

Chaotic roots of the modular multiplication dynamical system in Shor's algorithm

Abu Musa Patoary¹, Amit Vikram¹, Laura Shou,² and Victor Galitski^{1,3}

¹*Joint Quantum Institute and Department of Physics, University of Maryland, College Park, Maryland 20742, USA*

²*School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455, USA*

³*Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA*



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Shor's factoring algorithm, believed to provide an exponential speedup over classical computation, relies on finding the period of an exactly periodic quantum modular multiplication operator. This exact periodicity is the hallmark of an integrable system, which is paradoxical from the viewpoint of quantum chaos, given that the classical limit of the modular multiplication operator is a highly chaotic system that occupies the “maximally random” Bernoulli level of the classical ergodic hierarchy. In this work, we approach this apparent paradox from a quantum dynamical systems viewpoint, and consider whether signatures of ergodicity and chaos may indeed be encoded in such an “integrable” quantization of a chaotic system. We show that Shor's modular multiplication operator, in specific cases, can be written as a superposition of quantized A -baker's maps exhibiting more typical signatures of quantum chaos and ergodicity. This work suggests that the integrability of Shor's modular multiplication operator may stem from the interference of other “chaotic” quantizations of the same family of maps, and paves the way for deeper studies on the interplay of integrability, ergodicity, and chaos in and via quantum algorithms.

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Introduction. Shor's algorithm [1,2] to factorize an integer N is a cornerstone of quantum computation [3], being exponentially faster than all known classical factorization algorithms and capable of breaking RSA encryption [4], a widely used scheme for secure data transmission. Interestingly, the success of this algorithm hinges on a foundational tension with the very notion of “quantum chaos” [5]: the quantum modular multiplication operator at the core of Shor's algorithm [1–3] belongs to a class of quantum systems that have a strongly chaotic classical limit, but violate several expected signatures of “chaos” on quantization.

The quantization of classically ergodic, chaotic systems [5,6] is typically associated with spectral signatures such as nondegenerate energy levels and spectral rigidity [5,7–16]. Paradoxically, as indicated above, some quantizations [1,17] of certain canonical textbook examples of classically ergodic and chaotic systems [6]—such as modular multiplication $f_A(x) = (Ax \bmod N)$ on a 1D interval $x \in [0, N]$ (quantized in Shor's algorithm) and Arnold's cat map on the torus—are *exactly periodic* at long times with highly degenerate and orderly spectra [1,18], which is at odds with ergodic quantum dynamics [16]. This is because quantization itself is not a uniquely defined procedure, and several distinct quantum systems can have the same classical limit (e.g., Refs. [1,19–21] consider entirely different quantizations of $f_2(x)$

with different spectral properties). In particular, the (conventionally) “standard” quantization of each of the above maps [1,17] captures the dynamics of only a *measure-zero* subset of periodic orbits with a common (not necessarily fundamental) period [6,22]. This gives the appearance of early-time “chaos” on quantization via the exponential divergence of typical nearby orbits, but completely misses out on the full ergodic and chaotic classical dynamics at late times in the bulk of the phase space.

On the one hand, the example of Shor's algorithm demonstrates a possibly generic need to eliminate “quantum chaos” in the quantization of even a classically chaotic map, for its successful utilization in certain quantum algorithms. On the other, it also suggests the more fundamental question of whether appropriate manifestations of quantum ergodicity and chaos can be hidden in some way even in such nonergodic quantizations. Interestingly, a partial resolution to this question was noted in Refs. [23,24], where it was shown [24] that the unitary operator implementing modular multiplication by $A = 2$ in Shor's algorithm can be expressed as a superposition of quantized baker's maps [20,25], which may be regarded as “chaotic” quantizations of $f_2(x)$ [more precisely, of baker's maps [6] in a 2D phase space (x, p) whose action on the position coordinate $x \in [0, 1]$ is identical to $f_2(Nx)/N$] that by and large exhibit the expected signatures of quantum chaos and ergodicity [20,21].

