

Hamiltonian with Energy Levels Corresponding to Riemann Zeros

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A Hamiltonian with eigenenergy $E_n = \rho_n(1 - \rho_n)$ has been constructed, where ρ_n denotes the n -th non-trivial zero of the Riemann zeta function. To construct such a Hamiltonian, we generalize the Berry-Keating paradigm and encode number-theoretic information into the Hamiltonian using modular forms. Although our construction does not resolve the Hilbert-Pólya conjecture (since the eigenstates corresponding to E_n are *not* normalizable), it provides a novel physical perspective on the Riemann Hypothesis (RH). In particular, we propose a physical interpretation of RH, which could offer a potential pathway toward its proof.

Introduction-The Riemann zeta function, defined by the series $\zeta(s) := \sum_{n \geq 1} n^{-s}$, lies at the core of analytic number theory. For instance, the growth order of many arithmetic functions (e.g., the prime number counting function $\pi(x)$) depends on the analytic properties of $\zeta(s)$ [1, 2]. Among the properties of $\zeta(s)$, the distribution of its zeros is of utmost importance and interest. The famous Riemann Hypothesis (RH) asserts that [1]

$$\left\{ \begin{array}{l} \zeta(s) = 0 \\ 0 < \Re s < 1 \end{array} \right. \implies \Re s = \frac{1}{2}, \quad (1)$$

where the condition $0 < \Re s < 1$ excludes the so-called trivial zeros of $\zeta(s)$, which occur at the negative even integers.

Based on the RH, many related problems have been proposed. A physically motivated example is the Hilbert-Pólya conjecture (HPC), which, in physical terms, asks whether there exists a self-adjoint Hamiltonian¹ whose energy levels satisfy $E_n = P(\rho_n)$ for all $n \in \mathbb{N}^+$. Here ρ_n denotes the n -th non-trivial zero of the Riemann zeta function with $\Im \rho_n > 0$, and the function P must satisfy the condition $P(\rho_n) \in \mathbb{R} \iff \Re \rho_n = \frac{1}{2}$, for example, $P(\rho_n) := -i(\rho_n - \frac{1}{2})$ or $P(\rho_n) := (1 - \rho_n)\rho_n$ [3].

The HPC implies the RH; therefore, it is regarded as a potential pathway toward proving the RH and has attracted significant attention from many researchers in physics [4–10]. For instance, Michael Berry and Jonathan Keating proposed the classical Hamiltonian $H_{\text{BK}} := xp$ [4], with the aim of quantizing it (under an appropriate scheme) to obtain a quantum Hamiltonian that satisfies the requirements of the HPC [11], where x and p denote the canonical coordinate and momentum, respectively. Although naive quantization of H_{BK} fails to achieve this objective [7], it has nonetheless inspired a large body of subsequent work, in which researchers have attempted

to quantize or extend H_{BK} using various techniques [5–7, 9]. To date, however, these efforts have not succeeded in fully satisfying the requirements of the HPC.

We now propose a Hamiltonian by extending the Berry-Keating framework from a different perspective. By encoding number-theoretic information into its structure, our Hamiltonian admits a novel set of energy levels $E_n = \rho_n(1 - \rho_n)$. Although our model does not fully satisfy the HPC—since the corresponding eigenstates are not bound states—it nevertheless offers a fresh perspective on both the RH and the HPC.

The model- Motivated by the Berry-Keating paradigm, we introduce the following two-dimensional classical Hamiltonian:

$$H = Vp^2, \quad (2)$$

where $p^2 = p_x^2 + p_y^2$ with p_x and p_y the momenta along the x - and y -axes, respectively, and $V(x, y)$ is a spatially dependent function, which we refer to as *geometric potential*. The similarity between our Hamiltonian and H_{BK} lies in the fact that both are products of coordinate-dependent and momentum-dependent quantities. However, in our case we use p^2 instead of p to avoid singularities in the system. Moreover, unlike the one-dimensional Berry-Keating Hamiltonian, the two-dimensional nature of our Hamiltonian allows for the existence of classical closed trajectories [6]. This can be explicitly demonstrated by choosing $V(x, y) = x^2 + y^2$, for which the Hamiltonian's canonical equations admit circular orbit solutions.

Note that Hamiltonian (2) can be realized in specific physical systems, such as a heavy fermion with a position-dependent effective mass [12, 13], and a particle moving on a conformally flat surface with the metric $g_{ij} = \frac{1}{V}\delta_{ij}$ [14].

The quantization of Hamiltonian (2) faces an ordering ambiguity. Therefore, it is natural to employ a covariant quantization scheme, specifically the path-integral approach, which yields a formally Hermitian(symmetric) Hamiltonian [14–16]:

$$\hat{H} = -V^{\frac{1}{2}}\hat{\Delta}V^{\frac{1}{2}}, \quad (3)$$

¹ For simplicity, in this paper the term *Hamiltonian* implicitly refers to the quantum Hamiltonian. In formulas, we use a hat symbol ($\hat{\cdot}$) to emphasize its operator nature, thereby distinguishing it from the classical Hamiltonian which is a function.

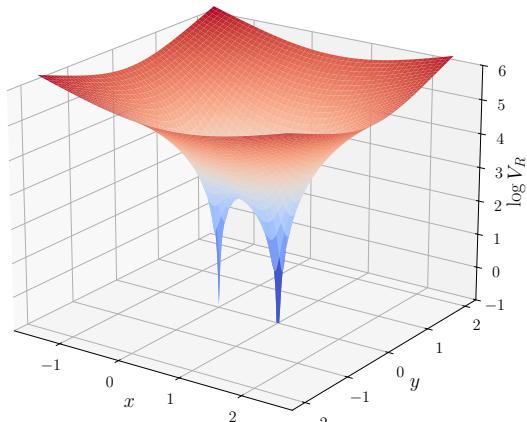


FIG. 1. The double well structure of the geometric potential $V_R(x, y)$. It can be clearly seen that there are two potential wells located at the origin and $(x, y) = (1, 0)$. Note here to demonstrate the structure of V_R we actually plot the logarithm of it.

where $\hat{\Delta} := \partial_x^2 + \partial_y^2$ is the Laplace operator.

Notably, our Hamiltonian exhibits fundamental differences from the conventional one, $H_C := p^2 + V$, in two critical aspects, even though both models describe a particle moving in a *potential* field.

First, the behavior of particles differs significantly where the potential tends to infinity. Consider a potential that asymptotically diverges at infinity. For the system governed by H_C , the particle is confined to a finite region because the momentum p will ultimately decrease to zero as the particle moves to the surface $V(x, y) = E$, where E is the energy of the system. Quantum mechanically, this implies that the states governed by $\hat{H}_C = -\Delta + V$ are always bound states.

