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## LETTER TO THE EDITOR

# Comparison between the exact and Brody repulsion function for the $\beta n^2$ spectrum

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**Abstract.** From the secular variation extraction of the nearest-neighbour spacing repartition function of the spectrum without an accumulation point in the part studied, an *ab initio* expression of the repulsion function is given. This expression is calculated for a  $\beta n^2$  spectrum and compared with the Brody semi-empiric repulsion function. The Brody parameters are not evaluated by fitting but calculated from the first and second moments of the nearest-neighbour spacing. Notable differences are found between the two expressions, differences which persist even for more complex spectra.

Since the early work of Thiele (1963) and Haarhoff (1963), we know how to approximate analytically the density of a Hermitian operator discrete spectrum by the use (under certain conditions of the Hermitian operator recalled below) of the inverse Laplace transform. The next step is the description of this discrete spectrum in the approximation of its  $k$ -spacing repartition function (' $k$ -spacing' for  $k$ th neighbour spacing).

The characterisation of the  $k$ -spacing repartition is important because classifications of intramolecular behaviour like  $\nu_{\text{VR}}$  (Felker and Zewail 1985) or searching in selective chemistry (Levine 1980) are based on the 'moments' of the state repartition on  $\mathbb{R}$  which control the intramolecular dynamics (Pechukas 1982).

The Wigner repulsion function (Wigner 1967) generalised by Brody (Brody *et al* 1981) and calculated by Berry within a semiclassical approximation (Berry and Tabor 1977) leads to a characterisation of the 1-spacing distribution (the nearest-neighbour spacing distribution) which is a 'semi-empiric' characterisation; the studies of the 1-spacing distribution and of the so-called repulsion parameters  $q$  have always been restricted for a given quantum spectrum to the best fitting of a states histogram after computer classification of the spacings (see for example Camarda and Georgopoulos (1983), Haller *et al* (1983) and Ishikawa and Yakawa (1985)).

We report in this letter preliminary work on the analytic approximation of the first-order repulsion function  $r_1(z, y)$  associated with the 1-spacing distribution. We recall below the spectrum decomposition method which leads to the  $k$ -spacing distribution and to the analytic formal expression of the repulsion function. The repulsion function associated with the simple ' $\beta n^2$  spectrum' is then explicitly calculated and compared with the one computed with the states histogram.

Later in this letter, the generalised repulsion function introduced by Brody is calculated directly from the knowledge of the spectrum without any histogram fitting and applied to the ' $\beta n^2$  spectrum'. Finally we compare this semi-empiric approximation

with the *ab initio* repulsion function calculated below and we present another example where the failure of the semi-empiric Brody repulsion function is much more important than in the ' $\beta n^2$ ' case.

Let us consider the discrete spectrum  $\sigma_{\text{disc}}(\hat{H}_X)$  of a semi-bound from below Hamiltonian  $\hat{H}_X$  with  $\sigma_{\text{disc}}(\hat{H}_X) \subset [w_X, +\infty[$ . The first interesting characteristic of  $\sigma_{\text{disc}}(\hat{H}_X)$  is the density of states  $\rho_X(x)$  which carries global information about the repartition of states on  $[w_X, +\infty[$ . A continuous approximation  $\bar{\rho}_X(x)$  of  $\rho_X(x)$  is directly obtained from the truncation (Thiele 1963)

$$\bar{\rho}_X(x) = \sum_{\text{pole } \mathbb{R}} \text{residue}(\text{Tr}|_{\sigma_{\text{disc}}(\hat{H}_X)}(\exp(-H_X \rho)) \exp(x\rho), \text{pole}) \quad (1)$$

of the  $(d/dx)(N_X(x))$  inverse Laplace transform if the  $\sigma_{\text{disc}}(\hat{H}_X)$  repartition function  $N_X(x)$  is majorable by  $\exp(\alpha x)$  with  $\alpha$  a constant. For another class of spectrum, this approximation can only be used when  $\sigma_{\text{disc}}(\hat{H}_X)$  has no accumulation point (Joachim 1985) with the reciprocal function of  $N_X(x)$  substituted to  $N_X(x)$  in (1).

To complete this global characterisation of  $\sigma_{\text{disc}}(\hat{H}_X)$ , generally called the secular variation characterisation of  $\sigma_{\text{disc}}(\hat{H}_X)$ , one introduces a local characterisation obtained by the elimination in  $N_X(x)$  of the absolute state position already contained in  $\bar{\rho}_X(x)$  by averaging.

