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Trace formula for an ensemble of bumpy billiards

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Abstract. We study the semiclassical quantization of an ensemble of billiards with a small random shape deformation. We derive a trace formula averaged over shape disorder. The results are illustrated by the study of supershells in rough metal clusters.

1. Introduction

Quantum billiards have been extensively studied as model systems having a chaotic or integrable classical dynamics (see e.g. [1]). They have also been considered as simple models for atomic nuclei or metal clusters. More recently they have been studied experimentally in ballistic microstructures [2, 3] and in microwave cavities [4]. In most of the experimental studies only an average shape for the equivalent billiard is determined. For instance, metal clusters have an underlying ionic background which implies an unavoidable degree of roughness of order of the interatomic distance, i.e. of order of the Fermi wavelength. For microstructures the roughness is mainly due to the irregularities in the depletion layer which can be estimated of being also of order of the Fermi wavelength [5]. Moreover clusters are produced in large amounts in molecular beams and one has to consider an ensemble of shapes. Similarly one also frequently considers an ensemble of microstructures (typically $\sim 10^5$) with a size dispersion ranging from 2% [6] up to 30% [3].

The mean free path in the experiments quoted above is larger than the typical distances in the system, thus the billiard model is still meaningful. Nevertheless it should be corrected due to shape irregularities. In this paper we make an attempt to study this phenomenon by considering an ensemble of billiards (in any dimension) obtained by a random deviation from a fixed initial shape (hereafter denoted as the perfect or unperturbed shape). We speak below of rough or bumpy billiards.

The paper is organized as follows: in sections 2 and 3 we derive a semiclassical trace formula averaged over the ensemble of rough billiards. As an illustration the method is applied in section 4 to study the supershell oscillations in rough metal clusters. We give our conclusions and make a comparison with previous works in section 5.

2. Green function in the presence of shape disorder

Modern semiclassics have made extensive use of trace formulae such as those derived by Gutzwiller in the context of quantum chaos (see [1] and references therein) or for quantum

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billiards by Balian and Bloch [7]. In these approaches the level density is obtained by computing the trace of the Green function $G(r_B, r_A, k)$, solution of the Helmholtz equation with Dirichlet or Neumann boundary conditions. It is written in the semiclassical limit as a sum of contributions arising from the classical orbits of the system. In the case of a billiard it reads schematically:

$$G(r_B, r_A, k) = \sum_{A \to B} \mathcal{D}(k) \mathrm{e}^{\mathrm{i}(kL - \mu\pi/2)} \tag{1}$$

where the sum is taken over the classical trajectories going from point A to point B. In (1) k is the wavevector and it is related to the energy by $\hbar k = \sqrt{2mE}$ (or $\hbar k = E/c$ for microwave cavities); μ is a Maslov index and $\mathcal{D}(k)$ an amplitude characterizing the trajectory of length L considered. A general expression for $\mathcal{D}$ can be found in [1, 7].

Let us now treat the case of the rough billiard. We consider that the shape disorder is weak enough so that a point r_C on the frontier of the bumpy billiard can be written unambiguously as

$$r_C = r_{C_0} + h(r_{C_0}) n_0 \tag{2}$$

where r_{C_0} is a point of the frontier of the perfect billiard and n_0 the normal at this point. h is a random displacement, the characteristics of which will be specified later.

Let us branch the perturbation (2) starting from a perfect billiard. The direct orbit going from A to B without bouncing on the boundary is not affected. If the shape modification is small enough (this will be made mathematically precise later) orbits experiencing only a few bounces will not be drastically altered (see figure 1). At first order in the semiclassical approximation we will consider that only the change in length is of importance, because it appears in the rapidly oscillating term $\exp(\mathrm{i}kL)$ of (1). The modification of the slowly varying amplitude $\mathcal{D}(k)$ is simply neglected. Long orbits, in contrast, experience many bounces and they may be completely different in the rough enclosure and the perfect billiard. They will also be drastically different from a bumpy billiard to another, and ensemble averaging will very efficiently damp their contribution. Hence it is legitimate in the semiclassical limit to work in a perturbative approach where the only extra contribution with respect to the perfect billiard is the modification of the length of the orbits in (1). The spirit of the present approach is very common (see e.g. [8–10]) and the results are similar to those obtained by other techniques (see below).