In this work, we show that this “embedding” of a superposition of “quantum chaotic” maps in the periodic modular multiplication map generalizes to an arbitrary multiplier A . The appropriate chaotic maps are direct generalizations of the 2D A -baker's maps [extensions of baker's maps whose 1D projection is $f_A(Nx)/N$], and these maps can be quantized in

terms of certain combinations of discrete Fourier transforms [20], when either $N + 1$ or $N - 1$ is a multiple of A . This establishes a rigorous correspondence between specific “ergodic” and “nonergodic” quantizations of $f_A(x)$ for arbitrary A , which may serve as a simple model for understanding the interplay of integrability, ergodicity, and chaos in different quantizations of the same system. We will now present the details of this correspondence, and subsequently discuss both its potential implications for studying the embedding of quantum chaos in Shor’s algorithm, and in extending the quantization of A -baker’s maps to arbitrary N .

Results. In the remainder of this Letter, we will refer to the exactly periodic quantum modular multiplication used in Shor’s algorithm simply as modular multiplication, without explicitly mentioning the qualifier “quantum”. Our main result [Eq. (8)] is to show that modular multiplication, in some specific cases, can be exactly written as a superposition of “chaotic” quantum A -baker’s maps. Modular multiplication U_A , given two co-primes N and A ($A < N$), is defined in an N -dimensional Hilbert space according to the equation

$$U_A|m\rangle = |mA \pmod{N}\rangle, \quad \text{for } m \in \{0, 1, \dots, N-1\}, \quad (1)$$

where $\{|0\rangle, |1\rangle, \dots, |N-1\rangle\}$ forms an orthonormal basis. U_A can be regarded as a quantization of $f_A(x)$, as a generic narrow wave packet of width $w \ll N$ centered at some x_0 remains narrowly distributed around the classical trajectory of x_0 up to an Ehrenfest time [26,27] $t_E \sim \ln(N/w)/\ln A$ determined by the Lyapunov exponent $\lambda = \ln A$. However, since N and A are co-primes, quantum modular multiplication is an exactly periodic unitary operator at longer timescales, which permutes the basis states according to Eq. (1).

The classical A -baker’s map, a generalization of the baker’s map, is a canonical example of an ergodic and chaotic system [28]. It maps a unit square to itself by stretching in one direction and compressing in the perpendicular direction in such a way that the total area of the square is preserved, and rearranging the stretched square to fit inside the unit square. The map is defined by the following transformation:

$$x \rightarrow x' = Ax - \lfloor Ax \rfloor, \quad (2)$$

$$p \rightarrow p' = \frac{p + \lfloor Ax \rfloor}{A}. \quad (3)$$

Here $(x, p) \in [0, 1] \times [0, 1]$ are phase space coordinates and $\lfloor x \rfloor$ denotes the integer part of x . The map is illustrated in Fig. 1. The unit square is divided into A rectangles of equal area as shown on the left side of Fig. 1. Each of the rectangles is stretched by a factor of A along the horizontal direction and by $1/A$ along the vertical direction. Then the rectangles are stacked on top of each other as shown on the right side of Fig. 1. When $A = 2$ the A -baker’s map reduces to the standard baker’s map [29].

As with any classical dynamical system, there is no unique way to quantize the A -baker’s map. Conventionally, the basic requirements are that the quantum map is unitary and it reduces to the classical map in the semiclassical limit. Several quantization procedures satisfying these requirements have been developed for the A -baker’s map [20,21,28,30–32]. In this Letter, we will use the quantization procedure developed

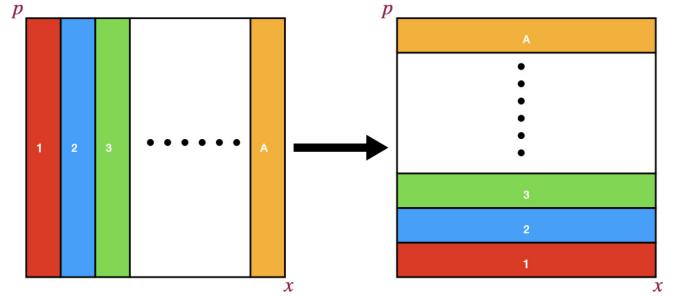


FIG. 1. The A -baker’s map transforms the unit square on the left to the one on the right. The unit square is divided into A rectangles which are marked by numbers from 1 to A . Each rectangle is stretched along the x axis and contracted along the p axis before the rectangles are stacked on top of each other.

