Some recent estimates on nodal sets and nodal domains in the high-energy limit

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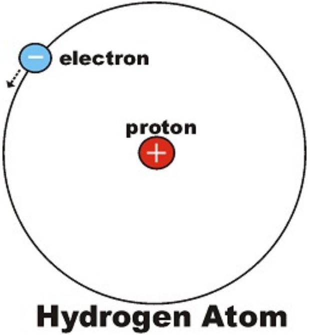
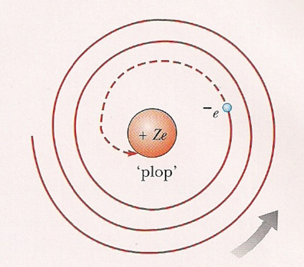
How does an atom look like?

Among other things, as a great leap of modelling, quantum mechanics resolves a puzzle about stability of atoms.
Prior to quantum mechanics, a hydrogen atom was roughly pictured as a 2-body planetary system, i.e. in terms of the classical Hamiltonian $H(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$, where $V(x) := -\frac{1}{|x|}$.



How does an atom look like?

That cannot be right as the electron would radiate energy and spiral into the nucleus.



So Bohr (1915) proposed a resolution by postulating that the electron can only occupy stable orbits with energies picked out by the Bohr-Sommerfeld quantization conditions.

Schrödinger's breakthrough

In *Quantisierung als Eigenwertproblem, Annalen der Physik, 1926*, Schrödinger modelled the energy states of the electron as eigenfunctions of the Schrödinger operator:

$$\hat{H}\phi_j := \left(-\frac{\hbar^2}{2}\Delta + V\right)\phi_j = E_j(\hbar)\phi_j, \tag{1}$$

where $\Delta = \sum \frac{\partial^2}{\partial x_j^2}$ is the Laplace operator; V is the potential, considered as a multiplication operator on $L^2(\mathbb{R}^3)$; $\hbar$ is Planck's constant.

Let us select an L^2-orthonormal basis of eigenfunctions $\{\phi_j\}$.

Stationary states

The time evolution of an energy state is given by the propagator:

$$U_\hbar(t)\phi_j := e^{-i\frac{t}{\hbar}\left(-\frac{\hbar^2}{2}\Delta+V\right)}\phi_j = e^{-i\frac{tE_j(\hbar)}{\hbar}}\phi_j. \tag{2}$$

Moreover, ϕ_j induces the probability density $|\phi_j(x)|^2 dx$, which is interpreted as *the probability of finding a particle at* x.

According to physicists, the *observable quantities* associated to the energy state ϕ_j are the above probability density, as well as, more generally, the matrix elements of observables

$$\langle A\phi_j, \phi_j\rangle, \tag{3}$$

where A is a self-adjoint (pseudo-differential) operator.

The factors of $e^{-i\frac{tE_j(\hbar)}{\hbar}}$ cancel, and so observables **remain constant** under the time evolution.

A resolution

Roughly speaking, modelling energy states by eigenfunctions ϕ_j resolves the paradox of particles which are simultaneously in motion and are stationary.

This comes at the price of trading the geometric (classical mechanical) Bohr model of classical orbits for eigenfunctions ϕ_j of the Schrödinger operator $\left(-\frac{\hbar^2}{2}\Delta + V\right)$.

How can we still retain the geometry and picture the stationary states of atoms, i.e. the eigenfunctions ϕ_j?

Some pictures of the hydrogen atom

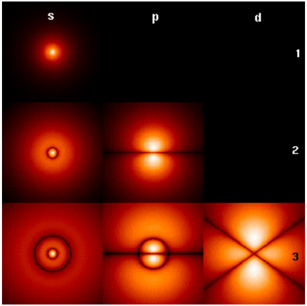


Figure: Intensity plots of energy states of the hydrogen atom.

In the Figure above, the brighter regions represent $|\phi_j(x)|^2$ being large, i.e. the most probable locations of an electron.

Question

How is ϕ_j distributed? How large can ϕ_j (i.e. its L^p-norms) be, relative to the energy $E_j(\hbar)$? How are the excursion sets $\Omega_{j,A,r} := \{x : |\phi_j(x)|^2 \geq A\hbar^{-r}\}$ distributed?

