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On quantisation using periodic classical orbits

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Abstract. Two approaches to semiclassical quantisation of integrable systems using periodic classical orbits are considered. They both lead to approximate formulae for the density of states function (a δ function at each energy level). The first, due to Gutzwiller, involves a sum over *isolated* stable periodic orbits of the system, and leads to the harmonic approximation to the eigenvalues. The second, due to Berry and Tabor, involves a sum over *families* of periodic orbits, and leads to the EBK ('torus') approximation to the eigenvalues.

Here, we extract a modified form of the Gutzwiller series from the Berry–Tabor series, by using a uniform approximation, and hence show that the complete spectrum involves both these series. The analysis demonstrates that genuine semiclassical quantisation rules for *generic* systems, using periodic orbits, will involve uniform approximation, which more closely reflects the underlying classical structure than do the existing stationary phase approximations.

1. Introduction

For a bounded integrable system with N freedoms the classical phase space is filled with N-dimensional hypersurfaces with the topology of N-tori (Arnol'd 1974). Any given trajectory lies on such a torus in phase space for all time. In the semiclassical limit (as $\hbar \to 0$) the quantum eigenvalues may be obtained by quantising these tori, as first realised by Einstein (1917). If $\boldsymbol{I} = (I_1, \ldots, I_N)$ are the action coordinates of the classical system, then the semiclassical eigenvalues are given by

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

where $\boldsymbol{\alpha}$ is the caustic index vector of the torus, and $\boldsymbol{m}$ is a vector of positive integers or zeros. (For a general review of torus quantisation see Berry (1982).) The density of states function (a δ function at each energy level) is then given by

$$d(E) = \sum_{\boldsymbol{m}} \delta\{E - H[\boldsymbol{I} = (\boldsymbol{m} + \tfrac{1}{4}\boldsymbol{\alpha})\hbar]\}. \tag{2}$$

Berry and Tabor (1976) show how to rewrite this as a sum over all periodic orbit tori in the classical system (these tori support N-dimensional families of similar periodic orbits). Their 'simple' semiclassical result is

$$d(E) = \bar{d}(E) + \frac{2}{\hbar^{(N+1)/2}} \sum_{\boldsymbol{M}}{}' \frac{\cos(2\pi \boldsymbol{M} \cdot \boldsymbol{I}^{\boldsymbol{M}}/\hbar - \frac{1}{2}\pi\boldsymbol{\alpha} \cdot \boldsymbol{M} + \frac{1}{4}\pi\beta_{\boldsymbol{M}})}{|\boldsymbol{M}|^{(N-1)/2} |\boldsymbol{\omega}(\boldsymbol{I}^{\boldsymbol{M}})| \, |K(\boldsymbol{I}^{\boldsymbol{M}})|^{1/2}} \tag{3}$$

where the indices $\boldsymbol{M}$ refer to the *topology* of the periodic orbit family; that is, the orbit makes M_i windings about the ith irreducible circuit of the torus, for $1<i<N$. The prime excludes the $\boldsymbol{M}=0$ term, which gives $\bar{d}(E)$, the smoothly varying average density; $\boldsymbol{\omega}(\boldsymbol{I}^{\boldsymbol{M}})$ is the frequency vector of the torus, $K(\boldsymbol{I}^{\boldsymbol{M}})$ is a scalar curvature of the energy surface in action space and $\beta_{\boldsymbol{M}}$ is a phase associated with this. For a system with two freedoms each term is of order $h^{-3/2}$.

Gutzwiller (1971) showed in general, even for non-integrable systems, that it is the periodic classical orbits which are important in understanding semiclassical spectra. He obtained a formula for $d(E)$ involving a sum over all isolated periodic orbits of the classical system. Such orbits, unlike periodic tori, occur in all classical systems, and they may be stable or unstable. An orbit is stable if neighbouring paths remain so as time passes, and unstable if they diverge. Unfortunately, Gutzwillers formula in the stable case is frequently divergent and the more sophisticated uniform approximation must be obtained. In those integrable systems which possess global action-angle variables, there are no unstable isolated orbits with finite period, but there are stable ones, which may be thought of as degenerate tori. Consequently, as a first step in understanding the uniform approximations we consider integrable systems in this paper.

The contribution to $d(E)$ from a stable isolated orbit, for *any* classical system with two freedoms, is given in Gutzwiller's theory by

$$\frac{\tau(E)}{2\pi\hbar}\sum_{m=1}^{\infty}\frac{\sin(mS(E)/\hbar-\frac{1}{2}m\lambda\pi)}{\sin\frac{1}{2}m\nu(E)} \tag{4}$$

where S is the action around the periodic orbit, ν is the stability angle, τ is the period and λ is the number of turning points along the orbit. Each term is of order h^{-1}, that is of lower order than the torus terms. The sum takes account of all repetitions, m, of the basic orbit. It is easy to generalise this result to higher dimensions (Miller 1975) but we restrict ourselves here to two freedoms.

