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The Hexagon Quantum Billiard

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A subset of eigenfunctions and eigenvalues for the hexagon quantum billiard are constructed by way of tessellation of the plane and incorporation of symmetries of the hexagon. These eigenfunctions are given as a double Fourier series, obeying C_6 symmetry. A table of the lower lying eigen numbers for these states is included. The explicit form for these eigenstates is given in terms of a sum of six exponentials each of which contains a pair of quantum numbers and a symmetry integer. Eigenstates so constructed are found to satisfy periodicity of the hexagon array. Contour read-outs of a lower lying eigenstate reveal in each case hexagonal 6-fold symmetric arrays. Derived solutions satisfy either Dirichlet or Neumann boundary conditions and are irregular in neighborhoods about vertices. This singular property is intrinsic to the hexagon quantum billiard. Dirichlet solutions are valid in the open neighborhood of the hexagon, due to singular boundary conditions. For integer phase factors, Neumann solutions are valid over the domain of the hexagon. These doubly degenerate eigenstates are identified with the basis of a two-dimensional irreducible representation of the C_{6v} group. A description is included on the application of these findings to the hexagonal nitride compounds.

KEY WORDS: Quantum billiards; hexagon; tessellation; basis functions; Dirichlet and Neumann boundary conditions; irreducible representations; nitride compounds.

1. INTRODUCTION

In the quantum-billiard problem, one examines solutions to the Schrödinger equation for a point particle which moves freely in a convex domain in the plane bounded by a perfectly reflecting surface.[(1–8)] The Schrödinger equation for the particle is given by (the Helmholtz equation)

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$$\Delta u(\mathbf{r})+k^2u(\mathbf{r})=0 \tag{1a}$$

$$u(D)=0 \tag{1b}$$

where D denotes the enclosing boundary. The energy of the particle is given by

$$E=\frac{\hbar^2k^2}{2m} \tag{1c}$$

where m denotes particle mass, Δ represents the Laplacian and $\mathbf{r}$ represents the displacement vector. Equations (1) apply equally to a clamped membrane[9] or thin plate[10] and TM modes in a metal-walled uniform waveguide.[11] It is known that four "elemental" polygons are integrable both classically and quantum mechanically.[6a, 7] These are: the triangles: $\pi(1/4, 1/4, 1/2)$; $\pi/3(1, 1, 1)$; $\pi(1/2, 1/3, 1/6)$ and the rectangle. The equilateral triangle quantum billiard is solved through tessellation of a parallelogram in the plane.[2] It has been stated[8] that any n-gon which tessellates the plane (through reflection, not translation) is integrable. This is valid for the elemental polygons listed above. However, it is only partially valid for the hexagon billiard. Classically, orbits which bisect a vertex of this billiard are singular. Consequently, the classical motion may be mapped onto a torus of genus greater than one.[12] For the hexagon quantum billiard, solution based on tessellation of the plane through odd reflection fails due to the property that a trivertex over 2π cannot be covered with two colors. Similarly, tessellation of a finite convex domain in the plane (as with the equilateral triangle billiard) fails for the hexagon. Furthermore, it has been established that the ground state of the hexagon quantum billiard is non-analytic in a neighborhood about a vertex.[6a] Thus, in general, the hexagon quantum billiard is non-integrable.

In the present work solutions are derived in terms of a double Fourier series in the plane, incorporating symmetries of hexagonal domains. Constraint equations are introduced to satisfy boundary conditions. Read-outs of solutions indicate that Dirichlet boundary conditions are approximately satisfied and result in improper complex eigenfunctions. On the other hand, for integer phase factors, Neumann boundary conditions are satisfied and corresponding eigenfunctions for the hexagon quantum billiard are real. However, as these solutions are finite sums of plane waves and the system is in general nonintegrable, they represent a subset of eigenfunctions. Difficulty in numerics in attaining Dirichlet boundary conditions may be attributed to discontinuous first derivatives across cusped boundaries. Applications of these results to two-dimensional thin films of compounds in the nitride group which typically are in the wurtzite (hexagonal) structure as well as gallium nitride hexagonal "quantum dots" are described.