In stark contrast, for the system described by Hamiltonian (2), the particle's momentum p never vanishes, even though it diminishes as V increases. This means that there always exist unbounded orbits. At the quantum level, we therefore expect the presence of scattering states, although their wave functions' modulus becomes very small near infinity.

Second, our model exhibits singularities at the zeros of the geometric potential V . Classically, the vanishing of V implies that the momentum p must diverge to infinity. Consequently, in the quantum regime, a physically admissible wave function should vanish at the zeros of V to satisfy regularity conditions.

Our goal is now to construct a geometric potential V that yields a set of eigenenergies corresponding to the Riemann zeros. Previous studies have provided several critical insights. For example, the statistical similarity between the distribution of zeta zeros and the eigenval-

ues of the Gaussian Unitary Ensemble (GUE) suggests that the desired geometric potential should correspond to a chaotic system [3, 17, 18]. Moreover, to "encode" the information of the zeta function into the Hamiltonian, we need to consider a geometric potential that possesses a number-theoretic structure [9]. Finally, since the zeta function satisfies the functional equation $\xi(1-s) = \xi(s)$ with $\xi(s) := \pi^{-\frac{s}{2}} \Gamma(\frac{s}{2}) \zeta(s)$, the required geometric potential must reflect this symmetry [19, 20].

For the above reasons, we consider the following geometric potential

$$V_R(x, y) = \left(\frac{\Im \tau(z)}{|\tau'(z)|} \right)^2 \quad (4)$$

with $z := x + iy \in \mathbb{C}$, $i := \sqrt{-1}$, $\tau'(z) = d\tau(z)/dz$ and

$$\tau(z) := i \frac{{}_2F_1\left(\frac{1}{6}, \frac{5}{6}, 1; \frac{1}{2}\left(1 + \sqrt{\frac{z}{z-1}}\right)\right)}{{}_2F_1\left(\frac{1}{6}, \frac{5}{6}, 1; \frac{1}{2}\left(1 - \sqrt{\frac{z}{z-1}}\right)\right)}, \quad (5)$$

where ${}_2F_1(a, b, c; z)$ is the Gauss hypergeometric function. Note that first, for any function $f(z)$, we restrict the argument range of z to $(-\pi, \pi]$. Second, for convenience, we will use both complex and two-dimensional real notations. Specifically, we always assume $z = x + iy$ and write $f(z) := f(x, y)$ for any function $f(x, y)$ defined on \mathbb{R}^2 . For example, we write $V_R(0) = V_R(0, 0)$ and $V_R(1) = V_R(1, 0)$.

This unconventional geometric potential meets our requirements for the following reasons. First, it describes a classically chaotic system, which can be demonstrated through both analytical approaches and numerical methods. Intuitively, as shown in Fig. 1, V_R possesses a double-well structure, which generally induces chaotic dynamics [21]. The two wells correspond to the two zeros of V_R , located at $(x, y) = (0, 0)$ and $(1, 0)$.

Second, the denominator in V_R exhibits a number-theoretic structure, since the inverse of $\tau(z)$ is given by

$$z(\tau) = \left(1 - \frac{E_4^3(\tau)}{E_6^2(\tau)} \right)^{-1}, \quad (6)$$

as provided by Ramanujan in his notebook [22], where $E_4(\tau)$ and $E_6(\tau)$ are the Eisenstein series defined by

$$E_{2k}(\tau) := \frac{1}{2\zeta(2k)} \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ (m,n) \neq (0,0)}} \frac{1}{(m+n\tau)^{2k}}. \quad (7)$$

By the modularity of Eisenstein series, one obtains [23]

$$z(\gamma\tau) = z(\tau), \quad (8)$$

where $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathbb{Z})$ and we define the action of γ on z by $\gamma z := \frac{az+b}{cz+d}$. Note that this property of $z(\tau)$ is key to our construction.

Finally, the numerator of V_R is designed to encode the functional symmetry of the zeta function. This feature, together with the second point mentioned above, will become evident when we solve the eigenenergy problem in the next section.

The eigenenergies- The time-independent Schrödinger equation corresponding to the geometric potential (4) is

$$\hat{H}_R \psi = E\psi , \quad (9)$$

where $\hat{H}_R := -V_R^{\frac{1}{2}} \hat{\Delta} V_R^{\frac{1}{2}}$ is the Hamiltonian. Note that, in general, we assume the eigenenergy $E \in \mathbb{C}$. Furthermore, to avoid singularities near the zeros of V_R , we impose the requirement that the wave function is everywhere bounded on \mathbb{R}^2 ; that is, there exists a constant $M \in \mathbb{R}^+$ such that

$$|\psi(x, y)| < M \quad (10)$$

holds for all $(x, y) \in \mathbb{R}^2$. We will now prove that the problem defined by Eq. (9) and (10) admits scattering state solutions, where the eigenenergy is discrete, and the energy levels satisfy $E_n = \rho_n(1 - \rho_n)$.

Using complex notation and changing the variables from z to τ , the Schrödinger equation (9) can be written in a much simpler form:

$$(\tau - \tau^*)^2 \frac{\partial}{\partial \tau} \frac{\partial}{\partial \tau^*} \phi(\tau) = E\phi(\tau) , \quad (11)$$

where $*$ denotes the complex conjugate and we have defined the *reduced wave function* $\phi(\tau) := \psi(z(\tau))V^{\frac{1}{2}}(z(\tau))$.

However, the coordinate transformation $z \rightarrow \tau$ is not one-to-one; multiple values of τ correspond to the same z . Therefore, additional constraints must be imposed to ensure that the values of ϕ are identical at all τ s corresponding to the same z . Specifically, by Eq. (8) and the definition of $\phi(\tau)$ one has

$$\phi(\tau) = \phi(\gamma\tau) . \quad (12)$$

Furthermore, we must analyze the wave function $\psi(z)$ near the zeros of V_R , specifically at $z = 0$ and $z = 1$, to check for potential singularities. An asymptotic analysis near $z = 0$ shows that (see Section III of Supplemental Material[24])

$$\psi(z) = [\phi(\mathbf{i}) + O(|z|)] \left[C|z|^{-\frac{1}{2}} + O(1) \right] , \quad (13)$$

where C is a non-zero constant. To satisfy boundary condition (10), it is both sufficient and necessary that $\phi(\mathbf{i}) = 0$. A similar asymptotic analysis for $z = 1$ gives $\phi(e^{i\frac{\pi}{3}}) = 0$. In conclusion, we have the boundary conditions

$$\phi(\mathbf{i}) = \phi(e^{i\frac{\pi}{3}}) = 0 \quad (14)$$

Note that \mathbf{i} and $e^{i\frac{\pi}{3}}$ occur here because the coordinate transformation $z \rightarrow \tau$ maps the zeros of V_R $z = 0$ and $z = 1$ to $\tau = \mathbf{i}$ and $\tau = e^{i\frac{\pi}{3}}$ respectively.

