NIUS Project Report

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Topic: *Nodal Line Statistics*

NIUS Physics Camp 12.2

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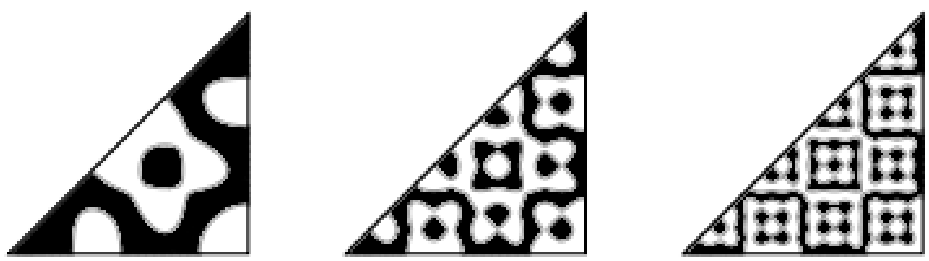
Introduction

The topic of the project work deals with the properties of nodal lines for regular but non-separable billiards and their statistics. We propose to study how these properties scale with the energy states of the system. So far we have begun to look at the total length of the nodal lines for a right angled isosceles triangle. The wave function, for the quantum numbers m and n, for this system, is well known implicitly

$$sin(mx)sin(ny) - sin(my)sin(nx) = 0$$

We have so far attempted to find either analytically or numerically, the total lengths of nodal lines so that we may study the variation of this property over m and n. The motivation for studying such a scaling lies partly in the close relation of quantum billiards with several other physical systems, and more so in the fact that the nodal lines can be naturally divided into families[1] that show evident geometric similarity over different sets of (m,n) within the same family. In case of the right angle isosceles triangle system the families consist of those (m,n) labelled by the same (c=m mod 2n) value for example some members of the family for c = 7 :



(a) (b) (c)

Figure: The pattern of nodal domains for (a) $\Psi_{7,4}$, (b) $\Psi_{15,4}$ and (c) $\Psi_{23,4}$.

Examples of various calculations for small m and n

Let $\psi(x,y) = sin(mx)sin(ny) - sin(my)sin(nx)$; then the total length of the nodal lines is given by integrating ,as a unit, the length of $|\nabla\psi(x,y)|^2$ over the nodal set, over the region of interest. Using the obvious symmetry we can take our region of interest to be $x \in [0,\pi]$,$x \in [0,\pi]$ and use a factor of half to get the required length. Also to restrict the integration to the nodal set only within the region of interest we can use the delta function $\delta(\psi(x,y) = 0)$. Thus the total length of the nodal lines is given by:

$$\frac{1}{2}\iint_S \delta(\psi(x,y) = 0)\frac{|\psi(x,y)|^2}{n.\nabla\psi(x,y)}\,dx\,dy$$

where S is the region $x \in [0,\pi]$,$x \in [0,\pi]$ and$n$ is for the variable that is left after using the δ function condition, i.e the parameter that is finally integrated over. The difficulty lies, however, in using the condition $\delta(\psi(x,y) = 0)$ to write the integrand in terms of one variable only. As an example to illustrate the calculation for total nodal length, consider the case, m=3;n=2.We have the $\delta(\psi(x,y) = 0)$ condition as:

$$sin(3x)sin(2y) = sin(3y)sin(2x)$$

Expanding each term and simplifying,while removing factors like sin(x), sin(y), and other inadmissible cases(we omit the algebraic manipulations here) we have:

$$cos^2(x) + cos^2(y) = \frac{1}{2}$$

From this last condition one can easily calculate $sin(2y)\,sin(3y)\,cos(2y)$ &$cos(3y)$ thus enabling us to right the integrand:

$$\frac{1}{2}\int \delta(cos^2x + cos^2y = \frac{1}{2})\cdot\left[1 + \left(\frac{2sin(3x)cos(2y) - sin(2x)cos(3y)}{3cos(3x)sin(2y) - 2cos(2x)sin(3y)}\right)^2\right]^{\frac{1}{2}}$$

in terms of x alone.The numerical value resulting from numerically evaluating the definite integral is also plausible.
A Sketch of the nodal lines for m=3, n=2 is given below:

Figure 1: Sketch of the nodal lines for m=3, n=2

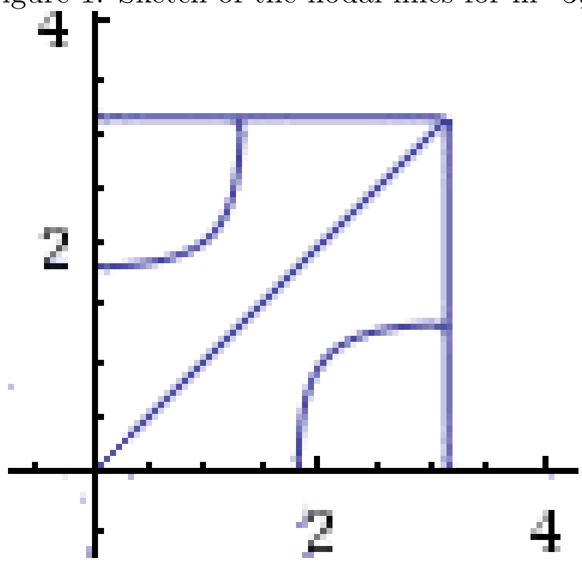
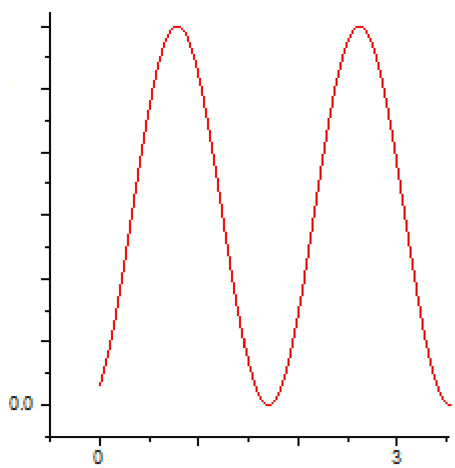


Figure 2: Graph of the integrand plotted as a function of x



This, and the nature of the graph of the integrand plotted as a function of x correspond to the wave function plot for these quantum number values(For example we see two peaks in the graph corresponding to the nodal line length in the upper triangle and then that in the lower triangle where the line is further along the x axis)

Modelling of the problem

Consider a wave function $\psi(r,t)$ r=x,y,z. The presence of a nodal line requires the vanishing of it's real and imaginary parts :

$$\psi(r,t) = R(r,t) + iN(r,t) = 0$$

This is thus the equation that any nodal set must satisfy. We now define two other loci: the loci of the points where the vorticity $\Omega(r,t)$ of the wave vanishes and the intensity stationary points where $\nabla|\psi^2| = 0$. We now show that intensity critical points are constrained to lie on the zero vorticity lines.

$$\Omega(r,t) = \nabla \times (Im(\psi^*)\nabla\psi = \nabla \times Im(R(r,t) - iN(r,t))\nabla\psi$$
$$= \nabla \times (-N(r,t))\nabla(R(r,t) + iN(r,t)) = \nabla \times (-N(r,t))(\nabla R(r,t) + i\nabla N(r,t))$$
$$= -\nabla \times (N(r,t)\nabla R(r,t) + iN(r,t)\nabla N(r,t))$$
$$= -(\nabla \times (N(r,t)\nabla R(r,t)) + \nabla \times (iN(r,t)\nabla N(r,t)))$$

now by using the formula:

$$\boldsymbol{\nabla \times (\psi \mathbf{A}) = \psi \nabla \times \mathbf{A} + \nabla \psi \times \mathbf{A}}$$

we have, writing R for R(r,t) and N for N(r,t):

$$\Omega(r,t) = -(N\nabla \times (\nabla R) + (\nabla N) \times \nabla R + iN\nabla \times (\nabla N) + i(\nabla N) \times \nabla N)$$

