Quantum Chaos: An Exploration of the Stadium Billiard Using Finite Differences

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Math 53: Chaos!
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Dartmouth College
December 4, 2009

Abstract

We investigate quantum chaos in chaotic billiards by modelling the square (non-chaotic) and the stadium (chaotic) billiards as 2D infinite square wells. We developed MATLAB code that uses grid points and the method of finite differences to numerically solve the Schrödinger equation for either case. We successfully obtained the "scar" structures in higher energy eigenfunctions for the stadium case, discovered by Joseph Heller in 1984. We also studied the eigenvalue spacings, and obtained the Poisson distribution for the square case and the GOE distribution for the chaotic case. Thus, we were able to demonstrate both features (scarring in eigenfunctions and GOE distribution in eigenvalue separation) that indicate the presence of chaos in the classical limit.

Background

For more than 80 years, predictions from quantum mechanics (QM) have been validated in laboratory experiments with infallible accuracy. QM is, to date, the most accurate description of nature in the limit where relativistic effects can be ignored. On the other hand, classical mechanics as formulated by Newton, Lagrange, Hamilton and others give accurate results for less than exotic, every-day length scales and energies (known as the classical limit), until we go much smaller and reach the molecular level where quantum effects become important. We expect the more general and accurate theory, QM, to reduce to the less general, classical mechanics, in the classical limit. This is Bohr's correspondence principle.

The phenomenon of deterministic chaos was discovered by Henri Poincaré in the late 18^{th} century when he was studying the seemingly erratic orbit of the moon in the 3-body system of Sun-Earth-Moon. The classical context in which chaos was discovered and also continued to study until late into the 20^{th} century naturally meant the definition of chaos in a dynamical

system was cast exclusively in classical terms: chaotic systems are those that have orbits that (i) are not asymptotically periodic and (ii) have positive Lyapunov exponent(s).

Note how chaos is formulated entirely in terms of orbits, i.e. the trajectory of a particle. But in QM, the particle does not have a definite position due to the Heisenberg Uncertainty Principle (in any finite potential, a particle has a finite likelihood to be anywhere at any moment in time due to quantum tunneling). Hence, the definition of chaos in classical mechanics does not carry over to QM. It is not even obvious what chaos would entail in the quantum world, if anything. What kind of behavior would a classically chaotic system produce if studied in the quantum regime? Also, from the other logical direction, would it be possible to look at quantum mechanical results (i.e. eigenfunctions and eigenvalues) of a system and deduce whether or not that system is classically chaotic?

Intuitively, one might expect that since most orbits of a chaotic system are dense in the phase space, the quantum eigenfunction would also be broadly, thinly and randomly smeared out and show no significant localization. Surprisingly,however, in many of the eigenfunctions corresponding to large eigenvalues, we see pockets of high probability densities in the coordinate space, often forming ornate patterns with various symmetries but no discernible similarity or connection with other eigenfunctions. Even more curiously, for some of these eigenfunctions, we can identify the pockets as lying along some of the unstable periodic orbits of the corresponding classical system. For this last subset of eigenfunctions, the pockets around the unstable orbits are known as ‘scars.’

One-Dimensional Square Infinte Potential Well

We began by solving the Schrodinger equation for the one-dimensional squre infinite potential well defined by the potential function

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le 1 \\ \infty & \text{otherwise} \end{cases}$$

and compared our numerical results with the exact results. Doing so allowed us to develop and test our method of finite differences code in a case much simpler than the stadium.

In computing solutions we began with the time-independent Schrödinger equation,

$$\frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi, \text{where } \nabla^2 = \frac{d^2}{dx^2}.$$

V = 0 everywhere inside the well, and we take $\frac{\hbar^2}{2m}$ to be unity so the Schrodinger equation simplifies to the Helmholtz equation

$$-\nabla^2\Psi = E\Psi$$

We approximated ∇^2as a matrix A that acts on a set of grid points. Using secant line approximations to the derivative we obtain

$$\left.\frac{d^2f}{dx^2}\right|_{x_n} \approx \frac{\left.\frac{df}{dx}\right|_{x_{n+1/2}} - \left.\frac{df}{dx}\right|_{x_{n-1/2}}}{h} \approx \frac{\frac{u_{n+1}-u_n}{h} - \frac{u_n-u_{n-1}}{h}}{h} = \frac{u_{n+1}-2u_n+u_{n-1}}{h^2}$$

where $h = x_n - x_{n-1}$ is the lattice spacing and $u_i = \Psi(x_i)$ as illustrated in Figure 1.

