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Exact Bogomolny sections for separable systems*

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Abstract. A good Poincaré section of a classical dynamical system defines a mapping that provides essential qualitative information about its orbits. Bogomolny's sections in quantum mechanics lead to an eigenvalue condition that depends on the Poincaré map in the semiclassical limit. The conditions for the construction of purely quantum mechanical Bogomolny–Green functions are discussed here with reference to separable systems. For appropriately chosen Green functions the ensuing eigenvalue condition is shown to be exact. This result is valid even if not a single classical orbit crosses the surface of section.

1. Introduction

The Poincaré surface of section is a valuable instrument of classical dynamics. If almost all the orbits cross the section, almost all the periodic orbits of the classical system will appear as periodic points of the Poincaré map. These periodic orbits and periodic points will proliferate exponentially with period in both the system and the map if they are chaotic. We likewise find that all the other principal qualitative features of the continuous system are deducible from the map in its reduced phase space.

The energy spectrum of a quantized system is related to the classical periodic orbits. In some special cases the correspondence is exact (the Selberg trace formula), whereas generally the relation is achieved by the Gutzwiller trace formula, which is a semiclassical approximation (Gutzwiller 1990). The following questions thus arise: If the eigenvalues are related to the periodic orbits and these intersect the Poincaré section, can we obtain the spectrum from a reduced quantum map defined on the section? Would this result be exact or only a semiclassical approximation?

The construction of a quantum map over a section, such that its Green function supplies the eigenvalues of the surrounding Hamiltonian, was achieved by Bogomolny (1990, 1992). In the first paper Bogomolny constructed directly a semiclassical Green function, but he later derived it from the convolution of two Green functions defined on either half space resulting from the section of the full space. Even so, the main effort was directed there to the derivation of the Gutzwiller trace formula as an expansion of the ensuing quantization condition. Because of this, semiclassical arguments permeate the discussion, obscuring a point of paramount importance: if the Bogomolny condition can be stated in exact quantum mechanical terms, then the conditions for finding a good Bogomolny section must depend only on the quantum mechanical features of the system. To invoke the classical orbit structure is important for the understanding of

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the semiclassical approximation of the eigenvalue condition, but it cannot precede the definition of the Green function.

The purpose of this paper is to discuss the construction of Bogomolny's section and eigenvalue condition prior to any semiclassical approximation. Section 2 presents a one-dimensional interpretation of the theory for general Sturm–Liouville problems, since these arise naturally in the separation of variables in the Schrödinger equation. This is compared with the deduction of the eigenvalue condition for higher dimensions, recapitulated in section 3. The one-dimensional Green functions constructed in section 2 are then used to construct the full auxiliary Green functions of separable systems in section 4.

The main result is that the general Green functions admitted in Bogomolny (1992) can lead to spurious zeros of the eigenvalue condition of separable systems. However, the use of purely outgoing (or purely incoming) Green functions renders Bogomolny's condition necessary and sufficient for these special systems even in the case that the section is only accessible through tunnelling. Section 6 discusses the difficulties of generalizing the exact theory to non-separable systems.

2. The eigenvalue problem in one dimension

In certain special cases it is possible to separate the variables of the time-independent Schrödinger equation in a given region V of L-dimensional configuration space. The energy eigenvalue problem is then reduced to the Sturm–Liouville problem (Smirnov 1964)

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[r(x)\frac{\mathrm{d}}{\mathrm{d}x}v(x,\lambda)\right]-[s(x)+\lambda t(x)]v(x)=0 \qquad (-a_2<x<a_1) \tag{2.1}$$

with the boundary conditions

$$\alpha_1 v(a_1,\lambda)+\beta_1\frac{\mathrm{d}v}{\mathrm{d}x}(a_1,\lambda)=0 \qquad \alpha_2 v(-a_2,\lambda)+\beta_2\frac{\mathrm{d}v}{\mathrm{d}x}(-a_2,\lambda)=0. \tag{2.2}$$

It makes no practical sense to solve an eigenvalue problem by means of the preliminary solution of two problems each of which is essentially identical to the given one. None the less, this is the basis of Bogomolny's general reduction of an eigenvalue problem to a condition on a single surface of section. In one dimension the surface reduces to a single point, $x=0$, without loss of generality. We thus consider a pair of Green functions on both sides of the origin satisfying the two related self-adjoint equations

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[r_1(x)\frac{\mathrm{d}}{\mathrm{d}x}g_1(x,x',\lambda)\right]-[s_1(x)+\lambda t_1(x)]g_1(x,x',\lambda)$$
$$=\delta(x-x') \qquad (-a_1'<x<a_1) \tag{2.3}$$

with

$$\alpha_1 g_1(a_1, x', \lambda) + \beta_1 \frac{dg_1}{dx}(a_1, x', \lambda) = 0$$
$$\alpha_1' g_1(-a_1', x', \lambda) + \beta_1' \frac{dg_1}{dx}(-a_1', x', \lambda) = 0 \tag{2.4}$$

and

$$\frac{d}{dx}\left[r_2(x)\frac{d}{dx}g_2(x, x', \lambda)\right] - [s_2(x) + \lambda t_2(x)]g_2(x, x', \lambda)$$
$$= \delta(x - x')(-a_2 < x < a_2') \tag{2.5}$$

with

$$\alpha_2' g_2(a_2', x', \lambda) + \beta_2' \frac{dg_2}{dx}(a_2', x', \lambda) = 0$$
$$\alpha_2 g_2(-a_2, x', \lambda) + \beta_2 \frac{dg_2}{dx}(-a_2, x', \lambda) = 0. \tag{2.6}$$

