JOURNÉES ÉQUATIONS AUX DÉRIVÉES PARTIELLES

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EIGENFUNCTIONS OF THE LAPLACIAN, QUANTUM CHAOS, AND COMPUTATION

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The following is an extended summary of the talk I gave in Saint Jean de Monts on 30 May 1995.

§I. Consider a freely moving particle (of mass m) on a compact Riemann surface S of negative curvature. The trajectory taken by such a particle is necessarily a geodesic. It is known, however, that when the curvature is negative, the geodesic flow on S is ergodic. The particle's dynamics will therefore be quite sensitive to the initial conditions. In common parlance, one says that the particle's dynamics are classically chaotic.

The question then arises: what manifestations of this chaotic behavior are seen at the quantum-mechanical level?

Those things that *are* seen can be loosely described as quantum chaos.

In view of the fact that quantum mechanics should tend to classical mechanics as $\hbar \longrightarrow 0$, it is a safe bet that something akin to ordinary chaos should be visible at least for those quantum-states (i.e. quantum-mechanical "particles") having a nonvanishing energy E as $\hbar$ tends to 0 .

The wave-function Ψ of a quantum-mechanical particle of energy E satisfies

$$(1.1) \qquad i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi = E \Psi \quad ,$$

where Δ is the Laplace-Beltrami operator on S . Upon taking $E = \hbar \nu$, we immediately get

$$\Psi = \varphi(P) e^{-i\nu t} \qquad (P \in S, \ t \in \mathbb{R})$$

and

$$(1.2) \qquad \Delta \varphi + \frac{2mE}{\hbar^2} \varphi = 0 \qquad on \quad S \ .$$

Since the probability that the "particle" lies in a box $A \overset{c}{=} S$ is

$$\int_A |\Psi|^2 dP \quad ,$$

the function φ needs to be square-integrable on S with L_2 norm **1** .

The occurrence of the combination $2mE/\hbar^2$ reflects the fact that the potential energy $V(P)$ is identically zero.

With $\lambda = 2mE/\hbar^2$, (1.2) becomes:

$$(1.3) \qquad \Delta\varphi + \lambda\varphi = 0 \quad on \quad S \; .$$

For energies bounded away from 0, taking $\hbar \longrightarrow 0$ simply means that we want λ to be large.

§II. The results we reported on in the talk pertained to the case of surfaces having constant negative curvature $\kappa = -1$ (i.e. the case of *hyperbolic* geometry).

In such a setting, it is customary to represent S as a quotient space $\Gamma \setminus H$, where H is the Poincaré upper half-plane and $\Gamma \subseteq PSL(2,\mathbb{R})$ is a Fuchsian group.

Bearing in mind that, on H , the hyperbolic metric has $ds = |dz|/y$ and area element $d\mu = y^{-2}dxdy$, equation (1.3) immediately becomes:

$$(2.1) \qquad \left\{ \begin{array}{l} y^2[\varphi_{xx} + \varphi_{yy}] + \lambda\varphi = 0 \quad for \quad z \in H \\[2mm] \varphi(Tz) = \varphi(z) \; , \quad T \in \Gamma \\[2mm] \int_{\Gamma\setminus H} |\varphi|^2 d\mu = 1 \end{array} \right\} \; .$$

This is precisely the setting of the Selberg trace formalism (as described, say, in [H1,H2,V]).

The main theoretical result currently known about eigenfunctions φ with large λ is the so-called equidistribution theorem of Shnirelman/Zelditch/Colin de Verdiere [Sh1,Sh2,Z1,C]. The result asserts that, *apart from* a "thin" sequence of exceptional eigenvalues λ_n satisfying $N[\text{bad } \lambda_n \overset{\le}{=} X] = o(X)$, one automatically has

$$(2.2) \qquad \lim_{n \to \infty} \int_A |\varphi_n|^2 d\mu = \frac{\mu(A)}{\mu(\Gamma\setminus H)}$$

for every Jordan measurable set $A \overset{\subseteq}{=} \Gamma \setminus H$. (It is believed that, in constant negative curvature, the exceptional λ_n-sequence is empty, but this remains to be proved. Cf. [LS,RS] .)

Getting a better grip on the distribution of the individual φ_n's , particularly when Γ has no special arithmetic properties, seems to be a very challenging problem.

For the time being at least, the surest way of obtaining new insight into this matter appears to be by way of numerical experimentation.

