

IFUSP/P-830

UNIVERSIDADE DE SÃO PAULO

INSTITUTO DE FÍSICA
CAIXA POSTAL 20516
01498 - SÃO PAULO - SP
BRASIL

PUBLICAÇÕES

IFUSP/P-830



QUANTUM SIGNATURE OF A PERIODIC ORBIT
FAMILY IN A HAMILTONIAN SYSTEM

C.P. Malta

Instituto de Física, Universidade de São Paulo

A.M. Ozorio de Almeida

Instituto de Física, Universidade de Campinas
C.P. 6165, 13081 Campinas, SP, Brazil

Março/1990

QUANTUM SIGNATURE OF A PERIODIC ORBIT FAMILY IN A HAMILTONIAN SYSTEM

C. P. Malta

Universidade de São Paulo,
 Instituto de Física,
 CP 20516, 01498 São Paulo, SP, Brazil.

and

A. M. Ozorio de Almeida

Universidade de Campinas,
 Instituto de Física,
 CP 6165, 13081 Campinas, SP, Brazil.

ABSTRACT

The periodic orbit family with the shortest period in a two dimensional anharmonic oscillator is responsible for oscillations in the smoothed density of states. We have computed the energy spectrum for a specific potential and compared the oscillations of the smoothed density of states with those predicted by semiclassical theory. We also verify that the 'scarred' intensity profile for these orbits is not affected by the period-doubling bifurcation cascade that breaks up the surrounding tori.

1. INTRODUCTION.

The formal semiclassical theory for the quantum energy spectrum, developed by Gutzwiller (1971), ascribes to each periodic orbit a term in the density of states. Generically, these orbits are embedded in families parametrized by the energy (or the period) and the phase of each contribution is basically the action S measured in units of Planck's constant \hbar . Balian and Bloch (1974) obtained similar results for the smoothed density of states, with the difference that in this case not all periodic orbits contribute but only those having period up to a finite value T , reciprocal to the energy smoothing δE according to the uncertainty principle $T\delta E \approx \hbar$. It follows that by increasing sufficiently the smoothing δE we can eliminate the contribution of all the periodic orbits so that only the average (or Weyl) density of states remains (see e.g. Berry, 1983, or Ozorio de Almeida, 1988, for reviews of these topics). By decreasing δE we can then incorporate the contribution of the family of periodic orbits with shortest period. The resulting smoothed density of states should exhibit, superposed on the averaged background, a nearly sinusoidal oscillation in energy with frequency $1/r$, where

$$r = dS/dE \quad (1)$$

is the period of the orbit.

The wave functions for these quantum states may also display 'scars' in the neighbourhood of the periodic orbits, as discovered by Heller (1984). These scars become particularly sharp if we superpose the intensity of all the wave functions in a range δE . Heller's theory for wave intensities was cast in a form quite analogous to the one for the spectrum by Bogomolny (1988) (see also Ozorio de Almeida, 1988). However, so far it is not certain whether the intensity peaks at a scar depend on the combined contribution of the many states in the range δE or whether they can be ascribed to a single strong state in this interval.

The formal semiclassical results that we are discussing cannot be completely verified by a calculation using a basis of states and a given value of Planck's constant. Conversely, the semiclassical results are useful only if they describe the approximate features of such particular quantum systems. It is therefore important to verify computationally which are the features of these theories that can be relied on in less than ideal conditions. So far most work has been concentrated on the easily accessible periodic orbits of billiard systems (as in Heller, 1984, Bogomolny, 1988). However, nonlinear oscillators,

$$H(x, y, p_x, p_y) = (p_x^2 + p_y^2)/2 + V(x, y) . \quad (2)$$

provide more realistic examples. Of these, the Hénon-Heiles potential is the most studied, but here we work with

$$V(x, y) = (x^2 + 3y^2)/2 - x^2 y + x^4/12. \quad (3)$$

This potential (codename MARTA) has a minimum at zero energy and two saddles at an energy of 0.75. The symmetry in x implies that $x = 0$, $p_x = 0$ is an invariant plane in phase space; hence this is foliated by the family of 'vertical' (y direction) periodic orbits. The potential along this plane is quadratic, so these orbits have constant period $\tau = 2\pi/\sqrt{3}$. Numerical studies of this system by Aguiar, Malta, Baranger and Davies (1987), show that this is the orbit with the lowest period below the saddle energy. Furthermore, this family generates a period-doubling bifurcation cascade starting at $E = 0.103$. Below this energy the motion in its neighbourhood is mainly regular, becoming locally chaotic at higher energies, though the system still exhibits invariant tori (Aguiar and Baranger, 1988).

