 J. Phys. A: Math. Gen. 10 371

(http://iopscience.iop.org/0305-4470/10/3/009)

J. Phys. A: Math. Gen., Vol. 10, No. 3, 1977. Printed in Great Britain.

Calculating the bound spectrum by path summation in action-angle variables

M V Berry†§ and M Tabor‡||

† Indian Institute of Science, Bangalore 560012, India

‡ H H Wills Physics Laboratory, Bristol University, Tyndall Avenue, Bristol BS8 1TL, UK

Received 24 September 1976

Abstract. The density of states $n(E)$ is calculated for a bound system whose classical motion is integrable, starting from an expression in terms of the trace of the time-dependent Green function. The novel feature is the use of action-angle variables. This has the advantages that the trace operation reduces to a trivial multiplication and the dependence of $n(E)$ on all classical closed orbits with different topologies appears naturally. The method is contrasted with another, not applicable to integrable systems except in special cases, in which quantization arises from a single closed orbit which is assumed isolated and the trace taken by the method of stationary phase.

1. Introduction

In a recent paper (Berry and Tabor 1976, to be referred to as I) we showed that the density $n(E)$ of quantum states for a bound system whose classical motion is multiply periodic can be closely approximated by a 'topological sum' over all the closed classical orbits at the energy E. The derivation proceeded by transforming the generalized Bohr–Sommerfeld quantum condition obtained by Einstein (1917), Brillouin (1926) and Keller (1958), a rigorous treatment of which was provided by Maslov (1972). Each closed orbit contributes an oscillatory variation to $n(E)$ (see also Balian and Bloch 1972, 1974), and the sum converges onto a series of delta functions at the bound state energies.

In this paper we derive again the central result of I, but by a different method, whose starting point is the expression for $n(E)$ in terms of the trace of the time-dependent Green function. There are several reasons for presenting this alternative derivation, arising from the fact that we use action-angle variables to describe the classical motion. In the first place the operation of taking the trace corresponds, in action-angle variables, to a trivial multiplication. This generalizes the known result (Rajaraman and Weinberg 1975) that the trace operation is trivial when a symmetry is present (see Gutzwiller 1970, for a particular example), the point being that action variables are often related to constants of the motion unconnected with any symmetry (examples are the moduli of velocity components in a rectangular box). In the second place the action-angle formalism shows in the clearest and most natural way how $n(E)$ depends

§ Permanent address: H H Wills Physics Laboratory, Bristol University, Tyndall Avenue, Bristol BS8 ITL UK.

|| Now at Department of Physical Chemistry, Hebrew University of Jerusalem, Jerusalem, Israel.

on all topologically different closed orbits with energy E as well as on all repeated traversals of each orbit. In the third place there is a different quantization method, devised by Gutzwiller (1971), which proceeds from the assumption that the closed orbits are isolated, so that the trace can be evaluated by the method of stationary phase; Gutzwiller's method, and later elaborations of it (Miller 1975, Voros 1976, Dashen *et al* 1974, 1975, Rajaraman 1975), are in general inapplicable to multiply periodic systems (even when these are non-separable), and this fact is most clearly brought out by the action-angle formalism. And in the fourth place the derivation is in parts not obvious and we think the subtleties are worth presenting.

2. Basic formalism

Consider a bound system with N degrees of freedom whose classical Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p})$ depends on the $2N$ canonical coordinates and momenta $\boldsymbol{q}$ and $\boldsymbol{p}$. Let $\hat{H}$ be the corresponding Hamiltonian operator. Then it is well known that the density of states, defined as

$$n(E) = \mathrm{Tr}\,\delta(E-\hat{H}), \tag{1}$$

can be expressed as

$$n(E) = \mathrm{Re}\frac{1}{\pi\hbar}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et/\hbar}\,\mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} = \mathrm{Re}\frac{1}{\pi\hbar}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et/\hbar}\int \mathrm{d}^N q K(\boldsymbol{q}, \boldsymbol{q}; t), \tag{2}$$

where K is the time-dependent Green function, defined as

$$K(\boldsymbol{q}_B, \boldsymbol{q}_A; t) = \langle \boldsymbol{q}_B | \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} | \boldsymbol{q}_A \rangle. \tag{3}$$