§III. To this end, it now becomes expedient to allow the consideration of surfaces $S = \Gamma \setminus H$ which are noncompact, but still of finite hyperbolic area.

Geometrically, this simply means that S is compact except for a finite number of hyperbolic punctures (i.e. cusps).

Cf. [H2,V] for the relevant spectral theory.

§IV. The groups I chose to experiment with were the Hecke triangle groups $\Gamma = \mathfrak{G}(2\cos\frac{\pi}{N}) = \mathfrak{G}_N$ generated by

$$z \longrightarrow -\frac{1}{z} \qquad and \qquad z \longrightarrow z + 2\cos\left(\frac{\pi}{N}\right) \qquad .$$

Here N is a positive integer ≥ 3 . Compare [HR] and [H3] .

The standard fundamental region for $\mathfrak{G}_N \setminus H$ is $\mathcal{F}_N = \{z \in H : |z| > 1 ,$ $|x| < \cos\frac{\pi}{N}\}$. From [H3] , one knows that $\mathfrak{G}_N$ is commensurable with $PSL(2,\mathbb{Z})$ if and only if $N = 3 , 4 , 6$. For all other N , $\mathfrak{G}_N$ is nonarithmetic (and has itself as its $PSL(2,\mathbb{R})$ – commensurator).

In line with the Sarnak–Phillips philosophy [PS,S2] , when $N \neq 3,4,6$, it is tacitly assumed that any φ under discussion is *odd* with respect to x .

The Shnirelman/Zelditch/Colin de Verdiere result (2.2) will continue to hold for $\mathfrak{G}_N \setminus H$ modulo this proviso : see [Z2] .

For $\lambda \neq 0$, each wave function φ necessarily admits a Fourier development of the form

$$(4.1) \qquad \varphi(x + iy) = \sum_{n \neq 0} d_n \sqrt{y} \, K_{iR}\left(\frac{2\pi|n|y}{\mathcal{L}}\right) e^{2\pi i n x / \mathcal{L}}$$

with $\lambda = \frac{1}{4} + R^2$, $R > 0$, and $\mathcal{L} = 2\cos\left(\frac{\pi}{N}\right)$. See [H2,H3] .

The trivial estimate for d_n asserts that $d_n = O(|n|^{1/2})$. This was recently improved in [S3,P].

Complementing this from the standpoint of the Rankin–Selberg theory (cf. [HR, eq. (6.10)]) is the fact that:

$$(4.2) \qquad \sum_{1 \leq |n| \leq X} |d_n|^2 \sim \beta X \qquad for \qquad X \longrightarrow \infty \qquad .$$

The coefficient β is a simple function of N, R, and $\|\varphi\|_2$.

§V. Though the method of [H3] was successfully used in computing a variety of relatively large R - values on general $\mathbb{C}_N$, the procedure is handicapped by its *in*ability to produce (even for small R) more than just the first few d_n .

This difficulty was overcome by replacing the old (collocation-based) algorithm with a new one which takes advantage of the fact that $\varphi(x+iy)$ is effectively a finite Fourier series [with $|n| \lesssim M(y)$] for each y . (^{1})

When the grid points $z_j = x_j + iy$ in the "defining" equation for $d_n \sqrt{y} \, K_{iR}\left(\frac{2\pi|n|y}{x}\right)$ are pulled back to $\mathcal{F}_N$ by virtue of φ's automorphy, it quickly becomes apparent that one obtains a *non-tautological* linear system for $\{d_n : |n| \lesssim M(y)\}$ so long as $y < \sin(\frac{\pi}{N})$. The fact that $\mathcal{F}_N$ remains above $y = \sin(\frac{\pi}{N})$ ensures that, in this system, everything basically just depends on solving for $\{d_k : |k| \lesssim M(\sin\frac{\pi}{N})\}$. The latter entails solving a system no bigger than $2M(\sin\frac{\pi}{N}) \times 2M(\sin\frac{\pi}{N})$.

As in [H3], the number R has to be adjusted in such a way so that, when solving the system for at least *two* different y - values, one obtains a solution vector free of any y - dependence.

Successively higher d_n are (then) obtained by taking y smaller and smaller.

§VI. This method seems to work quite well on the computer. R - values as high as 1000 were easily explored for $4 \lesssim N \lesssim 7$. For $\mathbb{C}_3$, R was pushed as high as 5000 .