Now, our task is to solve the problem defined by Eq. (11), Eq. (12) and Eq. (14). We first find $\phi_s^{(0)}(\tau) = (\Im\tau)^s$ as the solution to Eq. (11), although it fails to satisfy the modular condition (12). To resolve this, we modify $\phi_s^{(0)}$ by shifting and summing over the appropriate group elements as follows:

$$\phi_s(\tau) = \sum_{\gamma \in \Gamma_\infty \backslash SL(2, \mathbb{Z})} \phi_s^{(0)}(\gamma\tau) , \quad (15)$$

where $\Gamma_\infty := \begin{pmatrix} 1 & \mathbb{Z} \\ 0 & 1 \end{pmatrix}$ is a subgroup of $SL(2, \mathbb{Z})$, and $\Gamma_\infty \backslash SL(2, \mathbb{Z})$ is the left quotient group.

Through direct calculation, it can be shown that ϕ_s satisfies the modular condition in Eq. (12) and serves as an eigenstate of Eq. (9) with eigenenergy $E = s(1 - s)$. Moreover, it has a zeta function representation (see Section II of Supplemental Material [24]):

$$\phi_s(\tau) = \phi_s^{(0)}(\tau) \frac{\zeta_E(s, \tau)}{\zeta(2s)} , \quad (16)$$

where the Epstein zeta function is defined by

$$\zeta_E(s, \tau) = \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ (m,n) \neq (0,0)}} \frac{1}{|m\tau + n|^{2s}} . \quad (17)$$

Note that although the summation in Eq. (17) converges only for $\Re s > 1$, it can be analytically continued to the entire complex plane \mathbb{C} , except for a pole at $s = 1$. Additionally, since $\zeta(s)$ has a pole at $s = 1$, we require $s \neq \frac{1}{2}$, otherwise $\phi_s(\tau)$ would degenerate into the zero solution.

In the final step, we require the solution $\phi_s(\tau)$ to satisfy Eq. (14). We have

$$\frac{\zeta_E(s, \mathbf{i})}{\zeta(2s)} = \frac{\zeta_E(s, e^{i\frac{\pi}{3}})}{\zeta(2s)} = 0 . \quad (18)$$

By the analytic formulation of Gauss's quadratic reciprocity law, the two terms $\zeta_E(s, \mathbf{i})$ and $\zeta_E(s, e^{i\frac{\pi}{3}})$ can be decomposed as the product of the Riemann zeta function and Dirichlet L -functions [25]:

$$\begin{aligned} \zeta_E(s, \mathbf{i}) &= 4\zeta(s)L(\chi_{-4}, s) \\ \zeta_E(s, e^{i\frac{\pi}{3}}) &= 6\zeta(s)L(\chi_{-3}, s) , \end{aligned} \quad (19)$$

where χ_{-4} and χ_{-3} are Dirichlet characters defined by

$$\chi_{-m}(n) := \begin{cases} 1 & n \equiv 1 \pmod{m} \\ -1 & n \equiv m-1 \pmod{m} \\ 0 & \text{otherwise} \end{cases} .$$

Since both characters are odd (i.e., $\chi_{-4}(-1) = \chi_{-3}(-1) = -1$), the trivial zeros of $L(\chi_{-4}, s)$ and $L(\chi_{-3}, s)$ are located at negative odd integers, while the

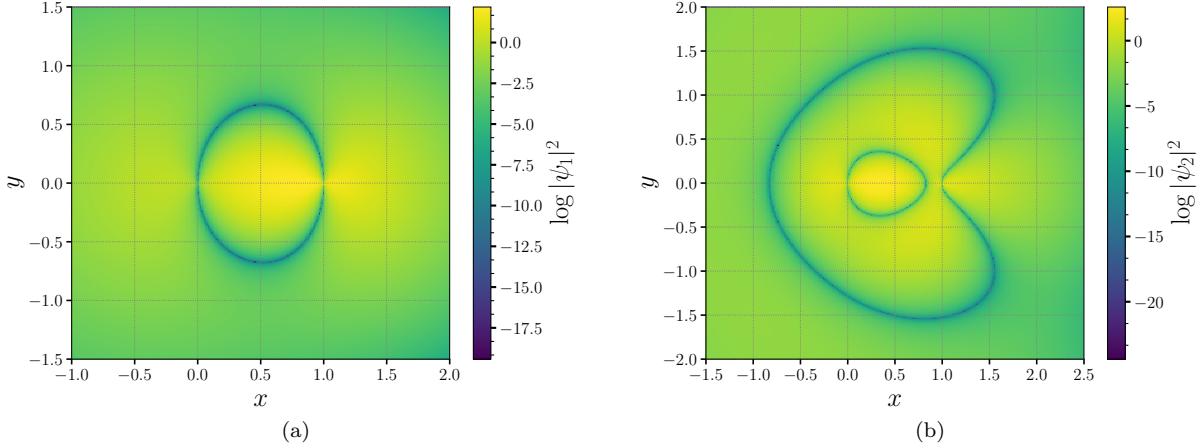


FIG. 2. The probability density of the first two eigenstates, corresponding to the first two Riemann zeros: (a) $\rho_1 = 0.5 + i14.13472\dots$ and (b) $\rho_2 = 0.5 + i21.02203\dots$, respectively, is shown. At the zeros of V_R , namely $z = 0$ and $z = 1$ (where $z := x + iy$), the wave function indeed vanishes. We plot the logarithm of the probability density so that the nodal line, on which the wave function $\psi(z)$ vanishes, is clearly visible.

trivial zeros of $\zeta(s)$ are located at negative even integers. Surprisingly, these trivial zeros are completely canceled out by the trivial zeros of $\zeta(2s)$ at negative integers. Thus, Eq. (18) and (19) imply that²

$$\zeta(s) = 0, \quad 0 < \Re s < 1. \quad (20)$$

Namely, by taking s to be the non-trivial zeros of the Riemann zeta function, the boundary condition (10) can be satisfied. As a consequence, the eigenenergy is discrete, and the energy levels are given by $E_n = (1 - \rho_n)\rho_n$.