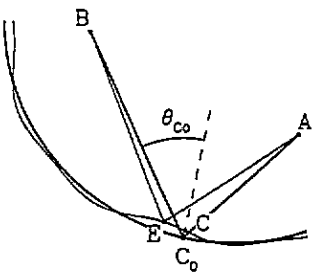

Figure 1. Classical orbits going from point A to point B with one bounce on the boundary. The bold curves correspond to the perfect billiard and the thin curves to the bumpy billiard. Point C_0 (resp. point E) is the point of specular reflection on the perfect (resp. bumpy) enclosure. θ_{C_0} is the normal reflection angle at C_0. C is the intersection of the normal at C_0 with the bumpy boundary.

If we denote by δL a modification in the length of an orbit due to surface roughness, using the notation in figure 1, for a single bounce trajectory one obtains

$$\delta L = (AE + EB) - (AC_0 + C_0B) \simeq (AC + CB) - (AC_0 + C_0B). \tag{3}$$

In (3) C_0 (resp. E) is the point of specular reflection in the perfect (resp. bumpy) billiard. Since $AE + EB$ is an extremum of the length, at first order it can be computed replacing E by a nearby point. This has been done in the right-hand side of (3) where point C was used, C being the intersection of the normal to the perfect billiard at C_0 with the bumpy frontier (see figure 1). This can easily be extended to orbits with n bounces and simple geometry yields

$$\delta L \simeq 2\sum_{j=1}^{n} h(r_{C_j})\cos\theta_{C_j} \tag{4}$$

where the sum is extended over all the bouncing points C_j of the classical trajectory on the boundary of the perfect billiard (θ_{C_j} is the normal angle of incidence at point C_j, see figure 1).

Then the semiclassical Green function in the rough billiard is written as

$$G(r_B, r_A, k) \simeq \sum_{A\to B}^{0} \mathcal{D}(k)e^{i(kL-\mu\pi/2)} \exp\left(2ik\sum_{j=1}^{n} h(r_{C_j})\cos\theta_{C_j}\right) \tag{5}$$

where the upper index 0 indicates that the sum is taken over the trajectories of the *perfect billiard.*

Careful derivation puts the following limitations to the use of equations (4) and (5):

(i) $|h|/L \ll |\nabla h| \ll 1$ or, in other words, L should be greater than the typical distance between two bumps, itself being greater than the amplitude of shape disorder. These restrictions ensure that replacing E by C in (3) is legitimate and that $\delta L \ll L$.

(ii) $k|h|^2 \ll L$ ensures that using the approximate length $L + \delta L$ in the semiclassical formula yields corrections which are indeed small compared to the main term (5).

(iii) One should also make sure that diffractive corrections to the leading-order semiclassics can be safely neglected. Hence, the typical distance between two bumps ($|h|/|\nabla h|$) should be larger than the wavelength ($1/k$). If not, the amplitude $\mathcal{D}(k)$ is significantly modified by the surface roughness.

Keeping in mind the physical examples given in the introduction one sees that among the above restrictions only the ones involving ∇h are not trivially satisfied. Indeed in the case of a large shape disorder the distance between two bumps is of order of the amplitude of a bump (then ∇h is of order 1) and also diffractive effects will have to be taken into account. Hence (5) is rigorously applicable only for small roughness (characterized by the restrictions (i), (ii) and (iii)). Nevertheless we will see in section 3 that in this limit the effects of the surface roughness are already very noticeable. Hence one can argue that when (5) is no longer valid the associated oscillations in the level density are already almost completely damped (see (12)).

