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Maximum entropy ansatz for transmission in quantum conductors: a quantitative study in two and three dimensions

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Abstract. — The transmission of electrons through a disordered conductor is described by a transmission matrix t. In random matrix theory the joint probability distribution of the eigenvalues of $t^\dagger t$ can be derived from a maximum entropy ansatz in which the mean eigenvalue density is given as a constraint. For a microscopic Anderson model, we examine the density for different shapes of the conductor (quasi–1d,2d, 3d). For the high transmission modes the form of the density is independent of disorder, size and dimensionality. We derive expressions for the eigenvalue correlations implied by the maximum entropy ansatz and compare these with the actual correlations of the Anderson model spectrum. We find that the correlations are qualitatively correct in all dimensions. However, the ansatz does not reproduce the weak system shape dependence of the universal conductance fluctuations (UCF), giving always results close to the quasi- 1d UCF- value. A careful study of the variances of different appropriate quantities indicates that the ansatz is quantitatively exact in quasi–1d over the whole spectrum of $t.t^\dagger$, but correctly describes the correlations in higher dimensions on intervals which are larger in the bulk of the spectrum than near the edge. We show that eigenvalues near the edge of the spectrum, corresponding to high transmission or reflection, remain correlated to associated non isotopically distributed eigenvectors.

1. Introduction.

Since the discovery of non self- averaging conductance fluctuations in mesoscopic conductors [1, 2], it has become necessary to reconsider various fundamental aspects of quantum electronic transport. In particular, the one-parameter scaling theory of localisation [3] has been challenged [4] on the ground that the conductance is not a self-averaging quantity, and that it is necessary to consider the full distribution of conductance rather than just the mean or typical value. Indeed it has been argued [4] that the large moments of the distribution show non-universal scaling behaviour, although this may not imply the absence of a universal limiting

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distribution [5] with a few system dependent parameters. A major difficulty in resolving such basic questions arises from the fact that most methods [6] permit the calculation of average quantities only, as opposed to, say, arbitrary n-point correlation functions.

One approach that provides the possibility of obtaining the full distribution of conductance is based on the theory of random matrices [7, 8]. It exploits the connection between conductance g and the eigenvalues $\{\lambda_a\}$ of a certain combination of transfer matrices describing the transport [9]. These eigenvalues are directly related to the eigenvalues of $t.t^\dagger$, where t is the transmission matrix of the disordered conductor. A global maximum entropy ansatz [8] then permits the calculation of the full eigenvalue distribution subject to a given constraint, e.g. their average density $\sigma(\lambda)$. The approach expresses this distribution in terms of a simple Coulomb gas analogy and provides a simple qualitative explanation for the universal conductance fluctuations (UCF) in the metallic regime [7], and for the effects [8, 10] of change of symmetry due to magnetic field or spin-orbit scattering [11].

However, despite strong qualitative hints [12, 13, 14], it has not so far been possible to demonstrate that the method is valid outside the quasi- 1d limit. Indeed exact quantitative agreement with the quasi- 1d UCF value for the variance of conductance has been obtained only by a mapping [15] on to an alternative model [16] which is valid in quasi-1d only [17]. It is therefore very important to clarify the validity of the global maximum entropy ansatz in higher dimensions.

In a first attempt [14] to address this issue, we studied the two point correlation functions of numerically unfolded spectra of microscopic 2d–Anderson models. In the bulk of the spectrum, the correlations were in agreement with universal expressions occurring in random matrix theory. However, since we are dealing with strictly positive eigenvalues, an important edge effect was discovered for the small positive eigenvalues and shown to yield a non universal contribution to their correlations. This effect, which though not in contradiction with the maximum entropy ansatz, did not allow us to exclude the possibility of dimensionality dependent corrections for the small eigenvalues.

In the present work, we present a second attempt to test the validity of the maximum entropy ansatz outside the quasi–1d limit. Instead of an uncontrolled numerical unfolding of the spectrum, we use an analytical (or a more accurate cubic spline) fit to the constraint containing the physical information and extend our study to three dimensions. We find that the functional form of the constraint does not depend on disorder, size or dimension for the small eigenvalues. This allows us to define a maximum entropy model where detailed information about the system is contained in a few quantities which parameterise a single particle potential $V(\lambda)$ for the eigenvalues. We show that within this model, it is possible to calculate explicitly and exactly any n-point correlation function for a given finite size system. Comparisons with independent numerical solutions of tight binding Anderson Hamiltonians allow us to put the global maximum entropy ansatz to the most stringent test. We restrict ourselves to the metallic regime (weak disorder case), leaving the localized regime (strong disorder case) for a separate publication [13].