The spectrum and the eigenfunctions of the MARTA potential can be calculated by diagonalizing the quantum MARTA Hamiltonian in the harmonic oscillator basis corresponding to the quadratic terms in the potential. In the following section we display the smoothed density of states of the spectrum corresponding to 595 states in the energy range $[0.0797, 0.1997]$ with $\hbar = 0.0029$, which thus includes the chaotic transition near the symmetry plane. Our numerical results are then compared with the predictions of periodic orbit theory.

In section 3 we display wave intensities, averaged over y , as functions of x . These can be compared with the wave intensities given by the hypothesis of Voros (1976, 1977) and Berry (1977) at the same energy, i.e. that which results from the assumption that the Wigner function is

a delta-function over the energy shell. Comparison with this average background reveals that individually scarred states are still present above the period-doubling bifurcation that destroys the neighbouring tori.

2. DENSITY OF STATES.

Below the saddle energy (0.75), the eigenvalue problem of the MARTA quantum system,

$$H\psi_i(x,y) = E_i\psi_i(x,y), \quad (4)$$

was solved by using the expansion

$$\psi_i(x,y) = \sum_{n=0}^{2N} \sum_{m=0}^N C_{nm}^i \varphi_n(x) \varphi_m(y), \quad (5)$$

where $\varphi_n(x)$ and $\varphi_m(y)$ are eigenfunctions of the one-dimensional harmonic oscillator Hamiltonians H_x and H_y ,

$$H_x = (p_x^2 + x^2)/2,$$

$$H_y = (p_y^2 + 3y^2)/2. \quad (6)$$

The prime in the summation means that only even n (even parity) or only odd n (odd parity) are included.

The value $n = N$, at which expansion (5) is truncated, is chosen according to the energy interval to be investigated, which, of course, has to be much below the saddle point energy. In this region we can neglect the connection with the continuum through tunneling under the saddles.

As already mentioned, one of the families of periodic orbits of the classical MARTA Hamiltonian (Aguilar, Malta, Baranger and Davies, 1987) is the so called vertical family which consists of harmonic oscillations of period $2\pi/\sqrt{3}$ in the y direction. This family undergoes a first period-doubling bifurcation at $E = 0.103$ and, in order to verify its effect on the level density, we calculated this level density in the energy interval $[0.0797, 0.1997]$. This range of energy is much below the saddle energy, therefore the expansion method with truncation can be safely used. Semiclassical results are obtained by using a small \hbar . However, too small a value of \hbar implies the diagonalization of too big a matrix, so the value $\hbar = 0.0029$ chosen by us represents a compromise. With this value the level spacing of the vertical harmonic oscillator is $\hbar \omega_y = 0.005$ and the above energy interval of energy contains 595 states. We made the truncation of expansion (5) at $N = 40$.

The density of states (histograms) as function of energy has been calculated in the above energy interval using $\delta E = 0.001$ and $\delta E = 0.002$. For the value of \hbar we are using, the number of states contained in such small δE is small giving rise to spurious fluctuations, but this problem

can be circumvented by making a Gaussian smoothing. We have used normalized Gaussians of half width equal to δE and the resulting smoothed level densities for $\delta E = 0.001$ and $\delta E = 0.002$ are displayed in figures 1 and 2, respectively. These densities were numerically obtained at energy points separated by 0.0005 and a line was drawn joining these points.

According to the periodic orbits theory, the density of states may be separated in two terms (Berry, 1983, Ozorio de Almeida, 1988),

$$d(E) = d_{av}(E) + d_{osc}(E), \quad (7)$$

where d_{av} is the average density of states (the so called Weyl term) corresponding to zero period orbits, and d_{osc} is the oscillatory term which incorporates the contribution of periodic orbits of period greater than zero.