We recall that (5) is only valid for short orbits. The contribution of long orbits in the bumpy billiard cannot be inferred from the motion in the perfect billiard. In order to have a formula rigorously applicable let us now damp the contribution of long orbits by performing an ensemble average of the Green function. The computation is straightforward and the average quantity reads

$$\langle G(r_B r_A, k)\rangle \simeq \sum_{A\to B}^{0} \mathcal{D}(k)e^{i(kL-\mu\pi/2)} \prod_{j=1}^{n} \chi(2k\cos\theta_{C_j}) \tag{6}$$

where χ is the characteristic function of the rough shape [11]. It is the Fourier transform of the probability density of the frontier displacement h:

$$\chi(s) = \int_{-\infty}^{+\infty} p(h) \mathrm{e}^{\mathrm{i}sh} \, \mathrm{d}h. \tag{7}$$

In (6) we have made the hypothesis that the bounces were separated by a distance larger than the correlation length of the shape disorder, i.e. $p(h(r_{C_1}), \ldots, h(r_{C_n})) = p(h(r_{C_1})) \times \cdots \times p(h(r_{C_n}))$. This restriction is not necessary but it simplifies the presentation. Following [10] one could think of deformations strongly violating this assumption: this would be the case, for instance, of an unperturbed circle going to a rough ellipse. In this case it will always be possible to use the present formalism if we consider the perfect ellipse as the unperturbed billiard.

Most authors (see [11]) choose a Gaussian distribution for h with standard deviation σ:

$$p(h) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{h^2}{2\sigma^2}\right) \qquad \text{and} \qquad \chi(s) = \exp\left(-\frac{s^2\sigma^2}{2}\right). \tag{8}$$

Note here that on the basis of equation (8) only one cannot check the validity of restrictions (i), (ii) and (iii) above; they mainly concern the correlation length of the random function h and not only the characteristic function χ which is our unique ingredient. The restrictions will be fulfilled if σ is smaller than the correlation length, itself being smaller than typical distances in the billiard.

The physics embodied in equation (6) can be simply interpreted by noting that the wave propagates as in a perfect billiard with, at each bounce, an extra damping factor $\chi(2k\cos\theta_{C_j})$ (i.e. $\exp(-2k^2\sigma^2\cos^2\theta_{C_j})$ in the Gaussian model (8)). The general form $\chi(2k\cos\theta_{C_j})$ is commonly obtained in Kirchhoff theory of wave scattering from rough surfaces [11]. As anticipated this damps very efficiently the contribution of orbits experiencing many reflections. The quantity $k\sigma\cos\theta_{C_j}$ is known as the Rayleigh parameter [12] and characterizes to what extent an incident wave is sensitive to surface roughness; as one would intuitively expect, the sensitivity is at a maximum for perpendicular incidence ($\cos\theta_{C_j} \simeq 1$) and short wavelengths ($k\sigma \gg 1$).

3. Trace formula in the bumpy billiard

The next step in the derivation of a trace formula is to compute the level density by taking the trace of the Green function:

$$\rho(k) = -\frac{2d_S k}{\pi} \operatorname{Im} \int \mathrm{d}^D r \, G(r, r, k) == -\frac{2d_S k}{\pi} \operatorname{Im} \operatorname{Tr} \hat{G}(k). \tag{9}$$

In (9) the integral extends over the interior of the billiard and D is the dimension of space. $\hat{G}(k)$ is the operator whose matrix elements in configuration space give $G(r_B, r_A, k)$. d_S accounts for a possible spin degeneracy (in this case $d_S = 2$, $d_S = 1$ otherwise).