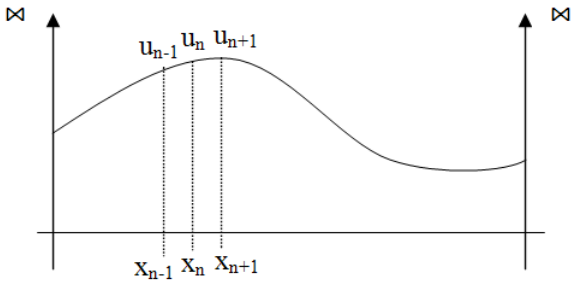

Figure 1: Illustration of quantities used in the method of finite differences.

Hence, the matrix A takes the form

$$\nabla^2 \approx A = \begin{bmatrix} -2 & & \cdots & & 0 \\ & \ddots & & & \\ \vdots & 1 & -2 & 1 & \vdots \\ & & & \ddots & \\ 0 & & \cdots & & -2 \end{bmatrix}$$

Computed solutions match theoretical solutions

$$\Psi_n = \sin(n\pi x)\,, E_n = n^2, n \in \mathbb{Z}^+$$

very well, with errors scaling as k^2, the scale factor depending on resolution. Deeper analysis of error scaling is reserved for the two-dimensional case.

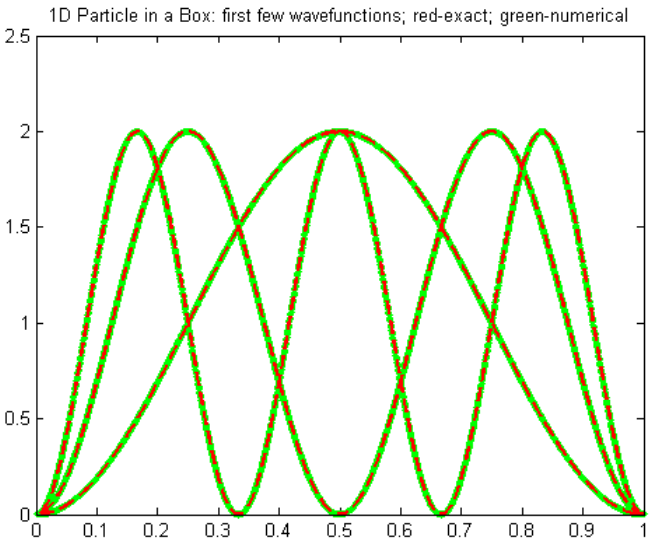

Figure 2: Calculated (green) and theoretical (red) wavefunctions of one-dimensional square infinite potential well for N=2000 degrees of freedom.

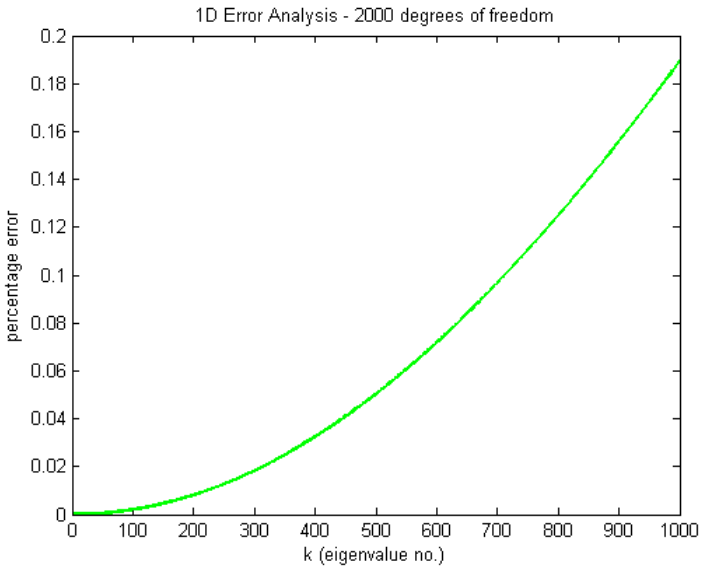

Figure 3: Eigenvalue errors for one-dimensional square infinte potential well for N=2000 degrees of freedom.