by Balazs and Voros (BV) [20]. In the BV quantization, one replaces the phase space of the classical map with a D -dimensional Hilbert space. Then one can consider discrete position ($|x_n\rangle$) and momentum ($|p_n\rangle$) bases with the boundary conditions $|x_{n+D}\rangle = e^{-2\pi i \beta} |x_n\rangle$ and $|p_{n+D}\rangle = e^{2\pi i \alpha} |p_n\rangle$. Finally one constructs a $D \times D$ unitary matrix which transforms the states in ways analogous to the classical transformation in Eqs. (2) and (3). This unitary matrix is the quantum A -baker’s map. The Hilbert space dimension D plays the role of \hbar^{-1} [20]. Therefore the semiclassical limit of this map is obtained by taking $D \rightarrow \infty$ which is equivalent to $\hbar \rightarrow 0$. We explain the associated procedures in detail in the Supplemental Material [33]. The quantum A -baker’s map, obtained using the BV procedure, is given by the following unitary matrix $B_A^{(0)}$ (block diagonal with q blocks of $F_{\frac{D}{A}}^{\alpha, \beta}$):

$$B_A^{(0)} = (F_D^{\alpha, \beta})^{-1} \bigoplus_{j=1}^q F_{\frac{D}{A}}^{\alpha, \beta}. \quad (4)$$

Here α, β are phases introduced in the boundary condition of position and momentum basis and $F_D^{\alpha, \beta}$ is a generalized discrete Fourier transform (DFT) matrix whose elements are

$$[F_D^{\alpha, \beta}]_{nm} = \frac{1}{\sqrt{D}} e^{-2\pi i (n+\alpha)(m+\beta)/D}. \quad (5)$$

For periodic boundary conditions ($\alpha = \beta = 0$), $F_D^{\alpha, \beta}$ reduces to the standard DFT matrix which we simply denote by F_D . Note that D/A in Eq. (4) should be an integer which requires D to be a multiple of A .

One can modify the A -baker’s map so that the rectangles on the right side of Fig. 1 are stacked differently, and then use the same BV procedure to quantize this modified map. For example, if all the rectangles on the right side of Fig. 1 are cyclically permuted by one step so that now 1 goes to A , 2 goes to 1, ..., 3 goes to 2, we get a different quantized map $B_A^{(1)}$. Similarly one can construct other quantum maps $B_A^{(2)}, B_A^{(3)}, \dots, B_A^{(A-1)}$ by cyclically permuting the horizontal rectangles by 2, 3, ..., $A - 1$ steps, respectively. The general

equation for the A -baker's map $B_A^{(k)}$ is

$$B_A^{(k)} = [F_D^{\alpha, \beta}]^{-1} \begin{bmatrix} 0 & \dots & k-1 & k & \dots & A-1 \\ 0 & \dots & 0 & F_D^{\alpha, \beta} & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & \dots & F_D^{\alpha, \beta} \\ F_D^{\alpha, \beta} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & F_D^{\alpha, \beta} & 0 & \dots & 0 \end{bmatrix}, \quad (6)$$

where $k \in \{0, 1, \dots, A-1\}$. When $k=0$ it reduces to Eq. (4).

With this background we can state our main result. Given two co-prime integers N and A such that $N = Aq \pm 1$ where q is an integer, the corresponding modular multiplication operator U_A^\pm can be written to act instead on $D = Aq$ states (rather than on $N = Aq \pm 1$ as usual). This operator is obtained in the case $N = Aq + 1$ by removing the state $|0\rangle$ which is always a fixed point, $U_A^+|0\rangle = |0\rangle$, and in the case $N = Aq - 1$ by adding a D th state $|D-1\rangle$, with the extension $U_A^-|D-1\rangle = |D-1\rangle$ which agrees with the original map defined in Eq. (1). The modular multiplication map dynamics are thus preserved, but the advantage is the number of states is now a multiple of A . With these conventions, the $Aq \times Aq$ representation of the modular multiplication operator U_A^\pm can be expressed as

$$U_A^\pm = F_{Aq}^{-1} \begin{bmatrix} F_q & \dots & F_q^{0, \mp \frac{A-1}{A}} \\ \vdots & \vdots & \vdots \\ F_q & \dots & F_q^{0, \mp \frac{A-1}{A}} \end{bmatrix} \odot \tilde{F}_{Aq}^\mp. \quad (7)$$