It is customary to separate the contribution of the quasi zero length orbits to which the semiclassical approximation (1) does not apply. These orbits contribute to the smooth part $\bar{\rho}(k)$ of the level density through the 'Weyl expansion' (see e.g. [13]). In three dimensions and for Dirichlet boundary conditions it reads

$$\bar{\rho}(k) = d_S \left(\frac{Vk^2}{2\pi^2} - \frac{Sk}{8\pi} + \cdots\right) \tag{10}$$

where V is the volume of the billiard and S its surface area. In the typical case of a bumpy sphere of radius R with disorder of type (8) the average $\langle\bar{\rho}(k)\rangle$ is easily computed; one

obtains $\langle V\rangle = 4\pi(R^3/3+\sigma^2 R)$ and $\langle S\rangle = 4\pi(R^2+\sigma^2)$. σ is supposed to be small compared to R, thus surface roughness poorly affects the smooth part of the spectrum: for practical computations we will approximate $\langle\tilde{\rho}(k)\rangle$ by the value $\tilde{\rho}(k)$ in the perfect billiard. We have given here a generic three-dimensional example but the same holds in any dimension.

A quantity of primary interest is the oscillatory part $\tilde{\rho}(k)$ of the level density. As shown by Gutzwiller [1] and Balian and Bloch [7], inserting the semiclassical Green function (1) in equation (9) and performing a non-trivial stationary phase analysis leads to a trace formula which reads schematically:

$$\tilde{\rho}(k) = \sum_{\text{PO}} \mathcal{A}(k)\sin(kL + \nu\pi/2). \tag{11}$$

The sum (11) extends over all the classical periodic orbits (POs) of the system. As in (1) $\mathcal{A}(k)$ is a slowly varying amplitude and ν a Malsov index characteristic of the PO of length L considered (see [1, 7]). Some POs may form continuous families, i.e. some orbits—forming a continuous set—may all have the same length and the same topology (such as the bouncing ball orbit in the stadium billiard or the POs in integrable enclosures). Two orbits of the same family differ only by their bouncing points. Each family is represented by a single term in the summation (11) but its amplitude is enhanced by additional powers of k with respect to the contribution of an isolated orbit. This is related in [14] to local (possibly global) continuous symmetries of the Hamiltonian.

If one now wishes to write a trace formula for a rough billiard in contrast to what happens for the Green function, the form (11) of $\tilde{\rho}(k)$ is different in the bumpy and in the perfect billiard. The reason is that some POs may appear in continuous families and roughening destroys these families. This can be illustrated with the following two-dimensional example: consider a rectangular billiard of which one edge—the upper one say—has been modified to adopt a sinusoidal shape. One of the important continuous families of POs in the perfect rectangle—the vertical bouncing ball—is reduced in the bumpy rectangle to only a couple of orbits (those hitting the sinusoidal upper edge at points with horizontal tangent). Nevertheless the level densities of the two systems are certainly very similar if the edge deformation is small. This type of problem has been recently addressed in [10, 15] and deserves careful treatment. For isolated orbits it might, in some cases, be explained semiclassicaly by the introduction of complex POs in the trace formula (see the discussion in [7] and also [16]). However, we can bypass these kind of subtleties when averaging over disorder because it is legitimate to permute the trace and the average: $\langle \operatorname{Im}\operatorname{Tr}\hat{G}(k)\rangle = \operatorname{Im}\operatorname{Tr}\langle\hat{G}(k)\rangle$. Hence $\langle\tilde{\rho}(k)\rangle$ can simply be computed by inserting the average $\langle G(r, r, k)\rangle$ in the trace (9). Since $\langle G(r, r, k)\rangle$ is evaluated by using the orbits of the perfect billiard, the saddle point can be performed in the usual manner and yields the average oscillating part of the level density:

$$\langle\tilde{\rho}(k)\rangle \simeq \sum_{\text{PO}}^{0} \mathcal{A}(k)\sin(kL + \nu\pi/2)\prod_{j=1}^{n}\chi(2k\cos\theta_{C_j}). \tag{12}$$

The index 0 in the summation indicates as before that all the quantities are evaluated in the unperturbed billiard. Hence n in (12) is the number of bounces of a PO in the perfect billiard, the θ's are the normal angle of incidence.

