Quasiclassical Surface of Section Perturbation Theory

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Perturbation theory, the quasiclassical approximation and Bogomolny's quantum surface of section method are combined for the first time. With this method, we can quantize the resonances and chaotic regions generically appearing in classical perturbation theory. As compared with existing techniques, our results and calculations are relatively simple and in reduced dimension, and they are readily visualized. We illustrate by applying the method to a class of problems of recent interest.

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Poincaré found that perturbation theory [PT] on an integrable classical system fails in two or more dimensions due to 'small denominators'. Kolmogorov-Arnol'd-Moser [KAM]¹ theory greatly illuminated the subject and showed that the breakdown of PT signals chaos, and leads to new, small, classical actions dependent on the perturbation parameter ϵ . Quantizing such a theory has been of interest². The comparison of Planck's constant h with these actions is then important to the quantization procedure, which is naturally carried out in the quasiclassical approximation, [QCA].

Phase space trajectories of an integrable system lie on invariant tori [IT]. Perturbation destroys all periodic orbits, on 'rational' tori, except for one or more stable and unstable orbits. The dense rational tori are labelled by rational numbers p/q. The tori near the rational ones are also destroyed, to a width in action $\sqrt{\epsilon}S_{pq}$. Topologically new IT are formed around the stable orbits while chaos develops near the unstable orbit and separatrix. The characteristic action S_{pq} generically drops off rapidly with q. The result is usually pictured, as in Fig.1, on a Poincaré surface of section [SS], a slice through the tori, where the structure of alternating stable and unstable orbits is called an 'island chain' or 'resonances'.

Chaos is conceptually important, but the phase space volume of the chaotic regions is smaller than any power of ϵ . This allows an order by order transformation of the Hamiltonian to a series in integrable 'normal form', which if truncated yields approximate IT, which can be quantized by EBK methods. This and related methods have been extensively used to find approximations to IT even though it is known that such a series does not converge. The method can be efficient numerically as well as providing some insight².

We here combine for the first time, PT, the QCA, and the powerful QCA-SS method of Bogomolny^{3,4}. We achieve quite complete and explicit results. Namely, we are able to find all the energy levels and SS-wavefunctions in a WKB approximation for small ϵ , provided h is not too small in a sense to be specified. We do not find or need to know the whole IT, but only its intersection with the SS. We also give some numerical checks.

Our SS method has the usual advantages. There is a reduction in dimension, most dramatically at d=2, which allows visualisation of the results, and provides a convenient formulation for general considerations. If the Poincaré SS map is simple, the calculations are relatively easy, but if it tedious to obtain the SS map, and numer-

ical results are the main focus, another method may be preferred. Our method can sometimes also be applied when the perturbation is not smooth enough or weak enough to permit a KAM analysis.

Our method based on ref.³, can also be seen as a "resummation" of the perturbed Berry-Tabor trace formula which yields approximations to the energy levels, rather than just correlations between them^{2,5}.

There has been recent interest in a number of problems susceptible to our technique⁶⁻⁹, and we have also learned of several ongoing efforts^{10,11}. These problems are related to a weakly deformed circular billiard. We adopt the notation of this case. The Helmholtz equation $(\nabla^2 + k^2) \Psi = 0$ is to be solved for eigenfunctions $\Psi = \Psi_a$ and eigenvalues $k = k_a$ with, say, Dirichlet conditions $\Psi_a(r,\theta) = 0$ on the boundary, ∂B . The latter is expressed in polar coordinates by $r(\theta) = R_0 + \epsilon \Delta R(\theta)$. These and similar boundary perturbations have heretofore been treated¹² by methods valid only for $k\sqrt{\epsilon} << 1$.