Two-Dimensional Square Infinite Potential Well

Having successfully computed eigenfunctions and eigenvalues of the one-dimensional square infinite potential well we move on to the two-dimensional case with potential given by

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le 1 \text{ and } 0 \le y \le 1 \\ \infty & \text{otherwise} \end{cases}$$

The two-dimensional Laplacian

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

is simply the sum of two one dimensional Laplacians. The matrix approximation A is therefore the sum of two matrices, one identical to the one-dimensional matrix and one with off diagonal elements a distance M+2 (rather than one) from the diagonal.

$$\nabla^2 \approx A = \begin{bmatrix} \cdots & 0 & 1 & \overbrace{\cdots \quad 0 \quad 1 \; \ddots}^{M+1} & -4 & \underbrace{1 \; \ddots \quad 0 \quad \cdots}_{M+1} & 1 & 0 & \cdots \end{bmatrix}$$

Using this matrix to find eigenfunctions requires us to represent two-dimensional wavefunctions as vectors. To accomplish this we discretize the two-dimensional square in the same fashion as the one-dimensional case but transform the two-dimensional grid into a vector

by stacking columns of the grid. This is the reason for the M+2 spacing (M+2 for M degrees of freedom plus boundary points on either side) of off-diagonal entries from the $\frac{\partial^2}{\partial y^2}$ term.

Wavefuntions of the two-dimensional square infinite potential well can be found using separation of variables and are therefore products of wavefunctions of the one-dimensional square infinite potential well.

$$\Psi_{n_x,n_y} = \sin(n_x \pi x)\sin(n_y \pi y),\ n_x, n_y \in \mathbb{Z}^+$$

Probability distributions of these wavefunctions are periodic and symmetric, hence relatively simple and show little localization – a feature common to all integrable systems.

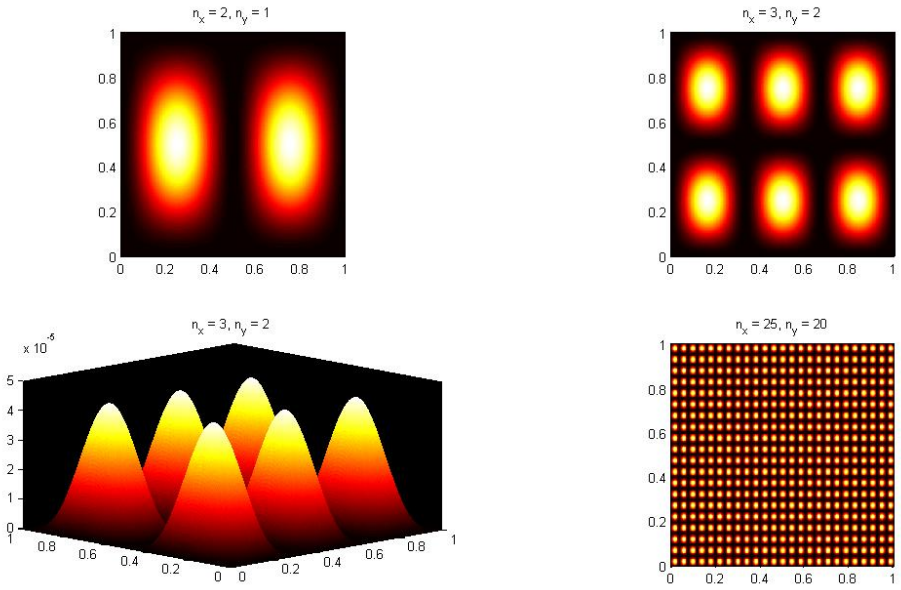

Figure 2: Probability distributions of two-dimensional square infinte potential well.

Energy levels of the two-dimensional square infinite potential well are sums of the one-dimensional values.

$$E = n_x^2 + n_y^2$$

Knowing these exact values we can see how the computed solutions compare. A plot of energy level errors is shown in Figure 3.

