

LETTERS AND COMMENTS

Comment on ‘Quantum chaos in elementary quantum mechanics’ by Yu Dabaghian and R Jensen

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Abstract

Algebraic, numerical and conceptual problems in a recently published paper by Dabaghian and Jensen (2005 *Eur. J. Phys.* **26** 423–439) are discussed. A convergent scheme for summing periodic orbits in the tunnelling regime is suggested.

In a recently published paper [1], Dabaghian and Jensen used a step-in-a-box potential to illustrate how complexity arises in elementary quantum mechanics and how quantum problems with transcendental spectral equations can nevertheless be solved analytically. With the help of many illustrations and historical references they make a problem at the forefront of scientific inquiry accessible to the non-specialist. In addition, the authors address the problem of obtaining explicit quantum energy levels in the tunnelling regime by inclusion of ghost orbits. Unfortunately, the procedures recommended in [1] yield divergent results. We propose a cure at the end of this comment. Throughout this comment we use the notation established in [1], but we use s_n for the action eigenvalues consistently throughout in order not to confuse s_1 and s_2 with the classical actions S_1 and S_2 .

The matrix

$$M = \begin{pmatrix} 0 & -e^{iS_1} & 0 & 0 \\ r e^{iS_1} & 0 & 0 & t e^{iS_2} \\ t e^{iS_1} & 0 & 0 & -r e^{iS_2} \\ 0 & 0 & -e^{iS_2} & 0 \end{pmatrix} \quad (1)$$

serves a dual purpose. We use it to correct (35) of [1] (factors of $1/\pi$ are missing and two of the signs are wrong) and to uncover the root cause of the divergence problem for $E < V$. With (1), we write (31) of [1] explicitly according to [2]

$$s_n^{(m)} = 2\pi n - \frac{\pi}{2} - \int_{\pi(n-1/2)}^{\pi(n+1/2)} \bar{N}(S) dS - \frac{1}{2\pi} \text{Im Tr} \sum_{l=1}^m \frac{1}{l} \int_{\pi(n-1/2)}^{\pi(n+1/2)} M^{2l}(S) dS, \quad (2)$$

where Tr denotes the trace of a matrix. Computing M^2 , M^4 and M^6 analytically (only three 4×4 matrix multiplications are required) shows that the corrected (35) of [1] reads

$$\begin{aligned}
 s_n^{(m=3)} = & 2\pi n - \frac{\pi}{2} - \int_{\pi(n-1/2)}^{\pi(n+1/2)} \bar{N}(S) dS + \frac{1}{\pi} \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} r(e^{2iS_1} - e^{2iS_2}) dS \\
 & - \frac{1}{\pi} \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \left(\frac{1}{2} r^2 e^{4iS_1} + t^2 e^{i(2S_1+2S_2)} + \frac{1}{2} r^2 e^{4iS_2} \right) dS \\
 & + \frac{1}{\pi} \text{Im} \int_{\pi(n-1/2)}^{\pi(n+1/2)} \left(\frac{1}{3} r^3 e^{6iS_1} + r t^2 e^{i(4S_1+2S_2)} - r t^2 e^{i(2S_1+4S_2)} - \frac{1}{3} r^3 e^{6iS_2} \right) dS.
 \end{aligned} \tag{3}$$

Carefully keeping track of signs and factors, (3) can also be obtained directly from (31) of [1]. With (3) and the corrected (37) of [1] (r and t^2 in (37) of [1] are stated incorrectly for $E < V$) we obtain $s_1^{(m)} = 2.6198, 2.6140, 2.6019, s_2^{(m)} = 5.5789, 5.2387, 5.1611, s_{17}^{(m)} = 53.4020, 53.4020, 53.4037$, where m ranges from 1 to 3. These results are inconsistent with seven out of nine entries in the $m = 1, 2, 3$ columns of table 1 of [1] to within the stated accuracy in table 1 of [1]. Because of this and a sign error in (39) of [1] it appears that all numerical results in (40) of [1] are incorrect to within the stated accuracy in (40) of [1].

