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Application of Bogomolny's transfer operator to a circular harmonic oscillator plus $1/r^2$ potential

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Abstract. Bogomolny's transfer operator has been used to find an analytical solution for the semiclassical energy eigenvalues of a simple two-dimensional integrable system. The system studied consists of a particle moving in an isotropic harmonic oscillator potential plus a $1/r^2$ potential. The classical trajectories are used to construct the transfer matrix, and an expression is derived for the eigenvalues of this matrix as a function of the energy. These eigenvalue curves yield the semiclassical energy eigenvalues for the quantum system, which turn out to be exactly the same as the results obtained by solving the Schrödinger equation. Some insight into this unexpected agreement is provided by considering an exact transfer operator. We show that when this operator is expanded in powers of Planck's constant, the leading term in the expansion is Bogomolny's transfer operator.

1. Introduction

For simple systems described by time-independent Hamiltonians, the correspondence between classical and quantum descriptions may be viewed as the problem of relating the trajectories of a classical system to the energy eigenvalues and eigenfunctions of its quantum analogue. Establishing this connection is complicated when the classical system is nonintegrable and shows chaotic behaviour, but many such systems have now been studied using the periodic orbit theory based on the Gutzwiller trace formula and related methods [1–11].

Another semiclassical approach, applicable to both integrable and nonintegrable systems, was formulated by Bogomolny [12, 13] in terms of a transfer operator and a suitably chosen Poincaré surface of section (PSS). The transfer operator is constructed using the classical trajectories that go from a given point on the PSS to another chosen point on the PSS, with at most one crossing of the PSS in between. (At the chosen points, the trajectories must cross the PSS in the same sense.) Usually, there is a small number of such trajectories, and this makes it relatively easy to calculate the transfer operator, or a finite approximation to it, leading to approximate energy eigenvalues for the analogous quantum system. Bogomolny's method has been found to give excellent results for a variety of integrable and nonintegrable systems [14–23]. In the case of the two-dimensional hydrogen atom, the transfer operator was calculated analytically [23]. It was found, however, that the energy eigenvalues were systematically shifted from the exact quantum eigenvalues as a result of an unwanted overall phase factor in the transfer operator.

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Clearly, it is of interest to find other simple systems for which the transfer operator can be obtained analytically. In the present paper we describe such a system and show that it yields results which agree with the exact quantum energy eigenvalues. To gain some understanding of why this occurs, we consider how Bogomolny's transfer operator is related to the exact transfer operator of the system.

2. The transfer operator and the determinantal equation

We begin with a brief description of Bogomolny's transfer operator. For a system with two freedoms, the PSS is simply a one-dimensional curve, and the transfer operator has the form

$$T(q'', q'; E) = \sum_{\text{cl.tr.}} \frac{1}{(2\pi i\hbar)^{1/2}} \left| \frac{\partial^2 S(q'', q'; E)}{\partial q'' \partial q'} \right|^{\frac{1}{2}} \exp[iS(q'', q'; E)/\hbar - i\nu\pi/2] \quad (1)$$

where q' and q'' are points located on the PSS. The summation is over all classical trajectories which cross the PSS only once in going from q' to q'' and have the normal component of the momentum in the same direction at q' and q'' . For each such trajectory one needs the action at energy E , denoted by $S(q'', q'; E)$, and the phase index ν , which is related to the number of points on the trajectory at which the semiclassical approximation is not valid.

One way of constructing a finite approximation to the T -operator in coordinate space is to divide the accessible part of the PSS into N cells, the i th cell centred on q_i having width Δ_i . In terms of the transfer operator $T(q_j, q_i; E)$ from q_i in cell i to q_j in cell j , the matrix element $T_{ij}(E)$ is defined to be

$$T_{ij}(E) = T(q_j, q_i; E)(\Delta_i \Delta_j)^{1/2}. \quad (2)$$

Then the condition for an energy eigenvalue is that

$$\det[\delta_{ij} - T_{ij}(E)] = 0. \quad (3)$$

We note that this equation will be satisfied whenever one of the eigenvalues of the T -matrix is equal to unity.