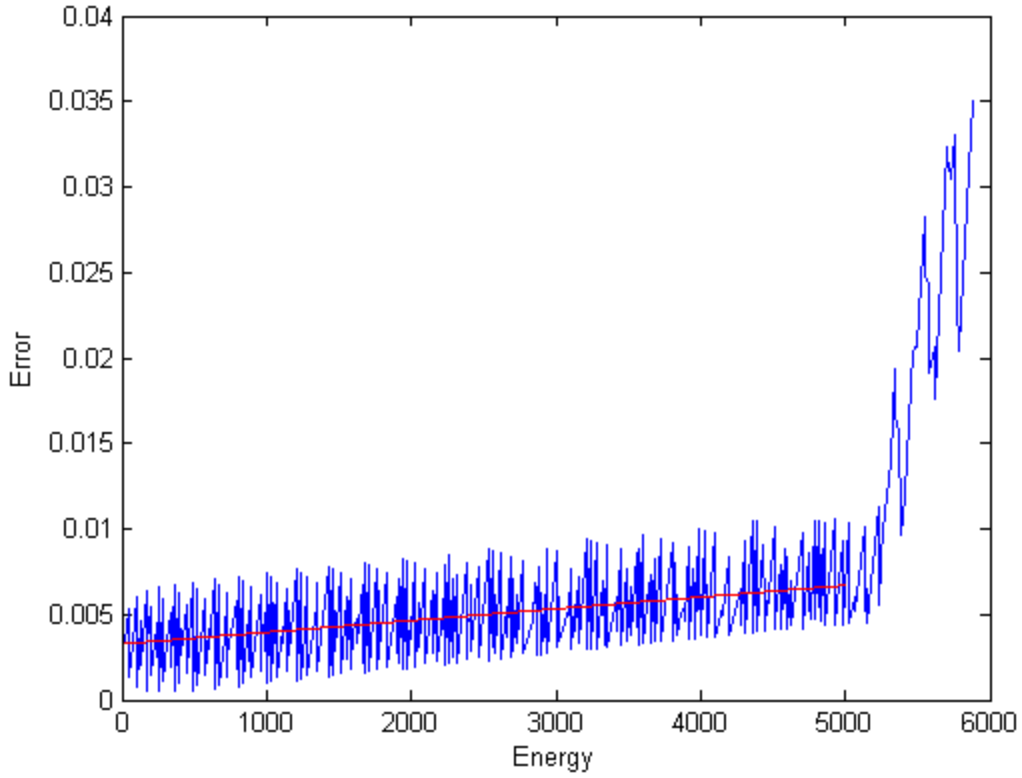

Figure 3: Energy level errors for two-dimensional square infinite potential well with 90,000 degrees of freedom.

Discarding the spike at the end (which is due to inaccuracies in the Matlab function eigs) we see that error scales linearly with energy, with the specific scale factor depending on resolution. This makes sense because in an area with zero potential the energy operator is equal to the kinetic energy operator which is proportional to the second derivative of the wave function i.e., the curvature. High curvature means the wavefunction is changing sharply over space and the discretization will fail to accurately capture these fine variations.

We might expect the error scaling factor to scale linearly with degrees of freedom i.e., as N^2 where N is the degrees of freedom in either the x- or y-direction. Running a numerical analysis (using the Matlab function polyfit) we see we actually do slightly better: errors scales approximately as $N^{1.9}$. Based on these results we can expect highly accurate results for the stadium billiard for several hundred energy levels using $NM \gtrsim 100{,}000$ degrees of freedom.

Indexing Stadium Lattice Nodes

The key numerical difference between the two-dimensional square infinite potential well and the stadium billiard is in the entires of the matrix A, which effectively encodes boundary

conditions constraining solutions of the Helmholtz equation. To encode the boundary condition we begin by traversing lattice points of the circumscribed rectangle of the stadium giving each point that falls within the stadium an index number which is stored in a map. We also create an inverse map from index numbers to points.

Now we can create A by traversing points in the index map and setting diagonals to -4 and entries corresponding to neighboring points within the stadium to 1. The neighboring points we test for the point (x_k, y_j) are: east, (x_{k+1}, y_j); west, (x_{k-1}, y_j); north, (x_k, y_{j+1}); and south, (x_k, y_{j-1}) again using our map to find the appropriate index for these points in rows of A.