Formula (12) is the most important result of the paper. It is valid for rough billiards in any dimension. It is interesting to note that when considering an integrable perfect billiard with *an ergodic perturbation*, the contribution of short orbits is correctly accounted for by equation (12), even without ensemble averaging. By ergodic, we mean that 'any statistical average taken over many different parts of one shape realization is the same as an

average over many realizations' [11]. In the case of integrable unperturbed billiards, all the orbits occur in families and the spatial integration (9) over a continuous family is—by the hypothesis of ergodicity—equivalent to ensemble averaging (this was certainly not the case in the simplified example above of sinusoidal deformation of a rectangle billiard because sine is not an ergodic function). We recall that this is not correct for long orbits which may be very different in the bumpy and the perfect billiard, in this case ensemble average is necessary to damp the associated oscillations.

To fix the ideas we apply (12) to a bumpy sphere of radius R. The total average level density $\langle\rho\rangle \simeq \bar{\rho} + \langle\tilde{\rho}\rangle$ is plotted on figure 2 for two values of the surface roughness in the Gaussian model (8): $\sigma = 0.04R$ and $0.06R$. The amplitude $\mathcal{A}(k)$ for each PO in the perfect sphere can be found in [7]. Seventy-five POs were included, with a maximum length of 26 times the radius. More precisely in the terminology of [7] the maximum values of the parameters are $t = 5$ and $p = 15$ (t being the winding number of an orbit around the centre and p the number of bounces). We also indicate with black arrows the location of the first 15 eigenlevels in the unperturbed sphere. One sees on the figure that in the lower part of the spectrum, the wavelength being large, surface irregularities do not perturb the eigenstates much and there is still a strong bunching of levels. This shell effect gradually disappears for increasing energies (when the wavelength becomes comparable with the amplitude of the disorder).

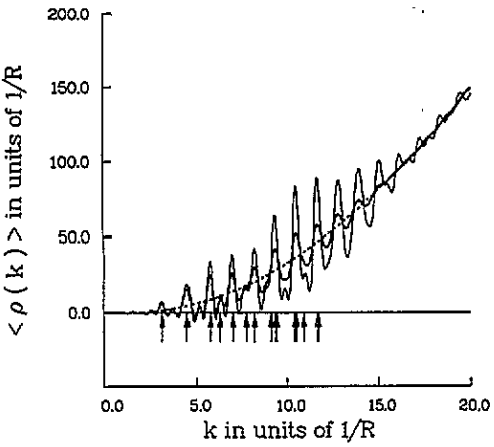

Figure 2. Total average level density in bumpy sphere for $\sigma = 0.04R$ (full curve) and $\sigma = 0.06R$ (bold curve). The broken curve represents the smooth term $\bar{\rho}(k)$. The black arrows indicate the location of the first 15 eigenlevels in the perfect sphere.

4. Supershells in rough metal clusters

In this section we illustrate the above results with the example of shell structure in metal clusters. Rough clusters will be described by a simple model first introduced in [17]: N electrons are moving independently in a bumpy sphere. The radius R of the perfect sphere scales with N so that the mean electronic density is kept constant and equal to its bulk value : $R = r_S N^{1/3}$, r_S being the Wigner–Seitz radius of the bulk material. The standard deviation from this average shape is of order of atomic distances i.e. of order r_S. Note that such irregularities are to be taken into account even if the cluster is 'liquid-like': the mean velocity of the ionic cores is always by several orders of magnitude smaller than the typical electronic Fermi velocity. Hence, as far as electronic motion is concerned, the ionic cores can be considered as frozen and this automatically implies a certain degree of surface roughness.

In the unperturbed sphere, due to the high symmetry of the potential there is a strong bunching of levels leading to shell structure and magic numbers (see e.g. [18]). This shell structure is modulated when the cluster size grows (it first disappears, then increases, etc). This is called the 'supershell structure' and was first noticed in [7] and seen experimentally by the Copenhagen group [19]. We will here study this effect in a rough cluster.

One of the most important observables when studying shell structure is the shell energy which is the oscillating part of the total energy. Shells are experimentally detected on a mass spectrum; roughly speaking clusters with relatively smaller total energy (corresponding to minima of the shell energy) are more stable and will be more numerous in a beam. This is also correlated with larger ionization potential, but for this observable shell effects decrease with cluster size, making its study more difficult.