In quantum language, we take units $R_0 = 1$, $\hbar = 1$, particle mass = 1/2, so k is the large dimensionless wavenumber, (equivalent to $1/\hbar$). We take ∂B as SS. Then Bogomolny's unitary operator is³

$$T(\theta, \theta'; k) = -\left(\frac{k}{2\pi i} \frac{\partial^2 L(\theta, \theta')}{\partial \theta \partial \theta'}\right)^{\frac{1}{2}} \exp\left(ikL\left(\theta, \theta'\right)\right) \quad (1)$$

where L is the chord distance between two points on ∂B , specified by polar angles. Expanding,

$$kL(\theta, \theta') = 2k \left| \sin \frac{\theta - \theta'}{2} \right| \left(1 + \epsilon \frac{\Delta R(\theta) + \Delta R(\theta')}{2} \right) + \dots$$
$$= k(L_0 + \epsilon L_2 + \dots)$$
(2)

The levels k_a of the system are given in QCA³ by solution of $\det(1 - T(k)) = 0$, a resummation of the trace formula. Our seemingly more difficult technique studies

$$\psi(\theta) = \int d\theta' T(\theta, \theta'; k) \psi(\theta'), \tag{3}$$

solvable only for $k = k_a$. $[\psi \approx \partial \Psi / \partial n \text{ on } \partial B.]$

A rule of thumb is that only phase space structures of area h or greater are reflected in the quantized system. Thus, if $\sqrt{\epsilon}S_{pq} << \hbar$ ordinary quantum perturbation theory works well. If $\sqrt{\epsilon}S_{pq} \geq \hbar$, ordinary perturbation theory breaks down as a number $\sqrt{\epsilon}S_{pq}/\hbar$ unperturbed quantum states are strongly mixed by the perturbation¹³.

We begin with what is usually the largest resonance, q=2, by making a WKB Ansatz $\psi(\theta)=\exp{(i\alpha f(\theta))}$ where $df/d\theta=f'\sim 1$ and $k>>\alpha>>k\epsilon$. This Ansatz represents a superposition of angular momentum states $|l|\sim\alpha<< l_{\rm max}=k$, and for $\alpha>1$ conveniently expresses the mix of states of low angular momentum needed to diagonalize the Hamiltonian

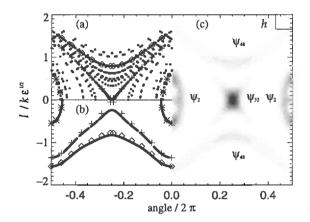


FIG. 1. SS [angular momentum vs angle] of orbits for a) 'stadium' and b) 'smoothed stadium' $\epsilon = 0.01$. Points on $l_{WKB}(\theta)$, for 'continuum', \diamondsuit , 'separatrix',+, and 'bound', *, values of E_m , respectively. Three orbits, each iterated 1000 times, coalesce into solid lines in b), where KAM applies. Orbits started at the symbols iterated forward and backward 15 times appear as dots in a) where KAM fails. Only short time structure is regular. c) Husimi plots for exact states of Fig. 2, as well as a 'scar' state ψ_{32} . Square has area h.

According to the stationary phase [S\Phi] method, the θ' integral of Eq.(3) is dominated by the region $\theta' \sim \theta \pm \pi$ where $kL_0 = 2k \left| \sin \frac{1}{2}(\theta - \theta') \right|$ is stationary. Expand $\sin \frac{1}{2}(\theta - \theta') \approx 1 - \frac{1}{8}\delta\theta^2$, $\delta\theta = \theta' - \theta - \pi$ to find

$$S(\theta, \theta') \equiv kL \approx 2k - \frac{1}{4}k\delta\theta^2 + k\epsilon(\Delta R(\theta) + \Delta R(\theta'))$$
 (4)

Regarding S as a classical generating function, we obtain the surface of section maps $(l', \theta') \rightarrow (l, \theta)$ found earlier, θ by θ by

Returning to Eq.(3), expand all functions of θ' about $\theta + \pi$. I.e. $f(\theta') \approx f(\theta + \pi) + \delta\theta f'(\theta + \pi)$ to order $\delta\theta$, since $\alpha << k$, and $\Delta R(\theta') \approx \Delta R(\theta + \pi)$, since $\alpha >> k\epsilon$. Doing the integral reduces Eq.(3) to

$$\exp[i\alpha f(\theta)] = i\exp\left[i\left(2k + (\alpha f')^2/k + k\epsilon V(\theta) + \alpha f(\theta + \pi)\right)\right]$$
 (5)

where $V(\theta) = \Delta R(\theta) + \Delta R(\theta + \pi)$.

