Statistics of Nodal Domains in Quantum Chaotic Eigenstates in the Semiclassical Limit

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GOALS AND DEFINITIONS

It has been conjectured that nodal domains in quantum chaotic eigenstates follow the same statistics as a random superposition of plane waves in the semiclassical or high energy limit [Bogolmony et al.]. This thesis seeks to provide strong numerical evidence for this conjecture by collecting empirical data at previously unseen accuracy.

A quantum chaotic eigenstate is a solution $u(\overrightarrow{x})$ of the Schrodinger equation

$$\triangle u(\overrightarrow{x}) + k^2 u(\overrightarrow{x}) = V(\overrightarrow{x})\, u(\overrightarrow{x}) \;\; for \; \overrightarrow{x} \in \Omega, \; k \in \mathbb{C}$$

(where $\triangle = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is the laplacian differential operator) on a "quantum chaotic" domain $\Omega \subset \mathbb{R}^2$. For Ω to be a quantum chaotic means that a classical point particle exhibits non-integrable dynamics, i.e. positive Lyapunov exponent [are these equivalent?], on Ω; additionally, we define $V(\overrightarrow{x})$ to be a step potential on Ω given by

$$V(\overrightarrow{x}) = \begin{cases} 0 & if \; \overrightarrow{x} \in \Omega \\ \infty & if \; \overrightarrow{x} \notin \Omega \end{cases}$$

which reduces the Schrodinger equation to the Helmholtz equation

$$\nabla^2 u(\overrightarrow{x}) + k^2 u(\overrightarrow{x}) = 0 \; for \; \overrightarrow{x} \in \Omega, \; k \in \mathbb{C}$$

$$u(\overrightarrow{x}) = 0 \; for \; \overrightarrow{x} \in \partial\Omega$$

where k is the wave number of the solution, which when squared is proportional to the energy of the eigenfunction. This energy corresponds to the kinetic energy of a quantum wave-particle in the domain Ω with a wavefunction given by $\Psi(\overrightarrow{x}) = u(\overrightarrow{x})$.

It is known that these chaotic eigenstates of the Schrodinger equation contain complex and irregular structures of nodal domains in the semiclassical limit, where a nodal domain $\eta \subseteq \Omega$ of an eigenfunction $u(\overrightarrow{x})$containing a point $\overrightarrow{x_0}$ is defined as the largest connected subset of Ω such that $sign(\overrightarrow{x}) = sign(\overrightarrow{x_0})$ for all $\overrightarrow{x} \in \eta$. Thus any eigenfunction can be partitioned into a set of nodal domains [introduce notation for this set? $\eta(\Omega)$?] allowing us to consider statistics of this set such as the mean and variance of the area[/measure] of a nodal domain or the mean length of a nodal domain.

The conjecture that these statistics in quantum chaotic eigenstates are identical to those of a random superposition of plane waves has an intuitive appeal based upon visual inspection of nodal domain sets for each case (Fig. 1). The goal of this thesis is to provide a strong numerical underpinning for this apparent correspondence by developing computational tools to collect large amounts of high accuracy data on nodal domains of quantum chaotic eigenstates.

METHODS

Due to the chaotic nature of the domains investigated herein, it is not possible to analytically solve the Schrodinger equation. In order to obtain eigenfunctions we therefore use numerical solutions, computed by a method first described by Vergini [2] and implemented in C by Barnett [3]. Vergini's method computes eigenfunctions on a discrete grid of points by solving the system of equations which arises when we place many sources of plane waves (including evanescent plane waves) of varying intensity just outside the domain boundary and requiring that the eigenfunction go to zero on the boundary $\partial\Omega$. Given the intensity of each plane wave source which satisfies the given boundary condition we compute the eigenfunction at each point by summing the plane waves giving a $\Theta\left(mn^2\right)$ runtime where m is the number of plane wave sources and n is the number of grid points in either the x- or y- direction, which is inversely proportional to the grid resolution $\Delta x = \Delta y$. This computation is relatively expensive and dominates total computation time, restricting us to work with relatively coarsely sampled eigenfunctions. Vergini's method does however scale well with k (independent of k?) allowing us to work with very high energy eigenfunctions ($k \sim 10^3$).

The development of efficient computational methods to identify and compute statistics of nodal domains has been the primary obstacle to verifying the random plane wave conjecture and is the focus of this thesis. Nodal domains are counted by fully exploring domains one at a time and marking grid points as explored and belonging to a particular domain. This method runs as $\Theta\left(n^2\right)$ where n is again the number of gridpoints in the x-direction but in practice is several hundred times faster than computing eigenfunctions. Because we are restricted to work with coarsely sampled eigenfunctions however, the naive approach to counting nodal domains is not always accurate. We may have scenarios where we are unable to resolve the way in which nodal domains cross one another (Fig. 2).

In order to resolve such ambiguities we can selectively interpolate our coarsely sampled eigenfunction to a much higher resolution within the small region containing the ambiguity. It can be shown that the functions $1 \cup \{\sin(n\theta) J_n(kr)\}_{n=0,2,4,\ldots}^{\infty} \cup \{\cos(n\theta) J_n(kr)\}_{n=1,3,5,\ldots}^{\infty}$ are a spanning set for the solution space of the Helmholtz equation where $J_n(r)$ is a Bessel function of the first kind. This observation allows us to interpolate by expanding our coarsely sampled function in terms of the given basis functions and sampling the expansion at high enough resolution to resolve the ambiguity. Preliminary investigations suggest that interpolation using ~ 20 terms can produce a local surrogate function $\tilde{u}_{\overrightarrow{x_0}}\left(\overrightarrow{x}\right)$ which can be upsampled to arbitrarily high accuracy with error norm $\left\|u - \tilde{u}_{\overrightarrow{x_0}}\right\|_{L_\infty[\omega]} \sim 10^{-?}$ where $\omega \subset \Omega$ is the domain we are upsampling on.

Upon completion of this project I intend to release my source code under an open source license so that it may be used to investigate related problems in the field of quantum chaos.