Here \odot denotes Hadamard or entry-wise product of two matrices defined as $(A \odot B)_{ij} = A_{ij}B_{ij}$ and $\tilde{F}_{Aq} = F_A^\mp \otimes J_q$ with J_q being a $q \times q$ matrix with all elements equal to 1, F_A^+ the $A \times A$ DFT matrix with no phase, F_A^- the conjugate of F_A^+ , and \otimes denoting tensor product. We analytically derive Eq. (7) in the Supplemental Material [33].

To extract the quantized A -baker's maps embedded in Eq. (7), we rewrite it as

$$U_A^\pm = \frac{1}{\sqrt{A}} \sum_{k=0}^{A-1} \tilde{B}_A^{\pm(k)}, \quad (8)$$

where $\tilde{B}_A^{\pm(k)}$ are quantized maps similar to the ones obtained in Eq. (6) but with some differences. Let us write the explicit form of $\tilde{B}_A^{\pm(k)}$ to identify the differences:

$$\tilde{B}_A^{\pm(k)} = F_{Aq}^{-1} \begin{bmatrix} 0 & \dots & k-1 & k & \dots & A-1 \\ 0 & \dots & 0 & F_q^{0, \mp \frac{k}{A}} & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & \dots & F_q^{0, \mp \frac{A-1}{A}} \\ F_q & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & F_q^{0, \mp \frac{k-1}{A}} & 0 & \dots & 0 \end{bmatrix} \odot \tilde{F}_{Aq}^\mp. \quad (9)$$

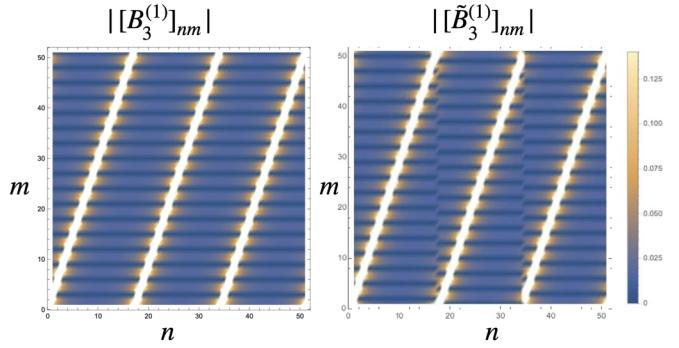


FIG. 2. The density plot of the absolute value of the matrix elements of $B_3^{(1)}$ (left) and $\tilde{B}_3^{(1)}$ (right) when $N = 52$. They are mostly identical except for minor difference in the cuts between the 3 segments. Both of them resemble the classical A -baker's map for $A = 3$. This is necessary but not sufficient to claim that $\tilde{B}_3^{(1)}$ reduces to the 3-baker's map in the semiclassical limit.

Comparing Eq. (9) with Eq. (6) we notice two main differences: (1) In $\tilde{B}_A^{\pm(k)}$, the inverse of F_{Aq} has no phase and the phases of each $q \times q$ DFT matrix are different but in $B_A^{(k)}$ all of them have the same phase. (2) The Hadamard product in Eq. (9) is absent in Eq. (6). Despite these differences, the evolution of states under the operators $\tilde{B}_A^{\pm(k)}$ is very similar to that of $B_A^{(k)}$ in the semiclassical limit, and we will call $\tilde{B}_A^{\pm(k)}$ *quantum A -baker's maps*. We note that if we plot the matrix elements of $\tilde{B}_A^{\pm(k)}$ they resemble classical Bernoulli maps in the same way as the $B_A^{(k)}$ do (Fig. 2), although as we explain shortly this is not a sufficient criterion.