For $x \geqslant 0$ the functions $r_1(x)$, $s_1(x)$ and $t_1(x)$ coincide with $r(x)$, $s(x)$ and $t(x)$, whereas the latter are identical to $r_2(x)$, $s_2(x)$ and $t_2(x)$ for $x \leqslant 0$. If we choose $x' < 0$, then $g_1(x, x', \lambda)$ is a solution of (2.1) for $x \geqslant 0$, satisfying the first boundary condition (2.2). We may analytically continue this solution as far as $x = -a_2$, if $r(x)$, $s(x)$ and $t(x)$ are analytic functions, but generally it will not satisfy the second condition (2.2). Likewise we may consider $g_2(x, x'', \lambda)$ with $x'' > 0$ as a solution (2.1) for $x < 0$ that satisfies the second condition (2.2).

Two solutions $v(x)$ and $w(x)$ of the linear equation (2.1) will be linearly dependent if and only if the Wronskian

$$v(x)\frac{d}{dx}w(x) - w(x)\frac{d}{dx}v(x) = \frac{c}{r(x)} \tag{2.7}$$

is identically zero. It follows that, if $r(0) \not\equiv 0$, the two Green functions defined above match within a scale factor at $x = 0$ to form a solution of the Sturm–Liouville problem for the λs such that

$$\tilde{g}(x', x'', \lambda) = \left[g_1(x, x', \lambda)\frac{d}{dx}g_2(x, x'', \lambda) - g_2(x, x'', \lambda)\frac{d}{dx}g_1(x, x', \lambda)\right]_{x=0} = 0. \tag{2.8}$$

Alternatively, we may say that (2.8) is the condition for the analytical continuation of $g_1(x, x', \lambda)$ to satisfy (2.1) and (2.2). All the functions satisfying (2.1) and the first condition (2.2) for $x > 0$ are proportional to $g_1(x, x', \lambda)$, so that condition (2.8) supplies all the eigenvalues λ_n of the Sturm–Liouville problem if we can guarantee that $g_1(x, x', \lambda_n)$ and $g_2(x, x'', \lambda_n)$ taken as functions of x are not identically zero. Conversely, it is evident that if either $g_i(x, x', \lambda) \equiv 0$ we obtain a spurious zero of this *one-dimensional Bogomolny condition*. In any case, we may take the limit $x' \to 0$ and $x'' \to 0$, so that $\tilde{g}(0, 0, \lambda) = 0$ is an eigenvalue condition defined on a single point corresponding to a surface of section in one dimension.

Though the theory in this section is entirely elementary, it will serve as an important reference for the ensuing discussion. It should then be emphasized that the $g_i(x, x', \lambda)$ are not the usual Green functions adopted in the treatment of Sturm–Liouville problems. It is customary to define the Green function for the problem (2.3), (2.4) with $\lambda = 0$ in (2.3). The resulting Green function is then used to turn the problem with $\lambda \neq 0$ into an integral equation.

Our Green functions $g_1(x, x', \lambda)$ and $g_2(x, x', \lambda)$ can easily be constructed in the usual way. If $v_1(x)$ is a function that satisfies the homogeneous version of (2.3) and the first condition (2.4), whereas $u_1(x)$ satisfies the same equation but the second boundary condition, then

$$g_1(x, x', \lambda) = \begin{cases} c_1 v_1(x) u_1(x') & (x \geqslant x') \\ c_1 v_1(x') u_1(x) & (x \leqslant x') \end{cases} \tag{2.9}$$

and we have a similar expression for $g_2(x, x', \lambda)$. Inserting these into (2.8), we obtain

$$\tilde{g}(x', x'', \lambda) = c_1 c_2 \left[v_1(0) \frac{\mathrm{d}v_2(0)}{\mathrm{d}x} - v_2(0) \frac{\mathrm{d}v_1(0)}{\mathrm{d}x} \right] u_1(x') u_2(x''). \tag{2.10}$$

Therefore, $\tilde{g}(x', x'', \lambda)$ is proportional to the Green function for the complementary Sturm–Liouville problem where the equation has coefficients $r_1(x)$, $s_1(x)$, $t_1(x)$ for $x < 0$ (with the corresponding boundary condition) and $r_2(x) \ldots$ for $x > 0$. However, the coefficient in (2.10) is not the correct one for this Green function; indeed, it vanishes when λ is an eigenvalue. The *complementary Green function* also vanishes if $u_1(x') = 0$ $u_2(x'') = 0$.

