Signatures of quantum chaos in the nodal points and streamlines in electron transport through billiards

K.-F. Berggren
Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden

K. N. Pichugin
Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia; Institute of Physics, Academy of Sciences, 16000 Prague, Czech Republic

A. F. Sadreev
Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden; Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

A. Starikov
Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

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Streamlines and the distributions of nodal points are used as signatures of chaos in coherent electron transport through three types of billiards: Sinai, Bunimovich, and rectangular. Numerical averaged distribution functions of the nearest distances between nodal points are presented. We find the same form for the Sinai and Bunimovich billiards and suggest that there is a universal form that can be used as a signature of quantum chaos for electron transport in open billiards. The universal distribution function is found to be insensitive to the way the averaging is performed (over the positions of the leads, over an energy interval with a few conductance fluctuations, or both). The integrable rectangular billiard, on the other hand, displays a nonuniversal distribution with a central peak related to partial order of nodal points for the case of symmetric attachment of the leads. However, cases with asymmetric leads tend to the universal form. Also, it is shown how nodal points in the rectangular billiard can lead to ''channeling of quantum flows,'' while disorder in the nodal points in the Sinai billiard gives rise to unstable irregular behavior of the flow. © *1999 American Institute of Physics.* [S0021-3640(99)00718-5]

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Billiards play a prominant role in the study of classical and quantum chaos.[1] Indeed, the nature of quantum chaos in a specific system is traditionally inferred from its its classical counterpart. Hence one may ask if quantum chaos is to be understood solely as a phenomenon that emerges in the classical limit, or are there some intrinsically quantal phenomena that can contribute to irregular behavior in the quantum domain? This is a question we raise in connection with quantum transport through ideal regular and irregular electron billiards.

The seminal studies by McDonald and Kauffmann[2] of the morphology of eigenstates in a closed Bunimovich stadium have revealed characteristic patterns of disordered, nondirectional, and noncrossing nodal lines. Here we will first discuss what will happen to patterns like these when input and output leads are attached to a billiard, regular or irregular, and an electric current is induced through the the billiard by an applied voltage between the two leads. For such an open system the wave function ψ is now a scattering state with both real and imaginary parts, each of which gives rise to separate sets of nodal lines at which either $\mathrm{Re}[\psi]$ or $\mathrm{Im}[\psi]$ vanish. How will the patterns of nodal lines evolve as, e.g., the energy of injected electrons is increased, i.e., more scattering channels become open? Could they tell us something about how the perturbing leads reduce the symmetry and how an initially regular billiard may eventually turn into a chaotic one as the number of open modes increases? Below we will argue that nodal points, i.e., the points at which the two sets of nodal lines intersect because $\mathrm{Re}[\psi]=\mathrm{Im}[\psi]=0$, carry important information in this respect. Thus we will study their spatial distributions and try to characterize chaos in terms of such distributions. The question we wish to ask is simply if one can find a distinct difference between the distributions for nominally regular and irregular cavities.

In addition, what other signatures of quantum chaos may one find in the coherent transport in open billiards? The spatial distribution of nodal points plays a decisive role in how the flow pattern is shaped. Therefore we will also study the general behavior of streamlines derived from the probability current associated with a stationary scattering state

$$\psi=\sqrt{\rho}\,\exp(iS/\hbar).$$

The time-independent Schrödinger equation can be decomposed as[3,4]

$$E=\frac{1}{2}mv^2+V+V_{QM}, \quad \nabla\rho\mathbf{v}=0, \quad m\dot{\mathbf{X}}=\nabla S.$$

The separate quantum streamlines are sometimes referred to as Bohm trajectories.[4] In this alternative interpretation of quantum mechanics it is thought that an electron is a ‘‘real’’ particle that follows a continuous and causally defined trajectory (streamline) with a well-defined position **X**, with the velocity of the particle given by the expressions above.