In the semiclassical approximation K depends on the classical paths from $\boldsymbol{q}_A$ to $\boldsymbol{q}_B$ in the time t. If the rth such path has coordinates and momenta $\boldsymbol{q}_r(t)$, $\boldsymbol{p}_r(t)$ the action W_r along it is

$$W_r(\boldsymbol{q}_A, \boldsymbol{q}_B; t) = \int_0^t \mathrm{d}t[\boldsymbol{p}_r(t)\cdot\dot{\boldsymbol{q}}_r(t) - H(\boldsymbol{q}_r(t), \boldsymbol{p}_r(t))]. \tag{4}$$

From this can be obtained the Nth-order determinant D_r defined as

$$D_r(\boldsymbol{q}_A, \boldsymbol{q}_B; t) \equiv \det\left(-\frac{\partial^2 W_r}{\partial q_{Ai}\partial q_{Bj}}\right) = \left(\frac{\mathrm{d}\boldsymbol{q}_B}{\mathrm{d}\boldsymbol{p}_{Ar}}\right)^{-1}, \tag{5}$$

where the suffixes i and j label components of $\boldsymbol{q}_A$ and $\boldsymbol{q}_B$ and where the right-hand member is the Jacobian between $\boldsymbol{q}_B$ and $\boldsymbol{p}_{Ar}$. If α_r is the number of caustics of the paths emanating from $\boldsymbol{q}_A$ that the rth path encounters *en route* to $\boldsymbol{q}_B$, the semiclassical Green function K_{sc} is

$$K_{\mathrm{sc}}(\boldsymbol{q}_B, \boldsymbol{q}_A; t) = \frac{1}{(2\pi\mathrm{i}\hbar)^{N/2}}\sum_r |D_r|^{1/2}\exp\left[\mathrm{i}\left(\frac{W_r}{\hbar} - \alpha_r\frac{\pi}{2}\right)\right]. \tag{6}$$

A derivation of this result, and an account of its long history, is given by Berry and Mount (1972).

3. Action-angle variables

The systems under consideration are multiply periodic. This means that they possess N independent constants of motion (i.e. they are integrable) and inhabit N-dimensional tori in the $2N$-dimensional phase space. Each such torus is labelled by action variables $\boldsymbol{I} = (I_1 \ldots I_N)$, and points on each torus are labelled by angle variables $\boldsymbol{\theta} = (\theta_1 \ldots \theta_N)$ in such a way that θ_i changes by 2π during the ith irreducible circuit of the torus. $\boldsymbol{\theta}$ and $\boldsymbol{I}$ are respectively the new coordinates and momenta in a canonical transformation from the original $\boldsymbol{q}$ and $\boldsymbol{p}$. In these new variables the Hamiltonian $H(\boldsymbol{I})$ is independent of the angles $\boldsymbol{\theta}$. Proofs of these assertions are given in appendix 26 of Arnol'd and Avez (1968).

Dynamics is very simple in action-angle variables. The actions $\boldsymbol{I}$ remain constant, and the system winds its way round the torus with angular velocities obtained from Hamilton's equation as

$$\dot{\boldsymbol{\theta}} = \nabla_{\boldsymbol{I}} H(\boldsymbol{I}) \equiv \boldsymbol{\omega}(\boldsymbol{I}), \tag{7}$$

where the defined quantities $\boldsymbol{\omega} = (\omega_1 \ldots \omega_N)$ are the N frequencies of the multiply periodic motion. It is trivial to integrate this equation and obtain implicitly the actions $\boldsymbol{I}_r(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B, t)$ specifying the torus on which the system moves on the rth path between configurations $\boldsymbol{\theta}_A$ and $\boldsymbol{\theta}_B$ in time t:

$$\boldsymbol{\theta}_B - \boldsymbol{\theta}_A = \boldsymbol{\omega}(\boldsymbol{I}_r)t. \tag{8}$$