The simplest example of the present theory is the one-dimensional Helmholtz equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} v(x) + k^2 v(x) = 0 \tag{2.11}$$

with the Dirichlet boundary conditions $v(a_1) = v(-a_2) = 0$. The easiest choice is then $r_1(x) = r_2(x) = r(x) = 1$, $s_1(x) = s_2(x) = 0$ and $t_1(x) = t_2(x) = -1$. The Green functions $g_1(x, x', \lambda)$ and $g_2(x, x', \lambda)$ will then depend exclusively on the choice of a_1' and a_2' and the boundary conditions there. It can be verified immediately that for the Dirichlet boundary conditions

$$g_1(x, x', k^2) = \begin{cases} \dfrac{\sin k(x - a_1) \sin k(x' + a_1')}{\sin k(a_1 + a_1')} & (x \geqslant x') \\ \dfrac{\sin k(x' - a_1) \sin k(x + a_1')}{\sin k(a_1 + a_1')} & (x \leqslant x') \end{cases} \tag{2.12}$$

and

$$g_2(x, x'', k^2) = \begin{cases} \dfrac{\sin k(x - a_2') \sin k(x'' + a_2)}{\sin k(a_2 + a_2')} & (x \geqslant x'') \\ \dfrac{\sin k(x'' - a_2') \sin k(x + a_2)}{\sin k(a_2 + a_2')} & (x \leqslant x''). \end{cases} \tag{2.13}$$

The eigenvalues of the original boundary value problem are

$$k_m = \frac{m\pi}{a_1 + a_2} \tag{2.14}$$

so we cannot use $a_1' = a_2$ and $a_2' = a_1$ lest g_1 and g_2 have singularities at the eigenvalues. The eigenvalues are correctly given by

$$\sin k(x - a_1) \cos k(x + a_2) - \sin k(x + a_2) \cos k(x - a_1) = \sin k(a_1 + a_2) = 0 \tag{2.15}$$

as given by (2.10). However, we also obtain spurious zeros for $k(x' + a_1') = m_1\pi$ and $k(x'' - a_2') = m_2\pi$. These extra zeros depend on our choice of x', x'', a_1' and a_2', but they are also present for alternatives to the Dirichlet boundary conditions.

The only way to avoid the spurious zeros in the one-dimensional Bogomolny condition is to push the boundaries a_1' and a_2' out to infinity. We can then construct the outgoing Green functions appropriate to our problem from the outgoing free Green function

$$g_0(x, x', k^2) = \frac{1}{2ik} \exp(ik|x - x'|) \tag{2.16}$$

by the method of images. Indeed, the Green function

$$g_1(x, x', k^2) = \frac{1}{2ik} [\exp(ik|x - x'|) - \exp(ik|x + x' - 2a_1|)] \tag{2.17}$$

is outgoing at $x \to -\infty$ and satisfies the Dirichlet boundary condition at $x = a_1$. For $x \geqslant x'$, g_1 has the same form as (2.9) with $c_1 = k^{-1}$, $v_1(x) = \sin k(x - a_1)$ as in (2.12), but $u_1(x') = \exp[ik(a_1 - x')]$. This choice of $u_1(x')$ is never zero, so it will not contribute spurious zeros to the eigenvalue condition. Choosing both g_1 and g_2 as outgoing Green functions over semi-infinite intervals guarantees that $\tilde{g} = 0$, as defined by (2.10), is a necessary and sufficient eigenvalue condition for the Helmholtz equation.

It is also instructive to use g_1 in the form (2.17) directly in (2.8) (without decomposing it into v_1 and u_1) together with g_2, obtained from (2.16) by exchanging $a_1 \to -a_2$. We then obtain

$$\tilde{g}(x'', x', k^2) = -\frac{1}{2ik} \{\exp(ik|x'' - x'|) - \exp[ik(|x'' - x'| + 2a_1 + 2a_2)]\} \tag{2.18}$$

which may be interpreted as the interference of the free Green function for direct motion from x' to x'' with the motion that bounces once on both walls on its way from x' to x''. It is this second motion which would correspond classically to a Poincaré map for $x' \to 0$ and $x'' \to 0$, so we can follow Bogomolny in considering the eigenvalue condition as

$$T(k^2) \equiv \exp[ik2(a_1 + a_2)] = 1. \tag{2.19}$$

(The direct motion degenerates to the identity as $x'' \to 0$ and $x' \to 0$.)

The above example can be generalized to any Sturm–Liouville problem that results from the separation of the Schrödinger equation. For non-singular boundary conditions at a_1' and a_2' we obtain real Green functions of the form (2.9) such that u_l and v_l are functions with nodes. As λ changes continuously, these nodes sweep through the origin,

generating unwanted zeros in (2.10). However, it is always possible to define the auxiliary Green functions such that the boundary conditions at a_1' and a_2' are singular, that is, g_1 and g_2 are outgoing Green functions.

3. The quantum Poincaré section

A Poincaré section in classical dynamics may be defined as a section Σ in the L-dimensional position space. This eliminates one coordinate, while the corresponding momentum is then constrained by the condition that energy is conserved. The position in the full configuration space will be denoted here by the lower case letter q, whereas the capital letter Q will be reserved for its restriction to an $(L-1)$-dimensional surface; likewise, the corresponding momenta will be p and P. All specific examples will be restricted to $L=2$, with $q=(x, y)$ even in the case of non-Cartesian coordinates. The section divides the accessible position space into two parts, V_1 and V_2, as depicted in

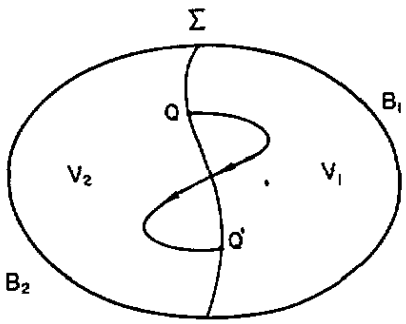

Figure 1. The accessible volume of configuration space, V, is divided by the section Σ into two regions, V_1 and V_2. The exterior boundary is then composed of B_1 and B_2.

figure 1. So for separable coordinates Σ corresponds to the surface $x=0$. Though represented as bounded in the figure, we may also consider the case where V_1 and $V_2 \to \infty$. However, for any given energy, it is presumed that the classical orbits are bounded and that they will repeatedly reintersect Σ. The first return Q' of each orbit originating on each point Q of Σ, such that the momentum transverse to Σ has the same sign, establishes the Poincaré map $(P, Q) \to (P', Q')$.