The asymptotic behavior of the obtained wave function ψ_n at infinity is crucial, as it determines the space in which the wave function resides. As $|z| \rightarrow \infty$, we have (see Section III of Supplemental Material[24])

$$\begin{aligned} \psi_n(z) &= A_n \frac{1}{|z|} \log(|12^3 z|)^{-\frac{1}{2}+d_n} \Omega_{d_n}(|z|) \\ &+ o\left(\frac{1}{|z|} \log(|z|)^{-\frac{1}{2}+d_n}\right), \end{aligned} \quad (21)$$

where $\Omega_{d_n}(|z|)$ is a bounded oscillatory term given by

$$\Omega_{d_n}(|z|) := \begin{cases} \log(12^3|z|)^{\pm i\omega_n} & \text{if } d_n > 0 \\ \cos(\omega_n \log(\log(12^3|z|)/(2\pi)) - \varphi_n) & \text{if } d_n = 0 \end{cases}$$

Here, $A_n \neq 0$ and $\varphi_n \in \mathbb{R}$ are constants depending on ρ_n , $d_n := |\Re \rho_n - 1/2|$ is the distance of the zeta zeros ρ_n to the line $\Re s = 1/2$, and $\omega_n = \Im \rho_n$ is the imaginary part of ρ_n .

As expected, the wave functions decay to zero as $|z| \rightarrow \infty$. The decay rate depends on the distance d_n , while the imaginary part of ρ_n (i.e., ω_n) acts as the frequency. However, the decay rate is not fast enough for ψ_n to be a bound state. One can verify that $\int_{\mathbb{R}^2} |\psi_n|^2 dx dy \rightarrow \infty$, which implies that the wave function ψ_n represents a scattering state.

To gain an intuitive understanding of the wave function, we numerically calculate the first two eigenstates and present them in Fig. 2. As expected, the two wave functions vanish at the zeros of V_R , namely $(0, 0)$ and $(1, 0)$, which is also consistent with our expectations (see Eq. (13)).

Discussion- It can be seen that the reality of E_n directly implies the RH. Writing $\rho_n = \frac{1}{2} + i\gamma_n$, we obtain $E_n = \frac{1}{4} + \gamma_n^2$, where $\gamma_n \in \mathbb{C}$ but cannot be purely imaginary. Hence, the reality of E_n necessitates the reality of γ_n , which is precisely equivalent to the RH.

Mathematically, however, standard spectral theory guarantees that bound states (which reside in a Hilbert space \mathcal{H}) possess real eigenvalues. In contrast, the wave function ψ_n describes a scattering state in the space of bounded functions $\mathcal{B}(\mathbb{R}^2)$, which falls outside the scope of traditional Hilbert space spectral theorems.

Here, we provide a possible path to prove that E_n is real. From the Schrödinger equation, one can derive the probability conservation equation (see Section IV of Supplemental Material[24]):

$$\dot{Q}(t) = - \oint_{\partial U} \mathbf{J} \cdot \mathbf{n} dl, \quad (22)$$

where $Q(t)$ is the probability of finding the particle in a region U , and \mathbf{J} is the probability current density vector. For a stationary wave function $\psi(z)e^{-iEt}$, the time

² Here, we assume that $L(\chi_{-4}, s)$ and $L(\chi_{-3}, s)$ do not share any non-trivial zeros. If they do, the common zeros would correspond to additional solutions in our model; however, these would not affect our main discussion.

derivative of $Q(t)$ is given by

$$\dot{Q}(t) = 2\Im(E)e^{2\Im(E)t} \int_U d^2z |\psi(z)|^2, \quad (23)$$

and the probability current density vector is given by

$$\mathbf{J} := e^{2\Im(E)t} (\psi^* \hat{\mathbf{v}} \psi - \psi \hat{\mathbf{v}} \psi^*), \quad (24)$$

with the velocity operator defined by $\hat{\mathbf{v}} := -iV_R^{\frac{1}{2}} \nabla V_R^{\frac{1}{2}}$.

For each ψ_n , suppose there exists a compact region $U_n \subset \mathbb{C}$ (which depends on n) such that 1. $\psi_n|_{\partial U_n} \equiv 0$; 2. $\int_{U_n} d^2z |\psi_n|^2 \neq 0$. Then, by Eq. (22)–(24), it follows that $\Im E_n = 0$. Since the wave function ψ_n is real analytic, it cannot vanish almost everywhere on any compact region, and thus the second condition is automatically satisfied. Consequently, to establish the reality of the eigenenergy, it suffices to identify a closed nodal line of the corresponding wave function, where a nodal line is defined as a curve along which the wave function vanishes.

We computed a number of wave functions ψ_n , and for each of them, a closed nodal line can be identified. For example, the "egg-shaped" curve shown in Fig. 2(a) and the "heart-shaped" curve shown in Fig. 2(b) serve as illustrations.

We now turn to the theoretical possibility of proving the existence of such nodal lines.

According to Eq. (14), $\tau = i$ and $\tau = e^{i\frac{\pi}{3}}$ are two zeros of the reduced wave function $\phi_{\rho_n}(\tau)$. Furthermore, one can prove that near $\tau = i$, the reduced wave function ϕ_{ρ_n} can be expressed as (see Section III of Supplemental Material[24]):

$$\begin{aligned} \phi_{\rho_n}(i + \eta) &= \alpha_n(\eta^2 + \eta^{*2}) + O(|\eta|^3) \\ &= 2\alpha_n((\Re\eta)^2 - (\Im\eta)^2) + O(|\eta|^3), \end{aligned} \quad (25)$$

where $\alpha_n \neq 0$ is a constant depending on ρ_n . If we ignore the higher-order terms, the nodal lines of the leading-order term $(\Re\eta)^2 - (\Im\eta)^2$ form a cross with $\tau = i$ as the vertex. Although this cross may be disrupted by higher-order terms (for example, $\phi(i + \eta) = (\Re\eta)^2 - (\Im\eta)^2 + i(\Re\eta)^3$), we can assume its existence and then explore what conclusions can be drawn.

When we map the τ -plane to the z -plane via Eq. (6), the four edges of this cross merge into two edges with $z = 0$ as the vertex. For the other point, $\tau = e^{i\frac{\pi}{3}}$, the situation is entirely analogous; thus, we may also assume two nodal lines with $z = 1$ as the vertex.