3. The circular harmonic oscillator with a $1/r^2$ potential

The system we have chosen to study is described by the classical Hamiltonian,

$$H = \frac{p_r^2}{2m_0} + \frac{L^2}{2m_0 r^2} + \frac{1}{2} m_0 \omega^2 r^2 + \frac{\alpha^2}{2m_0 r^2} \quad (4)$$

where m_0 is the mass of the particle, $p_r = m_0 \dot{r}$ is the radial component of the momentum, and $L = m_0 r^2 \dot{\theta}$ is the constant angular momentum. The strength of the $1/r^2$ potential has been written for convenience as $\alpha^2/(2m_0)$, where α has the dimensions of angular momentum. (We shall assume that $\alpha > 0$.) This Hamiltonian has been proposed as a simple exactly solvable model for an electron interacting with a second electron in a quasi two-dimensional quantum dot [24–26]. The harmonic potential serves to confine the electron to the region of the quantum dot, while the $1/r^2$ term is an average potential describing the repulsion from the second electron. The two-dimensional Schrödinger equation corresponding to this Hamiltonian is readily solved (see, for example, Flügge [27]), and the exact quantum energy eigenvalues are found to be

$$E(n, m) = \hbar\omega[2n + (m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} + 1] \quad (5)$$

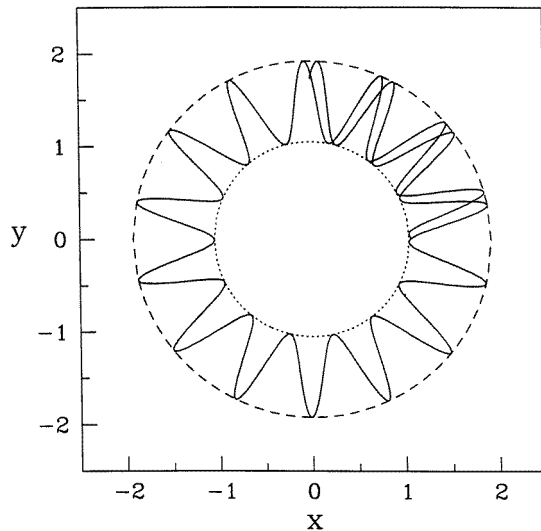


Figure 1. A typical classical trajectory of the circular oscillator plus $1/r^2$ potential. The outer and inner circles have radii r_+ and r_- respectively, given by equation (6).

where n takes the values $0, 1, 2, \dots$, and the angular momentum quantum number m is any positive or negative integer including zero. The corresponding eigenfunctions are confluent hypergeometric functions times $\exp(im\theta)$.

Let us consider the classical motion associated with the Hamiltonian (4). It is not hard to show that the minimum possible energy of the system is $E_{\min} = \omega\alpha$. For a given total energy $E > E_{\min}$ the radial motion occurs between r_- and r_+ given by

$$r_{\pm}^2 = \frac{E \pm [E^2 - \omega^2(L^2 + \alpha^2)]^{\frac{1}{2}}}{m_0\omega^2}. \tag{6}$$

In figure 1 we show a typical classical trajectory.

For this system a natural choice for the PSS is a circle. While any circle having a radius between r_- and r_+ would be satisfactory, we have chosen the circle of radius $r = r_+$ as the PSS. (Conceptually it would be desirable to choose the radius of the PSS to be $r_+ - \epsilon$, where ϵ is small and positive, as then the classical trajectories would actually *cross* the PSS. One could then let ϵ tend to zero at a later stage in the calculation.) The coordinate q in the transfer operator may be taken to be the angle θ from a chosen reference line. The PSS is divided into N cells of width $\Delta = 2\pi/N$, and the centres of the cells are situated at $\theta_j = j\Delta$, $j = 1, 2, \dots, N$. To construct the matrix element $T_{ij}(E)$ we require the trajectory at energy E connecting the points θ_i and θ_j on the PSS which does not touch the PSS at any point in between. We now show that when such a trajectory exists, it is unique and corresponds to a particular value of the angular momentum L .