Some pictures of the hydrogen atom

There are also illuminative plots of the **nodal hypersurfaces**, i.e. where the probability density of the particle's position vanishes.

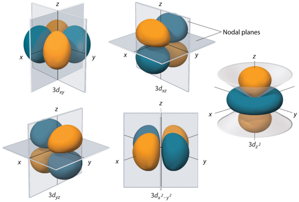


Figure: Nodal hypersurfaces, upon which $\phi_j(x)$ vanishes.

Question

How is the nodal set distributed as the energy gets larger? How large is the size of the nodal set?

Hydrogen atom under the quantum microscope

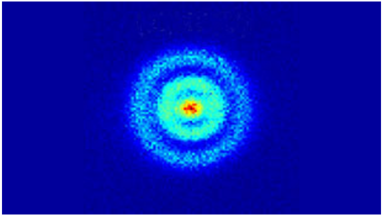


Figure: Nodal structure of an excited hydrogen atom.

In 2013, A. Stodolna, FOM Institute for Atomic and Molecular Physics, the Netherlands, M. Vrakking, the Max-Born-Institute in Berlin, Germany, etc, have shown that photoionization microscopy can directly obtain **the nodal structure of the electronic orbital of a hydrogen atom** placed in a static electric field.

The framework

We consider a smooth closed Riemannian manifold (M, g) of dimension n. Denote the Laplace-Beltrami operator acting on functions by Δ. It is well-known that Δ possesses a discrete spectrum of eigenvalues $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \to \infty$.

We are interested in the **asymptotic behaviour** as $\lambda_i \to \infty$ (i.e. in the high-energy limit) of the corresponding eigenfunctions

$$\Delta\phi_\lambda = \lambda\phi_\lambda. \tag{4}$$

On one hand, the idea is that the limit $\lambda \to \infty$ (corresponding to the semi-classical limit $\hbar \to 0$) should **capture the relation between classical and quantum mechanics**, i.e. between eigenfunctions and the the underlying Hamiltonian dynamics of the geodesic flow of (M, g).

Nodal sets and nodal domains

Roughly, we investigate the geometry of an eigenfunction ϕ_λ (level sets, localization, etc). The primary objects of concerns will be the following. Define the **nodal set** of an eigenfunction ϕ_λ as

$$N_\lambda := \{x \in M | \phi_\lambda(x) = 0\}. \tag{5}$$

The **nodal domains**, usually denoted by Ω_λ, are defined to be the connected components of the complement of the nodal set.

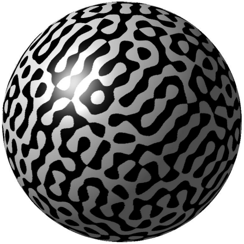


Figure: Nodal domains (the black and white regions) on $\mathbb{S}^2$.

Some questions

- How large can an eigenfunction ϕ_λ be in terms of λ? How large is the set where ϕ_λ is largest? What is the location of the set where ϕ_λ is largest?
- How large is the nodal set? How is it distributed? The variational characterization of eigenfunctions suggests that the nodal set becomes very dense as $\lambda \to \infty$.
- How large can a nodal domain be? How thin (in terms of its inner radius) can a nodal domain be?
- How many nodal domains are there?
- How does the underlying geometry affect the eigenfunction's asymptotic behaviour (e.g. the effect of curvature)?

Some results and major conjectures

Quantum Ergodicity (Colin de Verdière-Schnirelman-Zelditch)

Assume that M possesses an ergodic geodesic flow. Then, up to a density 1 subsequence, the probability measures $|\phi_j(x)|^2 dx$ converge weakly to the uniform measure $\frac{dx}{\mathrm{Vol}(M)}$.

Manifolds with maximal/minimal eigenfunction growth

Classification results due to Sogge-Zelditch and Toth-Zelditch.

Yau's conjecture

The hypersurface (Hausdorff) measure of the nodal set is asymptotically $\sim \sqrt{\lambda}$. Confirmed for real-analytic (M, g) by Donnelly-Fefferman (1988). In the smooth case major progress has been made by A. Logunov (2016).