The action W_r is easily found from (4) as

$$W_r(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B; t) = \boldsymbol{I}_r \cdot (\boldsymbol{\theta}_B - \boldsymbol{\theta}_A) - H(\boldsymbol{I}_r)t, \tag{9}$$

and the determinant D_r is from (5) and (8)

$$D_r(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B; t) = \left(\frac{\mathrm{d}\boldsymbol{\theta}_B}{\mathrm{d}\boldsymbol{I}_r}\right)^{-1} = \frac{1}{t^n \det(\partial\omega_i/\partial I_{rj})}. \tag{10}$$

These last two equations give the ingredients necessary to rewrite equation (6) for the Green function $K_{sc}(\boldsymbol{\theta}_B, \boldsymbol{\theta}_A; t)$ in angle coordinates. The notorious difficulties in setting up a fully-fledged quantum mechanics in action-angle variables (Carruthers and Nieto 1968) are not involved in *semiclassical approximations* and so do not affect the present work. For an application showing the power of 'action-angle semiclassical mechanics', and pertinent references, see Marcus (1971).

The density of states is given by equation (2). This involves the trace operation, that is integration over all configurations to which the system returns in time t. Now the angles $\boldsymbol{\theta}$ and $\boldsymbol{\theta} + 2\pi\boldsymbol{M}$, where $\boldsymbol{M}$ is an N-dimensional vector with integer components, represent the same configuration, so that in the semiclassical approximation the integral in (2) is

$$\int \mathrm{d}^N q\, K_{sc}(\boldsymbol{q}, \boldsymbol{q}; t) = \sum_{\boldsymbol{M}} \int_0^{2\pi} \mathrm{d}^N \theta\, K_{sc}(\boldsymbol{\theta} + 2\pi\boldsymbol{M}, \boldsymbol{\theta}; t). \tag{11}$$

The classical paths corresponding to each vector $\boldsymbol{M}$ are those which at time t have returned to the same point on their torus after making M_1 circuits of coordinate θ_1, M_2 circuits of coordinate θ_2, etc. Therefore the paths involved in the trace operation are all *closed*—when the system returns to the original configuration its 'momentum' $\boldsymbol{I}$ has not changed. This contrasts with the situation when (say) Cartesian coordinates $\boldsymbol{q}$ are employed to specify the system's configuration: then the momenta $\boldsymbol{p}$ are usually

different when the system returns to $\boldsymbol{q}$. It is clear that $\boldsymbol{M}$ labels the *topology* of the closed orbits, and will henceforth be used instead of the earlier label r, under the assumption that at most one torus contains orbits with topology $\boldsymbol{M}$ (in I we discuss briefly what happens in the interesting situation when this assumption is false).

The torus $\boldsymbol{I}_{\boldsymbol{M}}(t)$ containing orbits with topology $\boldsymbol{M}$ is determined (equation (8)) by

$$\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}}(t))t = 2\pi\boldsymbol{M}. \tag{12}$$

For the systems considered here, all components of $\boldsymbol{\omega}$ are positive. (This corresponds to convexity of the 'energy contours' on which $H(\boldsymbol{I})$ is constant in $\boldsymbol{I}$ space.) Moreover, in equation (2) t is never negative. Therefore equation (12) shows that there are no paths with topologies for which any component M_i of $\boldsymbol{M}$ is negative. The action is $W_{\boldsymbol{M}}(t)$ which from equation (9) is

$$W_{\boldsymbol{M}}(t) = 2\pi\boldsymbol{I}_{\boldsymbol{M}}(t)\,.\,\boldsymbol{M} - H(\boldsymbol{I}_{\boldsymbol{M}}(t))t, \tag{13}$$

while the determinant $D_{\boldsymbol{M}}(t)$ is given by (10) with $\boldsymbol{I}_r$ replaced by $\boldsymbol{I}_{\boldsymbol{M}}$.