These equations imply that the electron moves under the influence of a force which is not obtained entirely from the classical potential V but also contains a ‘‘quantum mechanical’’ potential

$$V_{QM}=-\frac{\hbar^2}{2m}\frac{\nabla^2\rho}{\rho}.$$

This quantum potential is large and negative, where the wave function is small, and becomes infinite at the nodal points of the wave function where $\rho(x,y)=0$. Therefore, the close vicinity of a nodal point constitutes a forbidden area for quantum streamlines contributing to the net transport from source to drain. When ρ does not vanish, S is single-valued and continuous. However at the nodal point where $\psi=0$, neither S nor ∇S

is well defined. The behavior of S around these nodal points is discussed in Refs. 3, 5, and 6. For our study the main important property of the nodal points of ψ is that probability current flows described by ''open'' streamlines cannot encircle a nodal point. On the contrary, they are effectively repelled from the close vicinity of the nodal points, in a way as if these were impurities.

The scattering wave functions ψ are found by solving the Schrödinger equation in the tight-binding approximation with Neumann boundary conditions outside the billiards, at a distance over which the evanescent modes have effectively decayed to zero. The energy of the incident electron is $\epsilon=20$, where $\epsilon=2E_F d^2 m^*/\hbar$, with E_F the Fermi energy, d the width of the channel, and m^* the effective mass.

An inspection of the two sets of nodal lines associated with the real and imaginary parts of the scattering wave function reveals the typical pattern of nondirectional, self-avoiding nodal lines found previously by McDonald and Kaufman[2] for an isolated, irregular billiard. However, in our case of a complex scattering function the nodal lines are not uniquely defined, because multiplication of the wave function by an arbitrary constant phase factor $\exp(i\alpha)$ would yield a different pattern. The nodal points, on the other hand, appear to helpful in this respect. They represent a new aspect of the open system and will obviously remain fixed upon a change in the phase of the wave function. Here we conjecture that the nodal points may serve as unique markers which should prove useful for a quantitative characterization of scattering wave functions for open systems.

To be more specific, we have considered a large number of realizations (''samples'') of nodal points associated with different kinds of billiards and present averaged normalized distributions of nearest distances between the nodal points. Figure 1 shows the distributions for open Sinai (a), Bunimovich (b), and rectangular billiards (c, d). The distributions are obtained as an average over 101 different values of energy belonging to a specific energy window in which the conductance undergoes a few oscillations as shown by the insets in Fig. 1. Cases (a), (b), and (c) correspond to two-channel transmission through the billiards, while case (d) pertains to five-channel transmission. The rectangular billiard is nominally maximal in area with a numerical size 210×100 and with the width of the leads equal to 10.

It is noteworthy that the distribution of nearest neighbors is distinctly different from the corresponding distribution for random points in the two-dimensional plane,[7,8]

$$g(r)=2\pi\rho r\ \exp(-\pi\rho r^2), \tag{1}$$

where the density ρ of random points is related to the mean separation $\langle r\rangle$ as $\rho=1/4\langle r\rangle^2$. This distribution is shown in Fig. 1a by the thin line, indicating an underlying correlation between the nodal points of the transport wave function through the Sinai billiard. In this sense quantum chaos is not randomness.

With slight deviations the Bunimovich billiard gives rise to the same distributions as the Sinai, as shown by Fig. 1a and 1b. Analysis of the distributions for lower energies ($\epsilon\approx20$, one-channel transmission) gives quite similar universal forms, as shown in Fig. 1a and 1b, but with more pronounced fluctuations because the number of nodal points is smaller at lower energies. Moreover, averaging over wider energy domains with a finer