Now, terms in this series diverge when $\frac{1}{2}m\nu(E)$ is a multiple of π. This is because a caustic of the classical propagator occurs along the periodic orbit after an integral number of periods. Then the argument leading to (4) breaks down, and the non-divergent uniform approximation is required. Gutzwiller appreciated this deficiency, and using an intuitive argument suggested that (4), when correctly modified, would lead to eigenvalues given by

$$S(E)=(2\pi m+\tfrac{1}{2}\nu(E)+\tfrac{1}{2}\pi\lambda)\hbar. \tag{5}$$

Miller (1975) pointed out that (4) may be rewritten in an exact way, giving an eigenvalue condition

$$S(E)=[2\pi m+(n+\tfrac{1}{2})\nu(E)+\tfrac{1}{2}\pi\lambda]\hbar. \tag{6}$$

Since $\nu h=\omega S'(E)$, where ω is the stability frequency, (6) is interpreted as the harmonic approximation to the true semiclassical eigenvalues (see also Voros 1976).

In figure 1, the action space of an integrable system is shown, with an energy contour $E=H(\boldsymbol{I})$ and its harmonic approximation. Eigenvalues of (1) are given by a lattice of points in $\boldsymbol{I}$ space, with spacing $\hbar$. The eigenvalues (5) are essentially limited to the I_1 axis. The harmonic eigenvalues (6) occur when the harmonic contour includes a lattice point. Clearly, for the integrable case, the eigenvalues (6) are a good approximation only where the harmonic contour closely approximates the true contour, that is, for low values of n. The reason that *all* values of n are predicted is that the

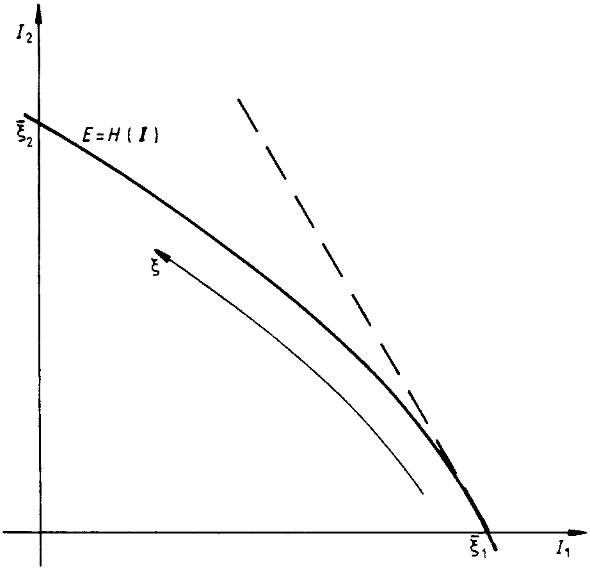

Figure 1. Energy contour $E = H(\boldsymbol{I})$ (full curve), and its harmonic approximation (broken curve). The integrals in (7) are over the coordinate ξ, with endpoints $\bar{\xi}_1$, $\bar{\xi}_2$. Real tori are represented by points in the positive quadrant, complex tori by points elsewhere.

divergent terms in (4) have not been treated uniformly. If this is done, then we show in § 2 that the uniformly modified path sum contributes only to those peaks in $d(E)$ which correspond to eigenvalues occurring where the harmonic contours are a good approximation to the true contours.

Now, stable isolated orbits also occur in generic classical systems (Arnol'd 1974) where there may be infinitely many. It seems likely that (6) also has limited validity in these cases, since it is still not clear how many harmonic eigenvalues to take from each orbit. This should become clearer if the divergent terms in (4) are replaced by uniform terms which take fuller account of the underlying classical structure near to a caustic. The non-divergent terms should still be valid, except perhaps for very long paths.

For integrable systems, our analysis below shows that when uniformly modified, Gutzwiller's path sum (4) extends beyond the harmonic approximation and contributes to the peaks in $d(E)$ corresponding to eigenvalues of (1) for thin tori. In so doing, we find that, for integrable systems, the Gutzwiller terms (4) are small corrections to the Berry–Tabor sum (3) which gives the complete semiclassical spectrum.

2. Isolated orbits in integrable systems with two freedoms

We use a uniform approximation derived by Berry and Tabor (1976) for the density of states in an integrable system, with two freedoms. It starts with a Poisson transformation of equation (2) which gives

$$d(E) = \bar{d}(E) + \sum_{\boldsymbol{M}}{}' \int_{\bar{\xi}_1}^{\bar{\xi}_2} \frac{\exp \mathrm{i}[(2\pi/\hbar)\boldsymbol{M}\cdot \boldsymbol{I}(\xi) - \frac{1}{2}\pi\boldsymbol{\alpha}\cdot\boldsymbol{M}]}{\hbar^2|\boldsymbol{\omega}(\xi)|}\,\mathrm{d}\xi. \tag{7}$$

The integrals (hereinafter denoted by $d_{\boldsymbol{M}}$) are over the energy contour in action space (figure 1), and $\boldsymbol{\omega}(\xi)$ is the frequency vector of the torus represented by the point ξ.