Now follows a point of crucial importance. The expressions just found for $W_{\boldsymbol{M}}$ and $D_{\boldsymbol{M}}$ are independent of $\boldsymbol{\theta}$. This means that the functions $K_{\mathrm{sc}}(\boldsymbol{\theta}+2\pi\boldsymbol{M}, \boldsymbol{\theta}; t)$ in equation (11) are also independent of $\boldsymbol{\theta}$, so that the integrals over $\boldsymbol{\theta}$ are trivial and simply give a factor $(2\pi)^N$. The reason for this great simplification is that the closed orbits with topology $\boldsymbol{M}$ are not isolated but form a continuous family covering the torus $\boldsymbol{I}_{\boldsymbol{M}}$.

The topology $\boldsymbol{M}=0$ is special: it corresponds to the 'paths of zero length' and can be shown to give the smoothly varying 'Thomas–Fermi' density of states $n_{\mathrm{TF}}(E)$ (for proofs see I or Berry and Mount 1972). Removing the term $\boldsymbol{M}=0$ from the summation in (11), and using equations (6), (10) and (13), the density of states (equation (2)) can now be written as

$$n(E) = \frac{(2\pi)^N}{\pi\hbar}\,\mathrm{Re}\,\frac{1}{(2\pi\mathrm{i}\hbar)^{N/2}}\sum_{\boldsymbol{M}}{}' \int_0^\infty \frac{\mathrm{d}t\,\exp\{[\mathrm{i}(2\pi\boldsymbol{I}_{\boldsymbol{M}}\,.\,\boldsymbol{M} - H(\boldsymbol{I}_{\boldsymbol{M}})t + Et)/\hbar] - \mathrm{i}\alpha_{\boldsymbol{M}}\,.\,\boldsymbol{M}\pi/2\}}{t^{N/2}\left|\det(\partial\omega_i/\partial I_{M_i})\right|^{1/2}}$$
$$+ n_{\mathrm{TF}}(E). \tag{14}$$

In this equation, $\boldsymbol{I}_{\boldsymbol{M}}$ is determined by equation (12), the prime on the summation denotes the exclusion of terms with any negative M_i and also the term $\boldsymbol{M}=0$, and $\boldsymbol{\alpha}_{\boldsymbol{M}}$, which replaces the caustic factor α_r in (6), is a vector in which each component α_{M_i} denotes the number of caustics of the family of paths encountered over each cycle i of the torus containing the paths with topology $\boldsymbol{M}$ (so that $\boldsymbol{\alpha}_{\boldsymbol{M}}\,.\,\boldsymbol{M}$ is the total number of caustics encountered along the whole path).

The convergence of the integrand of (14) for large t depends on the behaviour of $H(\boldsymbol{I})$ for small $\boldsymbol{I}$. If H begins with linear terms (as in the harmonic oscillator), the condition (12) has no solution as $t\to\infty$ for any finite non-zero $\boldsymbol{M}$—there are no closed orbits of any given topology with arbitrarily long period. Then the integrand of (14) is zero for large t. If H begins with terms quadratic in $\boldsymbol{I}$ (as in the particle in a box), closed orbits with arbitrarily long period do exist, and the integrands of (14) behave as $\exp(\mathrm{i}Et)/t^{N/2}$ as $t\to\infty$, which is sufficient to ensure the convergence of the integrals. (A faster convergence could be obtained by calculating not $n(E)$ but the smoothed function $n_\gamma(E)$, corresponding to replacing E by $E+\mathrm{i}\gamma$, introduced by Balian and Bloch (1972, 1974) and employed by us in I.)