Consider a bound interval  $[w_X, y]$  of  $[w_X, +\infty[$  without an accumulation point (if any in  $\sigma_{\text{disc}}(\hat{H}_X)$ ) and the associated repartition function  $n_X(x, y)$  defined by

$$n_X(x, y) = N_X(x)(1 - \Theta(x, y)) + N_X(y)\Theta(x - y) \quad (2)$$

with  $\Theta(x)$  the Heaviside function.

The self-correlation  $c_{\mu\mu}(z)$  of the density  $\mu = (d/dx)n_X(x, y)$  is only a function of the  $k$ -spacing repartition function where a  $k$ -spacing  $Z_k(j)$  is defined by  $Z_k(j) = x_{j+k} - x_j$ ,  $x_\alpha \in A(y)$  and  $A(y) = \sigma_{\text{disc}}(\hat{H}_X) \cap [w_X, y]$ :

$$\begin{aligned} c_{\mu\mu}(z) &= \int \mu(x)\mu(x-z) dz = \mathcal{F}^{-1}(|\mathcal{F}(\mu)|^2)(z) \\ &= s\delta_0 + \sum_{k=1}^{s-1} (N_X(y) - k)(\partial/\partial z)F_k^+(z, y) + \sum_{k=1}^{s-1} (N_X(y) - k)(\partial/\partial z)F_k^-(z, y) \end{aligned} \quad (3)$$

with  $\mathcal{F}$  the Fourier transform,  $s = \text{card}(A(y))$  and  $F_k^\pm(z, y)$  the  $k$ -spacing repartition functions defined by

$$F_k^\pm(z, y) = (N_X(y) - k)^{-1} \sum_{j=1}^{s-k} \Theta(z \mp Z_k(j)). \quad (4)$$

Then a local characterisation of the  $\sigma_{\text{disc}}(\hat{H}_X)$  properties restricted to  $[w_X, y]$  is reached by the extraction of the information carried by  $F_k^+(z, y)$  (or  $F_k^-(z, y)$  by symmetry) on  $\sigma_{\text{disc}}(\hat{H}_X)$ . The highest term considered in the spacing amplitude gives the precision of the local characterisation of  $A(y)$ .

Limiting the order to  $k=1$ , we have two methods to characterise the information on  $A(y)$  carried by  $F_1^+(z, y)$  for a fixed  $y$ : the characterisation of the 1-spacing distribution by its moments or by the extraction of the secular variation of  $F_1^+(z, y)$  with a truncation like (1). The repulsion function comes from the second method (see below) and the first one will be used later to deduce a semi-empiric value of the Brody repulsion parameter.

Because  $F_1^+(z, y)$  is a step normalised function on a subset of  $\sigma_{\text{disc}}(\hat{H}_X)$ , without an accumulation point by hypothesis, the truncation (1) can always be applied to the extraction of this secular variation, with (4) in (1) for  $k = 1$ , we obtain

$$\bar{F}_1^+(z, y) = (N_X(y) - 1) \sum_{\text{poles } \mathbb{R}} \text{residue} \left( \sum_{j=1}^{s-1} \exp[-\rho(Z_1(j) + z)] / \rho, \text{pole} \right). \quad (5)$$

Like  $F_1^+(z, y)$ ,  $\bar{F}_1^+(z, y)$  has bound variations and these variations decrease when  $\bar{F}_1^+(z, y)$  is closed to its upper bound. Then the variations in  $z$  of  $\bar{F}_1^+(z, y)$  are at least proportional to  $(1 - \bar{F}_1^+(z, y))$  and because  $\bar{F}_1^+(z, y)$  depends on the properties of  $A(y)$ , the proportionality coefficient must be a function of  $y$ , but also of  $z$ . This leads from the knowledge of  $\bar{F}_1^+(z, y)$  to the introduction of a function  $r_1(z, y)$  defined by

$$r_1(z, y) = -(d/dz)[\log(1 - \bar{F}_1^+(z, y))] \quad (6)$$

which gives after integration of (6) the well known expression for the  $f_1(z, y)$  1-spacing density function (Brody *et al* 1981)

$$f_1(z, y) = r_1(z, y) \exp \left( \int_0^z r_1(z', y) dz' \right). \quad (7)$$

The function  $r_1(z, y)$  (usually named the repulsion function (Brody *et al* 1981)) characterises, as an equivalent of  $\bar{F}_1^+(z, y)$  by definition, the secular variation of the 1-spacing repartition function. The principal interest of  $r_1(z, y)$  in the case of a well defined discrete spectrum is the expression proposed by Brody to approach this function which reduces the local characterisation of  $A(y)$  to a single parameter (see below).