Numerically, the Weyl term d_{av} is obtained by using a sufficiently big value of δE in the calculation of the density. The term d_{osc} is then obtained by subtracting the Weyl term from the total density $d(E)$. Therefore, the contribution to d_{osc} of the lowest period orbits may be analyzed by appropriately choosing the value of δE used in the calculation.

The Weyl term has been approximated by the Gaussian smoothed level density calculated using $\delta E = 0.04$ (see figure 3). So, using this approximation for d_{av} we obtained d_{osc} for $\delta E = 0.001$ and $\delta E = 0.002$. These results are displayed in figures 4 and 5, respectively (solid line).

In theory, each periodic orbit and all its repetitions contribute to d_{osc} . When a period n-upling occurs, new orbits are generated and the summation will include the n^{th} repetition of the original orbit plus all the new period n-upled orbits generated at the bifurcation. The vertical family is the family of periodic orbits of the classical MARTA potential (3) having the lowest period in the energy range under consideration. So, for the smoothing that we used, d_{osc} is basically obtained by considering only the contribution of the vertical family, without any repetition. In this approximation, d_{osc} is nearly a sinusoidal oscillation with the same period of the vertical family, therefore it can be approximated by

$$d_{osc}(E) = A \sin((2\pi/\hbar\omega_y) E + B). \quad (8)$$

The dominance of this period in d_{osc} is confirmed by the Fourier analysis shown in figure 4. The dashed curves displayed in figures 5 and 6 were obtained by fitting the corresponding d_{osc} to the above sin function.

It is important to note that the amplitude of a bifurcating orbit goes through a sharp peak (Ozorio de Almeida and Hannay, 1987). However, in this case of period doubling, the peak appears only for even repetitions, justifying the approximately constant amplitude over a narrow energy range in (8) for the first return of the orbit.

Now, d_{osc} obtained numerically incorporates the contributions of all periodic families having period up to $\hbar/\delta E$. It should be noted

that, depending on the energy value, already for a period twice the period of the vertical orbit, there are several orbits contributing to the density of states in the energy interval considered by us (Aguiar, Malta, Baranger and Davies, 1987). These contributions are not completely cancelled by the Gaussian smoothing in period. Therefore, it is quite remarkable that there should be such close agreement between the frequency of oscillation of d_{osc} and that of the approximation given by (8). As for the amplitude of d_{osc} , it should vary smoothly in the semiclassical limit, according to the theory. So, the large variations in amplitude observed in figures 5 and 6 cannot be accounted for in the semiclassical approximation (8), though it may result from the influence of the orbits with longer period.

3. AVERAGED WAVE INTENSITIES.

As we wanted to detect the existence of scars due to the vertical periodic family, we have calculated the state density distribution averaged over y , given by

$$\rho_i(x) = \int |\psi_i(x,y)|^2 dy = \sum_{\substack{n, n'=0 \\ \text{even}}}^N c_{n m}^i c_{n' m}^i \varphi_n(x) \varphi_{n'}(x). \quad (9)$$

(The odd parity states are zero at the origin and therefore cannot exhibit any scar due to the vertical family.)

So, this averaged wave intensity was calculated for those eigenstates with eigenvalues lying in the energy interval considered in section 2. The solid lines in figures 7, 8 and 9 show $\rho_i(x)$ corresponding to the eigenstates of energies 0.1040, 0.1043 and 0.1044, respectively. The dotted curves shown in these figures are the corresponding state density distributions $\rho_i^e(x)$, resulting from the use of the ergodic assumption (Voros, 1976, 1977), which in the case of two degrees of freedom Hamiltonian of type (2) is given by (Berry, 1977)

$$\rho_i^e(x) = \int dy \Theta(E_i - V(x,y)), \quad (10)$$

with Θ the step function.