Quantum ergodicity

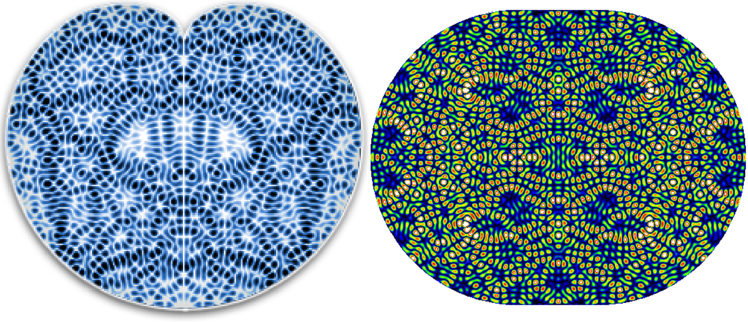


Figure: High-energy eigenfunctions on a cardioid and the Bunimovich stadium.

Quantum ergodicity

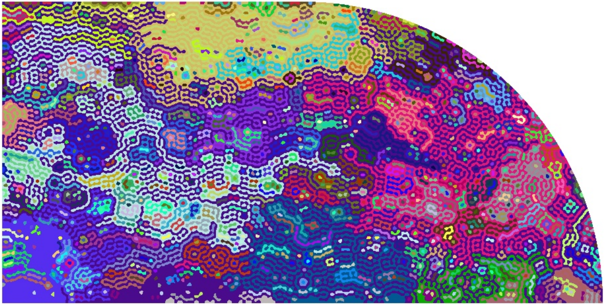


Figure: The different colours denote different nodal domains.

Global and local techniques

Roughly speaking, one may distinguish two major directions of investigation.

Local analysis

One works in a small wavelength ball B of radius $\sim 1/\sqrt{\lambda}$. After parametrizing the ball B using the unit ball B_1 in $\mathbb{R}^n$, the eigenequation $\Delta\phi_\lambda = \lambda\phi_\lambda$ becomes $\Delta\phi + \epsilon\phi = 0$, where $\epsilon > 0$ is small. That is, ϕ_λ is almost **harmonic** in B. Classical PDE techniques for harmonic functions in $\mathbb{R}^n$ can be applied. Examples include the works on Yau's conjecture of Donnelly-Fefferman, Nazarov-Polterovich-Sodin, Logunov, etc.

Global analysis

One applies global wave equation techniques and works with the wave propagator $e^{it\sqrt{\Delta}}$, Fourier integral operators, restriction theorems, etc. Vivid examples include the works of Zelditch, Sogge, Toth, etc.

Yau's conjecture

Stated formally, Yau's conjecture asserts that

$$C_1\sqrt{\lambda} \leq \mathrm{Vol}(N_\lambda) \leq C_2\sqrt{\lambda}, \tag{6}$$

where C_1, C_2 are constants which depend on (M, g) but not on λ.

Donnelly-Fefferman (1988): If (M, g) is **real analytic**, Yau's conjecture is true. A major insight is that an eigenfunction ϕ_λ can **be approximated by polynomials** of degree $\sqrt{\lambda}$. A technical argument shows that ϕ_λ is close to its average on most of the wavelength small cubes, i.e. the growth of the eigenfunction is controlled. This lead to tameness of the nodal geometry.

Yau's conjecture

Until recently, the bounds in Yau's conjecture for smooth (M, g) seemed quite non-optimal. The best known lower bounds (Colding-Minicozzi, Sogge-Zelditch) were polynomially decaying in λ and the best known upper bounds (Hardt-Simon) were exponentially exploding in λ.

In 2016, A. Logunov made a breakthrough and was able to prove the lower bound in Yau's conjecture and obtain a polynomially exploding upper bound. Roughly, his arguments, local and combinatorial in nature, exploited delicate harmonic function estimates, verifying a conjecture of Nadirashvili about harmonic functions.

The volume of a tube around the nodal set (real-analytic case)

M. Sodin and C. Fefferman posed the question about obtaining estimates on the volume of an at most wavelength in radius tubular neighbourhood around the nodal set.