This formula may also be obtained using the more general Green function approach to the density of states function (Gutzwiller 1970), as we explain in the appendix. Equation (7) is interpreted as a sum over closed orbit tori with topology $\boldsymbol{M}$. The simple semiclassical result (3) may be eventually regained if we let $\bar{\xi}_2 \to +\infty$ and $\bar{\xi}_1 \to -\infty$.

If a component of $\boldsymbol{\alpha}$ is zero then the energy surface never intersects the corresponding axis in $\boldsymbol{I}$ space and consequently one of the endpoints moves away to infinity. In what follows we assume that this is *not* the case. (Otherwise, it is trivial to modify the theory.)

It is assumed that each integral $d_{\boldsymbol{M}}$ has a single stationary point. (If the stationary point is outside the range of integration in (7), then the torus of topology $\boldsymbol{M}$ is not realised in phase space; it is called a *complex torus* since, if the motion is a libration, the turning points in coordinate space are imaginary.) The integrals may then be approximated uniformly in terms of

$$I = \int_{-\infty}^{\bar{\xi}} \mathrm{d}\xi\, g(\xi) \exp\left(\frac{\mathrm{i}}{\hbar} f(\xi)\right) \tag{8}$$

where $\mathrm{d}f/\mathrm{d}\xi$ is zero at one point only, ξ_c. Berry and Tabor obtain the uniform approximation

$$I \simeq \left[g(\xi_c)\left(\frac{\hbar}{|f''(\xi_c)|}\right)^{1/2} \int_{-\infty}^{\Lambda/\sqrt{\hbar}} \mathrm{d}x\, \exp(\tfrac{1}{2}\mathrm{i}\beta x^2)\right] \exp\left(\frac{\mathrm{i}}{\hbar} f(\xi_c)\right) + \frac{\hbar}{\mathrm{i}}\left[\frac{g(\bar{\xi})}{f'(\bar{\xi})} - \frac{g(\xi_c)}{\Lambda\beta}\left(\frac{1}{|f''(\xi_c)|}\right)^{1/2}\right] \exp\left(\frac{\mathrm{i}}{\hbar} f(\bar{\xi})\right) \tag{9}$$

where the prime indicates differentiation with respect to ξ, β is the sign of $f''(\xi_c)$ and

$$\Lambda = \pm[(2/\beta)(f(\bar{\xi}) - f(\xi_c))]^{1/2}.$$

Λ is positive if ξ_c is less than $\bar{\xi}$, and is always real.

It is now important to take this result a stage further using the formula

$$\frac{-\hbar}{\mathrm{i}\Lambda\beta} \exp\left(\frac{\mathrm{i}}{\hbar} f(\bar{\xi})\right) = \operatorname{sgn}\Lambda \left[\sqrt{\hbar} \exp\left(\frac{\mathrm{i}}{\hbar} f(\xi_c)\right) \int_{|\Delta|/\sqrt{\hbar}}^{\infty} \mathrm{d}x\, \exp(\tfrac{1}{2}\mathrm{i}\beta x^2) + \sqrt{\hbar}\mathrm{i}\beta \exp\left(\frac{\mathrm{i}}{\hbar} f(\xi_c)\right) \int_{|\Delta|/\sqrt{\hbar}}^{\infty} \frac{\mathrm{d}x}{x^2} \exp(\tfrac{1}{2}\mathrm{i}\beta x^2)\right] \tag{10}$$

which may be easily verified by noticing that the stationary points in the integrand are always outside the range of integration, and then using integration by parts.

We then find the uniform approximation

$$I(\bar{\xi}) = g(\xi_c)\left(\frac{2\mathrm{i}\pi\beta\hbar}{|f''(\xi_c)|}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} f(\xi_c)\right) \times \left[\Theta(\bar{\xi} - \xi_c) + \left(\frac{\mathrm{i}\beta}{2\pi}\right)^{1/2} \operatorname{sgn}(\bar{\xi} - \xi_c) \int_{|\Lambda|/\sqrt{\hbar}}^{\infty} \frac{\mathrm{d}x}{x^2} \exp(\tfrac{1}{2}\mathrm{i}\beta x^2)\right] + \frac{\hbar}{\mathrm{i}} \frac{g(\bar{\xi})}{f'(\bar{\xi})} \exp\left(\frac{\mathrm{i}}{\hbar} f(\bar{\xi})\right) \tag{11}$$

which is, of course, equivalent to (9).