We see that the wave intensities displayed in figures 7, 8 and 9 exhibit completely different characteristics. The state distribution in figure 7 exhibits caustic peaks which are the signature of quasiperiodic motion. The corresponding eigenvalue is just above 0.103 which is the energy value at which the vertical periodic family undergoes its first period-doubling bifurcation. The scarred wave intensity profile shown in figure 8 is virtually identical to the ones found below the bifurcation where the vertical orbit is stable. These scarred states are found near the quantized actions

$$\Delta S = n \hbar, \quad (11)$$

as previously discovered by M. Saraceno. The wave intensity displayed in Figure 9 seems to exhibit anticaustics (Berry, 1983), with the oscillations more or less following $\rho_1^e(x)$. However, as the classical underlying motion is not globally chaotic, further verification is required in order to confirm the presence of anticaustics.

ACKNOWLEDGEMENTS.

One of us (CPM) thanks the Center for Theoretical Physics at MIT, specially M. Baranger for the kind hospitality. We are indebted to Rudiger Wolff for helping in accessing the Livermore computer facilities.

We thank M A M de Aguiar for helpful discussions and useful comments G.G. Ragazzo for helping making some of the graphs. Last, but not least, we thank V.G. Franca for the final editing of the typed manuscript.

We acknowledge partial financial support from CNPq (Conselho de Desenvolvimento Científico e Tecnológico), USP (Universidade de São Paulo) and the US Department of Energy under Contract # DE-AC02-76ER03069.

REFERENCES.

- de Aguiar, M.A.M., Malta, C.P., Baranger, M. and Davies, K.T.R (1987) Ann.of Phys. 180, 167.
- de Aguiar, M.A.M. and Baranger, M. (1988), Ann.of Phys. 186, 355.
- Balian, R. and Bloch, C. (1974), Ann.of Phys. 85, 514.
- Berry, M.V. (1977), J. Phys. A: Math.Gen. 10, 2083;
(1983) "Chaotic Behaviour of Deterministic Systems", Les Houches, Session 36, ed. G. Ioss, R.G. Helleman and R. Stora. Amsterdam: North Holland, 171.
- Bogomolny, E.B. (1988), Physica D31, 169.
- Gutzwiller, M.C. (1971), J. Math. Phys. 8, 1979.
- Heller, E.J. (1984), Phys. Rev. Lett. 53, 1515.
- Ozorio de Almeida, A.M. and Hannay, J.H. (1987), J. of Phys. A20, 5873.
- Ozorio de Almeida, A.M. (1988), "Hamiltonian Systems: Chaos and Quantization", Cambridge Monographs on Mathematical Physics, Cambridge University Press.
- Saraceno, M., private communication.
- Voros, A. (1976), Ann. Inst. Poincaré A24, 31;
(1977), Ann. Inst. Poincaré A26, 343.

FIGURE CAPTIONS.

- Figure 1. Gaussian smoothed density of states $d(E)$ with $\delta E = 0.001$.
- Figure 2. Gaussian smoothed density of states $d(E)$ with $\delta E = 0.002$.
- Figure 3. The Weyl term $d_{av}(E)$, corresponding to the Gaussian smoothed density of states calculated with $\delta E = 0.04$.
- Figure 4. Fourier analysis of the smoothed density of states with $\delta E = 0.001$ (figure 1).
- Figure 5. The solid line is $d_{osc}(E)$ with $\delta E = 0.001$ and the dashed line is approximation (8) with $A = -7.290$ (standard deviation 0.653) and $B = -0.695$ (standard deviation 0.089), obtained by a least squares non-linear fit.
- Figure 6. The solid line is $d_{osc}(E)$ with $\delta E = 0.002$ and the dashed line is approximation (8) with $A = -3.364$ (standard deviation 0.440) and $B = -0.536$ (standard deviation 0.130), obtained by a least squares non-linear fit.
- Figure 7. The solid line is $\rho_i(x)$ for the eigenstate with $E = 0.1040$, exhibiting the caustic peaks characteristic of quasiperiodic motion
The dotted line is the corresponding $\rho_i^e(x)$.
- Figure 8. The solid line is $\rho_i(x)$ for the eigenstate with $E = 0.1043$, exhibiting a scar due to the vertical periodic family. The dotted line is the corresponding $\rho_i^e(x)$.
- Figure 9. The solid line is $\rho_i(x)$ for the eigenstate with $E = 0.1044$, apparently exhibiting anticaustics with oscillations that follow $\rho_i^e(x)$ (dotted line).