We generally used either the Cray-2 or the Cray-XMP at the Minnesota Supercomputer Center for this work.

As an indication of CPU time, we can report that, once R *and* the initial set of d_k are known, calculating d_n out to $n = 10^4$ (with $8 \sim 10$ place accuracy) typically takes several hours of machine time.

The "rub" of course is that $M(\sin\frac{\pi}{N})$ grows linearly with R . As such, the time needed to calculate R and the first few d_k eventually becomes prohibitive.

For $N = 3$ and $R \cong 5000$, the overall *conditioning*-level still seemed to be in pretty good shape, however. (^{2})

§VII. The new method has the further advantage that it is trivially restructured to apply to the (time-honored) case of holomorphic cusp forms F of even integral weight m on $\mathbb{C}_N \setminus H$.

(^{1}) Bear in mind here that $K_{iR}(X)$ begins to decay exponentially fast once X exceeds R .

(^{2}) Here $M(\sin\frac{\pi}{N}) \cong 970$.

For such functions, one has:

$$(7.1) \qquad F(Tz) = F(z)(cz+d)^m \quad , \quad T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathfrak{G}_N$$

and

$$(7.2) \qquad F(z) = \sum_{n=1}^{\infty} c_n e^{2\pi i n z/\mathcal{L}} \qquad .$$

An elementary manipulation shows that the coefficients c_n can always be taken to be *real* without loss of generality. It is also customary to replace F by $f \equiv y^{\frac{m}{2}} F$, so that:

$$(7.3) \qquad f(Tz) = f(z)\frac{(cz+d)^m}{|cz+d|^m} \quad for \quad T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathfrak{G}_N$$

and

$$(7.4) \qquad f(z) = \sum_{n=1}^{\infty} d_n \sqrt{y}\, k(ny) e^{2\pi i n x/\mathcal{L}}$$

where

$$c_n \equiv d_n n^{\frac{m}{2}-\frac{1}{2}} \quad , \quad k(y) \equiv y^{\frac{m}{2}-\frac{1}{2}} e^{-2\pi y/\mathcal{L}} \qquad .$$

The trivial bound for d_n is again $O(n^{1/2})$, with an improvement being available in $[G]$. In addition: (4.2) continues to hold for suitable $\mathcal{B}$.

The computational situation is now entirely similar to that of φ except for the fact that the automorphy condition (7.3) is a bit more complicated than before.

§VIII. The foregoing techniques were then used to carry out a series of experiments aimed at investigating two of the most likely manifestations of quantum chaos in the functions φ and F.

Since the case of $\mathfrak{C}_3$ was already dealt with in $[HA,HR,L]$, we were principally interested in what could be said for nonarithmetic $\mathfrak{C}_N$.

Our experiments ([3]) yielded the following conclusions:

[A] For any $\mathfrak{C}_N$, it would appear that the individual eigenfunctions φ_n become locally Gaussian distributed as $n \longrightarrow \infty$, in the sense that

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([3]) with $G_N \setminus H$ for $3 \leq N \leq 7$

$$(8.1) \qquad \lim_{n \to \infty} \frac{\mu\{z \in A : \varphi_n(z) \in [a,b]\}}{\mu(A)} = \frac{1}{\sigma\sqrt{2\pi}} \int_a^b e^{-u^2/2\sigma^2} \, du$$

holds for every Jordan measurable $A \overset{c}{=} \mathcal{F}_N$.

Here $\sigma = 1/\sqrt{\mu(\mathcal{F}_N)}$ in accordance with (2.2).

The possibility that (8.1) may hold was first raised nearly 20 years ago by M.Berry [B] in connection with domains in $\mathbb{R}^\nu$.

The heuristic justification for (8.1) outlined in [HR,§6] is readily adapted to $\mathfrak{C}_N$, but, for nonarithmetic groups, major problems loom because there are no *Langlands-type* lifts from $\mathfrak{C}_N \setminus H$ to GL(q) which would make the higher-correlation estimates involving d_n that are called for seem even remotely provable.

(One strongly suspects that there exists a better, more intrinsic, way of attacking this question.)

[B] For nonarithmetic $\mathfrak{C}_N$, it appears that in the case of both φ and F , the Fourier coefficients $\{d_n : n \geq 1\}$ will conform to Gaussian statistics of mean 0 and standard deviation $\sqrt{\eta\beta}$ as $n \to \infty$.