Let us regard the trajectory as a function $r(\theta)$ and write $\dot{r} = (dr/d\theta)\dot{\theta}$. Then,

$$m_0r^2\dot{r} = L\frac{dr}{d\theta}. \tag{7}$$

Using equation (4) to obtain \dot{r} , for a fixed energy E of the system, and integrating equation (7) over the trajectory from θ_i to θ_j , we obtain,

$$\theta_j - \theta_i = 2 \int_{r_-}^{r_+} \frac{L dr}{r[2m_0Er^2 - m_0^2\omega^2r^4 - (L^2 + \alpha^2)]^{\frac{1}{2}}} = \frac{L\pi}{(L^2 + \alpha^2)^{\frac{1}{2}}}. \tag{8}$$

For given angles θ_i and θ_j on the PSS, this equation can be solved to find the required value of L for the trajectory. However, it is clear from equation (6) that, for a given E , the maximum possible value of L must satisfy

$$L_{\max}^2 = E^2/\omega^2 - \alpha^2. \quad (9)$$

Hence, from equation (8), the maximum angular displacement in one mapping from the PSS to the PSS is

$$|\theta_j - \theta_i|_{\max} = \pi(1 - \omega^2\alpha^2/E^2)^{\frac{1}{2}}. \quad (10)$$

If the cells i and j are farther apart in angle than this, there is no classical trajectory connecting them at energy E , and the corresponding matrix element $T_{ij}(E)$ is zero.

To calculate the matrix element $T_{ij}(E)$ from equations (1) and (2), we require the action for the trajectory from θ_i to θ_j at energy E . After a short calculation we find

$$S(\theta_j, \theta_i; E) = 2 \int_{r_-}^{r_+} |p_r| dr + \int_{\theta_i}^{\theta_j} L d\theta = \pi E/\omega - \alpha[\pi^2 - (\theta_j - \theta_i)^2]^{\frac{1}{2}}. \quad (11)$$

The second derivative is

$$\frac{\partial^2 S}{\partial \theta_j \partial \theta_i} = -\frac{\pi^2 \alpha}{[\pi^2 - (\theta_j - \theta_i)^2]^{\frac{3}{2}}}. \quad (12)$$

Hence, when the trajectory from θ_i to θ_j exists, the matrix element is

$$T_{ij}(E) = \frac{\Delta}{(2\pi i\hbar)^{\frac{1}{2}}} \left(\frac{\pi^2 \alpha}{[\pi^2 - (\theta_j - \theta_i)^2]^{\frac{3}{2}}} \right)^{\frac{1}{2}} \times \exp\{i\pi E/(\hbar\omega) - i\alpha[\pi^2 - (\theta_j - \theta_i)^2]^{\frac{1}{2}}/\hbar - i\nu\pi/2\}. \quad (13)$$

Because of the rotational symmetry of the Hamiltonian, the matrix elements depend only on the angular difference $\theta = \theta_j - \theta_i$. As a result, the transfer matrix is a circulant matrix, for which the eigenvalues can be calculated analytically [22]. Setting the phase index ν equal to 2, corresponding to two classical turning points in the radial motion, and putting $\theta_{\max} = \pi(1 - \omega^2\alpha^2/E^2)^{\frac{1}{2}}$, as in equation (10), we define

$$t_n(E) = \frac{\Delta}{(2\pi i\hbar)^{\frac{1}{2}}} \left(\frac{\pi^2 \alpha}{(\pi^2 - \theta_n^2)^{\frac{3}{2}}} \right)^{\frac{1}{2}} \exp[i\pi E/(\hbar\omega) - i\alpha(\pi^2 - \theta_n^2)^{\frac{1}{2}}/\hbar - i\pi] \quad (14)$$

for $0 \leq \theta_n \leq \theta_{\max}$ and for $2\pi - \theta_{\max} \leq \theta_n \leq 2\pi$, while $t_n(E) = 0$ for $\theta_{\max} \leq \theta_n \leq 2\pi - \theta_{\max}$. Then the N eigenvalues of the T -matrix are [22]

$$\lambda_m(E) = \sum_{n=1}^N t_n(E) \exp(i2\pi mn/N) \quad m = 0, 1, \dots, N-1. \quad (15)$$