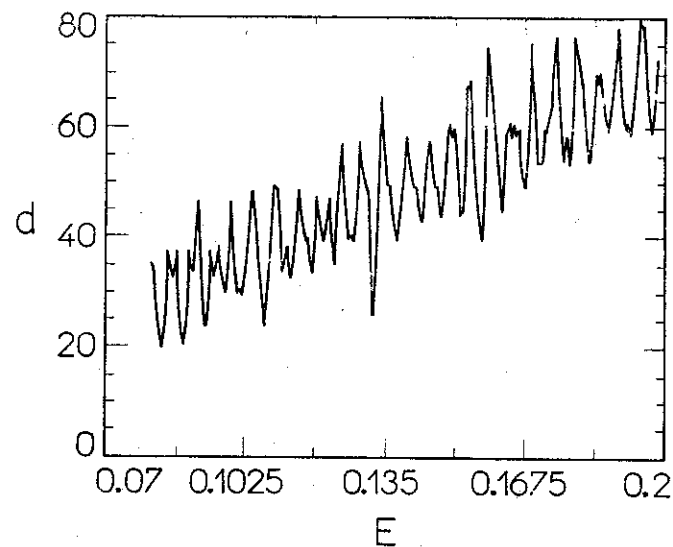


FIGURE 1

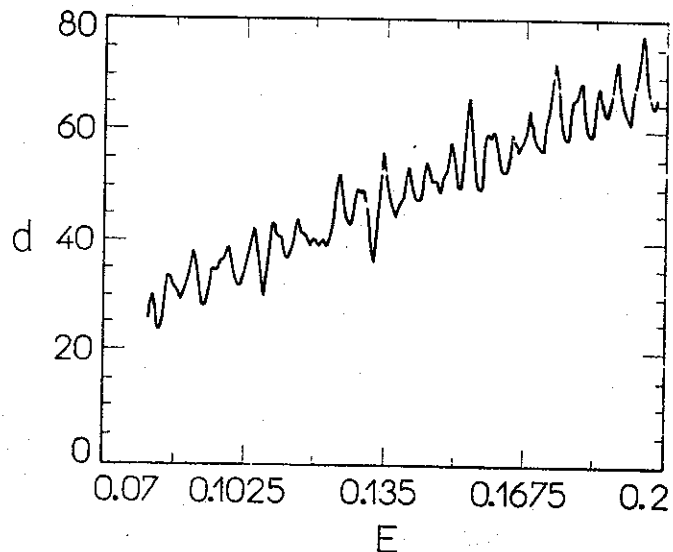


FIGURE 2