To compare the continuous  $r_1(z, y)$  defined by (6) with the approximation proposed in the literature, we need first of all the *ab initio*  $r_1(z, y)$ , that is, the repulsion function calculated directly from (8) with  $F_1^+(z, y)$  from (5). But not many such  $r_1(z, y)$  can be explicitly calculated. The  $r_1(z, y)$  extracted below comes from the Hamiltonian

$$\hat{H}_\beta = \sum_{n \in \mathbb{R}^*} \beta n^2 |n\rangle \langle n| \quad \beta \in \mathbb{R}^{+*}.$$

Elements of  $\sigma_{\text{disc}}(\hat{H}_\beta)$  are of the type  $\beta n^2$  and the 1-spacing element  $Z_1(n) = \beta(2n + 1)$  on the interval  $[\beta, x_s]$ ; truncation (5) and definition (6) leads, for the  $Z_1(n) = \beta(2n + 1)$  of  $\beta n^2$  spectra, to (see appendix 1)

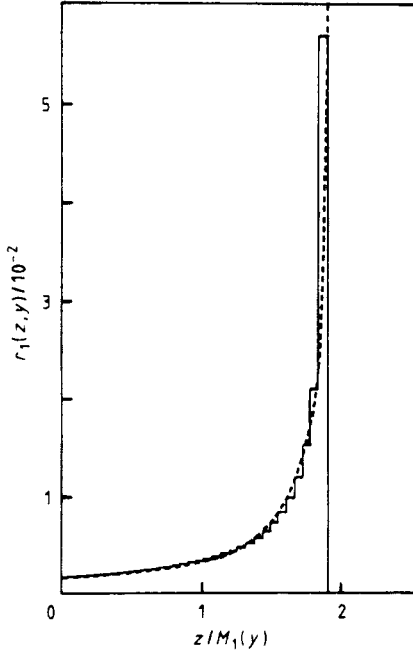
$$r_1(z, x_s) = \begin{cases} (2\beta N_\beta(x_s) - z)^{-1} & \text{for } 2\beta \leq z \leq 2\beta_s, \\ 0 & \text{for } z < 2\beta \text{ and } z > 2\beta_s. \end{cases} \quad (8)$$

The repulsion function (8) is represented in figure 1 with the function derived from the  $F_1^+(z, x_s)$  histogram.

The limiting factor in the *ab initio* calculation of  $r_1(z, y)$  is the secular variation extraction of  $F_1^+(z, y)$  because after the construction of the 1-spacing set directly from  $\sigma_{\text{disc}}(\hat{H}_X)$ , one needs to reordinate this set before the use of the truncation (5). Even for the Sinai billard  $\alpha n^2 + \beta m^2$  spectrum, the calculation of  $\bar{F}_1^+(z, y)$  is not trivial.

Then 'semi-empiric' approximations of  $r_1(z, y)$  are required. 'Semi-empiric' is taken here in the sense of the use of a parametrised continuous function for  $r_1(z, y)$  with the parameters calculated, computed from  $\sigma_{\text{disc}}(\hat{H}_X)$  or optimised from the  $\bar{F}_1^+(z, y)$  histogram.

To evaluate these parameters for the well known Brody repulsion function  $r_1(z, y) = a(q(y), y)z^{q(y)}$ ,  $q(y) \in \mathbb{R}$  one usually fits the  $f_1(z, y)$  calculated from the Brody  $r_1(z, y)$



**Figure 1.** Repulsion function for the  $\beta n^2$  spectrum on  $A(y) = [\beta, y]$  with  $\beta = 3$ ,  $y = 3 \times 10^4$  and  $M_1(y) = 303$ . The step function corresponds to the  $r_1(z, y)$  computed from the  $F_1^+(z, y)$  histogram and the dotted curve function to the *ab initio*  $r_1(z, y)$  calculated from (8).

introduced in (7) with the one computed from the  $F_1^+(z, y)$  histogram. The dependence on  $q(y)$  of  $a(y, q(y))$  may or may not be explicitly taken into account (see for example Camarda and Georgopoulos (1983), Haller *et al* (1983) and Ishikawa and Yakawa (1985)).