From the fact that $t_n(E) = t_{-n}(E) = t_{N-n}(E)$, it is easy to show that $\lambda_{-m}(E) = \lambda_m(E)$. Thus, although we shall restrict m to zero and the positive integers in what follows, each eigenvalue curve $\lambda_m(E)$ with m nonzero is doubly degenerate. (The curve for $m = 0$ is nondegenerate.) If we now put $\theta = 2\pi n/N$ and let N tend to infinity, we can convert the summation into an integral:

$$\lambda_m(E) = \frac{\pi\alpha^{\frac{1}{2}}}{(2\pi i\hbar)^{\frac{1}{2}}} \int_{-\theta_{\max}}^{\theta_{\max}} \frac{\exp[i\pi E/(\hbar\omega) - i\alpha(\pi^2 - \theta^2)^{\frac{1}{2}}/\hbar + im\theta - i\pi]}{(\pi^2 - \theta^2)^{\frac{3}{4}}} d\theta. \quad (16)$$

We evaluate the integral using the stationary phase approximation. The point at which the phase is stationary is found to be

$$\theta_0 = -\frac{m\pi}{(m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}}}. \quad (17)$$

After removing constant factors, the integral in (16) has the form

$$\int_{-\theta_{\max}}^{\theta_{\max}} \exp[ia(\theta - \theta_0)^2] d\theta \approx \int_{-\infty}^{\infty} \exp[ia(\theta - \theta_0)^2] d\theta = \left(\frac{\pi}{a}\right)^{\frac{1}{2}} \exp(i\pi/4) \quad a > 0. \quad (18)$$

From the Taylor expansion of the function in the exponential of equation (16) about the point θ_0 , the constant a is found to be

$$a = \frac{\hbar^2(m^2 + \alpha^2/\hbar^2)^{\frac{3}{2}}}{2\pi\alpha^2}. \quad (19)$$

Hence, the stationary phase approximation for the integral in (16) and the approximation resulting from extending the limits in (18) give the following simple result for the eigenvalues of the transfer matrix $T(E)$ as a function of E :

$$\lambda_m(E) = \exp\{i\pi[E/(\hbar\omega) - (m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} - 1]\} \quad m = 0, 1, \dots \quad (20)$$

Since an energy eigenvalue of the quantum system occurs whenever one of the T -matrix eigenvalues is equal to unity (see equation (3)), we obtain an energy eigenvalue whenever the quantity in square brackets in (20) is equal to an even integer. Then the energy eigenvalues are

$$E_{mn} = \hbar\omega[2n + (m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} + 1] \quad m = 0, 1, \dots \quad (21)$$

This equation is the same as the result for the exact quantum energies, equation (5). Note that the two-fold degeneracy corresponding to m and $-m$ for nonzero m , which exists in the quantum solution, is correctly given here, as was discussed following equation (15).

What are the allowed values of the integer n in equation (21)? In the solution of the radial Schrödinger equation, n can have only the values $0, 1, 2, \dots$ in order to make the series solution terminate, thereby avoiding a solution which would diverge exponentially with increasing r . However, in the semiclassical solution presented in this section, the only obvious requirement is that the energy is greater than the minimum classical energy $E_{\min} = \omega\alpha$. Thus, there seems to be no reason to rule out negative integer values for n such that, for given $\pm m$, $2n + (m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} + 1 \geq \alpha$. The lack of a good reason to exclude these negative values of n seems to be a failing of the present semiclassical method.

4. An exact transfer operator and its relation to the semiclassical transfer operator

At first sight it may seem surprising that we have obtained energy eigenvalues for our system using Bogomolny's transfer operator that are exactly the same as the energy eigenvalues of the Schrödinger equation. First of all, Bogomolny derived his transfer operator from a semiclassical Green function [12] which is certainly *not* an exact Green function for the quantum problem. Secondly, the integral in equation (16) was evaluated using the stationary phase approximation. Thus, it would appear that the effects of these approximations are cancelling out to give the correct quantum mechanical result.