2. ANALYSIS

We recall the following. Let R denote a symmetry operation of the Hamiltonian. It follows that if $u(\mathbf{r})$ is an eigenfunction of H with eigenenergy E, so is $u(R\mathbf{r})]$.[13] Thus, eigenstates exist which share symmetries with the Hamiltonian and for the present case, may be assumed to have C_6 symmetry.

2.1. Construction of Solutions

Consider that hexagons tessellate the plane (Fig. 1). The diameters of a hexagon of edge-length a, are: $d_1 = a\sqrt{3} < d = 2a$. Symmetry along the x axis has periodicity $d+a$ and periodicity d_1 along the y axis. Calling the eigenstate in each hexagonal domain $u(x, y)$, we write

$$u(x, y) = u[x+(a+d), y] \tag{2a}$$

$$u(x, y) = u[x, y+d_1] \tag{2b}$$

It follows that $u(x, y)$ may be expanded in the double Fourier series

$$u(x, y) = \sum_{n=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} b_{nq} \exp i \frac{2\pi}{a}\left[n\frac{x}{3} + q\frac{y}{\sqrt{3}} + a\Phi_{nq}\right] \tag{3}$$

where Φ_{nq} are constant phase factors. Substituting this solution into (1a) suggests that the form

$$k^2 = [(2\pi)^2/3a^2]\left[\frac{\bar{n}^2}{3} + \bar{q}^2\right] \tag{4}$$

for some characteristic $\bar{n}$ and $\bar{q}$ values, may be an eigenvalue for the eigenfunction $u(x, y)$.

As noted above, solutions in a neighborhood about a vertex are nonanalytic. Consequently, in such neighborhoods, the Laplacian cannot be taken inside the sum in (3) and resulting solutions are irregular in these neighborhoods. This observation together with the cusped property of solutions at the boundary of the billiard infer that solutions are regular in the open domain of the hexagon.

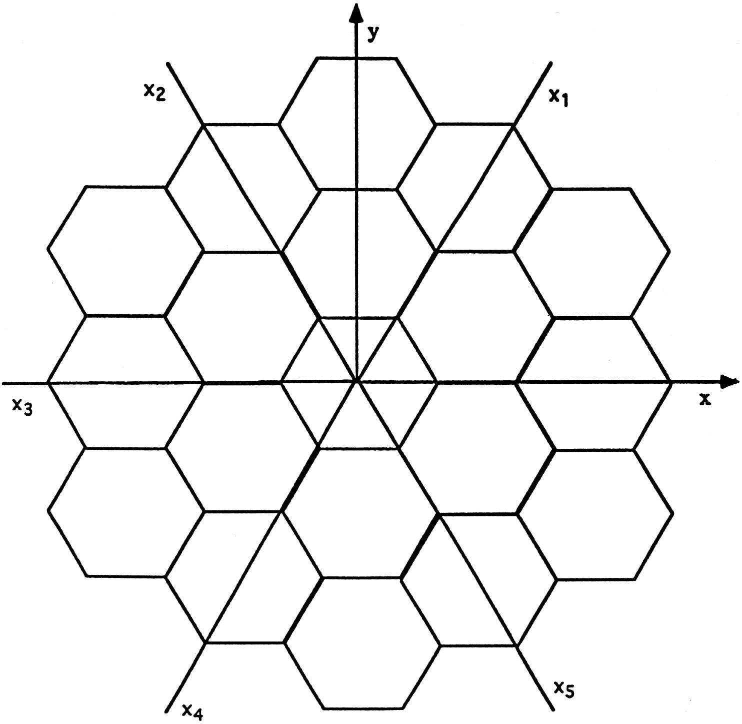

Fig. 1. Periodic array with 6-fold symmetry. New x-axes corresponding to rotations through $j2\pi/6$ ($j = 1, \ldots, 5, 6$) are shown as well.