Stadium Enery Levels

Transitioning from an integrable to nonintegrable system, we expect to see distinct changes in energy level distribution. Stadium energy levels should not follow a neat distribution but rather should reflect the classical chaos present in the nonintegrable system by following a pseudorandom distribution.

Literature on the subject has established that energy level spacings follow the Wigner distribution, the same distribution that is obeyed by spacings between eigenvalues of matrices in the Gaussian Orthogonal Ensemble (GOE) [3]. A GOE matrix consists of Gaussian elements with standard deviation 1 off the diagonal and $\sqrt{2}$ on the diagonal and mean 0 in both cases. A GOE matrix can be formed by taking an n-by-n matrix R with all elements Gaussians of mean 0 and standard deviation 1 and forming W given by

$$W = (R + R^T)/\sqrt{2n} \quad [4]$$

As n approaches infinity the distriubtion of spacings between eigenvalues of W approach the Wigner-Dyson distribution

$$W(s) = \frac{\pi}{2} s e^{-\frac{\pi}{4}s^2}$$

which falls to 0 at s = 0. In the context of energy levels of the stadium billiard this means that there are very few energy levels with close to the same energy. This contrasts with the integrable case where many energy levels are close together and spacings follow a Poisson distribution. [3]

Our results showed a clear Poisson distribution for the eigenvalues spacings of the two-dimensional square infinite potential well. To achieve an accurate Wigner-Dyson distrubtion for stadium eigenvalue spacings we plot only eigenvalues of wavefuntions that have odd-odd parity (i.e., antisymmetric through both axes), a technique known as desymmetrization originally utilized by McDonald and Kaufman [5]. To circumvent memory and time contraints, rather than finding many eigenvalues of a single billiard we parameterize the billiard by length in the x-direction and sum eigenvalue spacing distributions over many values of this parameter.

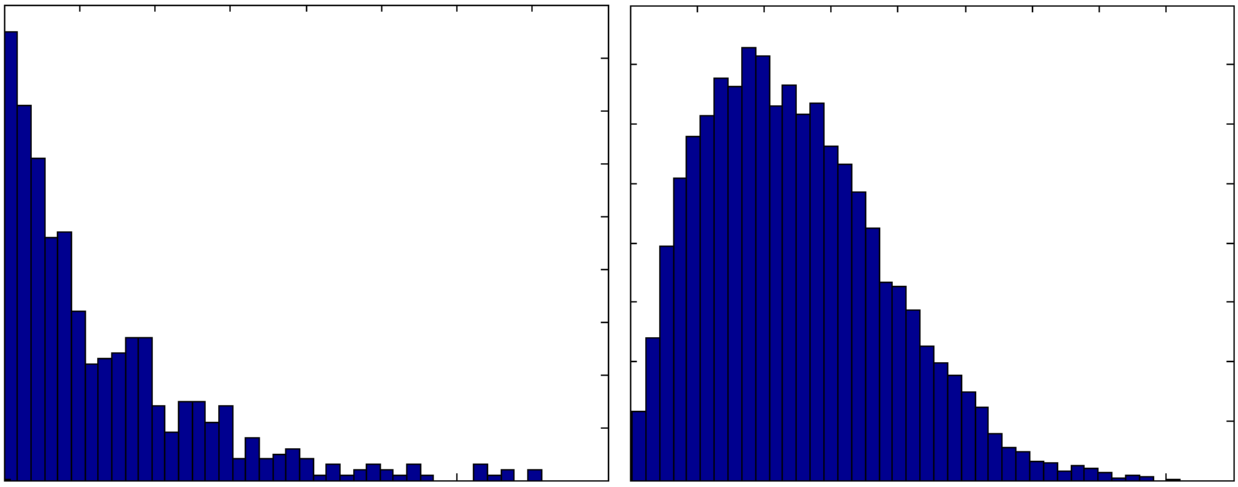

Figure 4: Eigenvalue spacings for two-dimensional square infinite potential well (left) and stadium (right).