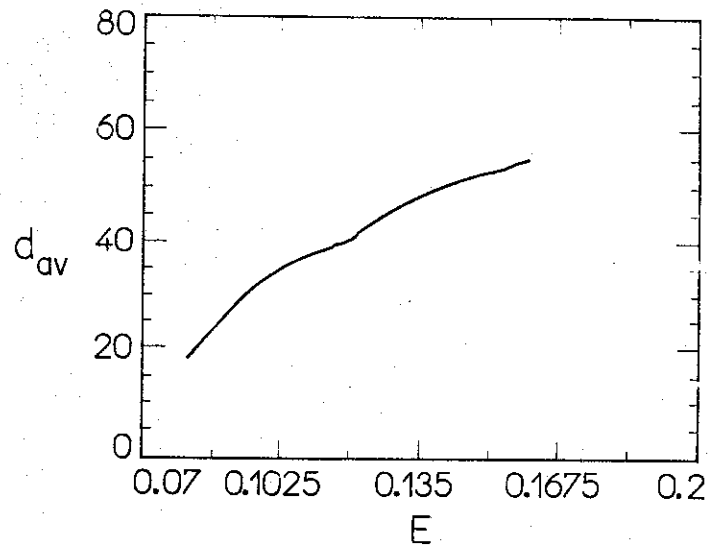


FIGURE 3

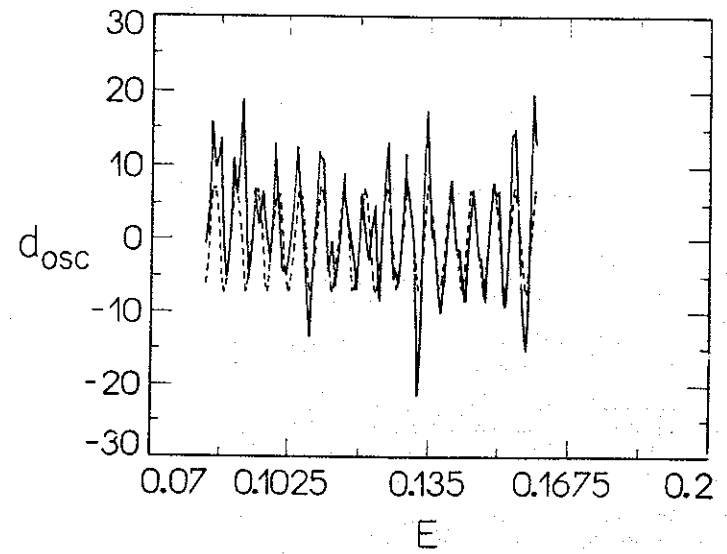


FIGURE 5

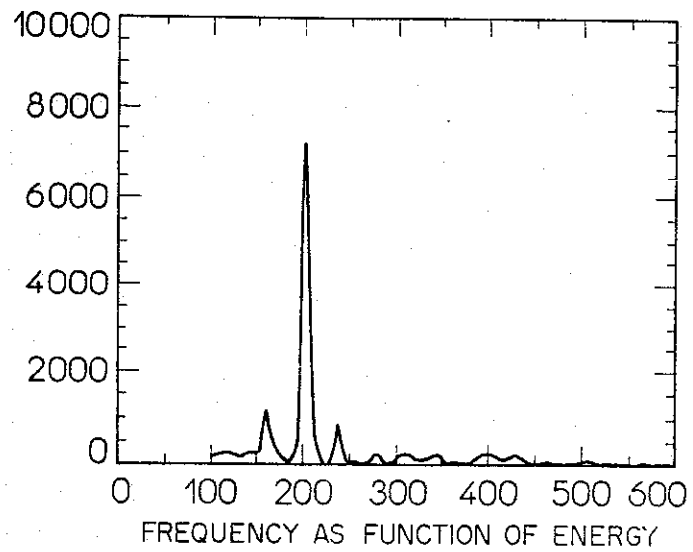