For Eq.(5) to hold, the exponents of order α must combine to give a constant c, i.e. $f(\theta + \pi) = f(\theta) + c$. Now take $\alpha = k\sqrt{\epsilon}$ so a solution is possible provided $(f')^2 + V(\theta)$ is a constant, which we call E_m . Thus

$$f(\theta) = \pm \int_{\theta_1}^{\theta} d\theta' \sqrt{E_m - V(\theta')}$$
 (6)

reminiscent of elementary WKB theory. The constant of integration is irrelevant. Notice $V(\theta) = V(\theta + \pi) \iff f(\theta + \pi) = f(\theta) + c$. We define $l_{WKB}(\theta) = \alpha f'(\theta)$, which is a simple leading order formula for the intersection of an IT, labelled by E_m , with the SS. The $S\Phi$ procedure on Eq.(3) is classically equivalent to the requirement that $(l_{WKB}(\theta'), \theta') \to (l_{WKB}(\theta), \theta)$ under the SS map.

Assuming for now that $E_m \geq V$, [a 'continuum' state], we must choose E_m such that $kb \int_0^{2\pi} d\theta' \sqrt{E_m - V(\theta')} = 2\pi m$ where m is integer, $b = \sqrt{\epsilon}$ and so $c = \pi m/kb$. The condition giving the energy is

$$\exp\left[i\left(2k + kb^2E_m + kbc + \pi/2\right)\right] = 1 = \exp(2\pi in)$$
 (7)

which has solutions $k=k_{n,m}$. For $\Delta R=0$, this reduces to $2k+m^2/k+\pi m=(n-\frac{1}{4})2\pi$ equivalent to Debye's approximation to Bessel's function, valid for k large and m/k small. Thus, we find states labelled m,n with m an integer angular quantum number satisfying $|m|<< k_{n,m}\approx \pi n$. There may be symmetries, for example time reversal which allows real wavefunctions. Then the states are $\psi=\cos\alpha f(\theta)$, $\sin\alpha f(\theta)$, which are degenerate at this level of approximation. This result allows an explicit estimate of ψ_l [angular momentum representation] which, for $|l|>k\sqrt{\epsilon}$, decays exponentially for smooth V and as l^{-4} for the stadium case^{7,9}.

If $E_m - V$ changes sign there are 'bound state' regions near the minima of V where $E_m > V$, which defines a region $\mathcal{B}: \theta_l < \theta < \theta_u$, where $\theta = \theta_{l,u}$ are 'classical turning points'. Take θ_l as the lower limit in Eq.(6). The quantization condition is now, approximately, $\sin(\alpha f(\theta_u)) = 0$, or $\alpha f(\theta_u) = m\pi$ and $\psi \approx 0$, $\theta \notin \mathcal{B}$. This treatment, which can be improved $f(\theta_u) = f(\theta_u) = f(\theta_u)$, effects on the amplitude of the wavefunctions and Maslov indices.

The bound states quantize the stable resonance islands and the continuum states quantize the unstable and perturbed KAM regions. A minimum in V is at a stable periodic orbit, and a maximum at an unstable one. 'Scars' of unstable orbits, Fig. 1c, are states with E_m just greater than the maximum V. Fig. 2 shows a WKB state and two indistinguishable numerically obtained states, all with the same value of $k\sqrt{\epsilon}$, one with $k\epsilon=1.8$ the other for $k\epsilon=0.18$. The state depends dominantly on $k\sqrt{\epsilon}$ and no qualitative changes occur at $k\epsilon\approx 1$. Husimi plots of these states are shown in Fig. 1c.