Here, in accordance with (4.2),

$$\eta = \begin{cases} 1/2 & \text{for } \varphi \\ 1 & \text{for } F \end{cases} .$$

[B'] It also seems reasonably likely that convergence of moments takes place for every $k \geq 1$, in the sense that:

$$(8.2) \qquad \sum_{1 \leq n \leq X} |d_n|^k \sim \frac{1}{\sqrt{\pi}} (2\eta\beta)^{k/2} \Gamma\left(\frac{k+1}{2}\right) X .$$

In particular: by letting k grow, it is immediately evident that one gets

$$(8.3) \qquad d_n = O(n^\varepsilon)$$

for every $\varepsilon > 0$. The Ramanujan-Petersson estimate would thus continue to hold

for nonarithmetic groups.

Relation (8.2) should be contrasted with the results in [MS,R1,R2,R3] .

[C] For arithmetic $\mathbb{C}_N$, Hecke operators exist and the functions φ , F can be taken to be Hecke eigenforms without loss of generality. In this case, the coefficients d_n satisfy *multiplicative* relations which cause primary interest to focus instead on the numbers d_p (at least after renormalizing things to ensure that $d_1 = 1$). Here p = prime .

The results we obtained for N = 4 , 6 were entirely analogous to those obtained earlier for N = 3 ; cf. [HA,St] . It continues to appear that the d_p satisfy Wigner's semicircle law

$$(8.4) \qquad \lim_{X \to \infty} \frac{N\{p \leq X : d_p \in [a,b]\}}{N\{p \leq X\}} = \frac{1}{2\pi} \int_a^b \sqrt{4 - u^2} \, du$$

for $-2 \leq a \leq b \leq 2$, as well as [in the case of φ] the apriori bound

$$(8.5) \qquad |d_p| \leq 2 \qquad .$$

Estimate (8.5) is of course a deep theorem in the case of F ; see [D] .

Properties (A) – (C) are consistent with the view that the wave-functions φ_n should look more and more like *random waves* as $n \longrightarrow \infty$. Some additional tests of (asymptotic) statistical independence and local energy density would be very desirable here, however. Cf. [HR,§5] and the references cited there.

Particularly in the case of nonarithmetic groups, where the d_n lack any kind of multiplicative structure, it is tempting to "explain" the presence of a Gaussian in (A) and (B) by the meta-mathematical statement that, *if* a limiting distribution does exist, it must "surely" be characterized by a maximum level of uncertainty (i.e. entropy). For given mean and standard deviation, however, *only* a Gaussian fits this bill. Cf. [Re,ShW,T] .

Bear in mind here that (2.2) and (4.2) are known.

When it comes to (8.2), this type of reasoning is no longer applicable. Cf., in particular, our earlier remark about Langlands-type lifts in item [A] .

In the case of (8.3), however, one can give a second approach as follows.

For simplicity, we restrict ourselves to φ . The thing to notice first is that:

$$\frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \varphi\left(\frac{z+j\mathcal{L}}{M}\right) \equiv \sum_{n \neq 0} d_{Mn} \sqrt{y} \, K_{iR}\left(\frac{2\pi|n|y}{\mathcal{L}}\right) e^{2\pi inx/\mathcal{L}} \quad .$$

Hence:

$$(8.6) \qquad d_M \sqrt{y} \, K_{iR}\left(\frac{2\pi y}{\mathcal{L}}\right) = \frac{1}{\mathcal{L}} \int_0^{\mathcal{L}} \left[\frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \varphi\left(\frac{z+j\mathcal{L}}{M}\right)\right] e^{-2\pi ix/\mathcal{L}} \, dx \quad .$$

The hope is that the bracketed term will have *bounded* L_2 norm for $y \stackrel{\sim}{=} M^{-\mathcal{E}}$ as $M \longrightarrow \infty$. This would immediately imply that $d_M = O(M^{\mathcal{E}/2})$.