Theorem (Jakobson-Mangoubi, 2007)

Let (M, g) be a real-analytic. Let T_ρ denote a tubular neighbourhood of radius ρ around the nodal set. Then there exist positive constants C_1, C_2, C_3 depending only on (M, g), such that

$$C_1 \rho \sqrt{\lambda} \leq \mathrm{Vol}(T_\rho) \leq C_2 \rho \sqrt{\lambda}, \tag{7}$$

whenever $\rho\sqrt{\lambda} \leq C_3$.

The idea was to exploit the machinery, developed by Donnelly-Fefferman, and to 'sneak-in' an additional parameter, which corresponds to the tubular neigbhourhood's radius.

The volume of a tube around the nodal set (smooth case)

Theorem (G.-Mukherjee, 2016)

Let (M, g) be a smooth closed Riemannian manifold. Then there exist constants C_1, C_2, C_3 depending only on (M, g), such that

$$C_1\lambda^{1/2-\epsilon}\rho \leq \mathrm{Vol}(T_\rho) \leq C_2\lambda^k\rho. \tag{8}$$

Here, $\epsilon > 0$ is some apriori chosen arbitrary small number; k is a positive constant, depending only on (M, g).

Roughly, the proof uses an iteration argument, exploiting estimates of Han-Lin on the growth/frequency of eigenfunctions, along with the recent results of A. Logunov.

The geometry of nodal domains

Some aspects of the geometry of nodal domains Ω_λ have been studied intensely.

- **The volume of a nodal domain**. Results by Donnelly-Fefferman and Mangoubi of the form

$$\frac{\mathrm{Vol}(\Omega_\lambda \cap B)}{\mathrm{Vol}(B)} \geq \frac{C}{\lambda^\alpha}, \tag{9}$$

  where α depends on dim M.
- **Thickness and 'straighntess' of nodal domains**. Techniques from Brownian motion due to S. Steinerberger.
- **The inner radius of a nodal domain**. Simple examples and empirical data suggest that the inner radius of a nodal domain should be of wavelength order, i.e. $\sim 1/\sqrt{\lambda}$.

Brownian motion tools

Using tools from Brownian motion, Steinerberger (2013) was able to prove that no nodal domain cannot be squeezed in a wavelength neighbourhood around a sufficiently flat hypersurface. A main insight is the use of **the Feynman-Kac formula**.

Let Ω_λ be e nodal domain and w.l.o.g. let $\phi_\lambda|_{\Omega_\lambda} > 0$. Setting $\Phi(t, x) := e^{-\lambda t}\phi(x)$, we see that Φ is a solution to the diffusion process

$$\begin{aligned}(\partial_t - \Delta)\Phi &= 0, \quad x \in \Omega_\lambda,\\ \Phi &= 0, \quad x \in \partial\Omega_\lambda,\\ \Phi &= \phi(x), \quad t = 0, \quad x \in \Omega_\lambda.\end{aligned}$$

The Feynman-Kac formula allows to express $\Phi(t, x)$ as an integral (expectation) over Brownian paths starting at x.

Brownian motion tools

Let $x_0 \in \Omega_\lambda$ be such that $\phi(x_0) = \max_{x \in \Omega_\lambda} \phi(x)$. Then

$$e^{-\lambda t}\phi(x_0) =: \Phi(t, x_0) = \mathbb{E}_{x_0}\left(\phi_\lambda(\omega(t))\psi_{\Omega_\lambda}(\omega, t)\right) \leq \\ \leq \|\phi\|_{L^\infty(\Omega_\lambda)}\mathbb{E}_{x_0}\left(\psi_{\Omega_\lambda}(\omega, t)\right) = \phi(x_0)(1 - p_t(x_0)). \quad (10)$$

Here $\omega(t)$ denotes an element of the probability space of Brownian motions starting at x_0. We define

$$\psi_{\Omega_\lambda}(\omega, t) = \begin{cases} 1, & \text{if } \omega([0,t]) \subset \Omega_\lambda, \\ 0, & \text{otherwise.} \end{cases} \quad (11)$$

Lastly, $p_t(x)$ is defined as the probability that a Brownian motion particle started at $x \in \Omega_\lambda$ will hit the boundary within time t.