Classical limit. To justify calling $\tilde{B}_A^{\pm(k)}$ a quantum A -baker's map, in the Supplemental Material [33] we determine the action of $\tilde{B}_A^{\pm(k)}$ on Gaussian states (“coherent states”) maximally localized at a point (x, p) in phase space. We show that $\tilde{B}_A^{\pm(k)}$ sends such a state to another coherent state localized close to the classical evolution location $(Ax - \lfloor Ax \rfloor, \frac{p + (\lfloor Ax \rfloor - k) \text{ mod } A}{A})$. We only do this for (x, p) away from the discontinuities of the classical A -baker's map; otherwise there can be diffraction effects [30,34,35]. The action on coherent states can be interpreted in terms of the Wigner or Husimi function in phase space: A state whose Wigner/Husimi function is localized near (x, p) is transformed by $\tilde{B}_A^{\pm(k)}$ to a state localized near the classical trajectory point $(Ax - \lfloor Ax \rfloor, \frac{p + (\lfloor Ax \rfloor - k) \text{ mod } A}{A})$. This correspondence between quantum and classical evolution is shown visually in Fig. 3.

Such an action on Gaussian states was used in [35] to prove a rigorous classical-quantum correspondence (Egorov-type theorem [35, Theorem 12]) for the original Balazs-Voros quantization of the baker's map. In the case here, we will be content with just analyzing the behavior of $\tilde{B}_A^{\pm(k)}$ on Gaussian states. Due to the varying phases in the DFT matrices in Eq. (9), the action on Gaussian states will be more complicated than in the original Balazs-Voros quantization. In particular, the quantum evolved state here is more accurately centered a small distance $\mathcal{O}_A(D^{-1})$ away from the classical trajectory point, though this will be sufficiently close for our purposes to the state actually centered at the classical trajectory.

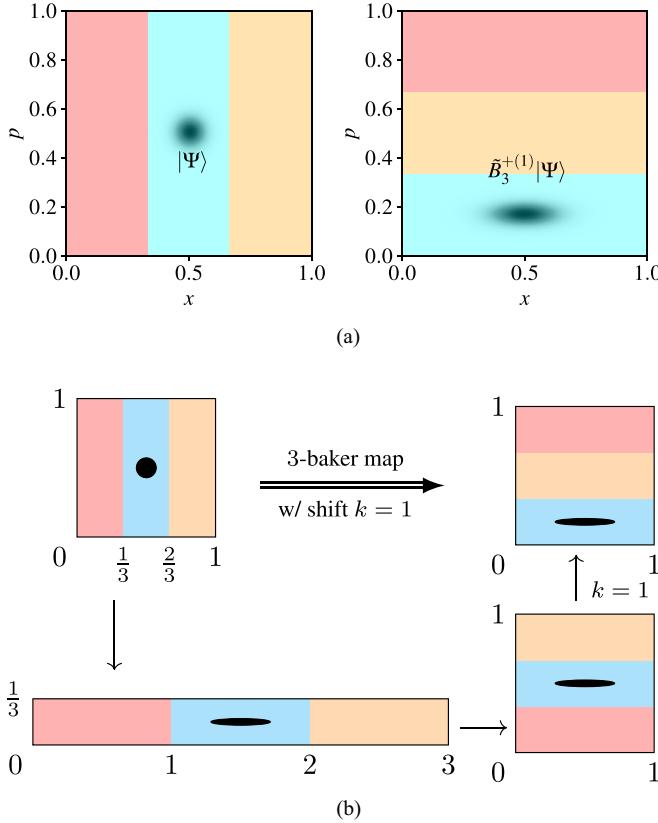


FIG. 3. Comparison of the quantum evolution under $\tilde{B}_3^{+(1)}$, and the classical evolution by the 3-baker's map with cyclic shift $k = 1$. (a) Phase space plots (Husimi functions) of the quantum evolution of a Gaussian state $|\Psi\rangle$ by $\tilde{B}_3^{+(1)}$, for $D = 150$. The colored rectangles are overlayed for easier comparison to (b). (b) Classical evolution of the unit square by the 3-baker's map with cyclic shift $k = 1$, which sends $(x, p) \mapsto (3x - [3x], \frac{p + (3x - 1) \text{ mod } 3}{3})$. The bottom row shows the intermediate components of the total transformation in the top row. The time-evolved quantum state $\tilde{B}_3^{+(1)}|\Psi\rangle$ shown in (a) follows the classical action shown in (b), and also displays the stretching in the x direction and shrinking in the p direction characteristic of the classical A-baker's map.