The functional

$$(8.7) \qquad U_M(x,y) \equiv \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} g\left(\frac{z+j\mathcal{L}}{M}\right)$$

is of interest for any automorphic g having mean 0 (on $\mathfrak{C}_N \setminus H$) and sensible behavior near $i\infty$. The essential point here is that the hyperbolic distance between successive $(z+j\mathcal{L})/M$ is

$$\cosh^{-1}\left[1 + \frac{\mathcal{L}^2}{2y^2}\right] \quad .$$

This quantity tends to infinity anytime $y \longrightarrow 0$. There is thus some chance that the $\mathfrak{F}_N$-pullbacks of the points $(z+j\mathcal{L})/M$ will get "thoroughly mixed", or decorrelated, as $(y,M) \longrightarrow (0, \infty)$.

Coupling the fact that $\mathfrak{C}_N \setminus H$ has no eigenvalues in $(0,1/4]$ with results like [S1] and [Ra] , one is led to expect *at least heuristically* that

$$(8.8) \qquad \frac{1}{\mathcal{L}} \int_0^{\mathcal{L}} U_M(x,y)\,dx \longrightarrow 0$$

and

$$(8.9) \qquad \frac{1}{\mathcal{L}} \int_0^{\mathcal{L}} U_M(x,y)^2 \, dx = \frac{1}{\mu(\mathfrak{F}_N)} \int_{\mathfrak{F}_N} g^2 \, d\mu + o(1) + O[y \log M]$$

anytime $y \longrightarrow 0$. The heuristics enter only in (8.9).

Assertions (8.8) and (8.9) clearly become interesting candidates for numerical experimentation anytime $y\log(M)$ starts to become small.

If one is lucky, the summands in (8.7) will begin to imitate independent random variables, and the distribution function of $U_M(x,y)$ on $0 \stackrel{\leq}{=} x \stackrel{\leq}{=} \mathcal{L}$ will tend to a *Gaussian* with mean 0 and standard deviation

(8.10)
$$\left\{ \frac{1}{\mu(\mathcal{F}_N)} \int_{\mathcal{F}_N} g^2 d\mu \right\}^{1/2}$$

as $M \longrightarrow \infty$.

These ideas were systematically tested for $N = 3, 5, 7$ using 16 very simple choices of g . (The restriction to *simple* g was necessary due to cpu-time concerns.) M was taken in the range $[10^6, 10^7]$.

The machines used were the Minnesota Cray-C90 and T3D/64 . In our largest jobs (~ 37 cpu hours each), we were able to look at $y = M^{-\beta}$ for $M \stackrel{\sim}{=} 10^7$ and β having size about .38 .

For $N = 5$ and 7 , the functions $U_M(x,y)$ were consistently found to have distribution *very* close to Gaussian, with standard deviation differing from (8.10) by no more than several % . One naturally suspects that these results are indicative of what happens for general g .

The hope voiced after (8.6) would thus seem to be in fairly good shape for nonarithmetic $\mathbb{C}_N$ (at least in those β - ranges we managed to reach).

For $N = 3$, however , these heuristics basically fell apart.

The reason for this lies in the fact that the functional U_M is essentially just the Hecke operator T_M . When $g = \varphi$, for instance, one effectively gets:

(8.11)
$$\frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \varphi\left(\frac{z+j\mathcal{L}}{M}\right) \stackrel{\sim}{=} (constant)\varphi(z) \qquad .$$

From this it follows that there is *no* chance of having $U_M[\varphi]$ manifest any type of Gaussian limit on $0 \stackrel{\leq}{=} x \stackrel{\leq}{=} \mathcal{L}$. Indeed, by applying [S1] to powers of φ , one quickly sees that the limiting distribution of $\varphi(x+iy)$ *with respect to* x must be just the spatial distribution of φ .

Relation (8.9) goes bad because the constant in (8.11) is not generally ± 1.

To understand what happens for a more general smooth g , one simply applies (8.11) to the individual components and eigenpackets making up the spectral decomposition of g . ([4])

We can summarize things by saying that the existence of Hecke operators basically induces *long-range correlations* in the "flow" $(z+j\mathcal{L})/M$ mod $\mathbb{C}_N$ (as $y \rightarrow 0$).

Such correlations seem to be absent when $\mathbb{C}_N$ is nonarithmetic.

([4]) Some finite set of these terms will of course carry the bulk of the information. (Note too that, when g is odd, the eigenpackets are absent.)

That absence causes (8.3) to take on the look of something that is true for "ergodic-theoretic" reasons.

§IX. Placing any one of the results in §VIII on a rigorous footing seems to be a tall order. New ideas definitely seem to be necessary. Perhaps some of these will come from PDE.

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