Brownian motion tools

Cancelling the factors of $\phi(x_0)$, one gets

$$p_t(x_0) \leq 1 - e^{-\lambda t}. \tag{12}$$

For small times $t \sim \epsilon/\lambda$, one has $p_t(x_0) \ll 1$, which can be interpreted as x_0 being situated deeply into the nodal domain.

Implications to 'squeezing' of nodal domains - Steinerberger (2013) and G.-Mukherjee (2016)

Suppose that a nodal domain is contained in a wavelength neighbourhood around a 'flat' submanifold. Classical hitting probabilities of Brownian motion would imply that $p_t(x_0)$ is large, i.e. a Brownian particle should exit the domain quickly. This contradicts the last estimate above.

An improvement of a result of E. Lieb

In a celebrated work of E. Lieb (*Invent. Math.*, 1983), an arbitrary domain $\Omega \subset \mathbb{R}^n$ was shown to possess an 'almost inscribed' ball (i.e. in the sense, that the 'non-inscribed' subset of the ball is relatively small in volume) of radius $\sim 1/\lambda_1(\Omega)$, where $\lambda_1(\Omega)$ is the first Dirichlet eigenvalue of Ω.

Using the derived estimate $p_t(x_0) \leq 1 - e^{-\lambda t}$ along with hitting probabilities due to Grigor'yan-Sallof-Coste (2002), in G.-Mukherjee (2016) we were able to improve Lieb's result by specifying that the almost inscribed ball can be positioned at a point of maximum of the first Dirichlet eigenfunction (w.l.o.g. assumed positive).

We also obtained an estimate of the decay of the non-inscribed subset as one shrinks the ball, and applied the result to nodal domains.

The inner radius of nodal domains (smooth case)

Due to Mangoubi, the following inradius estimates on a nodal domain are known.

Theorem (Mangoubi, 2006)

Let (M, g) be a smooth manifold of dimension n. Then

$$\frac{C_1}{\lambda^\beta} \leq \mathrm{inrad}(\Omega_\lambda) \leq \frac{C_2}{\sqrt{\lambda}}, \tag{13}$$

where $\beta = \frac{n+1}{4} - \frac{1}{2n}$ and C_1, C_2 are constants depending on (M, g). In particular, the estimates are sharp for surfaces.

The upper bound follows directly from the monotonicity of eigenvalues with respect to inclusion.
Note that the lower bound decays far quicker than the upper one in higher dimensions.

The inner radius of nodal domains (smooth case)

Briefly, the heart of the argument behind the lower bound on $\mathrm{inrad}(\Omega_\lambda)$ lies on **asymmetry estimates** of the form

$$\frac{\mathrm{Vol}(\{\phi_\lambda > 0\} \cap B)}{\mathrm{Vol}(B)} \geq \frac{C}{\lambda^\gamma}. \tag{14}$$

These can be proven via local techniques and classical elliptic PDE estimates.
One then **chops the nodal domain Ω_λ into cubes of size** $\sim \mathrm{inrad}(\Omega_\lambda)$ and uses a Poincare inequality (due to Maz'ya) and the asymmetry estimates above to obtain a **relation between the volume of one of the small cubes and λ** - this yields the lower bound on $\mathrm{inrad}(\Omega_\lambda)$.

Note that an improvement of the asymmetry would lead to a direct improvement of the inner radius and tame geometry of the nodal domains.

The inner radius of nodal domains (real-analytic case)

Theorem (G., 2016)

Let (M, g) *be real-analytic. Let* Ω_λ *be a nodal domain and w.l.o.g.* $\phi_\lambda|_{\Omega_\lambda} > 0$*. Then*

$$\frac{C_1}{\lambda} \leq \mathrm{inrad}(\Omega_\lambda) \leq \frac{C_2}{\sqrt{\lambda}}, \tag{15}$$

where C_1, C_2 *are depending only on* (M, g)*. Moreover, a ball of radius* $1/\lambda$ *can be inscribed not further than a wavelength distance from a maximum point of* ϕ_λ*.*

We note that the result of Mangoubi, does not specify the location of the inscribed ball.