For a well defined spectrum, a direct evaluation of these parameters is possible, without any fitting, from the moments  $M_n(y)$  of the 1-spacing distribution defined as

$$M_n(y) = \int_0^\infty z^n f_1(z, y) dz. \tag{9}$$

Such an evaluation of the Brody coefficient is more easily compared with the *ab initio* calculation because the fitting generally depends on the number of classes chosen to compute the  $f_1(z, y)$  histogram (Casati *et al* 1985).

After a choice of the  $r_1(z, y)$  semi-empiric expression, the moments  $\bar{M}_n(y)$  of the approximated  $f_1(z, y)$  are calculated as in (9) with the use of (7). By identification of the  $M_n(y)$  and the  $\bar{M}_n(y)$  at each order (this is the semi-empiric optimisation step), we obtain a system of equations. These solutions give the value of the parameters considered in the  $r_1(z, y)$  expression.

For the two Brody parameters  $r_1(z, y)$ , only the first- and the second-order moments have to be calculated:

$$\bar{M}_j(y) = \Gamma\left(1 + \frac{j}{q(y)+1}\right) \left(\frac{a(y, q(y))}{q(y)+1}\right)^{-j/(q(y)+1)} \quad \text{for } j = 1, 2 \tag{10}$$

from the properties of the Eulerian function with  $r_1(z, y) = a(y, q(y))z^{q(y)}$  substituted in (7).

For a fixed  $y$  and after identification of  $\bar{M}_j(y)$  with  $M_j(y)$ , this leads to the two coupled equations with  $q$  and  $a$  as unknowns:

$$\frac{M_2(y)}{M_1(y)} = \Gamma\left(1 + \frac{2}{q(y)+1}\right) \Gamma\left(1 + \frac{1}{q(y)+1}\right)^{-2} \quad (11)$$

$$a(y, q(y)) = (q(y)+1) \left[ \frac{1}{M_1(y)} \Gamma\left(1 + \frac{1}{q(y)+1}\right) \right]^{q(y)+1} \quad (12)$$

As is shown in figure 2 and because  $\eta = M_2(y)M_1(y)^{-2} \geq 0$ , equation (11) admits an unique solution belonging to  $]-1, +\infty[$  for a given  $\eta$ . The parameters  $q(y)$  carries through (11) the level of state non-equally spacing on  $A(y)$  because  $\eta - 1$  is equal to the 1-spacing distribution variance normalised by  $M_1(y)$ .

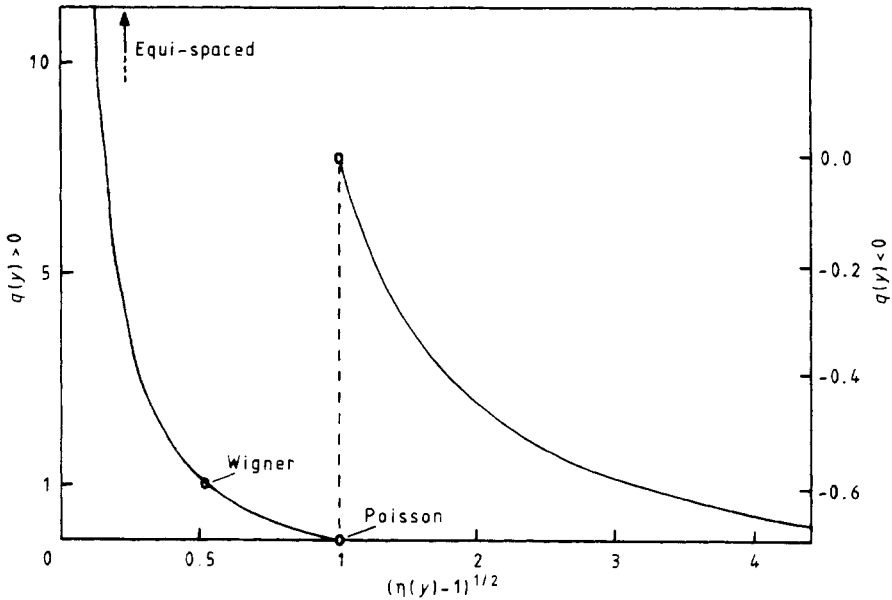


Figure 2. Evolution of the equation (11) solution  $q(y)$  as a function of the ratio  $M_2(y)/M_1^2(y)$  with  $\eta(y) = M_2(y)/M_1^2(y)$ . The  $q(y)$  corresponding to the well known Poisson and Wigner  $f_1(z, y)$  positions are shown.