FIGURE 4

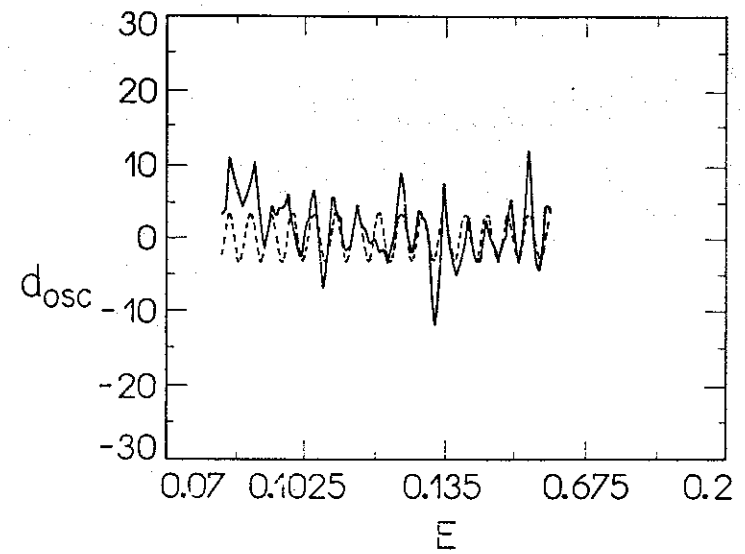


FIGURE 6

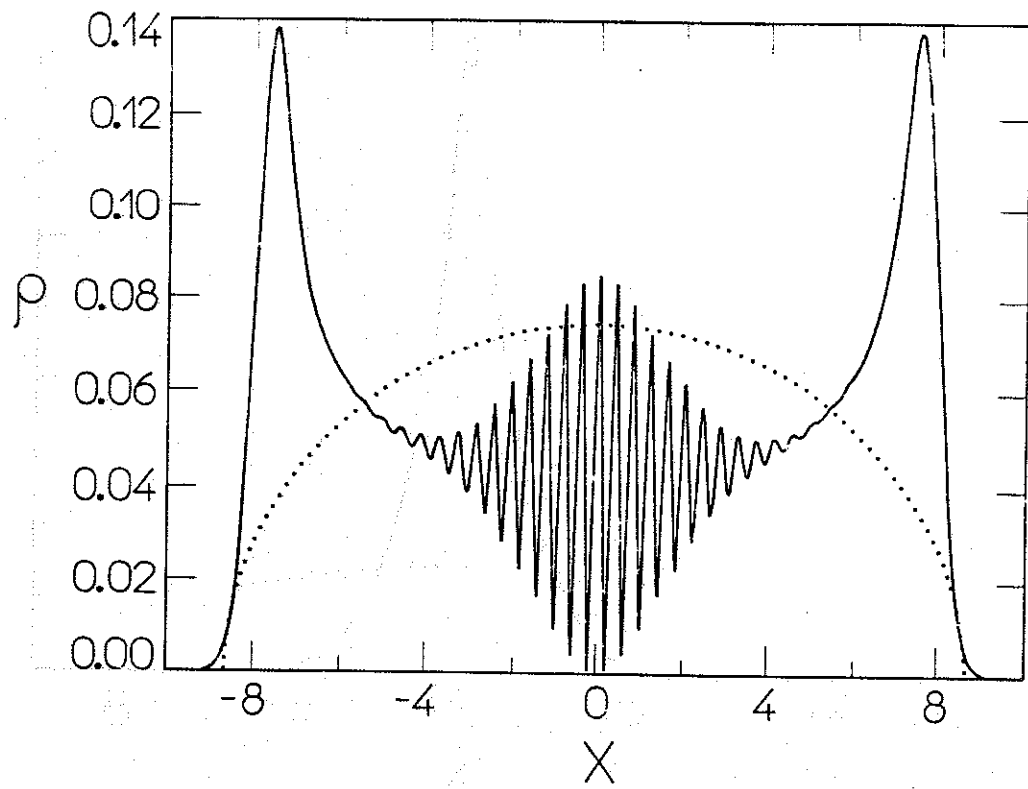