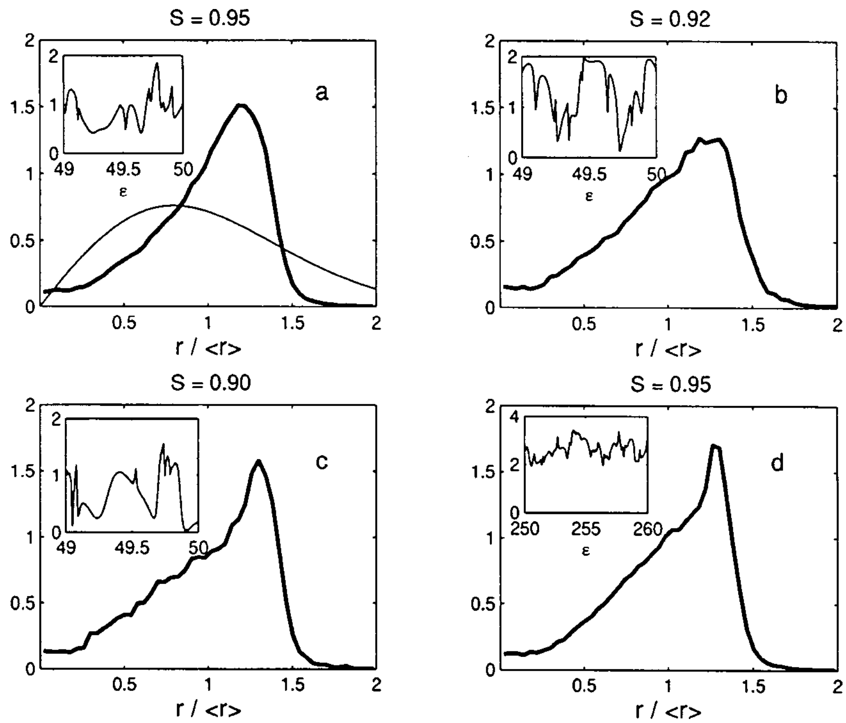

FIG. 1. Normalized distributions for nearest separations between nodal points (in units of the mean separation) averaged over an energy window for the chaotic Sinai (a) and Bunimovich billiards (b) and for two rectangular billiards (c, d). The Shannon entropy S is given for each separate case. Cases (a), (b), and (c) correspond to two-channel transmission and case (d) to five open channels. The corresponding conductance (in units of $2e^2/h$) versus energy is shown in the insets, which also define the energy window for each case. The distribution (1) for the nearest distances among completely random points is shown by thin line in (a).

grid or for higher energies gives no visible deviations from the distributions in Fig. 1a and 1b.

We considered also the Berry wave function of a chaotic billiard, which is accepted as a standard measure of quantum chaos:[9]

$$\psi(x,y)=\sum_j |a_j|\exp[ik(\cos\ \theta_j x+\sin\theta_j y)+\phi_j], \tag{2}$$

where $\theta_j, |a_j|$ and ϕ_j are independent random variables. We found that the distribution of nearest distances between the nodal points of (2) has completely the same form as for the Sinai billiard (Fig. 1a). On the other hand, an analysis of the nodal points of the wave function

$$\psi(x,y)=\sum_{k_x,k_y} \exp(ik_x x+k_y y) \tag{3}$$

with k_x, k_y distributed randomly leads to the distribution (1) of random points.

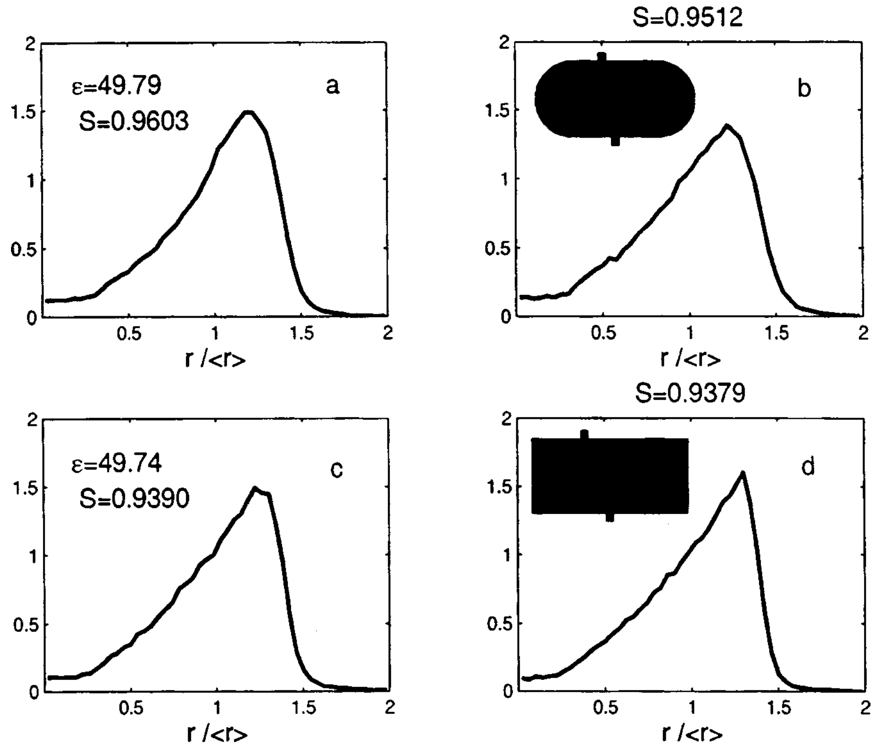

FIG. 2. Normalized distributions averaged over position of input lead for the Sinai billiard (a), over an energy window from $\epsilon=49$ to 50 for the Bunimovich billiard with asymmetric input lead (b), over lead positions for the rectangular billiard (c), and over an energy window for the rectangular billiard with asymmetric input lead (d).