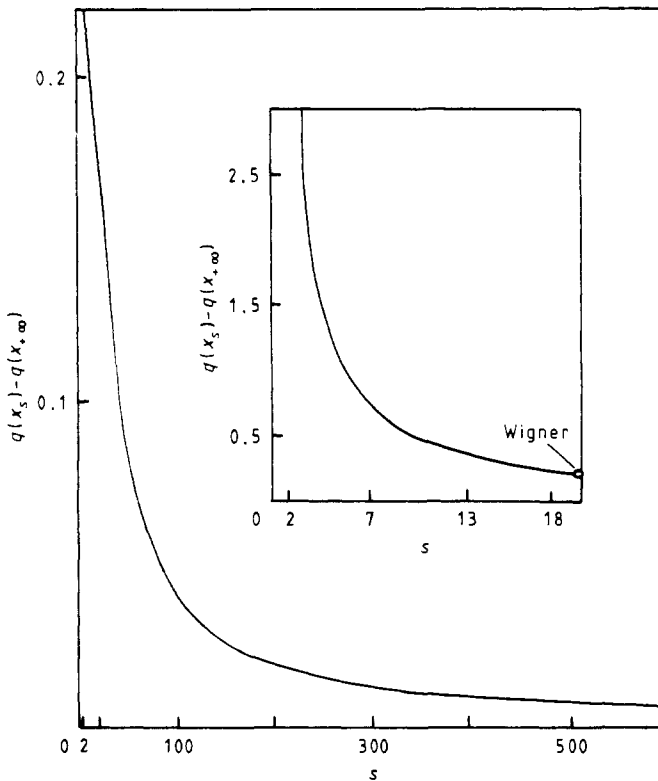
The important fact is that  $q(y)$  is not restricted to  $[0, 1]$  as proposed by Buch *et al* (1982) for fitted  $q(y)$ . With  $q(y)$  going from  $+\infty$  to  $-1$ , we come from equally spaced spectra, going to randomly spaced ones (the well known Poisson distribution with  $q = 1$ ), to reach spectra with an inhomogeneous distribution of states where aggregations of states exist.

Hydrogenic  $n^{-2}$  spectra, for example, belong to this class; for  $y = 2.5 \times 10^{-3}$ ,  $(\eta - 1)^{1/2} = 1.934$  and from figure 2  $q(y) = -0.443$ . Even vibrational spectra with a large number of modes can have negative  $q(y)$  values depending on the frequency mode repartition (Joachim 1986): for eight vibrational modes with a  $m^{1.5}$  repartition law on  $[600 \text{ cm}^{-1}, 4000 \text{ cm}^{-1}]$  and  $y = 2 \times 10^4 \text{ cm}^{-1}$ ,  $(\eta - 1)^{1/2} = 3.85$  and  $q(y) = -0.65$ .

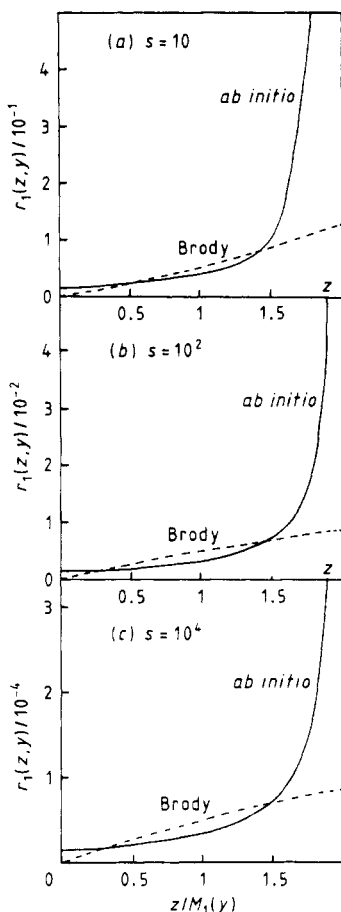
However, this explicit relation between the level of equally spacing spectra and  $q(y)$  does not mean that the Brody semi-empiric repulsion function optimised with (11) and (12) is a good approximation of the *ab initio*  $r_1(z, y)$ . It only means that for a well defined spectrum and after the direct computation of  $M_n(y)$ , one can obtain a 1-spacing distribution with only first and second moments equal to that of the spectrum. Higher-order moments of  $f_1(z, y)$  have not been used which may lead to a bad approximation for the inhomogeneous distribution of states.