Any nodal line that originates at $z = 0$ or $z = 1$ can only terminate at one of the points $z = 0$, $z = 1$, or $z = \infty$. By the asymptotic behavior given in Eq. (21), such nodal lines cannot end at $z = \infty$. Hence, only two scenarios remain possible: 1. Two nodal lines originate at $z = 0$ and terminate at $z = 1$; 2. One nodal line originates and terminates at $z = 0$, while another originates and terminates at $z = 1$. Examples of the first and second scenarios can be illustrated in Fig. 2(a) and Fig. 2(b), respectively. In both cases, the existence of at least one closed nodal line is guaranteed. We note that a nodal line may intersect itself or other nodal lines; however, this does not affect our conclusion.

The remaining issue is that one needs to conduct a detailed analysis of all the higher-order terms in Eq. (25) to ensure that they do not disrupt the cross. We numerically calculate a few wave functions and find that the cross exists in each of them(see Section IV of Supplemental Material [24]). However, significant effort is still required to analytically confirm the existence of the cross for all wave functions, and we leave this for future work.

In conclusion, we have constructed a novel Hamiltonian. Under the requirement that the wave function is bounded, this Hamiltonian admits $E_n = \rho_n(1 - \rho_n)$ as the eigenenergies of scattering states. Our construction offers a fresh physical perspective on both the RH and HPC. It suggests that the non-trivial zeros of the Riemann zeta function may be more closely associated with scattering states rather than bound states. Moreover, the study of scattering states—particularly bounded scattering states—could serve as a potential avenue for proving the RH.

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- [24] See Supplemental Material for rigorous definitions of the terms used in the main text, as well as details of certain calculations, which includes Refs. [23] and [26].
- [25] D. B. Zagier, *Zetafunktionen und quadratische Körper*, 1st ed., Hochschultext (Springer Berlin, Heidelberg, 1981) p. 144.
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Supplemental Material: Hamiltonian with Energy Levels Corresponding to Riemann Zeros

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In this supplementary material, we provide additional rigorous definitions of the terms used in the main text, as well as details of certain calculations. Specifically, the first section briefly reviews basic concepts from quantum mechanics and defines commonly used terms such as *eigenenergy* and *Hermitian*, in order to help readers with a mathematical background better understand the main text. The second section presents the Epstein zeta function representation of the wave function $\phi(\tau)$. The third section provides the asymptotic expansions used in the derivations, including the asymptotic formulas for V_R and for the wave function near $z = 0$, $z = 1$, and $z = \infty$. The last section derives the probability conservation equation and presents numerical results on the zero lines of $\phi(\tau)$ near $\tau = i$.

I. DEFINITIONS OF TERMS

A quantum system is typically described by a time-dependent vector $\Psi(t)$ (so-called wave function) in a linear space X , which satisfies the Schrödinger equation (in the unit $\hbar = 1$)

$$i\partial_t\Psi(t) = \hat{H}\Psi(t), \quad (\text{S1})$$

where \hat{H} is an operator referred to as (quantum) Hamiltonian, which acts on the linear space X and is determined by the system itself. For example, for a free particle in Euclidean space, the Hamiltonian is given by Laplacian $\hat{H}_f = -\frac{1}{2}\Delta$.

Given a time-independent Hamiltonian \hat{H} , we can define the eigenenergy and eigenstate as follows

Definition I.1. Let X be a linear space over \mathbb{C} (not necessarily normed space), and let $\hat{H} : D(\hat{H}) \rightarrow X$ be a Hamiltonian with domain $D(\hat{H}) \subseteq X$. A scalar $E \in \mathbb{C}$ is an eigenenergy of \hat{H} if there exists a non-zero element $\psi \in D(\hat{H})$ such that $\hat{H}\psi = E\psi$. And ψ is called the eigenstate of \hat{H} related to eigenenergy E .

Let ψ be a eigenstate of \hat{H} related to eigenenergy E , obviously $\Psi = \psi e^{-iEt}$ is the solution of Schrödinger Equation (S1). For this reason, $\hat{H}\psi = E\psi$ is usually referred to as the *time-independent Schrödinger equation*, and the eigenstate ψ is also called a *wave function*.

Remark I.2. Physically, a system described by an energy eigenstate ψ possesses a definite energy E , which is precisely the eigenenergy corresponding to ψ . Since energy must be real valued, we need to introduce additional conditions to ensure the real-valuedness of E . A common practice is to restrict $D(\hat{H})$ such that \hat{H} becomes a self-adjoint operator, thereby guaranteeing that

E is real. However, in some cases, this is not necessary, or even impossible. A striking example is the aforementioned Hamiltonian $\hat{H}_f = -\frac{1}{2}\Delta$ describing a free particle in Euclidean space \mathbb{R}^n . Its eigenstate e^{ax} has a domain of the entire space \mathbb{R}^n ; as long as the domain of H_f is restricted to the space of bounded functions, a must be a vector consisting of purely imaginary numbers, and the corresponding eigenvalue of e^{ax} is necessarily real. Yet, under the condition that the eigenstates are defined over the entire \mathbb{R}^n , it is impossible to find a non-trivial $D(\hat{H}_f)$ that makes \hat{H}_f self-adjoint.

Let ψ be the eigenstate of a Hamiltonian \hat{H} , if ψ is in Hilbert space, (thus it is normalizable), we say ψ is a *bound state*, otherwise it is a *scatter state*. To solve the time-independent Schrödinger equation, we generally need to introduce certain boundary conditions. These boundary conditions actually restrict the domain of the original \hat{H} . For convenience, we still denote the Hamiltonian after restricting its domain as \hat{H} . The set of all eigenenergies of \hat{H} (solved under some boundary conditions) is denoted as $\sigma(\hat{H})$. An eigenenergy $E \in \sigma(\hat{H})$ is said to be *discrete in $\sigma(\hat{H})$* if E is an isolated point in $\sigma(\hat{H})$; otherwise, $E \in \sigma(\hat{H})$ is said to be *continuous in $\sigma(\hat{H})$* . If $\sigma(\hat{H})$ contains only finitely many continuous points, then $\sigma(\hat{H})$ is said to be discrete. Discrete eigenenergies are generally referred to as *energy levels*.