The series (3) incorporates periodicity along only the x and y axes. To incorporate remaining periodicities, the following is noted. The hexagonal array of Fig. 1 is left unchanged by respective rotations through: ($\pi/3$, $2\pi/3$, π, $4\pi/3$, $5\pi/3$). For the first rotation through $\pi/3$ (for which the new x axis is labeled x_1 in Fig. 1) we write

$$u(x, y) = u(x/2 + \sqrt{3}\, y/2, -\sqrt{3}\, x/2 + y/2) \tag{5a}$$

For the second through $2\pi/3$ (new x axis labeled x_2 in Fig. 1) we write

$$u(x, y) = u(-x/2 + \sqrt{3}\, y/2, -\sqrt{3}\, x/2 - y/2) \tag{5b}$$

For the third rotation through $4\pi/3$ we write (new x axis labeled x_4 in Fig. 1)

$$u(x, y) = u(-x/2 - \sqrt{3}\, y/2, +\sqrt{3}\, x/2 - y/2) \tag{5c}$$

and for the fourth rotation through $5\pi/3$, there follows (new x axis labeled x_5 in Fig. 1)

$$u(x, y) = u(x/2 - \sqrt{3}\, y/2, +\sqrt{3}\, x/2 + y/2) \tag{5d}$$

The relation (5a) with (3) gives [n, q subscripts relate to the left side of 5(a–d)].

$$\begin{aligned} 2n &= n_1 - 3q_1, & 2n_1 &= n + 3q \\ 2q &= n_1 + q_1, & 2q_1 &= -n + q \end{aligned} \tag{6a}$$

The relation (5b) with (3) gives

$$\begin{aligned} -2n &= n_2 + 3q_2, & 2n_2 &= -n + 3q \\ 2q &= n_2 - q_2, & 2q_2 &= -n - q \end{aligned} \tag{6b}$$

The relation (5c) with (3) gives

$$\begin{aligned} 2n &= n_4 + 3q_4, & 2n_4 &= -n - 3q \\ 2q &= -n_4 - q_4, & 2q_4 &= n - q \end{aligned} \tag{6c}$$

The relation (5d) with (3) gives

$$\begin{aligned} 2n &= n_5 + 3q_5, & 2n_5 &= n - 3q \\ 2q &= -n_5 + q_5, & 2q_5 &= n + q \end{aligned} \tag{6d}$$

Invariance of the solution to reflection about either the x axis (labeled x_3 in Fig. 1) or the y axis indicates that

$$n = -n_3, \qquad q = -q_3 \tag{6e}$$

In the transformations, (6a)–(6e), the integer pairs (n_i, q_i) refer to rotation axes $\{x_i\}$, $i = 1, \ldots, 5$.

The starting solution (3) may be rewritten

$$u_{nq}(x, y) = \sum_{S(n,q)} b_{nq} \exp i \left\{ \frac{2\pi}{a} \left[n\left(\frac{x}{3}\right) + q\left(\frac{y}{\sqrt{3}}\right) + a\Phi_{nq} \right] \right\} \tag{7}$$

Table I. Lower-Lying Eigen-Number Pairs for the Hexagon Quantum Billiard

(n, q)	(n_1, q_1)	(n_2, q_2)	(n_3, q_3)	(n_4, q_4)	(n_5, q_5)	$3(ak/2\pi)^2$
$(1, -1)$	$(-1, -1)$	$(-2, 0)$	$(-1, 1)$	$(1, 1)$	$(2, 0)$	$4/3$
$(-1, 1)$	$(1, 1)$	$(2, 0)$	$(1, -1)$	$(-1, -1)$	$(-2, 0)$	$4/3$
$(3, 1)$	$(3, -1)$	$(0, -2)$	$(-3, -1)$	$(-3, 1)$	$(0, 2)$	4
$(-3, 1)$	$(0, 2)$	$(3, 1)$	$(3, -1)$	$(0, -2)$	$(-3, -1)$	4
$(2, 2)$	$(4, 0)$	$(2, -2)$	$(-2, -2)$	$(-4, 0)$	$(-2, 2)$	$16/3$
$(-2, 2)$	$(2, 2)$	$(4, 0)$	$(2, -2)$	$(-2, -2)$	$(-4, 0)$	$16/3$

The symbol $S(n, q)$ denotes summation over n, q values which satisfy the symmetry relations, (6a)–(6e). The phase constants Φ_{nq} come into play in establishing boundary conditions. Substituting the resulting form into (1) determines the related eigen k^2 value.