For the  $\beta n^2$  spectrum studied earlier, the  $q(y)$  solutions of (11) are given in figure 3 as a function of  $y$ . The  $\eta - 1$  ratio has been calculated directly from the  $Z_1(n)$  distribution and is equal to  $s(s-2)/3(s+1)^2$  for  $y = x_s$ . For low values of  $s$ ,  $q(x_s)$  is very sensitive to local properties of the  $\beta n^2$  spectrum and distinguishes well situations very close in  $\eta - 1$ . This is not the case for large  $s$  because  $\eta - 1$  tends to its asymptotic value  $\frac{1}{3}$  which means that  $\eta - 1$  is no more sensitive to local properties of the spectrum; the state density of the  $\beta n^2$  spectrum decreases and the characterisation of local properties loses its interest.

The *ab initio*  $r_1(z, y)$  and the Brody semi-empiric function, both calculated above for the  $\beta n^2$  spectrum, are given in figure 4 for three different  $y$  values with  $\beta = 3$ . For  $0.2M_1(y) < z < 1.5M_1(y)$  the *ab initio* and Brody  $r_1(z, y)$  are relatively close but do not have the same curvature. The semi empiric Brody approximation fails for low and



**Figure 3.** Value of the repulsion parameter  $q(y)$  for the  $\beta n^2$  spectrum as a function of  $s = \text{card}(A(y))$ . Each  $q(x_s)$  is a solution of (11) with  $\eta(x_s) - 1 = [s(s-2)]/[\beta(s+1)^2]$  and  $\beta = \frac{1}{3}$ . For  $A(y) = \sigma_{\text{disc}}(\hat{H}_\beta)$ ,  $q(x_{+\infty}) = 0.79148$  and for  $\text{card}(A(y)) = 2$ ,  $q(x_2) = +\infty$ .



**Figure 4.** Comparison between the *ab initio* and Brody semi-empiric  $r_1(z, y)$ . *Ab initio*  $r_1(z, y)$  are obtained from (8) and Brody semi-empiric  $r_1(z, y)$  from (11) and (12); (a)  $y = 300$ ,  $M_1(y) = 33$ ,  $q(y) = 1.254$  and  $a(y, q(y)) = 6.47 \times 10^{-4}$ , (b)  $y = 3 \times 10^4$ ,  $M_1(y) = 303$ ,  $q(y) = 0.8314$  and  $a(y, q(y)) = 4.21 \times 10^{-5}$ , (c)  $y = 3 \times 10^8$ ,  $M_1(y) = 300\,03$ ,  $q(y) = 0.7915$  and  $a(y, q(y)) = 1.38 \times 10^{-8}$ .

high  $z$  values. The failure is much more important for high  $z$  values; the *ab initio*  $r_1(z, y)$  gives a constant  $f_1(z, y)$  on  $[2\beta, 2\beta s]$  and the semi-empiric  $r_1(z, y)$  gives a decreasing exponential  $f_1(z, y)$ . Notice that no scaling effect appears between  $y = 10$  and  $y = 10^4$ .

Thus, the semi-empiric Brody  $r_1(z, y)$  is not a good approximation for the  $r_1(z, y)\beta n^2$  spectrum. The same problem exists also for more complex spectra, even for the well known  $\alpha m^2 + n^2$  spectra with  $\alpha$  an irrational number (see below) and is under investigation for vibrational spectra (Joachim 1986).

For this class of spectra, depending on the commensurability between the vibration frequency mode the 1-spacing distribution can be monomodal, bimodal or higher (Berry and Tabor 1977, Joachim 1985) and tends to be monomodal when the number of modes increases. Then the  $q(y)$  parameter cannot be used alone to characterise the local properties of all the types of vibrational spectra because the Brody  $r_1(z, y)$  leads by construction to monomodal  $f_1(z, y)$ .