On p 435 of [1] the authors state: ‘It turns out [11,12], that the correct way to obtain the m th approximation to the exact value of S_n [sic] is to include into sum (31) all the trajectories that reach the point $x = b$ m times or less.’ For later reference we call this summation prescription $P_>$. It is true only for $E > V$; it is incorrect for $E < V$.

First we prove that $P_>$ is indeed the correct summation prescription for $E > V$. As we saw in connection with the derivation of (3), use of M in (2) yields all periodic-orbit terms ordered precisely as required by $P_>$. For $E > V$ the matrix M is unitary. Thus, due to the convergence-generating factor $1/l$ in (2), $s_n^{(m)}$ converges as $m \rightarrow \infty$.

Now we use M to prove that $P_>$ of [1] is an incorrect summation prescription for $E < V$. Even though the substitution $\kappa \rightarrow i\kappa$ [1] turns M into a non-unitary matrix, it still produces the correct amplitudes of orbits and ghost orbits, and sums them precisely as required by $P_>$ if used in (2). Let us denote by λ_j , $j = 1, \dots, 4$, the four (complex) eigenvalues of M , and define λ_{\max} as the eigenvalue with the largest modulus, i.e. $|\lambda_{\max}| \geq |\lambda_j|$, $j = 1, \dots, 4$. Since M is non-unitary, it may happen that $|\lambda_{\max}| > 1$ with $\text{Im} \lambda_{\max} \neq 0$ in intervals of finite length inside the integration interval $J_n = [\pi(n-1/2), \pi(n+1/2)]$. In this case $|\text{Im} \text{Tr} \int (M^{2l}/l) dS| = |\text{Im} \sum_{j=1}^4 \int (\lambda_j^{2l}/l) dS| \sim |\text{Im} \int (\lambda_{\max}^{2l}/l) dS| \gg 1$ for large l and we have $|s_n^{(m)}| \rightarrow \infty$ for $m \rightarrow \infty$. This scenario indeed happens. For the example considered in [1] $|\lambda_{\max}| > 1$ in the open intervals $I_1 = (1.3064 \dots, s_1)$ and $I_2 = (3.8362 \dots, s_2)$. Since I_1 overlaps with J_1 and I_2 with J_2 , and in addition $\text{Im} \lambda_{\max} = 0$ only at a finite number of points, both $s_1^{(m)}$ and $s_2^{(m)}$ diverge for $m \rightarrow \infty$ if computed with M via (2). But since (2) implies $P_>$, both $s_1^{(m)}$ and $s_2^{(m)}$ diverge if summed according to the summation prescription $P_>$ of [1].

Since s_1 and s_2 are right at the edges of I_1 and I_2 , respectively, we cannot rescue the summation scheme of [1] by redefining the integration limits. However, in cases where $|\lambda_{\max}| > 1$, but very close to 1 (cases $n = 1, 2$ in the present context are examples), convergence is indeed observed over a large stretch of m before divergence sets in when more periodic orbits are included. In such cases $P_>$, restricted to a finite number of m , may be sufficient for some applications.

We found the mathematical reason for why $P_>$ of [1] yields divergent results for $E < V$. But (a) what is the physical reason? And (b) how can it be cured?

To answer these questions let us define four ‘channels,’ corresponding to a particle moving right (channel 1) or left (channel 2) in $0 < x < b$, or right (channel 3) or left (channel 4) in

$b < x < L$ of $V(x)$ (equation (6) of [1]). The matrix M can now be interpreted physically as the 4×4 scattering matrix describing the quantum flux in the four channels [2]. Its indices correspond one-to-one to the four channels, respectively [2]. In the language of scattering theory all four channels are open for $E > V$, explaining physically why for $E > VM$ (i) is four dimensional (ii) is the correct unitary description and (iii) implies, via (2), the correct summation prescription $P_>$.