The appearance of $\hbar$ in the denominator of the exponent in (14) makes the integrand a rapidly varying function of t under semiclassical conditions. Therefore the integral

can be evaluated by the method of stationary phase. The stationary point $t_{\boldsymbol{M}}(E)$ of (14) is given by

$$\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\text{phase of (14)}) = (2\pi\boldsymbol{M} - t\nabla_{\boldsymbol{I}}H)\cdot\frac{\partial \boldsymbol{I}_{\boldsymbol{M}}}{\partial t} - H(\boldsymbol{I}_{\boldsymbol{M}}) + E = E - H(\boldsymbol{I}_{\boldsymbol{M}}(t_{\boldsymbol{M}}(E))) = 0, \tag{15}$$

where the second equality holds by virtue of (7) and (12). This result is obvious: $t_{\boldsymbol{M}}(E)$ is the orbit time for which the contributing tori $\boldsymbol{I}_{\boldsymbol{M}}$ have energy E. The second derivative of the exponent in (14) is

$$\frac{1}{\hbar}\frac{\mathrm{d}}{\mathrm{d}t}(E - H(\boldsymbol{I}_{\boldsymbol{M}})) = -\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})\cdot\frac{\partial \boldsymbol{I}_{\boldsymbol{M}}}{\partial t}. \tag{16}$$

These results enable the stationary phase result to be written as

$$n(E) = n_{\mathrm{TF}}(E) + 2\,\mathrm{Re}\sum_{\boldsymbol{M}}{}' A_{\boldsymbol{M}}\exp\left\{\mathrm{i}\left[2\pi\boldsymbol{M}\cdot\left(\frac{\boldsymbol{I}_{\boldsymbol{M}}}{\hbar} - \frac{\boldsymbol{\alpha}_{\boldsymbol{M}}}{4}\right)\right]\right\}, \tag{17}$$

where the amplitudes $A_{\boldsymbol{M}}$ are defined by

$$A_{\boldsymbol{M}}^2 = \frac{(2\pi)^{N-1}}{\hbar^{N+1}\mathrm{i}^{N+1}t_{\boldsymbol{M}}^{N}|\det(\partial\omega_i/\partial I_{M_j})|\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})\cdot\partial\boldsymbol{I}_{\boldsymbol{M}}(t_{\boldsymbol{M}})/\partial t}. \tag{18}$$

4. Evaluating the amplitudes

The rather complicated manipulations in this section have the following aim: to eliminate from the amplitudes (18) all reference to the $t_{\boldsymbol{M}}$, and obtain an expression directly involving the Hamiltonian $H(\boldsymbol{I})$ and the geometry of the energy contours in $\boldsymbol{I}$ space, on which $H(\boldsymbol{I}) = E$.

From equation (12),

$$t_{\boldsymbol{M}}^{N} = t_{\boldsymbol{M}}t_{\boldsymbol{M}}^{N-1} = t_{\boldsymbol{M}}\frac{|2\pi\boldsymbol{M}|^{N-1}}{|\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})|^{N-1}}, \tag{19}$$

so that (18) becomes

$$A_{\boldsymbol{M}}^2 = \frac{|\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})|^{N-1}}{\hbar^{N+1}\mathrm{i}^{N+1}|\boldsymbol{M}|^{N-1}|\det(\partial\omega_i/\partial I_{M_j})|t_{\boldsymbol{M}}\,\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})\cdot\partial\boldsymbol{I}_{\boldsymbol{M}}/\partial t(t_{\boldsymbol{M}})}. \tag{20}$$

The denominator will be simplified using the fact that differentiating equation (12) with respect to t gives

$$\omega_i = -t\sum_j\frac{\partial\omega_i}{\partial I_j}\frac{\partial I_j}{\partial t}, \tag{21}$$

where suffixes denote components of vectors and where the labels $\boldsymbol{M}$ have been dropped for notational convenience. To solve these equations for the N unknowns $\partial I_j/\partial t$, it is convenient to introduce into $\boldsymbol{I}$ space a Cartesian coordinate system whose origin lies at $\boldsymbol{I}_{\boldsymbol{M}}$, in which one coordinate η_0 measures actions perpendicular to the energy contour at $\boldsymbol{I}_{\boldsymbol{M}}$, and the other $N-1$ coordinates $\boldsymbol{\eta} = (\eta_1 \ldots \eta_{N-1})$ measure actions in the tangent plane to the energy contour at $\boldsymbol{I}_{\boldsymbol{M}}$, as shown in figure 1.