The Fermi wavevector k_F and total energy E_{tot} are defined by

$$N = \mathcal{N}(k_F) = \int_0^{k_F} \rho(k)\,dk \qquad \text{and} \qquad E_{tot}(N) = \int_0^{k_F} \frac{\hbar^2 k^2}{2m}\rho(k)\,dk. \quad (13)$$

In (13) $\mathcal{N}(k)$ is the integrated level density or spectral staircase. As the level density, $\mathcal{N}$ can be written as the sum of a smooth quantity $\bar{\mathcal{N}}$ and an oscillating part $\tilde{\mathcal{N}}$. The same holds for k_F and E_{tot} considered as functions of N. The smooth terms are defined by

$$N = \bar{\mathcal{N}}(\bar{k}_F) = \int_0^{\bar{k}_F} \bar{\rho}(k)\,dk \qquad \text{and} \qquad \bar{E}_{tot}(N) = \int_0^{\bar{k}_F} \frac{\hbar^2 k^2}{2m}\bar{\rho}(k)\,dk. \quad (14)$$

As explained before we will identify the average smooth quantities $\langle \bar{E}_{tot} \rangle$ and $\langle \bar{k}_F \rangle$ with their value in the perfect sphere. On the basis of the Weyl expansion in the sphere and of (14) one obtains the following relations:

$$\bar{k}_F(N) = \kappa_F \left[1 - \frac{a_2}{3a_3}\left(\frac{N}{a_3}\right)^{-1/3} + \frac{a_2^2 - 3a_1a_3}{9a_3^2}\left(\frac{N}{a_3}\right)^{-2/3} + \cdots \right] \quad (15)$$

and

$$\bar{E}_{tot}(N) = \varepsilon_F \left[\frac{3a_3}{5}\left(\frac{N}{a_3}\right) - \frac{a_2}{2}\left(\frac{N}{a_3}\right)^{2/3} + \frac{a_2^2 - 2a_1a_3}{3a_3}\left(\frac{N}{a_3}\right)^{1/3} + \cdots \right] \quad (16)$$

where $a_3 = 2d_S/9\pi$, $a2 = -d_S/4$, $a_1 = 2d_S/3\pi$ (see [13]). κ_F and ε_F are the bulk Fermi wavevector and Fermi energy: $\kappa_F r_S = a_3^{-1/3}$ and $\varepsilon_F = \hbar^2\kappa_F^2/2m$.

The average oscillating part is obtained by subtracting (16) from the average total term. It is computed using the following approximation:

$$\langle \tilde{E}_{tot} \rangle = \left\langle \int_0^{k_F} \frac{\hbar^2 k^2}{2m}\rho(k)\,dk \right\rangle - \bar{E}_{tot} \simeq \int_0^{\langle k_F \rangle} \frac{\hbar^2 k^2}{2m}\langle \rho(k) \rangle\,dk - \bar{E}_{tot}. \quad (17)$$

The right-hand side of (17) can be considered as a simple first approximation of the exact result. It is made necessary by the difficulty mentioned above for estimating $\rho(k)$ in an individual rough cluster. We can invoke the hypothesis of ergodicity of surface disorder to make this approximation sound: for a cluster such as that created in a molecular beam one can argue that the individual level density will have a pattern very similar to the one displayed in figure 2 (cf the discussion in section 3). Hence, although in a given cluster $\rho(k)$ is exactly a sum of delta pics, the bunching of levels in an individual spectrum will disappear at the same wavelength as that predicted in the average $\langle \rho(k) \rangle$.