Table I includes a list of eigen numbers and related energies entering in the lower lying eigenstates of the hexagon quantum billiard. Quantum states corresponding to any row of elements in Table I have a common k^2 value. The sum $S(n, q)$ in (7) runs over all elements in a row.

Symmetries of the hexagon comprise the C_{6v} point group. This group has six irreducible representations ("irreps"). Four of the irreps are one dimensional and two are two dimensional. Wavefunctions whose eigen numbers are listed in Table I are two-fold degenerate and real. It follows that in the present work we have uncovered the basis functions for a two-dimensional irrep of the C_{6v} group. (Here one refers to symmetry related degeneracy, and not "accidental" degeneracy.[14]) In general, s-fold degenerate eigenfunctions of a system Hamiltonian that commutes with the symmetry operations of the system, comprise the basis functions of an s-dimensional irrep of that symmetry group.[13]

To within normalization, explicit expressions for eigenstates of the hexagon quantum billiard are given by (with edge-length $a = 1$ and expansion coefficients $b_{n,q} = 1$)

$$
\begin{aligned}
u_{nq}(x, y) = {} & \exp i2\pi\left[n\frac{x}{3} + q\frac{y}{\sqrt{3}} + \Phi_0^{(nq)}\right] + \exp i2\pi\left[n_1\frac{x}{3} + q_1\frac{y}{\sqrt{3}} + \Phi_1^{(nq)}\right] \\
& + \exp i2\pi\left[n_2\frac{x}{3} + q_2\frac{y}{\sqrt{3}} + \Phi_2^{(nq)}\right] + \exp i2\pi\left[n_3\frac{x}{3} + q_3\frac{y}{\sqrt{3}} + \Phi_3^{(nq)}\right] \\
& + \exp i2\pi\left[n_4\frac{x}{3} + q_4\frac{y}{\sqrt{3}} + \Phi_4^{(nq)}\right] + \exp i2\pi\left[n_5\frac{x}{3} + q_5\frac{y}{\sqrt{3}} + \Phi_5^{(nq)}\right]
\end{aligned} \tag{8}
$$

where (n_v, q_v) numbers and corresponding eigenenergies are given in Table I. Values of the symmetry $S(n, q)$ values in any eigenstate are determined from boundary conditions. These complex functions represent Bloch waves.

2.2. C_6 Periodicity

The eigenstates (8) have required C_6 periodicity. This property is illustrated explicitly for the first eigenstate of Table I. With phase-constants, Φ, set equal to zero we obtain

$$u_{1,-1}/2 = \cos 2\pi\left(\frac{x}{3} - \frac{y}{\sqrt{3}}\right) + \cos 2\pi\left(\frac{x}{3} + \frac{y}{\sqrt{3}}\right) + \cos 2\pi\left(\frac{2x}{3}\right) \tag{10a}$$

with eigenvalue (with edge-length a reinserted), $k^2 = (4\pi/3a)^2$. On the line $y = x/\sqrt{3}$ (at $\pi/6$ to the x-axis in Fig. 1), we obtain

$$u_{1,-1}/2 = 1 + 2\cos 2\pi\left(\frac{x}{3/2}\right) \tag{10b}$$

which has the period, $\Delta x = 3/2$. On the line $y = \sqrt{3}\,x$ (at $\pi/3$ to the x-axis in Fig. 1), we obtain

$$u_{1,-1}/2 = 2\cos 2\pi\left(\frac{x}{3/2}\right) + \cos 2\pi\left(\frac{2x}{3/2}\right) \tag{10c}$$

which has the period, $\Delta x = 3/2$. Note that these results apply as well to the axes $y = -x/\sqrt{3}$, and $y = -\sqrt{3}\,x$, respectively. On the line $y = 0$, $u_{1,-1}$ has the period $\Delta x = 3$. On the line $x = 0$, $u_{1,-1}$ has the period $\Delta y = \sqrt{3}$. Here is a recapitulation of periodicities for the hexagonal array (with $a = 1$).