FIGURE 7

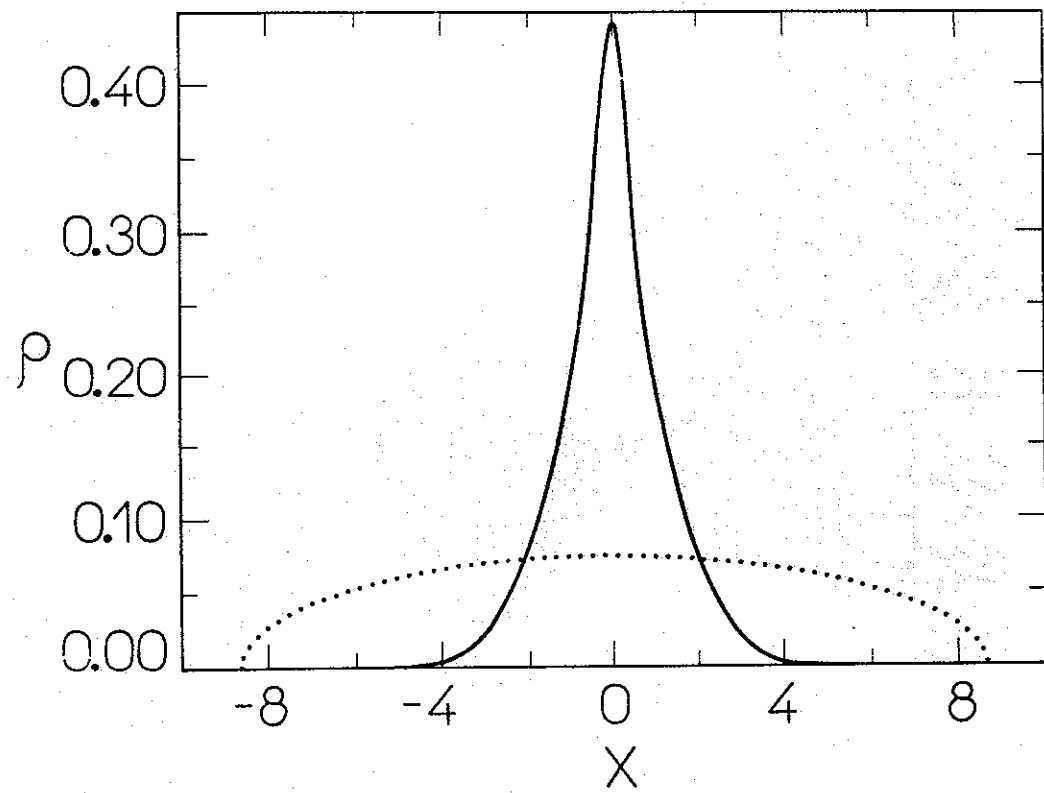


FIGURE 8

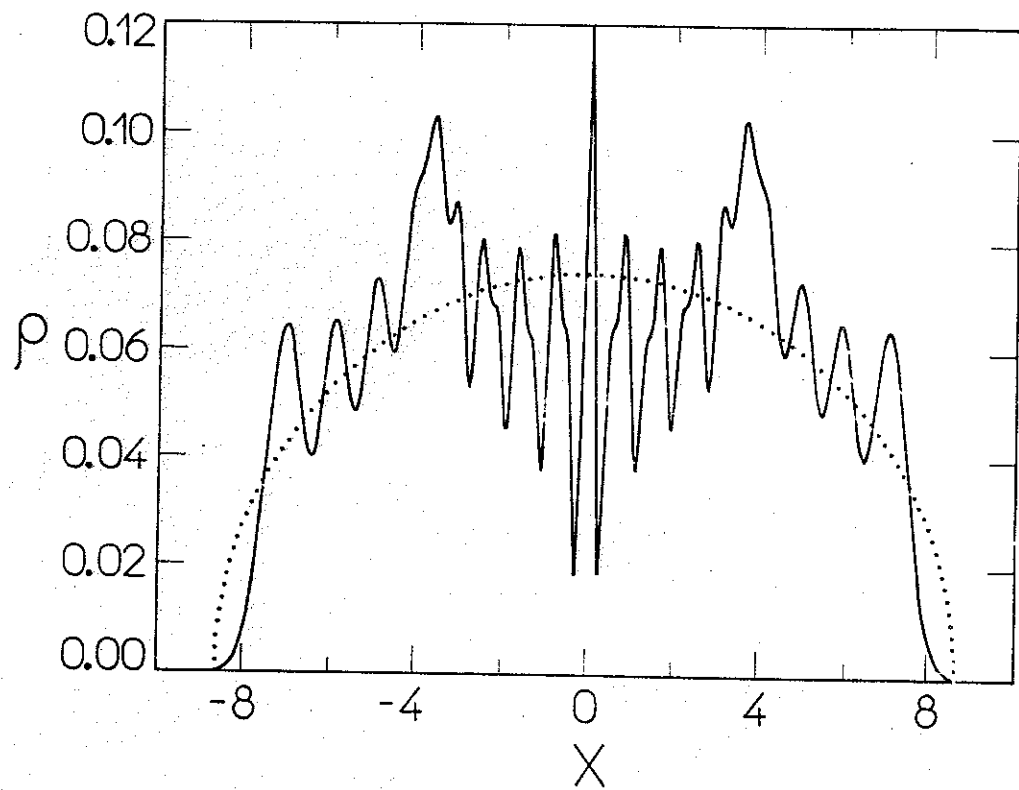


FIGURE 9