The construction of the Poincaré map is only possible if we know the classical motion in V_1 and V_2. Likewise, we can only construct a corresponding quantum map from the knowledge of the quantum mechanics in V_1 and V_2. In Bogomolny's procedure this is supplied by a pair of Green functions $G_1(q, q', E)$ and $G_2(q, q', E)$ with the following properties:

(i) $G_1(q, q', E)$ and $G_2(q, q', E)$ satisfy the inhomogeneous Schrödinger equation

$$(E-H(\hat{p}, q))G_j(q, q', E)=\delta(q-q') \tag{3.1}$$

inside the region V_j.

(ii) On the boundaries B_j of the V_j (see figure 1) the $G_j(q, q', E)$ obey the same boundary conditions as the eigenfunctions of $H(\hat{p}, q)$.

(iii) Both Green functions can be arbitrary on Σ.

In the subsequent argument there are points where it is necessary to extend $V_1 \to V_{1\varepsilon}$ beyond Σ up to $\Sigma_{1\varepsilon}$, as shown in figure 2, and $V_2 \to V_{2\varepsilon}$ in the same manner, so that

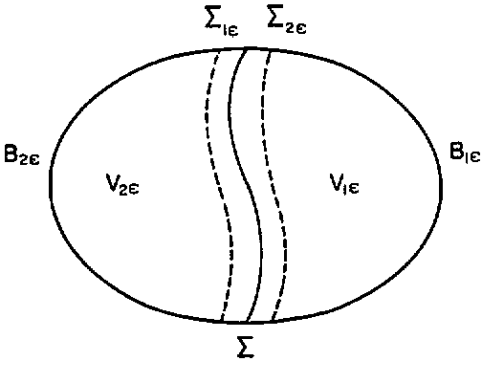

Figure 2. The volume $V_{1\varepsilon}$, with boundaries $B_{1\varepsilon}$ and $\Sigma_{1\varepsilon}$, includes the section Σ. The same is true of $V_{2\varepsilon}$.

$V_{1\varepsilon}$ and $V_{2\varepsilon}$ overlap. Condition (i) above will then apply to $V_{j\varepsilon}$, and condition (ii) then refers to the slightly larger boundaries.

In analogy to the treatment of the one-dimensional problem in the previous section, we may define the Green functions $G_j(q, q', E)$ as the solution of (3.1) in a region bounded by the closed surface $B_j + B_j'$, that includes V_j. The Hamiltonian must coincide with $H(\hat{p}, q)$ inside V_j, but it can be defined arbitrarily in the remaining accessible space. Evidently we may take B_j' out to infinity whether B_j is finite or not.

It is now necessary to make the hypothesis that any eigenfunction of the full problem

$$H(\hat{p}, q)\psi_n(q) = E_n\psi_n(q) \tag{3.2}$$

in $V_1 + V_2$, with specified boundary conditions on $B_1 + B_2$, can be written on the right side ($V_{1\varepsilon}$) in the form

$$\psi_{iE}(q) = \int_{\Sigma_{1\varepsilon}} G_1(q, Q, E)\mu_1(Q)\,\mathrm{d}Q. \tag{3.3}$$

In other words, $\psi_{1E}(q)$ has the form of a single-layer potential. Restricted to one dimension, this condition is simply that the wave function is proportional to $g_1(x, x', E)$. In this case it was found that, depending on the way that g_1 was defined and on the choice of x', $g_1(x, x', E)$ may be identically zero. So, even though (3.3) automatically satisfies the correct boundary value condition on B_1, we cannot assume that all solutions have the form (3.3).

The layer potential defined by (3.3) has a discontinuous derivative across $\Sigma_{1\varepsilon}$, just as $g_1(x, x', E)$ has a discontinuous derivative at $x = x'$. Because of this fact it cannot represent a smooth eigenfunction of the full problem on both sides of $\Sigma_{1\varepsilon}$. Suppose, though, that we can exactly match this wavefunction along Σ to $\psi_{2E}(q)$ defined in $V_{2\varepsilon}$ by (3.3) with the exchange of suffixes 1 and 2. We can now use the functions $\psi_E(Q) = \psi_{1E}(Q) = \psi_{2E}(Q)$ and $(\mathrm{d}\psi_E/\mathrm{d}n)(Q)$, where $(\mathrm{d}/\mathrm{d}n)$ denotes the normal derivatives to Σ, as initial values for a Cauchy problem for (3.2). Under very general conditions the solution exists and is unique (Smirnov 1964), so this coincides with both $\psi_{1E}(q)$ on the right and $\psi_{2E}(q)$ on the left. Since both of these wavefunctions satisfy the appropriate boundary conditions, the matched wavefunction is necessarily an eigenfunction.