$$\begin{aligned}\text{(curve; period):}\quad &(y = x/\sqrt{3}\,, \Delta x = 3/2); (y = \sqrt{3}\,x, \Delta x = 3/2);\\ &(y = 0, \Delta x = 3); (x = 0, \Delta y = \sqrt{3})\end{aligned} \tag{10d}$$

3. BOUNDARY CONDITIONS

At this point, it should be noted that two pieces of information have been inserted into the analysis: (a) The Fourier series (3) has proper periodicity in x and y directions. (b) The solutions (6), (8) have 6-fold rotational symmetry and stated periodicity on the six symmetric axes. These conditions are satisfied by a number of periodic arrays in the plane. This logic is borne out in a read-out of the eigenstate (10a) at $u=-1$, (Fig. 2a) where u is written for $u_{1,-1}/2$. This read-out exhibits an array of hexagons imbedded in 6-pointed stars with 6-fold symmetry that satisfies the periodicity conditions (10d). The contour map of $u(x, y)$ shown in Fig. 2b, illustrates a monotonic decay of the eigenstate from its maximum ($u=3$) at (0, 0) through the value -1 on the hexagon boundary to the minimum, -1.5, at triangle centers.

In an attempt to impose Dirichlet boundary conditions, $|u(x, y)|$ was computationally minimized on the boundary of a hexagon. Resulting phase

a

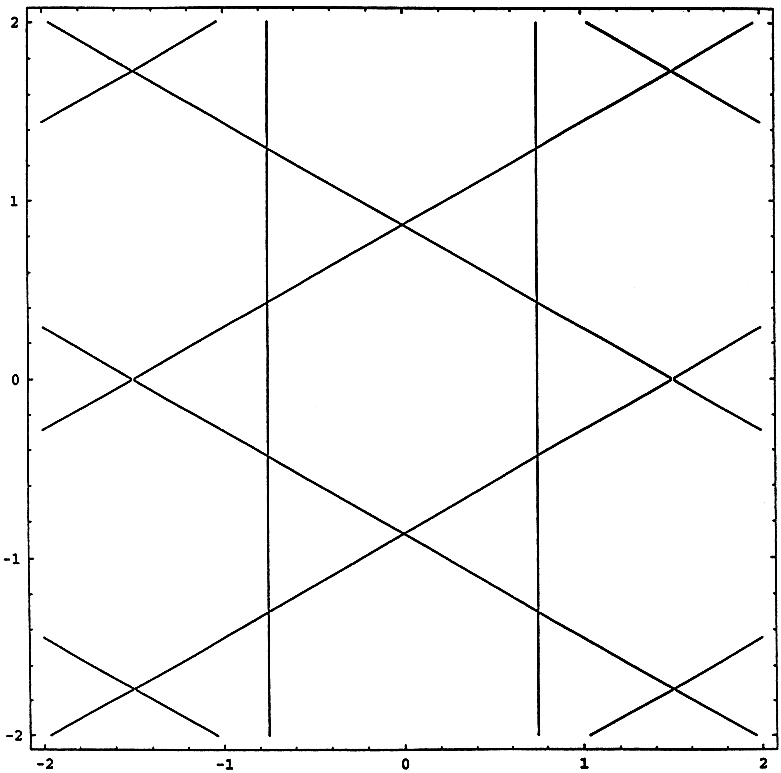

Fig. 2. (a) Contour lines of the eigenstate value, $u=-1$, exhibiting 6-fold symmetry composed of hexagons embedded in 6-pointed stars. (b) Contour map of the function $u(x, y)$ illustrating a monotonic decay of the function away from the center maximum, $u=3$ to the minimum value, -1.5, at triangle centers. The value $u=-1$ occurs in the region between the outer hexagon perimeter and the triangle domains.