An illustration is the stadium billiard^{7,9,10} which has two semicircular endcaps of radius R_B connected by parallel straight sides of length 2a. Then $\epsilon = a/R_B$ is assumed small and R_0 is taken as $R_0 \approx R_B + 2a/\pi$ while $\Delta R/R_0 \approx |\sin\theta| - 2/\pi$. This 'stadium' choice of ΔR has a discontinuous first derivative so KAM does not apply. The classical map deviates from the 'invariant' tori [given approximately by $l_{WKB}(\theta)$] after about $1/\sqrt{\epsilon}$ iterations, Fig. 1a. We also show results, Fig. 1b, for a 'smoothed stadium', a truncated Fourier series of the 'stadium' $\Delta R(\theta)$, where the orbit stays on an IT. The localization in this case was first⁷ thought to be dynamical localization in the presence of chaos analogous to Anderson localization¹⁴, but now^{9,10} [for $k\epsilon^2 < 1$] is attributed to Cantori. Our treatment has no need to invoke Cantori.

Classically the stadium is chaotic with no stable orbits. Orbits diffuse in angular momentum at long times. [Most SS returns follow l_{WKB} , but a fraction $\sim \sqrt{\epsilon}$ of these returns are near the kink at $\theta = 0, \pi$, and 'randomly' change E_m , on an angular momentum scale $\Delta l \sim k\epsilon$. This leads to a diffusion constant $D \propto \Delta l^2 \sqrt{\epsilon} \approx k^2 \epsilon^{5/2}$.] Our 'integrable' results are possible because it is the short time behavior, times up to the mean level separation of the mixing states which determines the quantization. That time, measured in SS returns, is, in this case, $\epsilon^{-1/2}$, provided l_{WKB} is approximately correct.

An average localization width in angular momentum, l_{σ} , where, [in effect] $l_{\sigma}^2 = \sum_a |c_a|^2 \int d\theta \, |\psi_a'|^2$ and c_a is the normalized zero angular momentum component of ψ_a has been numerically obtained⁹. We find the c_a 's are small for 'continuum' states, [Fig. 2] and the 'bound' states dominate. Then $l_{\sigma} \sim k \sqrt{\epsilon}$ for these states. Agreement with this result for fixed k and increasing ϵ , until $k\epsilon^2 \approx 1$ was obtained⁹. We show below that our theory should fail at that point. Ref.¹⁰ uses a different definition of l_{σ} and averages over different states, including high angular momentum states. Since classical phase space in this problem is hardly homogeneous, it is not surprising their results are different. Fig. 2 shows a high angular momentum state, away from a resonant torus, which has a much narrower distribution.

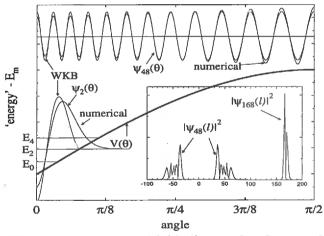


FIG. 2. 'Stadium' potential $|\sin\theta|$ vs angle. States and potential are symmetric about zero angle. Bound and continuum, WKB and exact states are shown, with zeroes at WKB 'energy' parameter E_m . $k\epsilon^{1/2}=42.3$ is fixed. Inset: Angular momentum representation of continuum state m=48 and exact state near angular momentum m=168.