But the curl of a gradient is 0, so we finally have:

$$\Omega(r,t) = (\nabla R) \times (\nabla N)$$

Thus any point satisfying $(\nabla R) \times (\nabla N) = 0$ must lie on a zero vorticity line. Consider now any intensity stationary point:

$$\nabla|\psi|^2 = 0 \Rightarrow \nabla(\psi^8\psi) = 0 \Rightarrow \nabla(R^2 + N^2) = 0 \Rightarrow R\nabla R + N\nabla N = 0$$

$$\Rightarrow \nabla R = -\frac{N}{R}\nabla N \Rightarrow \nabla R = \lambda \nabla N \Rightarrow \nabla R \times \nabla N = \lambda \nabla N \times \nabla N = 0$$

Thus all intensity stationary points lie on the $\Omega = 0$ lines. Furthermore the topology change undergone must occur when a nodal line meets such a zero vorticity line. We see that the sign of the vorticity changes across an intensity stationary point and that topological change events involve a confluence of all three of these features, thus intuitively since the sign of the vorticity must change across any such change event, hence the event itself in x,y,z,t must lie on the zero vorticity line. The proof that this is so is available in [3].

We now show an example as to how we can model the nodal line reconnection process as a two stage process involving locally coplanar hyperbolae, to show how all such reconnection processes can be written in a normal form, describing the switching of hyperbolas[2]:

$$\psi(r,t) = x^2 - y^2 + t + iz$$

Here the switching occurs at t=0 and the $\Omega = 0$ line is the z-axis.The meaning of 'normal form' is that any exchange of nodal lines which is stable under smooth perturbation of the wave function can be locally transformed, by smooth change of coordinates, into one described by something of the form $\psi(r,t) = x^2 - y^2 + t + iz$ Consider the wave function:

$$psi(r,t) = (x + i(z + \frac{1}{2}t))(y - i(z - \frac{1}{2}t))$$

which describes two nodal lines parallel to the x and y axes, approaching in the z direction with unit relative velocity and crossing at the origimn at t=0. We peturb the wave function by simply adding to it a complex constant,$a+ib$.

$$psi(r,t)_0 = (x + i(z + \frac{1}{2}t))(y - i(z - \frac{1}{2}t)) + a + ib$$

$$R(r,t) = xy + z^2 - \frac{1}{4}t^2 + a, \quad N(r,t) = z(y - x) + \frac{1}{2}t(x + y) + b$$

Direct calculation shows that the $\Omega = 0$ line is gin by$x = y, z = 0$.The topology change occurs when the nodal lines encounter this line and so these events must satisfy:

$$R(r,t) = x^2 - \frac{1}{4}t^2 + a = 0, \quad N(r,t) = tx + b$$

Eliminating x we get the bifurcation surface as an equation in t and the other unfolding parameters, a and b.

$$t^4 - 4at^2 - 4b^2 = 0$$

$$\Rightarrow t = t_{\pm} = \pm\sqrt{2(a + \sqrt{a^2 + b^2})}$$

The bifurcation set is everywhere smooth, except at a=b=t=0.We have the unstable reconnection represented by ψ_0 separated into two generic switching events at:

$$t = t_{\pm}, \quad x_{\pm} = y_{\pm} = -\frac{b}{t_{\pm}}, \quad z = 0$$

There is a self intersection line of the bifurcation surface away from which the events must occur at different times. On the self intersection line the events occur simultaneously but are spatially separated:

$$t_+ = t_- = 0, \quad x_{\pm} = y_{\pm} = \pm\sqrt{-a}, \quad z = 0$$

Choosing a=1,b=0 we expand ψ_0 about $_+ = +2$,we use the smooth transformation of coordinates:

$$t2 + T, \quad xX + Y, \quad yX - Y$$

Neglecting a T^2 term we now have:

$$\psi_0 = X^2 - Y^2 - Z^2 - T + 2i(zY + X)$$

And now removing the sub-dominant terms we have:

$$\psi_0 = -Y^2 - Z^2 - 2T + 2iX)$$

Apart from trivial scaling and rotation this is the same as the normal form:

$$\psi(r,t) = x^2 - y^2 + t + iz$$

We attempt to write the wave function of the system we are studying and find the zero vorticity lines:

$$\psi = sin(mx)sin(ny) - sin(my)sin(nx) + iz$$

$$\Omega = 0 \Rightarrow R\nabla R + N\nabla N = 0 \Rightarrow mcos(mx)sin(ny) - ncos(nx)sin(my) +$$
$$ncos(ny)sin(mx) - nmcos(my)sin(nx) + z = 0$$

assuming that:

$$\psi = sin(mx)sin(ny) - sin(my)sin(nx) + iz \neq 0$$

which we can assume as the points we are interested in, as described later would lie not on the nodal lines themselves as there is not intersection but only avoided intersection. Thus the points of interest lie between nodal lines where they just avoid intersecting. Now if we use:

$$ncos(ny)sin(mx) = nmcos(my)sin(nx) \& ncos(ny)sin(mx) = nmcos(my)sin(nx)$$

to substitute into the nodal line condition:

$$sin(mx)sin(ny) - sin(my)sin(nx) = 0$$

We get another relation that gives us another set of lines which should pass through the avoided intersection points:

$$cos(mx)cos(ny) - cos(my)cos(nx) = 0$$

Now the points about which we can attempt to try to write the nodal lines as pairs of hyperbolae, must lie on these lines. Furthermore if we assume that the points of expansion should be the centre of the hyperbolae, then we can find these points by considering the set of intersection points of these lines and the nodal lines themselves.
Here we show the plots for the nodal lines and the $\Omega = 0$ lines for m=11 and n=5, where Figure 1 shows the nodal set and Figure 2 the zero vorticity set.(see next page)

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ContourPlot[Sin[11x] Sin[5y] − Sin[5x] Sin[11y] , {x, 0, Pi} , {y, 0 , Pi} ]
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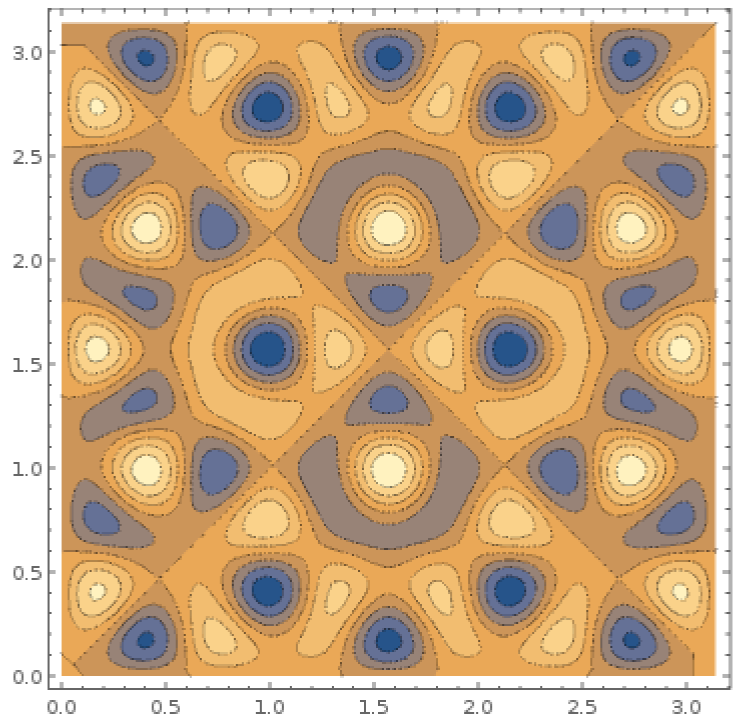