II. THE REDUCED WAVE FUNCTION $\phi_s(\tau)$

To prove that $\phi_s(\tau)$ defined by

$$\phi_s(\tau) = \sum_{\gamma \in \Gamma_\infty \setminus SL(2, \mathbb{Z})} \phi_s^{(0)}(\gamma\tau) \quad (\text{S2})$$

satisfy

$$(\tau - \tau^*)^2 \frac{\partial}{\partial \tau} \frac{\partial}{\partial \tau^*} \phi_s(\tau) = s(1-s)\phi_s(\tau), \quad (\text{S3})$$

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one just need to prove

$$(\tau - \tau^*)^2 \frac{\partial}{\partial \tau} \frac{\partial}{\partial \tau^*} \phi_s^{(0)}(\gamma \tau) = s(1-s) \phi_s^{(0)}(\gamma \tau). \quad (\text{S4})$$

For $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathbb{Z})$ we have

$$\phi_s^{(0)}(\gamma \tau) = \left[\Im \left(\frac{a\tau + b}{c\tau + d} \right) \right]^s = \left(\frac{\Im \tau}{|c\tau + d|^2} \right)^s. \quad (\text{S5})$$

It is straightforward to check that it satisfies Eq. (S4). The modularity $\phi_s(\tau) = \phi_s(\gamma \tau)$ is obvious, by the properties of group $SL(2, \mathbb{Z})$.

We will need some elementary knowledge of number theory to prove that $\phi_s(\tau)$ can be given by Epstein zeta function:

$$\phi_s(\tau) = \phi_s^{(0)}(\tau) \frac{\zeta_E(s, \tau)}{\zeta(2s)}. \quad (\text{S6})$$

Considering the Diophantine equation

$$-cx + dy = 1, \quad (\text{S7})$$

according to Bezout's Theorem, the necessary and sufficient condition for it to have integer solutions is that c and d are coprime, i.e., $\gcd(c, d) = 1$. Under this condition, its solutions can be expressed as $x = b' + nd, y = a' + nc$, where $n \in \mathbb{Z}$ and (b', a') is a particular solution, which is obtained by the Euclidean algorithm. In other words, each the element of $SL(2, \mathbb{Z})$ can be represented as

$$\gamma = \begin{pmatrix} a' + nc & b' + nd \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a' & b' \\ c & d \end{pmatrix}. \quad (\text{S8})$$

We actually decompose $SL(2, \mathbb{Z})$ to the product of $\Gamma_\infty := \begin{pmatrix} 1 & \mathbb{Z} \\ 0 & 1 \end{pmatrix}$ and the quotient group $\Gamma_\infty \backslash SL(2, \mathbb{Z})$. The element of the later can be uniquely determined by two coprime integers (c, d) . So by Eq. (S5) we have

$$\begin{aligned} \phi_s(\tau) &= \sum_{\gamma \in \Gamma_\infty \backslash SL(2, \mathbb{Z})} \phi_s^{(0)}(\gamma \tau) \\ &= \sum_{\gcd(c, d)=1} \frac{(\Im \tau)^s}{|c\tau + d|^{2s}} \\ &= \frac{(\Im \tau)^s}{\zeta(2s)} \sum_{k=1}^{\infty} \frac{1}{k^{2s}} \sum_{\gcd(c, d)=1} \frac{1}{|ck\tau + kd|^{2s}} \\ &= \frac{(\Im \tau)^s}{\zeta(2s)} \sum_{k \geq 1, \gcd(c, d)=1} \frac{1}{|kct + kd|^{2s}} \\ &= \frac{(\Im \tau)^s}{\zeta(2s)} \sum_{\substack{(m, n) \in \mathbb{Z}^2 \\ (m, n) \neq (0, 0)}} \frac{1}{|m + n\tau|^{2s}}. \end{aligned} \quad (\text{S9})$$

It is straightforward to check that $\phi_s(\tau)$ is an even function with respect to $\Re \tau$. We have

$$\begin{aligned} &\sum_{\substack{(m, n) \in \mathbb{Z}^2 \\ (m, n) \neq (0, 0)}} \frac{1}{|m + n\tau|^{2s}} \\ &= \sum_{\substack{(m, n) \in \mathbb{Z}^2 \\ (m, n) \neq (0, 0)}} \frac{1}{((m + n\Re \tau)^2 + (n\Im \tau)^2)^s} \\ &= \sum_{\substack{(m, n) \in \mathbb{Z}^2 \\ (m, n) \neq (0, 0)}} \frac{1}{((m - n\Re \tau)^2 + (-n\Im \tau)^2)^s} \\ &= \sum_{\substack{(m, n) \in \mathbb{Z}^2 \\ (m, n) \neq (0, 0)}} \frac{1}{((m + n(-\Re \tau))^2 + (n\Im \tau)^2)^s}. \end{aligned} \quad (\text{S10})$$

III. THE ASYMPTOTIC FORMULA

A. The asymptotic behavior of $V_R(z)$

We will give the asymptotic formula of V_R at its zeros ($z = 0$ and $z = 1$) and divergent points ($z = \infty$), since they are crucial in our analysis.

The Taylor expansions of $\tau(z)$ at $z = 0$ and $z = 1$ are given by

$$\tau(z) = \mathbf{i} + C_1 z^{\frac{1}{2}} + O(|z|), \text{ and} \quad (\text{S11})$$

$$\tau(z) = e^{\mathbf{i}\frac{\pi}{3}} + \mathbf{i}C_2(z-1)^{\frac{1}{3}} + O(|z-1|^{\frac{2}{3}}) \quad (\text{S12})$$

respectively, where we use C_n to represent a non-zero real constants. By the definition of $V_R(z)$, it follows that

$$V_R^{\frac{1}{2}}(z) = C_3 |z|^{\frac{1}{2}} + O(|z|), \text{ and} \quad (\text{S13})$$

$$V_R^{\frac{1}{2}}(z) = C_4 |z-1|^{\frac{2}{3}} + O(|z-1|) \quad (\text{S14})$$

hold for z near 0 and 1, respectively. Note that Eq. (S11) and (S12) imply that $\tau(0) = \mathbf{i}$ and $\tau(1) = e^{\mathbf{i}\pi/3}$, respectively.

The behavior of $V_R(z)$ at infinity can be obtained by the asymptotic expansion of ${}_2F_1$ at ∞ . However, it is complicated by the multi valuedness of ${}_2F_1$ in the region $|z| > 1$. A more convenient way is to consider

$$z(\tau) = \left(1 - \frac{E_4^3(\tau)}{E_6^2(\tau)} \right)^{-1}, \quad (\text{S15})$$

whose asymptotic expansion at ∞ is well known [1]

$$z(\tau) = -\frac{1}{12^3} e^{-2\pi \mathbf{i}\tau} + O(1), \quad (\text{S16})$$

as $\Im \tau \rightarrow \infty$. The inverse of Eq. (S16) gives

$$\tau(z) = \frac{\mathbf{i}}{2\pi} \log(-12^3 z) + O\left(\frac{1}{z}\right) \quad (\text{S17})$$

as $|z| \rightarrow \infty$. The asymptotic formula

$$V_R^{\frac{1}{2}}(z) = |z| \log(12^3|z|) + O(\log(|z|)) \quad (\text{S18})$$

follows.