As noted previously, the matrix elements of $\tilde{B}_A^{\pm(k)}$ in the position basis (and momentum basis) trace out the classical 1D action of the position (momentum) coordinate in the A-baker's map defined in Eqs. (2) and (3). This is not sufficient to conclude that $\tilde{B}_A^{\pm(k)}$ has the correct semiclassical behavior, as the Walsh baker's maps considered in [28] also display this behavior, but as shown in [36] are not quantizations of the baker's map. Checking the behavior in phase space, to ensure the quantizations entwine position and momentum together correctly, is thus necessary to understand the semiclassical limit.

Discussion. We have illustrated a specific “embedding” of quantum chaotic behavior in the periodic orbits of a classically ergodic, chaotic map via quantum superposition, by deriving an exact correspondence between the periodic modular-multiplication-by- A maps and “chaotic” A-baker's maps, for N such that either of $N \pm 1$ is a multiple of A . As will be shown in an upcoming work, this result generalizes to

other values of N albeit via a more complicated construction with two important implications.

First, in any practical implementation of Shor's algorithm, it is N that is given while A is chosen as per convenience, in contrast to the dynamical systems approach, in which a fixed A specifies the modular multiplication map while $N \rightarrow \infty$ through any subsequence of \mathbb{N} gives the classical limit. This means that a general result for N would be crucial if one is to understand the implications of this “embedding of quantum chaos” for Shor's algorithm (otherwise, choosing an A that is a factor of either of $N \pm 1$ would require the output of Shor's algorithm as applied to $N \pm 1$, introducing a circular element). Conversely, achieving such a generalization may provide a fuller picture of how certain perturbations affect the dynamics of Shor's algorithm, along the lines of the analysis in Ref. [24].

Second, from a fundamental quantum dynamical systems viewpoint, the study of quantized A -baker's maps has generally been restricted to Hilbert space dimensions that are multiples of A , due to a need to consider A copies of discrete Fourier transforms in, e.g., the Balazs-Voros quantization [20]. The above connection to modular multiplication in Shor's algorithm provides a promising avenue to generalize quantum A -baker's maps to a larger set of Hilbert space dimensions N , in particular any co-prime pair (A, N) , using *generalizations* of Fourier transforms. This also opens avenues for studying the semiclassical behavior of such generalized quantum A -baker's maps to explore atypicalities and any N -dependence in their “quantum chaos” signatures, noting that such atypicalities were observed for N a multiple of A in the Balazs-Voros quantization [20]. Further, A -baker's maps can be directly realized in quantum simulators using quantum Fourier transforms [37,38], which may allow the experimental detection of such atypical spectral signatures using recently developed measurement protocols for signatures of quantum ergodicity [39,40].

Finally, classical results in ergodic theory indicate that the above results relating different quantizations of the modular multiplication map $f_A(x)$ may generalize in some form to *arbitrary* sufficiently chaotic systems. This is due to Sinai's factor theorem [41,42], which implies that any ergodic and chaotic system, whose Kolmogorov-Sinai entropy [43] (sum of positive Lyapunov exponents) is at least $\ln A$, contains $f_A(x)$ as a factor [i.e., can be coarse grained to yield a system equivalent to $f_A(x)$]; a direct illustration is provided by the x -coordinate action of the A-baker's map (coarse-graining over p) being $f_A(x)$. Successfully implementing such a generalization in practice would depend on identifying suitable quantizations of a given chaotic system that capture the appropriate properties of its modular multiplication factor(s), and may provide further avenues for future work.

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