To supplement the averaging over energy we have also considered the positions of the leads. Figure 2a shows the normalized distribution of the nearest distances between nodal points for the Sinai billiard, obtained as an average over 101 positions of the input lead. It is seen that this distribution has the same form as the energy-averaged Sinai billiard in Fig. 1a. In the same way Fig. 2b shows the corresponding case of the Bunimovich billiard with an asymmetric input lead; this is to be compared with Fig. 1b. The asymmetric arrangement of leads allows a larger number of eigenstates of the Bunimovich billiard to participate in the electron transport because symmetry restrictions are relaxed.[10]

On the basis of Figs. 1 and 2 and comparison with the Berry wave function (2) we therefore argue that there is a universal distribution that characterizes open chaotic billiards. At this stage we conclude that the form of the distributions is insensitive to the averaging procedure, to the number of channels of electron transmission, and to the type of attachment of the leads. The mathematical form of the universal distribution constitutes an interesting problem that remains to be solved. So does a derivation of the random distribution associated with wave function in Eq. (3).

Let us now turn to the case of the nominally regular rectangular billiard. In Fig. 1c the distribution functions are given for the case of two-channel transmission with the same energy-averaging procedure as for the chaotic billiards. The nearest-neighbor distribution clearly displays a peak corresponding to a regular set of nodal points, in contrast to the other billiards discussed above. This feature is found even for very high energies around 250 (five-channel transmission). Therefore the rectangular dot with the two symmetrically attached leads displays considerable stability with respect to regular nodal points, in contrast to the chaotic Sinai and Bunimovich billiards.

As indicated, symmetric leads impose restrictions on how states inside the billiard are selected and mixed on injection of a particle. In Fig. 2c the result of averaging over the positions of the input lead is therefore shown for the rectangular billiard at a fixed energy chosen from the energy domain in Fig. 1c. As one might expect, the pronounced peak in the distribution function of nearest nodal points has now disappeared. Moreover, the distribution is close to the case of the Bunimovich billiard in Figs. 1b and 2b. Evidently the asymmetrical positioning of the leads disturbs the nominally regular billiard in a much more profound way, effectively lending it chaotic characteristics. To reconfirm this conclusion we have also performed calculations of the distribution of nodal points within the same energy domain and with the same number of energy steps as in Fig. 1c but for non symmetrical positions of the input lead. In fact, the distribution function of nearest distances in Fig. 2d demonstrates a close similarity with the position average of the nodal points. Therefore the nonuniversal behavior of the distribution function of nodal points for the rectangular billiard shown in Fig. 1c and 1d is the result of the fact that only a few symmetrical eigenstates take part in the transmission because of symmetry restrictions.

In order to give a quantitative measure of the disorder of nodal point patterns we consider the Shannon entropy S (Ref. 11) normalized for each specific billiard by the entropy of completely random points. Numerical values for S are specified in Figs. 1 and 2. As one might expect, for the same energy window there is a clear tendency towards maximal entropy for chaotic billiards. A similar tendency is clearly seen for the position average (Fig. 2). The case of a rectangular billiard with entropy 0.95 (Fig. 1d) is beyond the scope of this rule, because for five-channel transmission the number of nodal points substantially exceeds that for the other cases considered, irrespective of the type of billiard. Thus the Shannon entropy of nodal points is an important additional quantitative measure of quantum chaos for quantum transport through billiards.