B. The asymptotic behavior of wave function $\psi(z)$ and $\phi(\tau)$

The symmetry

$$\phi(\tau) = \phi(\gamma\tau) \quad (\text{S19})$$

has imposed the restrictions on the wave function $\phi(\tau)$ near the two points $\tau = i$ and $\tau = e^{i\pi/3}$. Let $\tau = i + \epsilon$ with $|\epsilon| \ll 1$ and

$$\gamma = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

then Eq. (S19) gives $\phi(i + \epsilon) = \phi(i - \epsilon) + O(|\epsilon|^2)$. This implies that near $\tau = i$, we have

$$\phi(\tau) = \phi(i) + O(|\tau - i|^2). \quad (\text{S20})$$

Consequently by Eq. (S11)) and the definition of $\psi(z)$, we have $\psi(z) = [\phi(i) + O(|z|)] V_R^{-1/2}(z)$. Finally by Eq. (S13), we have

$$\psi(z) = [\phi(i) + O(|z|)] \left[C_3^{-1} |z|^{-1/2} + O(1) \right], \quad (\text{S21})$$

where C_n represents a non-zero constant. Similarly, by considering

$$\gamma = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix},$$

for $\tau = e^{i\pi/3}$, one obtains

$$\psi(z) = [\phi(e^{i\frac{\pi}{3}}) + O(|z - 1|)] \times \left[C_4^{-1} |z - 1|^{-2/3} + O(|z - 1|^{-1/3}) \right] \quad (\text{S22})$$

Furthermore, under the condition that $\phi(i) = 0$, according to Eq. (S20), one can set

$$\phi_s(i + \eta) = \alpha\eta^2 + \beta\eta^{*2} + \gamma\eta^*\eta + O(|\eta|^3), \quad (\text{S23})$$

where $\eta := \tau - i$ and $|\eta| \ll 1$, α , β and γ are complex constants. Substitute Eq. (S23) into

$$(\tau - \tau^*)^2 \frac{\partial}{\partial \tau} \frac{\partial}{\partial \tau^*} \phi(\tau) = E\phi(\tau) \quad (\text{S24})$$

and take the leading order we get $\gamma \equiv 0$. Besides, by Eq. (S10), $\phi(\tau)$ is even function respect to $\Re\tau$, which implies that $\beta = \alpha$. So we get

$$\begin{aligned} \phi_s(i + \eta) &= \alpha(\eta^2 + \eta^{*2}) + O(|\eta|^3) \\ &= 2\alpha((\Re\eta)^2 - (\Im\eta)^2) + O(|\eta|^3). \end{aligned} \quad (\text{S25})$$

In addition, one can show that $\alpha \neq 0$.

When $\tau \rightarrow i\infty$, $\phi_s(\tau)$ has the following asymptotic formula[2]

$$\phi_s(\tau) = 2 \left((\Im\tau)^s + \frac{\xi(2-2s)}{\xi(2s)} (\Im\tau)^{1-s} \right) + O(e^{-2\pi\Im\tau}). \quad (\text{S26})$$

If $\Re s \neq 1/2$ we have

$$\begin{aligned} \phi_s(\tau) &= \text{Const.} \times (\Im\tau)^{\max(\Re s, 1-\Re s) \pm i\Im s} \\ &\quad + O((\Im\tau)^{\min(\Re s, 1-\Re s)}) \\ &= \text{Const.} \times (\Im\tau)^{\frac{1}{2}+d \pm i\omega} + o((\Im\tau)^{\frac{1}{2}+d}), \end{aligned} \quad (\text{S27})$$

where d is distance from s to the line with real part $1/2$, $\omega := \Im s$. If $\Re s = 1/2$ we have

$$\begin{aligned} \phi_s(\tau) &= 2(\Im\tau)^{\frac{1}{2}+i\omega} + 2 \frac{\xi(1-2i\omega)}{\xi(1+2i\omega)} (\Im\tau)^{\frac{1}{2}-i\omega} + O(e^{-2\pi\Im\tau}) \\ &= 2(\Im\tau)^{\frac{1}{2}} (e^{i\omega \log \Im\tau} + e^{i(2\varphi - \omega \log \Im\tau)}) + O(e^{-2\pi\Im\tau}) \\ &= 2(\Im\tau)^{\frac{1}{2}} e^{i\varphi} (e^{i(-\varphi + \omega \log \Im\tau)} + e^{i(\varphi - \omega \log \Im\tau)}) \\ &\quad + O(e^{-2\pi\Im\tau}) \\ &= 4e^{i\varphi} (\Im\tau)^{\frac{1}{2}} \cos(\omega \log \Im\tau - \varphi) + O(e^{-2\pi\Im\tau}), \end{aligned} \quad (\text{S28})$$

where we have use the fact that $|\xi(z)| = |\xi(z^*)|$ and set $\xi(1-2i\omega)/\xi(1+2i\omega) = e^{2i\varphi}$. Gather Eq. (S27)-(S28), Eq. (S16), and Eq. (S18) we obtain the asymptotic formula

$$\begin{aligned} \psi(z) &= A \frac{1}{|z|} \log(|12^3 z|)^{-\frac{1}{2}+d} \Omega_d(|z|) \\ &\quad + o\left(\frac{1}{|z|} \log(|z|)^{-\frac{1}{2}+d}\right), \end{aligned} \quad (\text{S29})$$

where $\Omega_d(|z|)$ is defined by:

$$\Omega_d(|z|) := \begin{cases} \log(12^3|z|)^{\pm i\omega} & d > 0 \\ \cos\left(\omega \log\left(\frac{\log(12^3|z|)}{2\pi}\right) - \varphi\right) & d = 0, \end{cases}$$

$A \neq 0$ and $\varphi \in \mathbb{R}$ are two constants rely on s , $d := |\Re s - 1/2|$ is the distance of s to the line $\Re s = 1/2$, and $\omega = \Im s$ is the imaginary part of s .