Stadium Wave Functions

Wavefunctions of the stadium billiard exhibit a surprising amount of localization. Looking at trajectories of the classical case, one might expect wavefunctions to be relatively unlocalized, as classical trajectories appear to fill the stadium relatively uniformly with no discernable patterns. There are of course certain classical trajectories in the stadium that stand out, namely low-period periodic orbits. These orbits are of course unstable as the stadium is a chaotic billiard, so in general they appear very infrequently for arbitrary starting conditions.

Nonetheless these unstable periodic orbits are manifest in the quantum wavefunctions of the stadium billiard as “scars,” a term coined by Eric Heller who has shown the presence of these scars to follow from basic principles.[6] It should be made clear that scars corresponding to unstable period orbits are not visible in all wavefunctions but do appear fairly regularly (Heller claims “about half the states have one or more recognizable scars,” though we saw a proportion closer to a quarter) in high energy solutions. Furthermore, even in those wavefunctions that do not display scars corresponding to unstable period orbits, there is almost always a relatively high degree of localization. Typical scar patterns are shown in Figure 5.

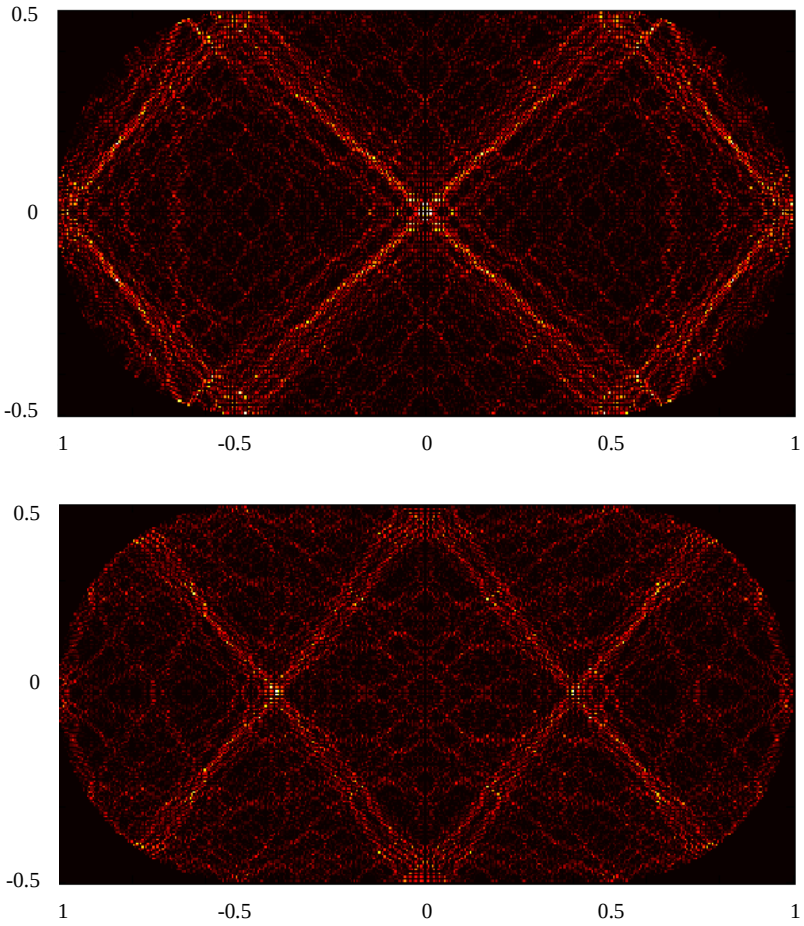

Figure 5: Scars in the stadium billiard corresponding to classical period orbits of period 6 (top) and period 3 (bottom).

Conclusion

We have obtained results in strong agreement with previous research in the field, demonstrating the connection between classical and quantum chaos. Primary manifestations of this connection are seen in energy level spacing distributions and scarring in wave functions. In contrasting integrable and nonintegrable billiards, we have demonstrated the specific routes by which chaos is manifest is quantum systems.

In a future project, we could explore how the eigenfunctions and eigenvalues change as we slowly vary the stadium parameter, changing the shape from disk to elongated stadium. Furthermore, it would be interesting to explore other chaotic (e.g. Sinai billiards) and non-chaotic (e.g. disk) billiard shapes in order to establish the generality of the features of the representative systems that have been analyzed here.

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