Lowering the energy through $E = V$ into the tunnelling regime $E < V$, channels 3 and 4 close, and the 4×4 matrix M has to be replaced by a unitary 2×2 scattering matrix to describe the flux in the two remaining open channels 1 and 2. Thus use of $P_>$ for $E < V$ is now revealed as equivalent to using a non-unitary 4×4 scattering matrix instead of a unitary 2×2 scattering matrix in a formalism designed for unitary scattering matrices [2]. This provides the physical reason for the divergences and answers question (a).

Addressing question (b), we note that the summation prescription $P_>$ of [1] can be restated equivalently using the binary L/R code defined in [1] (see also p 436 of [1]). $P_>$: the m th approximation $s_n^{(m)}$ of s_n is obtained by including in $s_n^{(m)}$ all periodic orbits coded by symbolic words of length $\leq m$, written with the two symbols L and R. Figure 5 of [1] serves as an excellent illustration. For instance, to compute $s_n^{(2)}$ with $P_>$, we include the orbits L, R, LL, LR and RR (first two panels of figure 5 of [1]), i.e. orbits coded by words of length 1 and 2.

However, in order to obtain convergent results in the tunnelling regime $E < V$, we have to sum the orbits differently. For $E < V$ a convergent theory of ghost orbits based on a unitary 2×2 scattering matrix is proposed in [3]. Reference [3] addresses a scaling version of $V(x)$, but the principles are the same. Equation (7) of [3] in conjunction with the second paragraph on p L566 of [3] implies the following summation prescription for $E < V$. $P_<$: the m th approximation $s_n^{(m)}$ of s_n is obtained by including in $s_n^{(m)}$ all periodic orbits coded by words containing m or fewer symbols L and any number of symbols R. For instance, in order to compute $s_n^{(1)}$ for $E < V$, we have to include the orbits L, LR, LRR, LRRR, ..., i.e. an infinite number of orbits coded by words containing one symbol L and any number of symbols R. The orbit LRR, e.g., is illustrated in the panel on the right of figure 7 of [1]. ‘Pure ghosts’ [3], i.e. periodic orbits that travel exclusively in the classically forbidden, right-hand region $b < x < L$ of $V(x)$, contribute too. They are coded by words containing only the symbol R (zero symbols L). The pure ghosts R and RR (after correcting $RR \rightarrow R$ ($LL \rightarrow L$) in the first panel) are illustrated in figure 7 of [1]. According to [3] pure ghosts contribute to $\bar{N}(S)$ and may be summed first.

Thus the cure of the divergence problems for $E < V$ is to use M , or (15) of [1], to generate the amplitudes of orbits and ghost orbits, and then to sum them according to (31) of [1] with $P_<$. This answers question (b).

In summary, while $P_>$ is the correct prescription for summing orbits for $E > V$, $P_>$ is incorrect for $E < V$ and has to be replaced with $P_<$ to obtain convergent results. The two summation prescriptions $P_<$ and $P_>$, respectively, differ in a fundamental way. While according to $P_>$ ($E > V$) it suffices to sum a finite number of periodic orbits to obtain $s_n^{(m)}$, $P_<$ ($E < V$) requires that an infinite number of periodic orbits has to be summed, even though m is finite. Compared with $P_>$, $P_<$ represents a nontrivial reordering of terms.

As noted by the authors of [1], proved by the 19th century mathematician Bernhard Riemann, and illustrated in the case of the nonequivalent summation prescriptions $P_<$ and $P_>$ here, the result of a conditionally convergent sum depends crucially on the ordering of its terms. Thus, in addition to providing a valuable review of the new field of explicit periodic-orbit expansions, the step-in-a-box potential of [1] provides a physically relevant illustration of Riemann’s theorem accessible with the tools of elementary quantum mechanics.

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