The matching of both the wavefunction and its normal derivatives along Σ implies that

$$\psi_{1E}(Q)\frac{\mathrm{d}\psi_{2E}(Q)}{\mathrm{d}n}-\psi_{2E}(Q)\frac{\mathrm{d}\psi_{1E}(Q)}{\mathrm{d}n}$$
$$=\int_{\Sigma_{1\varepsilon}}\mathrm{d}Q_1\int_{\Sigma_{2\varepsilon}}\mathrm{d}Q_2\,\mu_1(Q_1)\Big[G_1(Q,Q_1,E)\frac{\mathrm{d}}{\mathrm{d}n}G_2(Q,Q_2,E)$$
$$-G_2(Q,Q_2,E)\frac{\mathrm{d}}{\mathrm{d}n}G_1(Q,Q_1,E)\Big]\mu_2(Q_2)=0. \tag{3.4}$$

Thus, if the representation (3.3) for an eigenfunction exists, we obtain a matching condition for the eigenvalues E_n. Indeed, the square brackets in (3.4) have the same structure as in the eigenvalue condition (2.8), if we notice that taking the limit $\varepsilon\to 0$ fixes Q_1 and Q_2 on Σ, which is simply the origin in one dimension. However, we cannot immediately divide away the unknown functions μ_1 and μ_2, so it is better to review Bogomolny's original procedure.

The idea is to use only one layer potential (3.3) and to extend it to the other side. In Bogomolny (1992) it is presumed from the start that the resulting ψ_{1E} is an eigenfunction, but then it becomes impossible to assess whether the method provides a sufficient eigenvalue condition. In the one-dimensional problem it is obvious how to extend the solution smoothly from one side to the other for any energy. For higher dimensions we have two ways. The Helmholtz equation has analytic solutions (Smirnov 1964) and hence we may use analytic continuation. In the general case we can solve the Cauchy problem in V_2 using $\psi_1(Q)$ and $(\mathrm{d}/\mathrm{d}n)\psi_1(Q)$ on Σ as initial conditions. The resulting smooth solution on V_1+V_2 that satisfies the correct boundary condition on B_1 will be referred to simply as $\psi_E(q)$ from now on.

To obtain the condition on $\mu(Q)$ for $\psi_E(q)$ to be an eigenfunction of the full boundary value problem, we now combine (3.1) and (3.2) to obtain Green's identity, with the aid of Stokes's theorem as in Bogomolny (1992):

$$\frac{\hbar^2}{2}\int_{B_2+\Sigma}\mathrm{d}Q\left\{\psi_E(Q)\frac{\partial}{\partial n}G_2(q'',Q,E')-G_2(q'',Q,E')\frac{\partial\psi_E}{\partial n}(Q)\right\}$$
$$+(E'-E)\int_{V_2}G_2(q'',q',E')\psi_E(q')\,\mathrm{d}q'=0 \tag{3.5}$$

where the point q'' is chosen in V_1 (and hence outside V_2) and $(\partial/\partial n)$ is the outward normal derivative to the boundary. If $G_2(q,q',E)$ has no pole at $E'=E$, we may eliminate the second integral by choosing $E'=E$. Thus, Green's identity is reduced to

$$\int_{B_2}\mathrm{d}Q\left\{\psi_E(Q)\frac{\partial}{\partial n}G_2(q'',Q,E)-G_2(q'',Q,E)\frac{\partial\psi_E}{\partial n}(Q)\right\}$$
$$+\int_{\Sigma}\mathrm{d}Q\left\{\psi_E(Q)\frac{\partial G_2}{\partial n}(q'',Q,E)-G_2(q'',Q,E)\frac{\partial\psi_E}{\partial n}(Q)\right\}=0. \tag{3.6}$$

If $\psi_E(q)$ is indeed an eigenfunction, the first integral in (3.6) cancels, since both ψ_E and G_2 satisfy the same boundary condition on B_2. It is now possible to insert (3.3)

into (3.6), since $\psi_E = \psi_{1E}$ on Σ. Therefore, changing the order of integration, we obtain

$$\int_{\Sigma_{1E}} \tilde{G}(q'', Q', E)\mu_1(Q')\,\mathrm{d}Q' = 0 \tag{3.7}$$

where

$$\tilde{G}(q'', Q', E) = \frac{\hbar^2}{2}\int_{\Sigma} \mathrm{d}Q \left\{ G_1(Q, Q', E)\frac{\partial}{\partial n} G_2(q'', Q, E) - G_2(q'', Q, E)\frac{\partial}{\partial n} G_1(Q, Q', E) \right\}. \tag{3.8}$$

By restricting q to lie on $\Sigma_{2\varepsilon}$ we now obtain eigenvalues of the full problem as a compatibility condition for (3.7) to have a solution

$$\det[\tilde{G}(Q'', Q', E)] = 0 \tag{3.9}$$

i.e. the operator $\tilde{G}$, taking functions on $\Sigma_{1\varepsilon}$ to those on $\Sigma_{2\varepsilon}$, must have a zero eigenvalue at the energy E_n. By taking the limit $\varepsilon \to 0$, (3.9) becomes a condition on the Green function for the Poincaré section Σ.