From the extension of Lieb's result in G.-Mukherjee (2016) we are able to **specify the position of a maximal inscribed ball** in Mangoubi's result - that is, at points where ϕ_λ reaches a maximum.

The inner radius of nodal domains (real-analytic case)

Sketch of the lower bound

- At a maximal point one can almost inscribe a wavelength cube Q up to a certain error set S, which is relatively small in volume. In particular, S contains **the set** $Q \cap \{\phi_\lambda < 0\}$ which should therefore also **be small in volume**.

The inner radius of nodal domains (real-analytic case)

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- At a maximal point one can almost inscribe a wavelength cube Q up to a certain error set S, which is relatively small in volume. In particular, S contains **the set** $Q \cap \{\phi_\lambda < 0\}$ which should therefore also **be small in volume**.
- Chop Q into even smaller cubes of size $\sim 1/\lambda$.
  Real-analyticity and polynomial approximation implies that **at least over** 90% of the small cubes ϕ_λ has bounded growth - these are the **good** cubes.

The inner radius of nodal domains (real-analytic case)

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- By elliptic estimates, bounded growth in a small cube C implies controlled geometry of the nodal set and that $\mathrm{Vol}(\{\phi_\lambda > 0\} \cap C) \sim \mathrm{Vol}(\{\phi_\lambda < 0\} \cap C)$ if the nodal set intersects C deeply enough.

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- If the nodal set intersects deeply each of the small good cubes, the set $\{\phi_\lambda < 0\}$ will **pick up volume and contradict the first step**. Hence, there is a non-intersected cube.

The inner radius of nodal domains (real-analytic case)

Some remarks

- One might try to directly rule out the error set S through a propagation of smallness estimate. Work in progress.
- The techniques and tools in the smooth case are still far from the real analytic case - one simply cannot find that many large enough good cubes. The growth of ϕ_λ may be wild on many of the cubes.
- Possible applications of the lower inradius bound: e.g. in G.-Mukherjee (2016) we were able to obtain interior cone conditions through the inradius bound of nodal domains on $\mathbb{S}^{n-1}$.

The inner radius of nodal domains (real-analytic case)

Some remarks

- It is natural to ask whether and how the **global geometry of** M affects the inradius estimate. In G. (2016) we give log-type improvements for manifolds with negative curvature - the observation uses a small scale quantum ergodicity result of H. Hezari (2016).
- The bounds on the inradius are related to the distribution of L^2 norm - in G. (2016) we show that if a nodal domain has most of its L^2-mass in good cubes, then its inner radius is large.

References

1. H. Donnelly, C. Fefferman, "Nodal sets of eigenfunctions on Riemannian manifolds.", Inventiones mathematicae 93.1 (1988): 161-184.
2. C. Sogge, S. Zelditch, "Riemannian manifolds with maximal eigenfunction growth", Duke Math. J., Volume 114, Number 3 (2002), 387-437.
3. S. Zelditch, Uniform distribution of eigenfunctions on compact hyperbolic surfaces. Duke Math. J. 55 (1987), no. 4, 919941.
4. D. Mangoubi, Local asymmetry and the inner radius of nodal domains, Comm. Partial Differential Equations 33 (2008), no. 9, 1611-1621.
5. S. Steinerberger, Lower bounds on nodal sets of eigenfunctions via the heat flow, Communications in Partial Differential Equations, 39 (2014).

References

1. A. Logunov, "Nodal sets of Laplace eigenfunctions: polynomial upper estimates of the Hausdorff measure", 2016.
2. A. Logunov, "Nodal sets of Laplace eigenfunctions: proof of Nadirashvili's conjecture and of the lower bound in Yau's conjecture", 2016.
3. B. Georgiev, M. Mukherjee, "Nodal Geometry, Heat Diffusion and Brownian Motion", 2016.
4. B. Georgiev, M. Mukherjee, "Tubular neighbourhoods, cone conditions and inradius estimates", 2016.
5. B. Georgiev, "On the lower bound of the inner radius of nodal domains", 2016.