A different way of looking at the situation, however, is to think of the semiclassical transfer operator, given by equation (1), as being the leading term of an expansion of

an exact transfer operator in powers of \hbar . (We define an exact transfer operator to be one which, through a determinantal equation such as (3), yields the exact quantum energy eigenvalues. It is not known whether such an operator always exists.) This point of view was suggested in the work of Gaspard and Alonso [30, 31] where they obtained the most important correction terms for the Gutzwiller trace formula [1, 2] in the framework of periodic orbit theory. Finding an exact transfer operator appears to be a difficult problem for a generic system. Prosen [32] has derived a quantum Poincaré mapping which reduces to Bogomolny's transfer operator in the semiclassical limit ($\hbar \rightarrow 0$), but his result is formal and difficult to exploit. Fortunately, for the present problem the rotational symmetry makes it easy to obtain a simple expression for an exact transfer operator. (An exact transfer operator has also been derived for another system having circular symmetry—the annulus billiard [33].) In the remainder of this section we shall write down an exact transfer operator for our system, and show that Bogomolny's semiclassical transfer operator is the leading term of an expansion in powers of \hbar .

As in the previous sections of the paper, the PSS is chosen to be the circle of radius r_+ given by equation (6). The rotational symmetry implies that the mapping from (r_+, θ') to (r_+, θ'') depends only on the angle $\theta = \theta'' - \theta'$. In terms of this angle, we have found an exact transfer operator at energy E to be

$$T^{\text{exact}}(\theta; E) = \sum_{m=-\infty}^{\infty} \frac{1}{2\pi} \exp\{i\pi[E/(\hbar\omega) - (m^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} - 1]\} \exp(-im\theta) \quad (22)$$

with $-\pi \leq \theta \leq \pi$. This definition should be interpreted in the sense of distributions, since classically the infinite sum over m does not exist. To verify that this yields the exact quantum energies, without approximations, suppose the PSS is divided into N equal cells of width $\Delta = 2\pi/N$. From equation (2) one can define the matrix elements corresponding to (22), and hence obtain an $N \times N$ matrix $T^{\text{exact}}(E)$ which has the form of a circulant. The eigenvalue curves of this matrix can be found by using equation (15), with $t_n(E)$ replaced by the corresponding matrix element of (22). If one then lets $N \rightarrow \infty$, the sum in (15) is converted into an integral which is easily evaluated. One obtains the equation for $\lambda_m(E)$ in equation (20), without having made any approximations. (The finite matrix approximation for $T^{\text{exact}}(E)$ has been removed by letting $N \rightarrow \infty$.) Thus, with the help of the step leading from (20) to (21), we see that the transfer operator (22) yields the exact quantum energy eigenvalues.

To obtain a semiclassical approximation to (22) we use the Poisson summation formula in the form [34, 35],

$$\sum_{m=-\infty}^{\infty} f(m) = \sum_{M=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) \exp(i2\pi Mx) dx. \quad (23)$$

This enables us to write

$$T^{\text{exact}}(\theta; E) = \sum_{M=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[ig_M(x)] dx \quad (24)$$

where

$$g_M(x) = \pi[E/(\hbar\omega) - (x^2 + \alpha^2/\hbar^2)^{\frac{1}{2}} - 1] + (2\pi M - \theta)x. \quad (25)$$

Let us attempt to evaluate the integrals in (24) by using the stationary phase approximation. For the integral involving $g_M(x)$, the condition $g'_M(x) = 0$ has the solution

$$x_M = \frac{\alpha(2\pi M - \theta)}{\hbar[\pi^2 - (2\pi M - \theta)^2]^{\frac{1}{2}}}. \quad (26)$$

However, for θ in the range $-\pi \leq \theta \leq \pi$, this is real only for the case $M = 0$. This means that when $|M| \neq 0$, a stationary point does not exist on the x -axis, implying that the corresponding integrals cannot be evaluated by the stationary phase method. Therefore, let us keep only the $M = 0$ term in the summation in (24). Truncating the Taylor expansion of $g_0(x)$ about its stationary point x_0 at $(x - x_0)^2$, we obtain the result

$$T^{\text{exact}}(\theta; E) \approx \frac{1}{(2\pi i \hbar)^{\frac{1}{2}}} \left(\frac{\pi^2 \alpha}{(\pi^2 - \theta^2)^{\frac{3}{2}}} \right)^{\frac{1}{2}} \exp\{i\pi E/(\hbar\omega) - i\alpha(\pi^2 - \theta^2)^{\frac{1}{2}}/\hbar - i\pi\}. \quad (27)$$

If we set $\theta = \theta_j - \theta_i$ in this expression and compare it with equation (13), using equation (2) to extract the operator from the matrix element $T_{ij}(E)$, we see that this expression is precisely Bogomolny's transfer operator for our system. This is the main result of this section.