There are two possible problems with this eigenvalue condition. It is possible that not all eigenfunctions of the full problem can be expressed in the form (3.3), in which case (3.9) is not a necessary condition. On the other hand, if the operator G_1 in (3.3) has a zero eigenvalue for a given energy, (3.7) will also be zero for the corresponding eigenfunction $\mu_1(Q)$. Then Bogomolny's condition will not be sufficient, since it will have spurious zeros. This is the situation that turned up in one-dimensional Sturm–Liouville problems, so it will be investigated in the next session for the special case of separable systems.

4. Separable systems

All the cases where the Schrödinger equation is separable in two or three dimensions are discussed by Morse and Feschbach (1953). Rather than attempt some fancy notation to cover all cases, it is more instructive to consider two simple but typical examples.

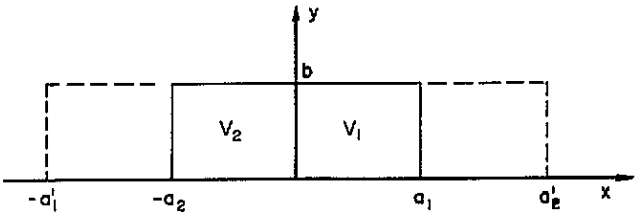

Figure 3. The rectangular billiard has Dirichlet boundary conditions at $y=0$ and b, and at $x=a_1$ and $-a_2$. The auxiliary Green function G_1 has Dirichlet boundary conditions at the same values of y and $x=a_1$ and $(-a_1')$, whereas G_2 satisfies the same boundary conditions at $x=a_2'$ and $(-a_2)$.

The first is the rectangular box of width a_1+a_2 and height b as shown in figure 3. We may either consider the billiard problem where $V=0$, or the separable problem where

$V(q) = V(x, y) = V_x(x) + V_y(y)$. The Schrödinger equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x, y) + [E - V_x(x) - V_y(y)]\psi(x, y) = 0 \tag{4.1}$$

(in units where $\hbar^2/2m = 1$) then has solutions $\psi(x, y) = X(x)\,Y(y)$, where

$$\frac{d^2}{dy^2}\,Y(y) + [\alpha^2 - V_y(y)]\,Y(y) = 0 \tag{4.2}$$

and

$$\frac{d^2}{dx^2}\,X(x) + [E - \alpha^2 - V_x(x)]X(x) = 0. \tag{4.3}$$

To test Bogomolny's eigenvalue condition for this system, let us choose Dirichlet boundary conditions and the section Σ to be the segment of the y-axis within the box. We may then obtain G_1 as the Green function for a similar box with the same height, but with boundariers at a_1 and $-a_1'$ and G_2 as the Green function for the box with boundaries at a_2' and $-a_2$. We then obtain one-dimensional Dirichlet problems for (4.2) and (4.3) with eigenfunctions $\langle y|n\rangle$, $\langle x|m\rangle_1$ and $\langle x|m\rangle_2$ such that in the case of a billiard ($V = 0$)

$$\begin{aligned} \langle y|n\rangle &\propto \sin\frac{n\pi y}{b} \\ \langle x|m\rangle_j &\propto \sin\frac{m\pi x}{a_j + a_j'}. \end{aligned} \tag{4.4}$$

The spectral representation of the Green functions is then

$$G_j(x, y, x', y', E) = \sum_{nm} \frac{\langle x|m\rangle_j\langle y|n\rangle\langle n|y'\rangle\langle m|x'\rangle_j}{E - E_n - E_{jm}} \tag{4.5}$$

where in the case of a billiard $E_n = \alpha^2 = (n\pi/b)^2$ and $E_{jm} = (m\pi)^2/(a_j + a_j')^2$. But, if we now recall that the spectral representation of the one-dimensional Green functions of section 2 is just

$$g_j(x, x', \lambda) = \sum_m \frac{\langle x|m\rangle_j\langle m|x'\rangle_j}{E - \lambda} \tag{4.6}$$

we may rewrite (4.5) as

$$G_j(x, y, x', y', E) = \sum_n G_{jn}(x, x', E)\langle y|n\rangle\langle n|y'\rangle \tag{4.7}$$

where

$$G_{jn}(x, x', E) = g_j(x, x', E - E_n). \tag{4.8}$$

So the two-dimensional Green functions are diagonal in the n-representation (i.e. the vertical momentum representation, tangent to the section) and the diagonal elements are the Sturm–Liouville Green functions.

The layer potentials (3.3) have the form

$$\psi_{1E}(x, y) = \int_0^b \mathrm{d}y'\, G_1(x, y, -\varepsilon_1, y')\mu(y'). \tag{4.9}$$

So, if we insert (4.5) in this integral, using (4.7) and (4.8), and define

$$\mu_n = \int_0^b \mathrm{d}y'\, \langle n | y' \rangle \mu(y') \tag{4.10}$$

we have

$$\psi_{1E}(x, y) = \sum_n \mu_n \langle y | n \rangle g_1(x, -\varepsilon, E - E_n). \tag{4.11}$$

The first problem to be faced is that, though the set of eigenfunctions $\langle y | n \rangle$ is orthogonal, it is not complete for square-integrable functions in the interval $(0, b)$. For instance, in the case that $V = 0$, the complete set includes cosines as well as the sines in (4.4). Thus, it is possible to choose $\mu(y)$ orthogonal to all the $\langle y | n \rangle$ and hence obtain $\psi_{1E} = 0$ for all energies.