Then $\langle \tilde{E}_{tot} \rangle$ can be computed with the following scheme: one first determines $\langle k_F \rangle$ by numerical inversion of the first term of equation (13) (with $\langle \rho \rangle$ replacing ρ) and the integral of the second term is then computed numerically. One can also evaluate the asymptotic

behaviour of the integrals (13) to get an analytical expression. For this purpose the exact Fermi wavevector in written as $k_F = \bar{k}_F + \tilde{k}_F$, where $\bar{k}_F$ is given by (15) and $\tilde{k}_F$ is supposed to be small. Then performing on $\mathcal{N} = \bar{\mathcal{N}} + \tilde{\mathcal{N}}$ a first-order limited expansion one gets

$$\mathcal{N}(k_F) \simeq \bar{\mathcal{N}}(\bar{k}_F) + \tilde{k}_F \left(\frac{d\bar{\mathcal{N}}}{dk}\right)_{\bar{k}_F} + \tilde{\mathcal{N}}(\bar{k}_F) + \tilde{k}_F \left(\frac{d\tilde{\mathcal{N}}}{dk}\right)_{\bar{k}_F}. \tag{18}$$

Since $\mathcal{N}(k_F) = \bar{\mathcal{N}}(\bar{k}_F) = N$ by definition (see (13, 14)) one obtains

$$\tilde{k}_F \simeq -\frac{\tilde{\mathcal{N}}(\bar{k}_F)}{\bar{\rho}(\bar{k}_F) + \tilde{\rho}(\bar{k}_F)}. \tag{19}$$

This expression can be evaluated by keeping only the leading order of $\tilde{\mathcal{N}}$ (obtained by integration of (11)) and neglecting the oscillatory term at the denominator. Then averaging over disorder yields:

$$\langle \tilde{k}_F \rangle \simeq \frac{1}{\bar{\rho}(\bar{k}_F)} \sum_{PO}^{0} \frac{\mathcal{A}(\bar{k}_F)}{L} \cos(\bar{k}_F L + \nu\pi/2) \prod_{j=1}^{n} \chi(2\bar{k}_F \cos\theta_{C_j}). \tag{20}$$

Then the shell energy $\tilde{E}_{tot}$ is computed from the difference between the total energy and its smooth part:

$$\begin{aligned} \tilde{E}_{tot} = E_{tot} - \bar{E}_{tot} &= \int_{\bar{k}_F}^{k_F} \frac{\hbar^2 k^2}{2m} \bar{\rho}(k)\, dk + \int_{0}^{k_F} \frac{\hbar^2 k^2}{2m} \tilde{\rho}(k)\, dk \\ &\simeq \tilde{k}_F \frac{\hbar^2 \bar{k}_F^2}{2m} \bar{\rho}(\bar{k}_F) + \int_{0}^{\bar{k}_F} \frac{\hbar^2 k^2}{2m} \tilde{\rho}(k)\, dk + \tilde{k}_F \frac{\hbar^2 \bar{k}_F^2}{2m} \tilde{\rho}(\bar{k}_F). \end{aligned} \tag{21}$$

In (21) we replaced the integrals by their large N approximations. The dominant contribution is obtained by integrating by parts the integral appearing in the last term of (21); this cancels due to relation (19). After averaging over disorder the next order reads:

$$\langle \tilde{E}_{tot} \rangle \simeq -\frac{\hbar^2 \bar{k}_F}{m} \langle \tilde{\mathcal{F}}(\bar{k}_F) \rangle \simeq \frac{\hbar^2 \bar{k}_F^2}{2m} \sum_{PO}^{0} \frac{2\mathcal{A}(\bar{k}_F)}{\bar{k}_F L^2} \sin(\bar{k}_F L + \nu\pi/2) \prod_{j=1}^{n} \chi(2\bar{k}_F \cos\theta_{C_j}). \tag{22}$$

$\mathcal{F}(k)$ is a primitive of $\mathcal{N}(k)$ which has been estimated at first order on the right-hand side of equation (22). This formula gives an accurate approximation of the value of $\langle \tilde{E}_{tot} \rangle$ computed numerically; the result is shown in figure 3 for the Gaussian model (8) and for several values of the surface roughness ($\sigma/r_S = 0$, 0.1, 0.2 and 0.3). The broken curve corresponds to equation (22) and the full curve to numerical evaluation of the integrals (13), (17). Here the integration adds an extra smoothing compared to figure 2 and one does not need to take into account so many orbits; the figure includes 35 POs up to a length $L = 12R$. In fact a very reasonable result can be obtained with only the seven shortest orbits; however, we have included more orbits here to have an accurate description of the shell effect in the supershell region $N^{1/3} \simeq 8$.