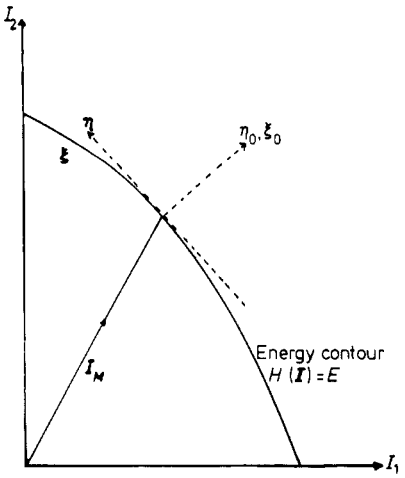

Figure 1. Coordinate systems in space of actions $\boldsymbol{I}$, illustrated for the case of two degrees of freedom: $(\eta_0, \boldsymbol{\eta})$ are Cartesians whose origin is $\boldsymbol{I}_M$ and $\boldsymbol{\eta}$ are $N-1$ coordinates in the tangent plane to the energy contour at $\boldsymbol{I}_M$, and $(\xi_0, \boldsymbol{\xi})$ are curvilinear coordinates where $\boldsymbol{\xi}$ are $N-1$ coordinates in the energy contour.

In these coordinates, the fact that $\boldsymbol{\omega}$ is perpendicular to the energy contour (this follows from equation (7)) means that

$$\omega_0 \doteq |\boldsymbol{\omega}|, \qquad \omega_1 = \omega_2 = \ldots = \omega_{N-1} = 0. \tag{22}$$

Therefore Cramer's rule applied to (21) gives, for the component of $\partial \boldsymbol{I}/\partial t$ along η_0,

$$t\frac{\partial \eta_0}{\partial t} = \frac{-|\boldsymbol{\omega}| \det(\partial \omega_i/\partial \eta_j)}{\det(\partial \omega_i/\partial I_j)}, \tag{23}$$

where the determinant in the numerator is of order $N-1$ (i.e. i and j run from 1 to $N-1$) and the determinant of order N in the denominator is the same as that appearing in the denominator of (20). The scalar product in (20) is

$$\boldsymbol{\omega} \cdot \frac{\partial \boldsymbol{I}}{\partial t} = |\boldsymbol{\omega}| \frac{\partial \eta_0}{\partial t}, \tag{24}$$

so that, using (23), equation (20) becomes

$$A_M^2 = \frac{|\boldsymbol{\omega}(\boldsymbol{I}_M)|^{N-3}}{\hbar^{N+1} i^{N+3} |\boldsymbol{M}|^{N-1} \det(\partial \omega_i/\partial \eta_j)} \tag{25}$$

where we have used the fact, which follows from our earlier assumption that there is at most one torus with topology $\boldsymbol{M}$, that the energy contour is convex so that the determinant in the denominator of (23) is positive definite.

Now a curvilinear coordinate system is introduced into $\boldsymbol{I}$ space, in which $N-1$ coordinates $\boldsymbol{\xi} = (\xi_1 \ldots \xi_{N-1})$ measure position on the energy contour and ξ_0 measures perpendicular distance from the contour, as shown in figure 1. Of course, very close to $\boldsymbol{I}_M$ this coincides with the system $(\eta_0, \boldsymbol{\eta})$ previously defined. The $N-1$ quantities $\partial \boldsymbol{I}/\partial \xi_i$

$(1 \leqslant i \leqslant N-1)$ are unit tangent vectors on the energy contour, so that they are perpendicular to $\boldsymbol{\omega}$, i.e.

$$\boldsymbol{\omega} \cdot \frac{\partial \boldsymbol{I}}{\partial \xi_i} = 0 \qquad (1 \leqslant i \leqslant N-1). \tag{26}$$

Differentiating with respect to ξ_j gives

$$\frac{\partial \boldsymbol{\omega}}{\partial \xi_j} \cdot \frac{\partial \boldsymbol{I}}{\partial \xi_i} = \frac{\partial \omega_i}{\partial \xi_j} = -\boldsymbol{\omega} \cdot \frac{\partial^2 \boldsymbol{I}}{\partial \xi_i \, \partial \xi_j}. \tag{27}$$