This problem disappears if we restrict the layer density to have the same boundary condition as $\langle y | n \rangle$. For this set of functions the $\langle y | n \rangle$ form a complete basis, so the coefficients μ_n uniquely define $\mu(y)$ and vice versa. Now, the solution of (4.3) that satisfies the correct boundary condition at $x = a_1$ is proportional to $g_1(x, -\varepsilon, E - E_n)$ as discussed in section 2, so that (4.11) represents the complete set of functions that satisfy the correct boundary condition along B_1, except for the energies where $g_1(x, -\varepsilon, E - E_{n_0}) = 0$. For each of these particular energies we may choose $\mu(y) \propto \langle y | n_0 \rangle$ and hence obtain a spurious zero of the Bogomolny condition.

The above considerations basically apply to any other separable system. In the case of a radially symmetric potential, the Schrödinger equation

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right]\psi(r, \theta) + [E - V(r)]\psi(r, \theta) = 0 \tag{4.12}$$

separates into the pair of equations

$$\frac{\mathrm{d}^2}{\mathrm{d}\theta^2} F(\theta) + n^2 F(\theta) = 0 \tag{4.13}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \left(rE - \frac{n^2}{r}\right)R(r) = 0. \tag{4.14}$$

In the case of a Dirichlet problem for a ring centred on the origin, n will be an integer for $F(\theta)$ to be periodic, but this is not necessary if the problem includes only a segment of the ring. In any case, we can define the Bogomolny section to lie on the curve $r = r_0$, within the ring, and then define $x = r - r_0$ and $v(x) = R(r)$ so as to apply the Sturm-Liouville theory in section 2.

Associating $y = \theta$ we can again obtain the Green functions G_j in terms of the spectral decomposition (4.5) with

$$\langle y | n \rangle = \mathrm{e}^{\mathrm{i}ny} \tag{4.15}$$

and, in the case of a billiard,

$$\langle x \mid m\rangle_j = A_m J_n[E_{jm}^{1/2}(x+r_0)] + B_m Y_n[E_{jm}^{1/2}(x+r_0)] \tag{4.16}$$

where J_m and Y_n are Bessel and Neumann functions (Abramowitz and Stegun 1964) and the energies E_{jm} are the eigenvalues of the Sturm–Liouville problem with Dirichlet boundary conditions at $x=a_j$ and $x=a_j'$. We now define the layer potential (4.9) as a function of the layer density. Everything goes through as before, but we note that in the case of eigenfunctions of the full ring we will automatically use a periodic $\mu(y)$. Thus, there is no possibility of a density that is orthogonal to the basis formed by the $\langle y \mid n\rangle$.

In all the cases where the boundary value problem is separable and the surface of section is a coordinate surface $x=0$ for one of the coordinates that achieves the separation, we may express the wavefunctions for $x \geqslant -\varepsilon_1$ in terms of one-dimensional Green functions (4.11). Using the decomposition (4.7) of the auxiliary Green functions, Bogomolny's complementary Green function becomes

$$\begin{aligned}
&\tilde{G}(\varepsilon_2, y'', -\varepsilon_1, y', E) \\
&\quad = \frac{\hbar^2}{2} \sum_{n'n''} \langle y'' \mid n''\rangle \langle n' \mid y'\rangle \left\{ G_{1n'}(x, -\varepsilon_1, E) \frac{\mathrm{d}}{\mathrm{d}x} G_{2n''}(\varepsilon_2, x, E) \right. \\
&\qquad \left. - G_{2n''}(\varepsilon_2, x, E) \frac{\mathrm{d}}{\mathrm{d}x} G_{1n'}(x, -\varepsilon_1, E) \right\}_{(x=0)} \int_0^b \mathrm{d}y \, \langle n'' \mid y\rangle \langle y \mid n'\rangle \\
&\quad = \frac{\hbar^2}{2} \sum_n \langle y'' \mid n\rangle \langle n \mid y\rangle \tilde{g}(\varepsilon_2, -\varepsilon_1, E - E_n).
\end{aligned} \tag{4.17}$$

This is a diagonal operator in the n-representation, hence the Bogomolny condition (3.9) reduces to

$$\tilde{g}(\varepsilon_2, -\varepsilon_1, E - E_n) = 0 \tag{4.18}$$

for some n. It was shown in section 2 that a sufficient condition for an eigenvalue of the Sturm–Liouville problem is (2.8), which is identical to (4.18); hence Bogomolny's condition is a sufficient condition for the two-dimensional eigenvalue problem.

If we choose auxiliary Green functions $G_j(x, x', \lambda)$ that are outgoing at the free border instead of standing waves, we can eliminate spurious zeros. Bogomolny's condition is then necessary as well as sufficient. These outgoing Green functions were obtained explicitly for the one-dimensional Helmholtz equation (2.11) that results in the solution of Helmholtz's equation in a rectangle. These exact eigenvalues were also obtained by Lauritzen (1993) within the semiclassical approximation. For the Helmholtz equation in a ring, the outgoing Green functions are obtained by choosing the functions $u_j(x)$ in (2.9) as Hankel functions (Abramowitz and Stegun 1964) instead of real combinations of Bessel and Neumann functions.