This is used to write down the uniform approximation to the integrals in (7),

$$d_{\boldsymbol{M}} \simeq \left(\frac{1}{\boldsymbol{M}\cdot\boldsymbol{I}''(\xi_c)}\right)^{1/2}\frac{1}{|\boldsymbol{\omega}(\xi_c)|\hbar^{3/2}}\left(\chi(\bar{\xi}_2,\bar{\xi}_1)+J\right)\exp \mathrm{i}\left(\frac{2\pi}{\hbar}\boldsymbol{M}\cdot\boldsymbol{I}(\xi_c)+\frac{\pi\beta}{4}-\frac{\pi}{2}\boldsymbol{\alpha}(\xi_c)\cdot\boldsymbol{M}\right)$$
$$+\frac{1}{2\pi\mathrm{i}\hbar}\left[\frac{1}{|\boldsymbol{\omega}(\bar{\xi}_2)|\boldsymbol{M}\cdot\boldsymbol{I}'(\bar{\xi}_2)}\exp \mathrm{i}\left(\frac{2\pi}{\hbar}M_2I_2(\bar{\xi}_2)-\frac{\pi}{2}\boldsymbol{\alpha}(\bar{\xi}_2)\cdot\boldsymbol{M}\right)\right.$$
$$\left.-\frac{1}{|\boldsymbol{\omega}(\bar{\xi}_1)|\boldsymbol{M}\cdot\boldsymbol{I}'(\bar{\xi}_1)}\exp \mathrm{i}\left(\frac{2\pi}{\hbar}M_1I_1(\bar{\xi}_1)-\frac{\pi}{2}\boldsymbol{\alpha}(\bar{\xi}_1)\cdot\boldsymbol{M}\right)\right] \tag{12}$$

where

$$J=\operatorname{sgn}(\bar{\xi}_2-\xi_c)\int_{|\Lambda_2|/\sqrt{\hbar}}^{\infty}\frac{\mathrm{d}x}{x^2}\exp(\tfrac{1}{2}\mathrm{i}\beta x^2)-\operatorname{sgn}(\bar{\xi}_1-\xi_c)\int_{|\Lambda_1|/\sqrt{\hbar}}\frac{\mathrm{d}x}{x^2}\exp(\tfrac{1}{2}\mathrm{i}\beta x^2),$$
$$\Lambda_i=\pm[(4\pi/\beta)(M_iI_i(\bar{\xi}_i)-\boldsymbol{M}\cdot\boldsymbol{I}(\xi_c))]^{1/2}$$

and

$$\chi(\bar{\xi}_2,\bar{\xi}_1)=\begin{cases}1 & \text{for } \bar{\xi}_1<\xi_c<\bar{\xi}_2,\\ 0 & \text{otherwise.}\end{cases}$$

Now for ξ_c away from the endpoints $J\sim O(\hbar^{3/2})$ and hence is asymptotically negligible with respect to the other terms. We are then left with the first term which is the 'simple' Berry–Tabor result (3) for a torus of topology $\boldsymbol{M}$, and the last terms which are expressed solely in terms of quantities evaluated on the boundaries, $\bar{\xi}_1$ and $\bar{\xi}_2$. These are consequently related to the stable isolated orbits of the system (there are typically two for an integrable system with two freedoms (which admits global action-angle variables), one for $I_1=0$ ($\xi=\bar{\xi}_1$) and another for $I_2=0$ ($\xi=\bar{\xi}_2$). If a component of $\boldsymbol{\alpha}$ is zero, then there is no corresponding isolated orbit, as previously mentioned, and the boundary term vanishes).

Near to the boundary, J becomes large and it may be shown that it uniformly 'sews' together the solutions for $\xi_c \gtrless \bar{\xi}_i$.

To obtain Gutzwiller's result (4) it is necessary to rewrite the last terms in (12) using the periods τ_1, τ_2 and the stability angles ν_1, ν_2 of the isolated orbit. Call the term associated with the boundary at $\bar{\xi}_2$, $d_{\boldsymbol{M}}^{\mathrm{io}2}$, i.e.

$$d_{\boldsymbol{M}}^{\mathrm{io}2}=\frac{1}{2\pi\mathrm{i}\hbar|\boldsymbol{\omega}(\bar{\xi}_2)|\boldsymbol{M}\cdot\boldsymbol{I}'(\bar{\xi}_2)}\exp \mathrm{i}\left(\frac{2\pi}{\hbar}M_2I_2(\bar{\xi}_2)-\frac{\pi}{2}\boldsymbol{\alpha}(\bar{\xi}_2)\cdot\boldsymbol{M}\right). \tag{13}$$

The frequency vector is easily written as

$$\boldsymbol{\omega}(\bar{\xi}_2)=\tau_2^{-1}(\nu_2,2\pi).$$

To find $\boldsymbol{I}'(\bar{\xi}_2)$ we use the facts that it is a unit tangent vector of the energy contour, and $\boldsymbol{\omega}(\bar{\xi}_2)$ is perpendicular to the energy contour at $\bar{\xi}_2$; $\boldsymbol{\omega}\cdot\boldsymbol{I}'(\bar{\xi}_2)=0$ and $|\boldsymbol{I}'(\bar{\xi}_2)|=1$.

This gives

$$\boldsymbol{I}'(\bar{\xi}_2)=(-2\pi,\nu_2)(4\pi^2+\nu_2)^{-1/2}$$

and

$$|\boldsymbol{\omega}(\bar{\xi}_2)|\boldsymbol{M}\cdot\boldsymbol{I}'(\bar{\xi}_2)=(-2\pi M_1+\nu_2M_2)/\tau_2. \tag{14}$$

Now, the components of $\boldsymbol{\alpha}$ are always even (for smooth potentials; in fact if any are odd then the Gutzwiller formula (4) needs to be modified). The component α_1 represents the number of directed caustics of neighbouring tori lying alongside the primitive isolated orbit represented by $\bar{\xi}_2$. We assume that $\alpha_1 \neq 0$, otherwise the isolated orbit is not realised; so we consider only $\alpha_1 = 2, 4, 6$, etc. But sufficiently near to the isolated orbit the neighbouring tori are always elliptical so that at $\bar{\xi}_2$, α_1 may be taken as 2.