IV. THE PROBABILITY CONSERVATION EQUATION, ZERO LINES, AND THE COORDINATE TRANSFORMATION $z \rightarrow \tau$

A. The probability conservation equation

For a stationary wave function $\psi(z)$, we consider the complete wave function $\Psi(z, t) = \psi(z)e^{-iEt}$, which satisfies the complete Schrödinger equation

$$i\dot{\Psi}(z, t) = \hat{H}_R \Psi(z, t), \quad (\text{S30})$$

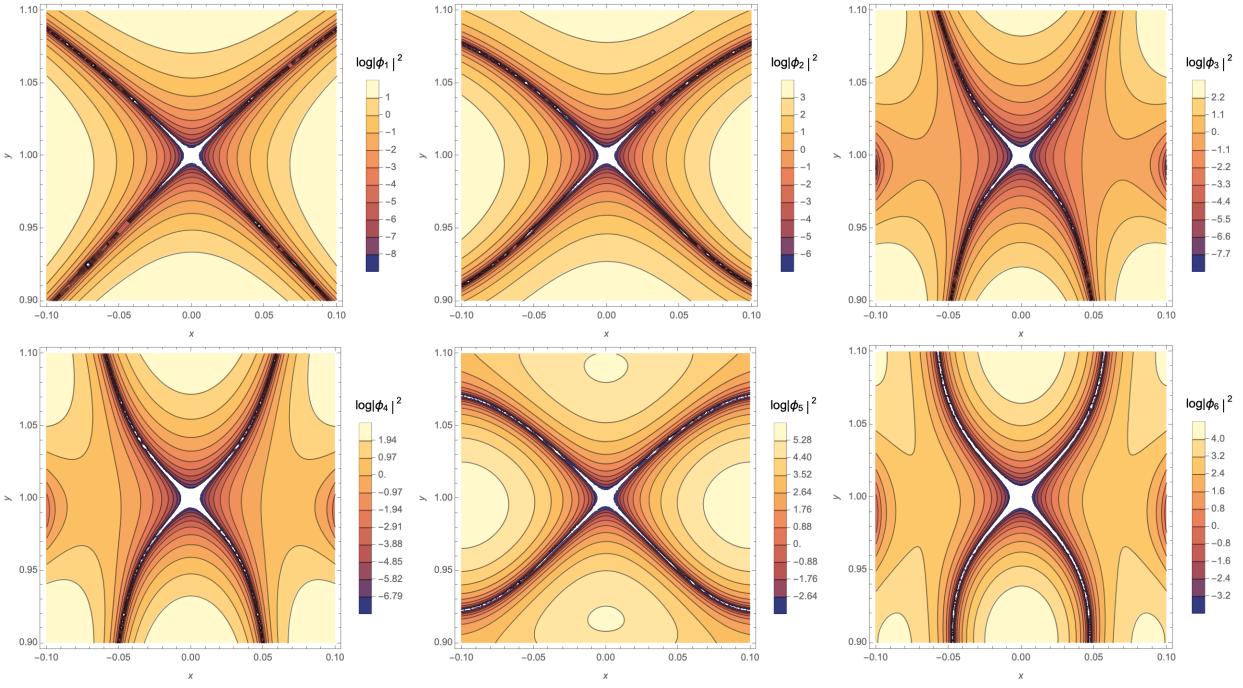


FIG. 1. The first six wave function $\phi_{\rho_n}(\tau)$ near $\tau = i$. In the plot we use ϕ_n to represent ϕ_{ρ_n} for simplicity. For each of them, the cross of zero curve exists. We plot the logarithm of the probability density so that the zero line is clearly visible.

where \cdot denote the derivative respect to time t , and generally we will suppose the eigenenergy $E \in \mathbb{C}$. From Eq. (S30) we have

$$\dot{\rho} = -i(\Psi^* \hat{H}_R \Psi - \Psi \hat{H}_R \Psi^*) , \quad (\text{S31})$$

where $\rho := \Psi^* \Psi$ the probability density. By the definition of H_R we obtain

$$\dot{\rho} = -\nabla \cdot \mathbf{J} , \quad (\text{S32})$$

where \mathbf{J} the probability current density vector defined by

$$\begin{aligned} \mathbf{J} &:= \Psi^* \hat{\mathbf{v}} \Psi - \Psi \hat{\mathbf{v}} \Psi^* \\ &= e^{2\Im(E)t} (\psi^* \hat{\mathbf{v}} \psi - \psi \hat{\mathbf{v}} \psi^*) \end{aligned} \quad (\text{S33})$$

with the velocity operator defined by $\hat{\mathbf{v}} := -iV_R^{1/2} \nabla V_R^{1/2}$. To gain a more practical form of Eq. (S32), one can integrate it over a compact region $U \subset \mathbb{C}$ and obtain

$$\dot{Q}(t) = - \oint_{\partial U} \mathbf{J} \cdot \mathbf{n} dl . \quad (\text{S34})$$

By definition, $\rho = \Psi^* \Psi = e^{2\Im(E)t} |\psi|^2$. One obtains

$$\begin{aligned} \dot{Q}(t) &:= \int_U d^2 z \dot{\rho} \\ &= \int_U d^2 z \frac{d}{dt} [e^{2\Im(E)t} |\psi(z)|^2] \\ &= 2\Im(E) e^{2\Im(E)t} \int_U d^2 z |\psi(z)|^2 . \end{aligned} \quad (\text{S35})$$

B. The zero lines

We calculated the first six reduced wave functions $\phi(\tau)$ and observed the cross structure of their zero curves near $\tau = i$, as shown in Fig. 1.

C. The coordinate transform $z \rightarrow \tau$

By the definition of geometric potential V_R , the Schrödinger equation $H_R \psi = E\psi$ can be written in complex notation

$$\frac{(\tau(z) - \tau(z)^*)^2}{\tau'(z)\tau'(z)^*} \frac{\partial}{\partial z} \frac{\partial}{\partial z^*} \tilde{\psi}(z) = E\tilde{\psi}(z) \quad (\text{S36})$$

where $*$ denotes the complex conjugate, $\partial/\partial z := (\partial_x - i\partial_y)/2$, $\partial/\partial z^* := (\partial_x + i\partial_y)/2$ and we have defined $\tilde{\psi} := V_R^{1/2} \psi$. Now we change the variables from z to τ , and define the reduced wave function $\phi(\tau) := \tilde{\psi}(z(\tau))$, Eq. (S36) can be written in a quite simple form

$$(\tau - \tau^*)^2 \frac{\partial}{\partial \tau} \frac{\partial}{\partial \tau^*} \phi(\tau) = E\phi(\tau) \quad (\text{S37})$$

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- [1] F. Diamond and J. Shurman, *A First Course in Modular Forms*, 1st ed., Graduate Texts in Mathematics (Springer New York, NY, 2005) pp. XVI, 450.
 - [2] H. Iwaniec, *Spectral Methods of Automorphic Forms*, 2nd ed., Graduate Studies in Mathematics, Vol. 53 (American Mathematical Society, Providence, RI, 2002).