Figure 3: the nodal lines for m=11, n=5

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ContourPlot[Cos[11x] Cos[5y] − Cos[5x] Cos[11y] , {x, 0, Pi} , {y, 0 , Pi} ]
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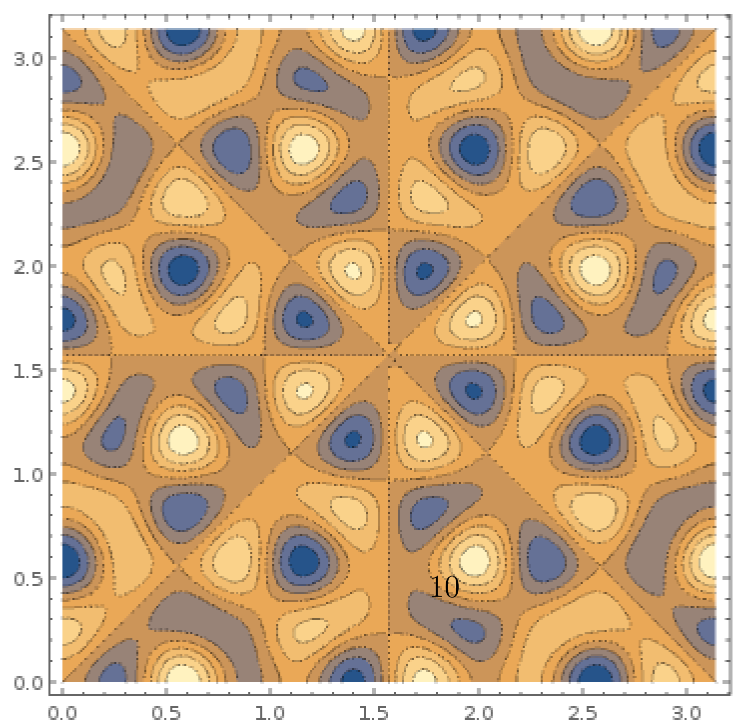

Figure 4: the zero vorticity lines for m=11, n=5

If we attempt to model the wave function for the isosceles right angled triangle as a st of nodal lines avoiding intersection at a set of points about which they can be modeled as locally coplanar hyperbolae then the approximation is expected to improve for larger m and n as the number of avoided intersections is expected to increase.

Possible future work

The idea of modelling the nodal lines as a set of approximate hyperbolas is motivated by the fact that the nodal sets of systems like the one under study show avoided re-connections and this tendency increases with the increase in the energy state of the system; furthermore it has also been shown that nodal lines evolving over time can be approximated as locally coplanar hyperbolas around intersection points[2]. It is planned to study the feasibility of such a modelling for the problem at hand i.e the question to be investigated is that can we show that for the system at hand we can approximate the nodal lines as hyperbolas about avoided intersection points.
Moreover it is proposed to search for other patterns in the nodal line structure of the system, in particular patterns related to the known subdivision into families so as to enable the studying of the scaling total nodal length with the quantum numbers. Possible relations, recurrences, other approximations, or indeed any other analytical or numerical techniques to facilitate the gathering of useful information or demonstrating properties of the solutions of $sin(mx)sin(ny) - sin(nx)sin(my) = 0$ will also be explored.
Another idea is to attempt to represent the total nodal line length as an integral in one variable only by generalizations of or techniques motivated by results for particular m and n, some of which have been stated in earlier sections, possibly initially solving this problem for particular families of $c = (m)mod(2n)$.
Other possible scalings such as those of curvature of the nodal lines or other properties of interest may also be investigated.
Meanwhile I plan to keep on studying other related papers and working on these and other ideas as suggested by my mentor.

Acknowledgement

I would like to thank my mentor, Dr. Sudhir Jain, for introducing me to so many new and exciting ideas and giving me a chance to work on this fascinating topic. I would also like to thank my co-mentor, Dr. Praveen Pathak as well as Dr. Anwesh Mazumdar for their invaluable help throughout my stay at HBCSE. This was my first experience of working on a problem alongside people doing actual research, and it was wonderful. I thank the NIUS Programme and everyone involved in it for making all this possible.

References

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[2] M. V. Berry, M. R. Dennis; Reconnections of wave vortex lines; European Journal of Physics

[3] M. V. Berry, M. R. Dennis; Topological events on wave dislocation lines: birth and death of loops, and reconnection;J.Phys:A Math. Theor.