The component α_2 is the number of caustics of neighbouring tori lying across the isolated orbit at $\bar{\xi}_2$, that is, α_2 is the number of turning points, λ_2, along the isolated orbit. Consequently,

$$\pi \boldsymbol{\alpha}(\bar{\xi}_2) \cdot \boldsymbol{M} = 2\pi M_1 + \lambda_2 \pi M_2. \tag{15}$$

Using (13)–(15), we find

$$d_{\boldsymbol{M}}^{\mathrm{io2}} = \frac{-\tau_2}{2\pi \mathrm{i}\hbar} \frac{(-1)^{M_1}}{2\pi M_1 - \nu_2 M_2} \exp \mathrm{i}\left(\frac{2\pi}{\hbar} M_2 I_2(\bar{\xi}_2) - \frac{\pi}{2}\lambda_2 M_2\right). \tag{16}$$

Now comes a vital point: every periodic torus (real or complex) on the energy contour contributes an isolated orbit term like (16). For a particular repetition M_2, the assumptions of the theory ensure that there is precisely one real or complex torus on the energy contour for every integer M_1. Hence, to find the isolated orbit term for M_2 repetitions, we must sum (16) over all M_1 to get

$$\frac{-\tau_2}{2\pi \mathrm{i}\hbar} \exp \mathrm{i}\left(\frac{2\pi}{\hbar} M_2 I_2(\bar{\xi}_2) - \frac{\pi}{2}\lambda M_2\right) \sum_{M_1=-\infty}^{\infty} \frac{(-1)^{M_1}}{2\pi M_1 - \nu_2 M_2}. \tag{17}$$

This is valid provided no contributing torus $\boldsymbol{M}$ is 'too close' to the isolated orbit; otherwise $2\pi M_1 - \nu_2 M_2$ is near to zero for some M_1, and J in (12) becomes large.

Assuming this does not occur, we do the sum using the standard formula,

$$\operatorname{cosec} z = \sum_{k=-\infty}^{\infty} \frac{(-1)^k}{z - \pi k}. \tag{18}$$

The terms $\pm M_2$ are summed. (These correspond to traversing the closed orbit forwards and backwards.) The result is

$$\frac{\tau_2}{2\pi\hbar} \frac{\sin[(2\pi/\hbar) M_2 I_2(\bar{\xi}_2) - \frac{1}{2}\pi\lambda M_2]}{\sin \frac{1}{2}\nu_2 M_2} \tag{19}$$

which is precisely a term in Gutzwiller's series (4).

We have noted that this result is invalid where $2\pi M_1 - \nu_2 M_2$ is near to zero. However, by referring to the uniform approximation (12) we may quite easily obtain the correct form for such terms.

Integrating J by parts gives

$$J = \frac{\sqrt{\hbar}}{\Lambda_2} \exp\left(\frac{\mathrm{i}}{\hbar}(2\pi M_2 I_2(\bar{\xi}_2) - 2\pi \boldsymbol{M} \cdot \boldsymbol{I}(\xi_c))\right) - \frac{\operatorname{sgn} \delta}{\mathrm{i}\beta} \int_{|\Lambda_2|/\sqrt{\hbar}}^{\infty} \exp(\tfrac{1}{2}\mathrm{i}\beta x^2) + \mathrm{O}(\hbar^{3/2}) \tag{20}$$

where $\delta = \bar{\xi}_2 - \xi_c$.

The first term cancels with the term $d_{\boldsymbol{M}}^{\mathrm{io2}}$ on the boundary. The second term reduces the torus term by a factor $\frac{1}{2}$.

Consequently for small $2\pi M_1 - \nu_2 M_2$, $d_{\boldsymbol{M}}^{\mathrm{io2}}$ varies uniformly, giving on the boundary

$$d_{\boldsymbol{M}}^{\mathrm{io2}} \underset{\xi_c \to \bar{\xi}_2}{\simeq} \frac{\tau_2}{2} \left(\frac{1}{|\boldsymbol{M} \cdot \boldsymbol{I}''(\bar{\xi}_2)|}\right)^{1/2} \frac{\exp \mathrm{i}[(2\pi/\hbar) M_2 I_2(\bar{\xi}_2) + \frac{1}{4}\pi\beta - \frac{1}{2}\nu_2 M_2 - \frac{1}{2}\pi\lambda_2 M_2]}{\hbar^{3/2}(4\pi^2 + \nu_2^2)^{1/2}}. \tag{21}$$

Now since $\boldsymbol{M}$ is perpendicular to the energy contour at $\bar{\xi}_2$, and $2\pi M_1 \simeq \nu_2 M_2$,

$$\boldsymbol{M} \cdot \boldsymbol{I}''(\bar{\xi}_2) \simeq (M_2/2\pi)(\nu_2 + 4\pi^2)^{1/2} \hat{\boldsymbol{n}}(\bar{\xi}_2) \cdot \boldsymbol{I}''(\bar{\xi}_2),$$

where $\hat{\boldsymbol{n}}(\bar{\xi}_2)$ is a unit vector perpendicular to the energy contour $\bar{\xi}_2$.