b

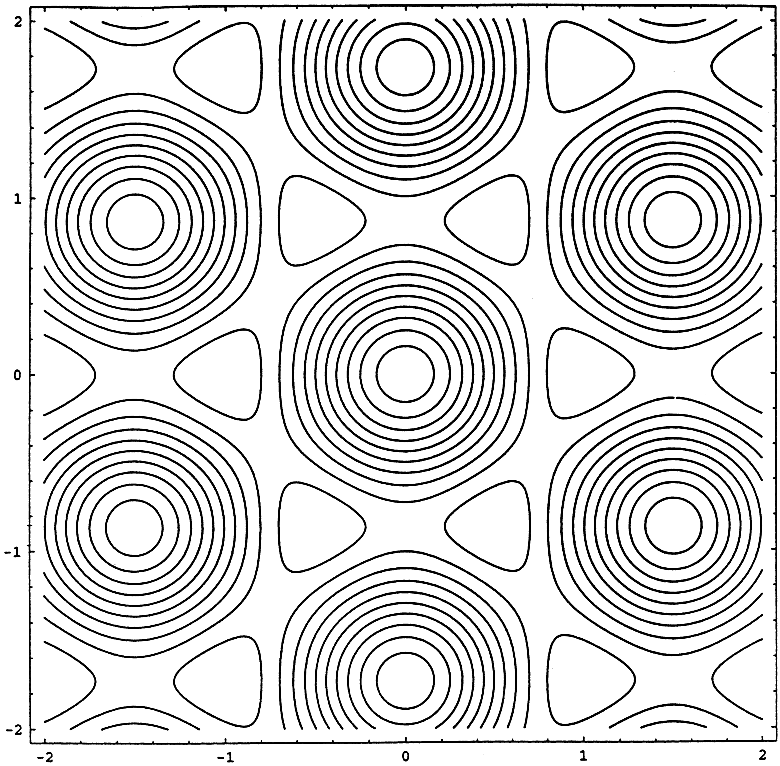

Fig. 2. (Continued).

constants are given by: $\Phi_0 = -0.027$, $\Phi_1 = -0.1873$, $\Phi_2 = -0.354$, $\Phi_3 = -0.527$, $\Phi_4 = -0.854$, $\Phi_5 = -0.6873$. The resulting read-out of the contours of $|u(x, y)|$ is shown in Fig. 3 in which it is seen that 12 zero islands lie on a hexagonal boundary. As noted above, this computational weakness is attributed to discontinuities of the first derivative across hexagon boundaries. As boundary phase constants were imposed in this calculation the hexagonal array of Fig. 1 reappears. Eigenfunctions corresponding to the preceding phase constants are complex.

3.1. Neumann Boundary Conditions

To impose Neumann boundary conditions, the following technique was employed. One sets