As we have said, the streamlines are strongly affected by the positions of the nodal points. Superficially they play the role of impurities. It is therefore of interest to determine whether the streamlines behave differently for regular and irregular situations, and for this reason we will consider a few typical examples, starting with two well-defined systems: the nominally regular rectangle and the irregular Sinai billiard. Figure 3a shows the flow lines in the case of the rectangular billiard. The features of the flow lines connecting the input and output leads are remarkable. It is clearly seen how the flow (trajectories) effectively ‘‘channel’’ through a ‘‘nodal crystal,’’ avoiding the individual nodal points. This picture is evidently very different from semi-classical physics and periodic orbit theory.[12] In Fig. 3 only contributions to the net current are displayed. In addition there are also vortical motions centered around each nodal point.

The other extreme, the completely chaotic Sinai billiard, is shown in Fig. 3b. Because the nodal distribution is now irregular also, the streamlines form an irregular pattern when finding their way through the rough potential landscape. Since a streamline

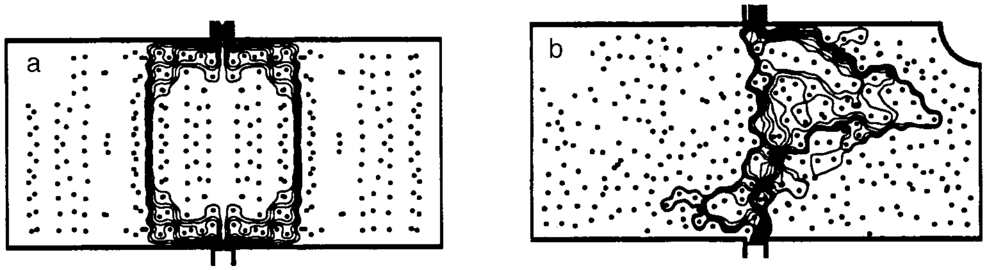

FIG. 3. Streamlines and positions of vortices (nodal points) at maximum conductance $(2e^2/h)$ for (a) the rectangle with $\epsilon=20.44$ and (b) for the Sinai billiard with $\epsilon=20.79$.

cannot cross itself, Fig. 3 brings to mind the classical example of meandering rivers in a flat delta landscape. As is well known, slight changes in the topography, for example, by moving only a few obstacles to new positions, may induce completely new flow patterns in a sometimes dramatic ways. In the same way slight variations of the energy, for example, may affect the quantum streamlines in the Sinai billiard in an endless way, occasionally forming more collected bunches connecting the two leads in a more focused way than in Fig. 3b. The same type of behavior has also been obtained for a two-dimensional ring in which a tiny variation of the external magnetic flux induce drastic changes of the flow lines and, as a consequence, the Aharonov–Bohm oscillations become irregular.[13]

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[1] T. Guhr, A. Müller-Groeling, and H. A. Weidenmüller, Phys. Rep. **299**, 189 (1998).
[2] S. W. McDonald and A. N. Kaufman, Phys. Rev. Lett. **42**, 1189 (1979); Phys. Rev. A **37**, 3067 (1988).
[3] J. O. Hirschfelder, C. J. Goebel, and L. W. Bruch, J. Chem. Phys. **61**, 5456 (1974).
[4] P. R. Holland, *The Quantum Theory of Motion. An Account of the de Broglie-Bohm Causal Interpretation of Quantum Mechanics*, Cambridge University Press, Cambridge, 1993.
[5] H. Wu and D. W. L. Sprung, Phys. Lett. A **183**, 413 (1993).
[6] P. Exner, P. Ŝeba, A. F. Sadreev *et al.*, Phys. Rev. Lett. **80**, 1710 (1998).
[7] B. I. Shklovskii and A. L. Efros, *Elctronic Properties of Doped Semiconductors*, Chapter 3, Springer-Verlag, Berlin–New York, 1984.
[8] J. R. Eggert, Phys. Rev. B **29**, 6664 (1984).
[9] M. V. Berry, Philos. Trans. R. Soc. London, Ser. A **287**, 237 (1971).
[10] I. V. Zozoulenko and K.-F. Berggren, Phys. Rev. B **56**, 1 (1997).
[11] A. Garcimartin, A. Guarino, L. Bellon, and S. Giliberto, Phys. Rev. Lett. **79**, 3202 (1997).
[12] M. Brack and R. K. Bhaduri, *Semiclassical Physics*, Addison-Wesley, Reading, Mass., 1997.
[13] K. N. Pichugin and A. F. Sadreev, Phys. Rev. B **56**, 9662 (1997).

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