It is of some interest to consider the corrections that arise when the $M = 0$ integral is evaluated in a better approximation. Corrections to the basic stationary phase approximation can be generated in a systematic way by expanding $g_0(x)$ to higher powers in $(x - x_0)$. The integrand then becomes multiplied by a factor of the form

$$\begin{aligned} \exp[ib(x - x_0)^3 + ic(x - x_0)^4 + \dots] \\ \approx 1 + ib(x - x_0)^3 + ic(x - x_0)^4 - (b^2/2)(x - x_0)^6 + \dots \end{aligned} \quad (28)$$

The integral involving any odd power on the right-hand side is zero because the integrand is an odd function of $(x - x_0)$. The integrals involving the last two terms shown in (28) can be worked out by repeatedly differentiating both sides of the relation

$$\int_{-\infty}^{\infty} \exp[-i|a|(x - x_0)^2] dx = \left(\frac{\pi}{|a|} \right)^{\frac{1}{2}} \exp(-i\pi/4) \quad (29)$$

with respect to the parameter $|a|$. The net result of retaining the terms shown in (28) is to multiply the right-hand side of (27) by the factor

$$\left(1 - i \frac{3c}{4|a|^2} - i \frac{15b^2}{16|a|^3} \right) = \left(1 - i \frac{3\hbar}{8\alpha(\pi^2 - \theta^2)^{\frac{1}{2}}} + O(\hbar^2) \right). \quad (30)$$

Thus, denoting the right-hand side of equation (27) as $T^{\text{Bog}}(\theta; E)$, we have shown that

$$\begin{aligned} T^{\text{exact}}(\theta; E) &= T^{\text{Bog}}(\theta; E) \left(1 - i \frac{3\hbar}{8\alpha(\pi^2 - \theta^2)^{\frac{1}{2}}} + O(\hbar^2) \right) \\ &+ \sum_{|M| \neq 0} \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[ig_M(x)] dx. \end{aligned} \quad (31)$$

We have not attempted to evaluate the integrals involving $|M| \neq 0$.

5. Discussion

We have studied a simple two-dimensional integrable system consisting of an isotropic harmonic oscillator potential and a $1/r^2$ potential. Using a suitably chosen Poincaré surface of section, and taking advantage of the circular symmetry, we were able to derive an expression for the eigenvalues of Bogomolny's transfer matrix as a function of energy. This leads to semiclassical energy eigenvalues for the quantum system which are exactly the same as the eigenvalues obtained by solving the Schrödinger equation. It is worth mentioning at this point that other methods for obtaining approximate energy eigenvalues also yield the exact quantum energies for this particular system. We have shown that both

Einstein–Brillouin–Keller (EBK) quantization (see, for example, [2, p 214]) and the WKB approximation as modified by Langer [28, 29] lead to the exact quantum energies given by equations (5) or (21).

Some insight into the situation is provided by the analysis of section 4, where it was shown that Bogomolny's semiclassical transfer operator can be obtained from an exact transfer operator by making two approximations. First, only the $M = 0$ term was retained in the summation of equation (24). Secondly, the expansion of $g_0(x)$ about the stationary point x_0 was truncated after the term in $(x - x_0)^2$. Corrections to the second approximation were shown to be of a higher order in \hbar . The contributions from the terms with $|M| \neq 0$, however, have not been investigated. Nevertheless, it seems clear (though not rigorously demonstrated) that corrections to Bogomolny's semiclassical transfer operator are of a higher order in \hbar . Likewise, it seems very likely that corrections to the stationary phase evaluation of the integral in equation (16) are of a higher order in \hbar . (A partial examination of these corrections, along the lines of the last section, supports this idea.) If these conjectures are correct, both types of corrections would lead to additions to the semiclassical energy eigenvalues (the right-hand side of (21)) which are of the order of \hbar^2 or higher. It follows that when no corrections are included, the result is just E_{mn} given by equation (21). When viewed in this way, it is not so surprising that the semiclassical energy eigenvalues from Bogomolny's transfer operator are the same as the exact quantum energies.

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