At the point $\boldsymbol{I}_{\boldsymbol{M}}$ of interest, first derivatives with respect to $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ are identical, so that the determinant in (25) is

$$\det\left(\frac{\partial \omega_i}{\partial \eta_j}\right) = \det\left(\frac{\partial \omega_i}{\partial \xi_j}\right) = (-1)^{N-1} \det\left(\boldsymbol{\omega} \cdot \frac{\partial^2 \boldsymbol{I}}{\partial \xi_i \, \partial \xi_j}\right) = (-1)^{N-1} |\boldsymbol{\omega}|^{N-1} K(\boldsymbol{I}_{\boldsymbol{M}}), \tag{28}$$

where $K(\boldsymbol{I})$ is the *scalar curvature* of the energy contour, defined in § 3 of I. Let $\beta_{\boldsymbol{M}}$ be the excess of positive over negative eigenvalues of the matrix $\boldsymbol{\omega} \cdot \partial^2 \boldsymbol{I} / \partial \xi_i \, \partial \xi_j$. Then there are $(N-1-\beta_{\boldsymbol{M}})/2$ negative eigenvalues, and

$$K = (-1)^{(N-1-\beta_{\boldsymbol{M}})/2} |K|. \tag{29}$$

Thus equation (25) for the amplitudes becomes, finally,

$$A_{\boldsymbol{M}}^2 = \frac{\mathrm{e}^{\mathrm{i}\pi\beta_{\boldsymbol{M}}/2}}{\hbar^{N+1} |\boldsymbol{M}|^{N-1} |\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})|^2 K(\boldsymbol{I}_{\boldsymbol{M}})}. \tag{30}$$

For the density of states, equation (17) gives

$$n(E) = n_{\mathrm{TF}}(E) + \frac{2}{\hbar^{(N+1)/2}} \sum_{\boldsymbol{M}}{}' \frac{\cos\{2\pi \boldsymbol{M} \cdot [(\boldsymbol{I}_{\boldsymbol{M}}/\hbar) - \frac{1}{4}\boldsymbol{\alpha}_{\boldsymbol{M}}] + \frac{1}{4}\pi\beta_{\boldsymbol{M}}\}}{|\boldsymbol{M}|^{(N-1)/2} |\boldsymbol{\omega}(\boldsymbol{I}_{\boldsymbol{M}})| \sqrt{|K(\boldsymbol{I}_{\boldsymbol{M}})|}}. \tag{31}$$

This is identical with equation (21) of I which we derived from the quantization rule for multiply periodic systems.

5. Discussion

A thorough discussion of equation (31) was given in I, together with computations demonstrating its high degree of numerical accuracy. The central result of this work is that for classically integrable systems a single closed classical orbit is of no quantal significance, but the torus in phase space formed by the continuous family of which the orbit is a member contributes a term to $n(E)$ that varies smoothly with energy in an oscillatory manner. The bound states, which give delta functions in $n(E)$, arise only on summing over all the tori that contribute with energy E, i.e. all families of topologically different orbits and repeated circuits of the same orbit.

In sharp contrast with these results is the picture presented by a different quantization method, currently enjoying some popularity. On the assumption that the closed

orbits of the system are isolated, Gutzwiller (1971) evaluates the trace in equation (2) by the method of stationary phase, and obtains a quantization condition involving the stability parameters of a single classical orbit and a single quantum number arising from repeated circuits of the orbit. By considering harmonic deviations from the single closed orbit, later authors (Miller 1975, Voros 1976, Dashen *et al* 1974, 1975) show how $N-1$ further quantum numbers can be introduced.