$$|\varphi|^2 = (\mathrm{Re}\, u)^2 + (\mathrm{Im}\, u)^2 \tag{11a}$$

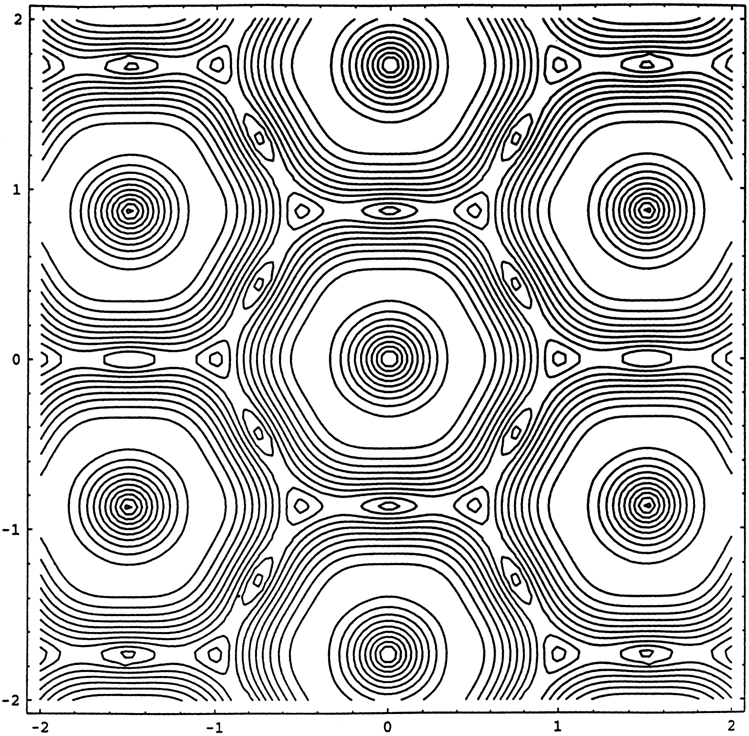

Fig. 3. Contour map of the eigenstate $|u(x, y)|$ corresponding to partially satisfied Dirichlet boundary conditions showing 12 zero islands distributed about a hexagon.

and then constructs

$$\nabla\, |\varphi|^2 \cdot \mathbf{n}(D) = 0 \tag{11b}$$

where $\mathbf{n}$ is normal to the boundary $D(x, y)$. The sum of the left side of (11b) over 27 equally spaced points on the hexagonal boundary is computationally minimized. Resulting phase constants, Φ_{nq}, stemming from these Neumann boundary conditions are all integers corresponding to real eigenfunctions.

Summation over the equally spaced 27 boundary points is E-85. Readouts of the contour of $|\varphi(x, y)|^2$ are shown in Fig. 4. [The fact that Φ_{nq} phase constants are integers for this case indicates that the wavefunction (7) are solutions with $\Phi_{nq} = 0$. This property is consistent with precision of these numerics.] Solutions so constructed maintain irregular behavior in

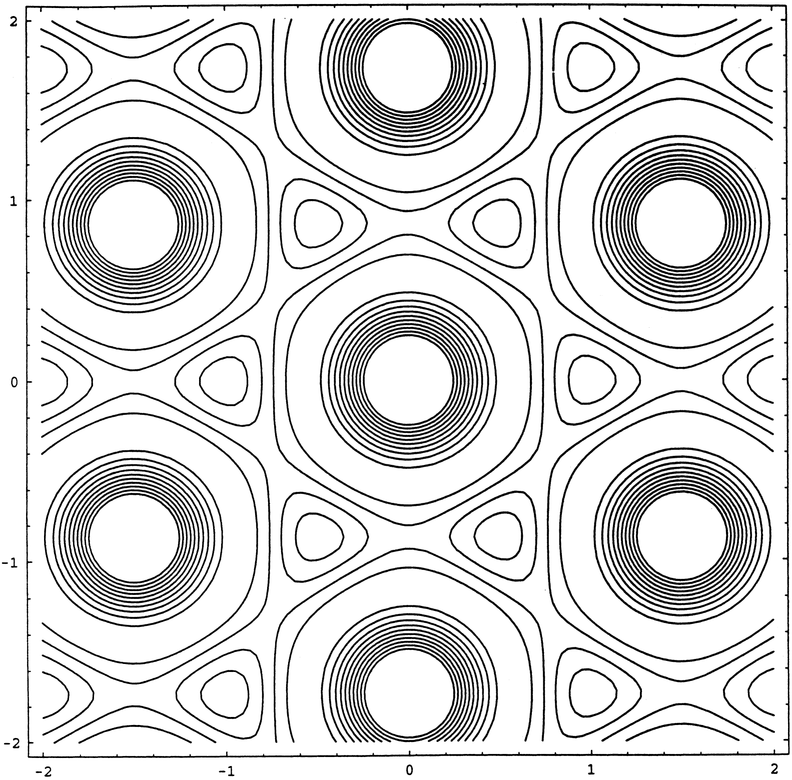

Fig. 4. Contour map of the eigenstate $|u(x, y)|$ corresponding to satisfied Neumann boundary conditions. Central domains correspond to relatively large positive values. The value $u'(x, y) = 0$ occurs on the hexagon defined by triangle centers.

neighborhoods of vertices. However, these solutions have zero normal derivatives at straight boundaries and are otherwise continuous in these domains. It is noted that Neumann boundary conditions are satisfied if and only if at least one of the following integer (n, q) relations 6(a)–(e), hold: $n = 0$, $q = 0$, $n = \pm q$, $n = \pm 3q$. These conditions are satisfied for the related values listed in Table 1.