We turn to general angular momenta and higher orders in ϵ . We first look for solutions of the form $\psi = \exp(iG(\theta'))$, where $G = l\theta' + k(\epsilon f_2 + \epsilon^2 f_4 + \ldots)$. The f's are 2π -periodic and $l \leq k$ is integer. This, if successful, is a usual PT for G. The $S\Phi$ angle is $\theta' \approx \theta + \Theta_l$ where $\Theta_l = -2\mathrm{sign}(l)\cos^{-1}(l/k)$. Expanding as before the order $k\epsilon$ condition is

$$f_2(\theta + \Theta_l) - f_2(\theta) = \tilde{L}_2(\theta). \tag{8}$$

We use \tilde{l}_2 and $\tilde{L}_2(\theta)$ as the constant and variable parts of $L_2(\theta, \theta + \Theta_l)$. The constant part $k \in \tilde{l}_2$ contributes to the phase of Eq.(7). Eq.(8) is solved in terms of $r \neq 0$ Fourier components, i.e. $f_{2r} = (\exp(ir\Theta_l) - 1)^{-1} \tilde{L}_{2r}$. This a good solution unless the denominator is excessively small. It never strictly vanishes since $\Theta_l/2\pi$ is an irrational number. However, if Θ_l is close to $\Theta_{pq} = 2\pi p/q$, where p/q is a rational number, [corresponding to the strongly perturbed rational tori of classical perturbation theory], then the denominator will be small if r is a multiple of q. It will still be a good solution if \tilde{L}_{2r} vanishes or is sufficiently small. Generically \tilde{L}_{2r} decreases rapidly for large r. If the small denominators are thus compensated by small numerators, this perturbation theory can be carried to higher orders by the methods described below. If not, we need to refine the approach along the lines of our first Ansatz which corresponds to q=2.

We are thus motivated to consider

$$\psi = \exp\left[i\left(l_{pq}\theta' + k(bf_1 + b^2f_2 + b^3f_3 + \ldots)\right)\right]$$
 (9)

The [non-integer] angular momentum l_{pq} is chosen to make the stationary point $\theta'=\theta+\Theta_{pq}$. Expanding as before, the order b requirement is $f_1(\theta+\Theta_{pq})-f_1(\theta)+l_{pq}\Theta_{pq}/kb=c=$ constant implying f_1' is q-periodic, i.e. periodic with period Θ_{pq} . At order b^2 we have

$$\sigma_{pq}^{-1} (f_1')^2 + \tilde{L}_2(\theta) + f_2(\theta + \Theta_{pq}) - f_2(\theta) = E_m \quad (10)$$

where $\tilde{L}_2(\theta)$ is the variable part of $L_2(\theta, \theta + \Theta_{pq})$, $\sigma_{pq} = \left|\sin\frac{1}{2}\Theta_{pq}\right|$ and E_m is to be determined. We divide Eq.(10) into q-periodic and non q-periodic parts. The nonperiodic terms f_2 and \tilde{L}_2 must combine to give a q-periodic result, thus

$$f_2(\theta + \Theta_{pq}) - f_2(\theta) + \tilde{L}_2(\theta) = \tilde{V}_q(\theta)$$
 (11)

where $\bar{V}_q(\theta)$ is to be determined. We 'q-average' both sides giving $\bar{V}_q(\theta) = \frac{1}{q} \sum_{j=1}^q \tilde{L}_2(\theta + j\Theta_{pq})$. Expressed in Fourier components, $\bar{V}_q(\theta) = \sum_l \tilde{L}_{2ql} e^{iql\theta}$ and $f_2(\theta) = \sum_l (1 - e^{il\Theta_{pq}})^{-1} \tilde{L}_{2l} e^{il\theta} + \bar{f}_2(\theta)$. The prime indicates that integers l divisible by q are not included in the sum and $\bar{f}_2(\theta)$ is an q-periodic function not yet determined. Then

$$f_1(\theta) = \pm S_{pq}^{1/2} \int_0^\theta d\theta' \sqrt{E_m - \bar{V}_q(\theta')}$$
 (12)

and considerations like those discussed earlier for q=2 fix the quantization of E_m . The size of \bar{V}_q , which decreases rapidly with q, determines if powers of $\sqrt{\epsilon}$ rather than ϵ are needed.