It is important to note that these outward Green functions, which are necessary for the full validity of Bogomolny's condition for separable systems, correspond in the semiclassical limit to the Green functions used by Bogomolny (1992). Indeed, though the Green functions defined over finite regions also satisfy the three *a priori* stipulations of section 3, the existence of another arbitrary boundary multiplies the number of classical paths that start at $\Sigma_{1\varepsilon}$ and return to $\Sigma_{2\varepsilon}$ in the complementary problem.

Conversely, even the exact complementary Green function can be split into two components (2.18) in the case of the rectangle. One is the direct propagator and the other describes the motion that proceeds by bouncing once off both walls.

For sufficiently large n we obtain $E_n > E$. The one-dimensional problem then reduces to the heat conduction equation instead of the wave equation; in other words, $G_m(x, x', E)$ describes decaying modes instead of propagating modes. These modes are not related to any zero eigenvalues of $\tilde{G}$. Indeed, it is evident that $\tilde{g}(x'', x', k^2)$ given by (2.18) is never zero when k is imaginary.

Consider now the case where $V_y(y) = 0$ in (4.2), but $V_x(x)$ is a symmetric double-well potential in (4.3). There will then be levels that are bound to the wells, that is, they are oscillatory only in finite regions to the right and to the left of the Poincaré section at $x = 0$. Not a single classical orbit will cross the section in the motion corresponding to these states, nonetheless, an appropriate definition of the Green functions furnishes the necessary and sufficient eigenvalue condition in the Bogomolny theory. Thus, in this case the eigenvalues would be said to depend on orbits that tunnel to and from the section. Let us now consider the limit $x'' = \varepsilon_2 \to 0$ and $x' = -\varepsilon_1 \to 0$. The complementary Green function for the rectangle is then

$$\tilde{G}(0, y, 0, y', E) = 2\mathrm{i} \sum_n \sqrt{E - E_n}[T(E - E_n) - 1]\langle y \mid n\rangle \langle n \mid y'\rangle \tag{4.19}$$

with T defined by (2.19). This operator leaves invariant the subspace of functions $\langle y \mid n\rangle$ with $n \leqslant N$, such that $E_n < E$. Furthermore, we can define the unitary operator

$$\mathbb{T}(y, y', E) = \sum_{n=0}^{N} T(E - E_n)\langle y \mid n\rangle \langle n \mid y'\rangle \tag{4.20}$$

which accounts for the quantum Poincaré map. Just as the classical Poincaré map is defined over a finite region in the phase plane, its quantum version propagates a finite Hilbert space. Though we can define arbitrary squared integrable functions on the section Σ, it is only their projection onto a finite subspace that will propagate to a function with the same norm. The rest of these functions will decay into the evanescent modes.

5. Conclusions

Can we generalize quantum surfaces of section to non-separable systems? The indications from the semiclassical theory developed by Bogomolny (1992) are very encouraging. Even so, there may be aspects of the exact theory that differ qualitatively from its semiclassical approximation. What constitutes a good surface of section? The coordinate surfaces that were used in the previous section do not necessarily satisfy Bogomolny's intuitive criterion that almost all classical orbits must cross it. The exact criterion cannot depend on the classical orbits, so it is better to define a good surface of section as one where all the eigenfunctions can be expressed as layer potentials (3.3).

When we perturb a system from separability, a lot of the structure found in section 4 will be lost, but the overall division into modes that oscillate at least in some regions and those that merely decay away from Σ should be maintained, if it is at all possible to generalize the exact theory. The dimension of the Hilbert space of the functions $\mu(Q)$, for which the layer potential propagates, is finite, but will increase with E.

Another danger for generalizations is that of further spurious zeros in the eigenvalue condition. The problem is that the second integral in (3.6) could cancel, without $\psi_E(q)$ satisfying the correct boundary condition. Consider, for instance, the case of the Dirichlet boundary condition on B_2. Then Bogomolny's condition would be satisfied if

$$\Psi(q) = \int_{B_2} \mathrm{d}Q' \frac{\partial G_2}{\partial n}(q, Q', E)\psi_E(Q') = 0. \tag{5.1}$$

Therefore, if we consider $\psi_E(Q|_{B_2})$ as the density for a double-layer solution of Helmholtz's equation, Bogomolny's condition will be satisfied if $\Sigma_{2\varepsilon}$ is a nodal surface of $\Psi(q)$. Since $\psi_E(Q'|_{B_2})$ depends linearly on $\mu_2(Q)$, we obtain a linear equation for spurious zeros.

These extra zeros cannot arise for coordinate sections of separable systems, since the n dependence is a multiplicative factor of the integral for each orthogonal mode. Hence, in this special case the integral over $x = -a_2$ only cancels if $\psi_E(Q')$ satisfies the boundary condition.

Whatever the difficulties of generalizing Bogomolny's condition, we can see that it is an exact algorithm for calculating energy eigenenergies of separable systems. It is true that the absence of spurious eigenvalues can only be guaranteed by a more restricted definition of the auxiliary Green functions than in Bogomolny's original work, but this only brings them more in line with his semiclassical theory.

Another important feature of the semiclassical theory is the unitary Poincaré map. This was only obtained for a very restricted example in which the quantum mechanics coincides with its semiclassical limit (Lauritzen 1993)). It therefore requires further work to extricate the unitary map from the complementary Green function, even for more general separable systems.

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