It is difficult to assess the applicability of the work of these authors in this paper and in I, because the closed orbits are not isolated (they fill tori) and moreover there are infinitely many topologically different closed orbits at each energy (any discussion based on the harmonic oscillator in several dimensions, or on the Coulomb potential, is irrelevant here, because these systems are degenerate in that *all* their orbits are closed and moreover have the same topology). A good illustration of this point is provided by the particle in a two-dimensional rectangular box with sides a and b, where the levels are exactly known. It is easy to prove the following results: the actions I_x and I_y picked out by the quantum condition do not correspond to closed classical orbits if a/b is irrational, and correspond to only an infinitesimal fraction of the closed orbits if a/b is rational. Moreover if the closed orbits are made the basis of quantization an infrared catastrophe ensues, because there are infinitely many closed orbits with the 'ground state' action h for a single traversal, and their energies diminish to zero as their topological complexity (number of pairs of x and y reflections before closure) increases! However, for most integrable systems there will be some parts of the spectrum for which Gutzwiller's methods can be applied to give an approximate description. As explained by Voros (1976) these are the contributions from the degenerate tori which do indeed contain just one closed orbit (they form the 'cores' of the whole concentric system of tori with energy E); an example is the circular orbit in the minimum of the effective potential for a particle bound by a central force.

About generic non-integrable classical systems that are far from integrable ones, little is known. But a great deal is known about quasi-integrable classical systems whose non-integrability consists of a generic perturbation (see Arnol'd and Avez 1968 and the useful review by Ford 1975). For such systems the closed orbits are indeed isolated; half of them are stable, and surrounded by manifolds of multiply periodic orbits (i.e. tori in phase space). This would seem to justify the application of the method of stationary phase, provided the total phase space volume occupied by such tori exceeds h^N (see the related discussion by Percival 1976). However, since such isolated closed orbits arise from the break-up of the 'unperturbed' tori of closed orbits, there will in general be not just one but a large number of these orbits, with different topologies, and it is hard to see how any quantum condition arising from the properties of a single closed orbit can be correct. The other half of the isolated closed orbits are unstable and surrounded by orbits pathologically distributed and stochastic in character as in an ergodic system, which are not confined to tori in phase space, and it seems unlikely that the method of stationary phase, based as it is on the assumption that isolated orbits are embedded in a smoothly varying environment, can be employed to take the trace.

Acknowledgments

One of us (MVB) thanks Professor K P Sinha for the hospitality of the Indian Institute of Science where this paper was written and Professor R Rajaraman for helpful discussions. The other (MT) was supported by an SRC research grant.

References

Arnol'd V I and Avez A 1968 *Ergodic Problems of Classical Mechanics* (New York: Benjamin)
Balian R and Bloch C 1972 *Ann. Phys., NY* **69** 76–160
—— 1974 *Ann. Phys., NY* **85** 514–45
Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315–97
Berry M V and Tabor M 1976 *Proc. R. Soc.* A **349** 101–23
Brillouin L 1926 *J. Phys. Radium* **7** 353–68
Carruthers P and Nieto M M 1968 *Rev. Mod. Phys.* **40** 411–40
Dashen R F, Hasslacher B and Neveu A 1974 *Phys. Rev.* D **10** 4114–29
—— 1975 *Phys. Rev.* D **11** 3424–50
Einstein A 1917 *Verh. Dt. Phys. Ges.* **19** 82–92
Ford J 1975 *Fundamental Problems in Statistical Mechanics* vol. 3, ed. E G D Cohen (Amsterdam: North-Holland) pp 215–55
Gutzwiller M C 1970 *J. Math. Phys.* **11** 1791–806
—— 1971 *J. Math. Phys.* **12** 343–58
Keller J B 1958 *Ann. Phys., NY* **4** 180–8
Marcus R A 1971 *J. Chem. Phys.* **54** 3965–79
Maslov V P 1972 *Theorie des Perturbations et Methodes Asymptotiques* (Paris: Dunod) (original Russian edition 1965)
Miller W H 1975 *J. Chem. Phys.* **63** 996–9
Percival I C 1976 *Adv. Chem. Phys.* **36** in the press
Rajaraman R 1975 *Phys. Rep.* **21** 227–313
Rajaraman R and Weinberg E J 1975 *Phys. Rev.* D **11** 2950–66
Voros A 1976 *Ann. Inst. Henri Poincaré* A **24** 31–90