As for the  $\beta n^2$  spectrum, higher-order moments of the 1-spacing and moments of the other  $k$ -spacing are needed to construct a more accurate semi-empiric repulsion function which covers the monomodal and the others. We have no means to say for example that the bimodal case is 'artificial' (Buch *et al* 1982) because it is not the spectrum which needs to be adapted to the Brody repulsion function but this semi-empiric approximation which needs to be improved for the local characterisation of a large class of well defined spectra.

Another interesting point is the difference between the calculated solution from (11) and the optimised solution by fitting  $q(y)$ . They are not always equal even for a random distribution of states: for  $6 \times 10^3$  states with a uniform law on  $[1, 500]$  and  $y = 499.91$ , the calculated  $q(y) = 10^{-2}$  and the optimised  $q(y) = 0.0$ . But for a Sinai  $\sqrt{2}m^2 + n^2$  billiard spectrum and  $y = 9218.779$  ( $\text{card}(A(y)) = 6 \times 10^3$ ) the calculated  $q(y) = 4 \times 10^{-2}$  and the optimised  $q(y) = 0.0$ . This confirms that the Poisson law is not completely adapted for the description of the local properties of the Sinai billiard spectrum (Casati *et al* 1985).

It seems from simulations that these differences between calculated and optimised  $q(y)$  can be used to appreciate the degree of validity of the Brody semi-empiric approximation. But this needs demonstration and not only simulations (Joachim 1986).

### Appendix. Expression of $r_1(z, y)$ for the $\beta n^2$ spectrum

For a  $\beta n^2$  spectrum, the Laplace transform of  $F_1^+(z, y)$  gives

$$\mathcal{L}(F_1^+(z, y)) = (N_\beta(y) - 1)^{-1} \frac{\exp(-\beta p)[\exp(-2\beta p) - \exp(-2\beta s p)]}{p(1 - e^{-2\beta p})} \quad (\text{A1})$$

with  $s = \text{card}(A(y))$ .

The residue  $u(x)$  of the second-order pole in  $p = 0$  for an analytic function  $f(p)$  of the form

$$f(p) = \frac{\exp(-ap) \exp(xp)}{p[1 - \exp(-bp)]} \quad (\text{A2})$$

is  $u(x) = [(x - a)/b] + \frac{1}{2}$  which must be taken equal to zero in our case for  $x < a - \frac{1}{2}b$  to obtain a positive function for  $z > 0$ . This result applied to (A1) leads from the truncation (5) to

$$\bar{F}_1^+(z, y) = \begin{cases} 0 & \text{for } z \leq 2\beta \\ \frac{z - 2\beta}{2\beta(N_\beta(y) - 1)} & \text{for } 2\beta \leq z \leq 2\beta s \\ \frac{s - 1}{N_\beta(y) - 1} & \text{for } z > 2\beta s. \end{cases} \quad (\text{A3})$$

The expression (8) of  $r_1(z, y)$  is then obtained from (A3) used in the definition (6).

### References

- Berry M V and Tabor M 1977 *Proc. R. Soc. A* **356** 375  
 Brody T A, Flores J, French J B, Mello P A, Pandey A and Wong S S M 1981 *Rev. Mod. Phys.* **53** 385

- Buch V, Gerber R B and Ratner M A 1982 *J. Chem. Phys.* **76** 5397  
Camarda M S and Georgopoulos P D 1983 *Phys. Rev. Lett.* **50** 492  
Casati G, Chirikov B V and Guarneri I 1985 *Phys. Rev. Lett.* **54** 1350  
Felker P M and Zewail A H 1985 *J. Chem. Phys.* **82** 2961, 2975  
Haarhoff P C 1963 *J. Mol. Phys.* **101**  
Haller E, Köppel H and Cederbom L S 1983 *Chem. Phys. Lett.* **101** 215  
Ishikawa T and Yakawa T 1985 *Phys. Rev. Lett.* **54** 1617  
Joachim C 1985 *Thesis Dissertation ENSAE* no 103  
— 1986 to be published  
Levine R D 1980 *Chem. Phys. Lett.* **76** 254  
Pechuckas P 1982 *J. Phys. Chem.* **86** 2241  
Thiele E 1963 *J. Chem. Phys.* **39** 3258  
Wigner E P 1967 *SIAM Rev.* **9** 1