Hence the contribution to $d(E)$ for an integrable system which replaces (19) when this form diverges is

$$\frac{\tau_2}{\hbar^{3/2}}\left(\frac{2\pi}{M_2 \hat{\boldsymbol{n}} \cdot \boldsymbol{I}''(\bar{\xi}_2)}\right)^{1/2} \frac{\cos[(2\pi/\hbar)M_2 I_2(\bar{\xi}_2) + \frac{1}{4}\pi\beta - \frac{1}{2}\nu_2 M_2 - \frac{1}{2}\pi\lambda_2 M_2]}{\nu_2 + 4\pi^2}. \qquad (22)$$

It can be verified that the remaining non-divergent terms in the sum over M_1 in (17) give zero.

It is important to realise that this expression is no longer associated entirely with the isolated orbit. It represents the combined contribution of the isolated orbit and the thin torus with topology (M_1, M_2) which surrounds it. As always with uniform approximations the individual contributions are no longer separable. The torus dominates in (22), since it is a *family* of orbits; this is the reason it is of order $h^{-3/2}$, as are the simple Berry–Tabor terms (3) (in the case of two freedoms).

Clearly we must associate the Gutzwiller series (4), in the integrable case, with only thin torus eigenvalues of (1). Consequently, we have seen how the harmonic approximation (6) is to be modified in the integrable case, when the Gutzwiller series is treated uniformly.

We should point out that for a different underlying classical structure (for instance, in a quasi-integrable system) the uniform approximation might be very different.

3. Discussion

We have shown that for integrable systems the Gutzwiller contributions to $d(E)$ are correction terms to the Berry–Tabor theory. This is achieved in a way that allows us to replace the divergent terms in Gutzwiller's series (where his argument breaks down) by uniform terms (22). The corrected series is interpreted as contributing to those peaks in the simple Berry–Tabor sum (3), which correspond to thin tori eigenvalues in (1); the isolated orbit terms are connected only with this part of the spectrum, and the full spectrum is given by the Berry–Tabor theory (which as we have seen includes the Gutzwiller terms). This contrasts with the harmonic approximation to $d(E)$ (Miller 1975) which gives a complete set of eigenvalues using only the isolated orbit terms.

For an integrable system of N (greater than two) freedoms, there will be boundary manifolds in phase space of all dimensions less than N, which may be treated in a similar uniform manner to the above. The Gutzwiller isolated orbit terms, suitably generalised, are then seen to be corrections to the simple Berry–Tabor formula (3) for boundary manifolds of dimension one.

I emphasise that the uniform approximation (22) is valid only for integrable systems. For generic systems new uniform approximations must be devised that take account of the underlying classical structure. This is the subject of continuing study.

Finally, a comment about unstable isolated orbits. Gutzwiller (1971) also derived a formula for these, analogous to (4),

$$\frac{\tau}{2\pi\hbar} \sum_{m=1}^{\infty} \frac{\cos m(S/\hbar - \frac{1}{2}l\pi)}{\sinh \frac{1}{2}m\nu}$$

where l is the number of caustics along the basic periodic orbit. In generic systems this series must also be corrected when periodic orbits of the same action are nearby in phase space, and ν is zero. However, in ergodic systems where nearly all periodic orbits are isolated and unstable the periodic orbits are all well separated and we would expect (23) to be valid for all these paths. In fact, Gutzwiller (1980) and Berry (1981) have both recently considered specific ergodic systems in which they demonstrate the validity of (23) in the ergodic case.

In summary, then, it is clear that integrable systems should be semiclassically quantised using the Berry–Tabor theory and ergodic systems using the Gutzwiller theory for unstable orbits. However, all the systems in between (which includes the quasi-integrable case) require that new uniform approximations be devised for the periodic orbit expansion of the density of states.

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Appendix. Green function approach, using action-angle variables

Here we show how to find the series (7) for the density of states, by using the semiclassical Green function. In general, for any bound system with N freedoms, the density of states function is given by

$$d(E)=\frac{\mathrm{Re}}{\pi\hbar}\int_0^\infty \mathrm{d}t\, k(t)\exp\left(\frac{\mathrm{i}}{\hbar}(E+\mathrm{i}\varepsilon)t\right) \tag{A1}$$

where $k(t)$ is the function $\mathrm{Tr}\exp[-(\mathrm{i}/\hbar)\hat{H}t]$, and $\hat{H}$ is the Hamiltonian operator.

There are great difficulties in setting up a *fully fledged* quantum mechanics in action-angle variables, but these do not affect the semiclassical formulae. Hence we may use these variables to find the approximation of the trace, $k(t)$.