As an example of an eigenstate with $\Phi_{nq} = 0$, we consider the state $u_{1,-1}/2$ given by (10a) and confirm analytically that this wavefunction satisfies Neumann boundary conditions on the boundaries of the hexagon array. Due to six-fold symmetry of the wavefunction, it suffices to verify these conditions on one parallel set of boundaries of the array. We label $u_{1,-1}/2 \equiv u$ and with (10a) obtain

$$\partial u/\partial x = -\frac{2\pi}{3}\left[\sin 2\pi\left(\frac{x}{3}-\frac{y}{\sqrt{3}}\right)+\sin 2\pi\left(\frac{x}{3}+\frac{y}{\sqrt{3}}\right)+\sin 2\pi\left(\frac{2x}{3}\right)\right] \tag{12a}$$

$$\partial u/\partial y = -\frac{2\pi}{3}\left[\sin 2\pi\left(\frac{x}{3}-\frac{y}{\sqrt{3}}\right)+\sin 2\pi\left(\frac{x}{3}+\frac{y}{\sqrt{3}}\right)\right] \tag{12b}$$

We verify Neumann boundary conditions on the top and bottom segments of hexagons, where $\partial u/\partial y = 0$ at constant intervals of y. With (12b) there results

$$\frac{x}{3}-\frac{y}{\sqrt{3}}=\frac{x}{3}+\frac{y}{\sqrt{3}}+s \tag{12c}$$

$$y=\frac{\sqrt{3}}{2}s \tag{12d}$$

where s is a positive or negative integer. Substituting this value into (12a) and expanding resulting forms gives

$$\partial u/\partial x \propto \left[\sin 2\pi\left(\frac{2x}{3}\right)\cos\left(\frac{2\pi s}{2}\right)-\cos 2\pi\left(\frac{2x}{3}\right)\sin\left(\frac{2\pi s}{2}\right)+\sin 2\pi\left(\frac{2x}{3}\right)\right] \tag{12e}$$

This form vanishes providing s is odd, which with (12d) gives the correct constant y-values of top and bottom segments of hexagons (Fig. 1).

As such (doubly degenerate) solutions, corresponding to integer phase constants, are valid over the domain of the hexagon (excluding infinitesimal neighborhoods about vertices), it follows that they comprise a two-dimensional basis for the C_{6v} group.

The last column of eigenvalues is consistent with (4) where $\bar{n}$ and $\bar{q}$ represent the lead (n, q) values in the table.

4. APPLICATIONS

These findings have application to two-dimensional thin films of compounds in the nitride group which typically are in the wurtzite (hexagonal) structure.[15] The wave functions described herein represent stationary Bloch waves in such hexagonal arrays with Neumann boundary conditions relevant. Furthermore, it has been reported that GaN "quantum dots" are hexagonal, for which case eigenfunctions constructed with Dirichlet boundary conditions are appropriate.[16] Nitride compounds are growing in importance in high-power semiconductor devices as well as in wide-band optical emitters.[17]

CONCLUSIONS

A subset of eigenfunctions and eigenenergies were obtained for the hexagon quantum billiard in terms of a double Fourier series with related C_6 symmetry. Dirichlet solutions are valid over an open domain of the hexagon and are approximate. Neumann solutions corresponding to integer phase constants are valid over the closed domain of the hexagon (excluding vertices) and comprise the basis of a two-dimensional irreducible representation of the C_{6v} group. A table of the lower-lying eigen numbers of this quantum billiard was included as well as the explicit form of eigenstates given in terms of six exponentials, six pairs of quantum numbers and six symmetry integers. Eigenstates so constructed were found to satisfy all six C_6 periodicities. A number of read-outs of contours of a lower lying eigenstate all revealed 6-fold symmetry patterns comprised either of contiguous hexagons or hexagons embedded in 6-pointed stars. A description was included of the application of these findings to quantum dots or thin films composed of hexagonal nitride compounds.

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