Order b^3 is more complicated: $L_2(\theta, \theta')$ and f_2 are expanded to $\delta\theta$, f_1 to $\delta\theta^2$ and L_0 to $\delta\theta^3$. The integral of Eq.(3) is thus

$$\int d\delta\theta \exp\left[\frac{-ik}{3!}L_0^{\prime\prime\prime}\delta\theta^3 + \frac{ik}{2}(L_0^{\prime\prime} + bf_1^{\prime\prime})\delta\theta^2 + iF^{\prime}\delta\theta\right]$$
(13)

where $F' = kbf'_1 + kb^2F'_2$ with $F'_2 = f'_2 + L'_2$. We denote derivatives evaluated at $\theta' = \theta + \Theta_{pq}$ by primes. [This

integral is done over a region near the original stationary point. The new stationary point coming from $\delta\theta^3$ is not meaningful.] The width of contributing angles $\delta\theta$ is of order $k^{-1/2}$ which is small. However, the shift of the center of the contributing region is expressed by a power series in b whose leading term is $-bf_1'/L_0''$. If $kb^2 \geq 1$, the shift cannot be neglected. Thus, to order b^3 we require

$$\frac{L_0'''}{3!} \left(\frac{-f_1'}{L_0''}\right)^3 - \frac{1}{2} f_1'' \left(\frac{f_1'}{L_0''}\right)^2 - \frac{f_1' F_2'}{L_0''} + c_3$$

$$= -f_3(\theta + \Theta_{pq}) + f_3(\theta) \tag{14}$$

where c_3 is a constant. Let $F_2' = \bar{f}_2' + A(\theta)$, where A has already been determined by lower order considerations. Eq.(14) can only be satisfied if the q-average of the left hand side vanishes. This determines \bar{f}_2' by

$$\bar{f}_2' = -\bar{A}_q + \frac{L_0'' c_3}{f_1'} - \frac{1}{2} f_1'' \frac{f_1'}{L_0''} + \frac{L_0'''}{3!} \left(\frac{f_1'}{L_0''}\right)^2.$$

This expression must also have vanishing angular average, since \bar{f}'_2 is the derivative of a periodic function, which determines c_3 . Thus f_2 is determined up to an irrelevant integration constant, and, then as before, f_3 is determined up to an q-periodic function.

If $kb^3 << 1$, we may stop here. If not, we can continue finding higher order corrections, expanding to higher powers of $\delta\theta$ and keeping the terms L_4, L_6, \ldots in the expansion of the phase of the T operator. The series will be effectively terminated at order n when $kb^n << 1$. However, the method may break down sooner, indicating a change in the fundamental physics.

In the case $\Delta R = |\sin \theta|$, there are δ -function singularities in f_1''' and L_2'' . These large derivatives invalidate the expansion. Thus in the Bunimovich problem we expect our solution to break down when $k\epsilon^2 > 1$.

In principle, we can use this technique to study perturbations of any two dimensional integrable system. 'Simply' use action angle coordinates I_1 , I_2 , Θ_1 , Θ_2 , and take as surface of section $\Theta_1 = 0$. The T operator will have a phase $k(S_0(\Theta_2 - \Theta_2') + \epsilon S_2(\Theta_2, \Theta_2') + \ldots)$ and the rest is pretty much the same as above. Other coordinates may be more convenient in practice, however. The circle is nice because the action-angle coordinates are immediate. On the other hand, harmonic oscillators coupled perturbatively need special treatment².

There are other applications of this technique in non-perturbative settings, in which certain classes of eigenstates can be found. The germ of the method first appeared in the study of the ray splitting billiard¹⁵, and it can be used to find the well known 'bouncing ball' states in the [large ϵ] stadium billiard.

We have thus produced a fairly general theory allowing us to find the effect of perturbations on integrable quantum systems which exploits the quasiclassical approximation and the surface of section technique. If the perturbation classically gives rise to resonances big enough to influence the quantum problem, we must expand in the square root of the small parameter. If the resonances are small, a simpler expansion works.

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