Firstly, we find the semiclassical propagator in angle coordinates; this is defined by

$$K_{\mathrm{sc}}(\boldsymbol{\theta}_B,\boldsymbol{\theta}_A;t)=\langle\boldsymbol{\theta}_B|\exp[-(\mathrm{i}/\hbar)\hat{H}t]|\boldsymbol{\theta}_A\rangle. \tag{A2}$$

The vectors $|\boldsymbol{\theta}\rangle$ are, of course, only valid semiclassically. We now use the relation

$$\hat{1}=\int_R \mathrm{d}\boldsymbol{I}'\,|\boldsymbol{I}'\rangle\langle\boldsymbol{I}'| \tag{A3}$$

where the integral is over all real tori (a complex torus is labelled by real actions $\boldsymbol{I}$, but is not realised in phase space). This gives

$$K_{\mathrm{sc}}(\boldsymbol{\theta}_B,\boldsymbol{\theta}_A;t)=\int_R \mathrm{d}\boldsymbol{I}'\,\langle\boldsymbol{\theta}_B|\boldsymbol{I}'\rangle\langle\boldsymbol{I}'|\boldsymbol{\theta}_A\rangle\exp\left(\frac{-\mathrm{i}}{\hbar}H(\boldsymbol{I}')t\right). \tag{A4}$$

The action variables $\boldsymbol{I}$ are given by

$$I_i=\frac{1}{2\pi}\oint_{\gamma_i}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q}+K_i, \tag{A5}$$

where γ_i is the ith irreducible circuit of the torus, and K_i is a constant, whose value does not affect the classical mechanics. We will find, however, that for semiclassical mechanics there is a convenient choice for K_i which vanishes as $\hbar \to 0$.

Now the amplitude of the semiclassical torus states $\langle \boldsymbol{\theta} | \boldsymbol{I} \rangle$ is clearly independent of $\boldsymbol{\theta}$ since the density of phase points is constant over the torus. The phase, ϕ, may be found from the general prescription

$$\phi(\boldsymbol{Q}) = \frac{1}{\hbar} \int_{\boldsymbol{Q}_0}^{\boldsymbol{Q}} \boldsymbol{P}(\boldsymbol{Q}) \cdot \mathrm{d}\boldsymbol{Q} - \frac{\pi}{2}(\text{no of directed } \boldsymbol{Q} \text{ caustics from } \boldsymbol{Q}_0 \text{ to } \boldsymbol{Q}) \tag{A6}$$

where $(\boldsymbol{P}, \boldsymbol{Q})$ are canonical coordinates. Since there are no θ-caustics the phase of $\langle \boldsymbol{\theta} | \boldsymbol{I}' \rangle$ is simply $\boldsymbol{I}' \cdot (\boldsymbol{\theta} - \boldsymbol{\theta}_0)/\hbar$.

We will now require that the phase change, $\Delta_i \phi$, on going round the ith irreducible circuit of the torus is independent of the canonical coordinates used to compute it. For *any* non-singular coordinates the number of $\boldsymbol{Q}$ caustics is α_i; hence

$$\Delta_i \phi = \frac{1}{\hbar} \oint_{\gamma_i} \boldsymbol{p} \cdot \mathrm{d}\boldsymbol{q} - \frac{\pi}{2} \alpha_i, \tag{A7}$$

which implies that we choose K_i as $-\alpha_i \hbar/4$ for semiclassical approximations.

Hence, from (A4) we find, after normalising the torus states,

$$K_{\mathrm{sc}}(\boldsymbol{\theta}_B, \boldsymbol{\theta}_A; t) = \frac{1}{(2\pi\hbar)^N} \int_{-\alpha_1 \hbar/4}^{\infty} \mathrm{d}I_1' \ldots \int_{-\alpha_N \hbar/4}^{\infty} \mathrm{d}I_N' \exp\left(\frac{\mathrm{i}}{\hbar}[\boldsymbol{I}' \cdot (\boldsymbol{\theta}_B - \boldsymbol{\theta}_A) - H(\boldsymbol{I}')t]\right). \tag{A8}$$

Upon changing variables to $\boldsymbol{I} = \boldsymbol{I}' + \boldsymbol{\alpha}\hbar/4$, we find

$$K_{\mathrm{sc}}(\boldsymbol{\theta}_B, \boldsymbol{\theta}_A; t) = \frac{1}{(2\pi\hbar)^N} \int_+ \mathrm{d}\boldsymbol{I} \exp \mathrm{i}\left[\left(\frac{\boldsymbol{I}}{\hbar} - \frac{\boldsymbol{\alpha}}{4}\right) \cdot (\boldsymbol{\theta}_B - \boldsymbol{\theta}_A) - \frac{H(\boldsymbol{I})t}{\hbar}\right] \tag{A9}$$

where the integration domain is the positive quadrant of $\boldsymbol{I}$ space.