We see in figure 3 that the shell structure is very sensitive to surface irregularities in the small amplitude. Nevertheless roughness reduces all oscillations without modifying the qualitative features of the supershells. Hence the present approach legitimates the usual explanation of supershell effects in rough metal clusters as being due to the interference of the square and triangular orbits [7, 19], although these orbits might not exist in an individual cluster. Including temperature effects and quantitatively comparing them with the experimental results could fix an order of magnitude for the irregularities of the surface of large metal clusters. A very rough estimate based on separation energies for small clusters gives the value $\sigma \sim 0.2 r_S$ [20].

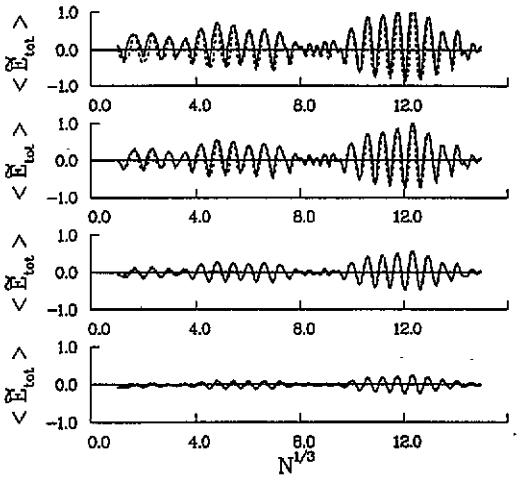

Figure 3. Average oscillating part of the total energy is rough metal clusters as a function of $N^{1/3}$ for several values of surface roughness : $\sigma/r_S = 0$ (upper graph), 0.1, 0.2 and 0.3 (lower graph). $\langle \tilde{E}_{tot} \rangle$ is expressed in units of the bulk Fermi energy ε_F. The full curve corresponds to numerical evaluation of the integrals (13), (17) and the broken curve to equation (22).

5. Discussion

In this paper we have studied the oscillating part of the level density in billiards with small size shape irregularities and we have derived a semiclassical trace formula averaged over shape disorder. The important feature of the level density is the gradual disappearance of the oscillations with increasing energy: when the wavelength is of order of the typical size of the surface defects this induced a shift in the eigenenergies which leads after averaging to a structureless level density.

The same type of approach has recently been used to study, within the semiclassical approximation, the role of families of orbits broken by a small perturbation of an initial shape having a local continuous symmetry. The authors of [15] studied the bouncing ball orbit in a deformed stadium billiard and in [10] a general trace formula is derived accounting for the role of broken families. In the present work, the main difference is the inclusion of an ensemble average yielding a formula which is also valid for isolated orbits. Moreover averaging damps the contribution of long orbits to which the simple perturbation technique (4), (5) does not apply. This averaging method is motivated by the experimental techniques of mesoscopic and cluster physics.

The method has been applied to study supershell oscillations in metal clusters using a model accounting for the irregularities of the surface due to the underlying ionic structure. It is also of interest in ballistics microstructures with shape irregularities [21].

The problem of surface roughness of metal clusters has recently been addressed using another approach: in [22] the effect of disorder is represented via addition to the Hamiltonian of a random matrix perturbation (cf [23]). The results for the average level density and shell oscillations are qualitatively very similar to what is presented here. In addition the authors of [22] argue that these effects could explain experimental shifts in the measured mass distribution. Note that in [22] and also in the present study the effects of temperature are indirect: although the usual temperatures reached in experiments are small compared to the Fermi energy (one remains in the very degenerate limit $k_B T \ll \varepsilon_F$) they are sufficient to

induce a disorder of the ionic arrangement which has a sizeable effect on the shell structure.

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