The integrand in (A9) has a stationary point at $\boldsymbol{I}^*$ given by

$$\boldsymbol{\theta}_B - \boldsymbol{\theta}_A = \boldsymbol{\omega}(\boldsymbol{I}^*)t. \tag{A10}$$

Evaluating the integral by the method of stationary phase then leads to

$$K_{\mathrm{sc}}(\boldsymbol{\theta}_B, \boldsymbol{\theta}_A; t) \simeq \frac{1}{(2\pi \mathrm{i}\hbar t)^{N/2}} \left|\det \frac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}\boldsymbol{I}}\right|^{-1/2} \exp \mathrm{i}\left[\left(\frac{\boldsymbol{I}^*}{\hbar} - \frac{\boldsymbol{\alpha}}{4}\right) \cdot (\boldsymbol{\theta}_B - \boldsymbol{\theta}_A) - \frac{H(\boldsymbol{I})t}{\hbar}\right]. \tag{A11}$$

Upon placing $\boldsymbol{\theta}_B = \boldsymbol{\theta}_A + 2\pi\boldsymbol{M}$ this gives the formula used by Berry and Tabor (1977) to evaluate the trace in (A1). They then use this to regain the simple semiclassical result (3). However, it is clear that the stationary phase method misses the contributions from the boundaries of the integration domain in (A9), so we will proceed by using the integral representation.

Due to the periodicity of the angle coordinates the trace is

$$\begin{aligned} k(t) &= \sum_{\boldsymbol{M}} \int_0^{2\pi} \mathrm{d}\boldsymbol{\theta}\, \langle \boldsymbol{\theta} + 2\pi\boldsymbol{M} | \exp(-\mathrm{i}\hat{H}t/\hbar) | \boldsymbol{\theta} \rangle \\ &= \frac{1}{(2\pi\hbar)^N} \sum_{\boldsymbol{M}} \int_0^{2\pi} \mathrm{d}\boldsymbol{\theta} \int_+ \mathrm{d}\boldsymbol{I} \exp \mathrm{i}\left(\frac{1}{\hbar}(2\pi\boldsymbol{M} \cdot \boldsymbol{I} - H(\boldsymbol{I})t) - \frac{\pi}{2}\boldsymbol{\alpha} \cdot \boldsymbol{M}\right). \end{aligned} \tag{A12}$$

Since the integrands do not involve $\boldsymbol{\theta}$, the $\boldsymbol{\theta}$-integrals merely introduce a factor $(2\pi)^N$. Hence, using (A1) and (A12), the density of states function is

$$d(E) \simeq \bar{d}(E) + \frac{\mathrm{Re}}{\pi\hbar^{N+1}} \int_0^\infty \mathrm{d}t \exp\left(\frac{\mathrm{i}t}{\hbar}(E + \mathrm{i}\varepsilon - H(\boldsymbol{I}))\right)$$

$$\times \sum_{\boldsymbol{M}}{}' \int_+ \mathrm{d}\boldsymbol{I} \exp \mathrm{i}\left(\frac{2\pi}{\hbar}\boldsymbol{M} \cdot \boldsymbol{I} - \frac{\pi}{2}\boldsymbol{\alpha} \cdot \boldsymbol{M}\right). \tag{A13}$$

Since the $\boldsymbol{M}$ sum is *real* and the real part of the t integral is $\pi\hbar\delta(E - H(\boldsymbol{I}))$ we find that

$$d(E) \simeq \bar{d}(E) + \frac{1}{\hbar^N} \sum_{\boldsymbol{M}}{}' \int_+ \mathrm{d}\boldsymbol{I}\, \delta(E - H(\boldsymbol{I})) \exp \mathrm{i}\left(\frac{2\pi}{\hbar}\boldsymbol{M} \cdot \boldsymbol{I} - \frac{\pi}{2}\boldsymbol{M} \cdot \boldsymbol{\alpha}\right). \tag{A14}$$

Following Berry and Tabor (1976), we rewrite the integral in curvilinear co-ordinates $(\xi_0, \boldsymbol{\xi})$ where ξ_0 is perpendicular to the energy contour $E = H(\boldsymbol{I})$ and $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_{N-1})$ is parallel to the energy contour. This gives

$$d(E) \simeq \bar{d}(E) + \frac{1}{\hbar^N} \sum_{\boldsymbol{M}}{}' \int_{\bar{\boldsymbol{\xi}}_1}^{\bar{\boldsymbol{\xi}}_2} \mathrm{d}\boldsymbol{\xi} \frac{\exp \mathrm{i}[(2\pi/\hbar)\boldsymbol{M} \cdot \boldsymbol{I}(\boldsymbol{\xi}) - \frac{1}{2}\pi\boldsymbol{\alpha} \cdot \boldsymbol{M}]}{|\boldsymbol{\omega}(\boldsymbol{I}(\xi))|} \tag{A15}$$

where $|\boldsymbol{\omega}(\boldsymbol{I}(\xi))| = |\partial H/\partial \xi_0|$ and $\bar{\boldsymbol{\xi}}_1$, $\bar{\boldsymbol{\xi}}_2$ are the boundary values of $\boldsymbol{\xi}$.

For two freedoms this result easily specialises to (7). The advantage of using the integral form (A9) for $K_{\mathrm{sc}}(\boldsymbol{\theta}_B, \boldsymbol{\theta}_A; t)$ over the stationary phase result (A11) is that it enables us to find the series of integrals for $d(E)$, (A15), which we may evaluate uniformly. If we use (A11), on the other hand, we may only find the simple semiclassical result (3).

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