This paper is organized as follows: in section 1 we review how the eigenvalue distribution is determined from the average eigenvalue density by the global maximum entropy ansatz. In section 2 we identify how the shape of the conductor enters the formulation by studying the densities of quasi–1d, 2d and 3d microscopic models which obey the known dimensionality dependence of UCF. For simplicity we focus attention on systems under applied magnetic field (unitary case) and show in section 3 how the correlation functions are given in terms of a set of orthogonal polynomials. Further we derive a general method for determining these polynomials. (We point out that arbitrary n-point correlation functions could be obtained and analyzed for possible non-universal scaling behavior at the tail of the distribution [4].) In section 4, the

two point correlation functions calculated from the global ansatz are compared with those obtained directly from the microscopic model. We present illustrative curves of the two point correlations functions in the bulk and at the edges of the spectrum, which do not show within the statistical accuracy a failure of the maximum entropy model in any dimension. In section 5, the conductance fluctuations implied by the random matrix model are calculated. We obtain in all dimensions variances close to the quasi–1d UCF value, showing that the real spectra are a little less rigid in two and three dimensions than assumed by the theory. These variances have been obtained both from transmission, which mainly probes the correlations at the lower edge of the spectrum, and from reflection which probes the upper edge of the spectrum. Cutting off the contribution to the transmission or reflection of eigenvalues smaller than a certain value, we compare the cut–off dependence of the fluctuations given by the microscopic calculations and by the theory. We find that the theory clearly provides a more accurate description for quasi–1d systems than for 3d systems. A careful analysis of the eigenvalue fluctuations indicates that the discrepancy is due to an overestimation of the correlations between the bulk and the two edges of the spectrum in higher dimensions. In section 6 we review the current understanding of the validity of a random matrix description of the Hamiltonian matrix, where the Thouless energy E_c defines a relevant scale for the spectrum. We propose a corresponding scale $\lambda_c(\lambda)$ for the transmission spectrum and we discuss how such a concept could be based on the appropriate time scales characterizing the transmission and reflection modes. We also discuss a possible generalization of our global maximum entropy approach in which more general constraints involving the eigenvectors are imposed. This leads us to investigate one of the underlying assumptions of the maximum entropy ansatz: that of an isotropic distribution of eigenvectors invariant under unitary transformation and uncorrelated with the eigenvalues. We find that for the microscopic model the eigenvectors are not fully randomized as assumed. A "memory effect" persists in the diffusive regime: good (bad) transmission remains slightly correlated with incoming modes of the outside leads having a large (small) longitudinal kinetic energy. Since the assumption of completely random eigenvectors implies an infinite range logarithmic interactions between the eigenvalues, we suggest that a screening of these interactions could result from the imposition of appropriate constraints on the eigenvectors.

1. The global maximum entropy model for transmission.

A quantum conductor can be viewed as a complex N–channel elastic scatterer and the scattering of electrons at the Fermi energy described by a $2N * 2N$ transfer matrix M. The usual Landauer approach to quantum transport in a two–probe geometry allows us to express [9] the conductance g (in units of e^2/h) in terms of the N doubly degenerate real positive eigenvalues $\{\lambda_a\}$ of the matrix

$$X = \frac{M.M^\dagger + (M.M^\dagger)^{-1} - 2\mathbf{1}}{4} \tag{1}$$

as

$$g = 2\sum_{a=1}^{N} \frac{1}{1+\lambda_a} \tag{2}$$

The factor two takes the spin degeneracy into account and $\mathbf{1}$ is the $2N \times 2N$ identity matrix. Denoting by t and r the $N \times N$–transmission and reflection matrices, the eigenvalues T_a and R_a of $t.t^\dagger$ and $r.r^\dagger$ can also be simply expressed in terms of the $\{\lambda_a\}$:

$$T_a = \frac{1}{1+\lambda_a} \tag{3}$$

$$R_a = \frac{\lambda_a}{1+\lambda_a} \tag{4}$$

The total transmission and reflection coefficient $T = \sum_{a=1}^{N} T_a$ and $R = \sum_{a=1}^{N} R_a$ satisfy from current conservation: $T + R = N$. This yields for the variances:

$$\mathrm{var}(T) = \mathrm{var}(R) = \frac{\mathrm{var}(g)}{4} \tag{5}$$

Within the global maximum entropy ansatz [8] the distribution of the $\{\lambda_a\}$ has the form

$$P(\{\lambda_a\}) = \prod_{a,b}^{N} |\lambda_a - \lambda_b|^{\beta} \prod_{c=1}^{N} \exp[-\beta . V(\lambda_c)]. \tag{6}$$

For systems where time reversal symmetry is broken $\beta = 2$. For time reversal symmetric systems $\beta = 1$ in the absence of strong spin orbit scattering. We omit from the present study the case $\beta = 4$ corresponding to strong spin orbit scattering [11]. The distribution (6) is obtained by taking the "most random statistical ensemble", for the X–matrix distribution with the average eigenvalue density $\sigma(\lambda)$ imposed as a constraint. In a mean field approximation it is possible to show that:

$$V(\lambda) = \int_0^{\infty} \sigma(\lambda') \ln|\lambda - \lambda'| \mathrm{d}\lambda' \tag{7}$$

For the derivation we refer the reader to the work by Wigner [18] on the semi- circle law characterizing the densities of the Gaussian ensembles. We may rewrite the distribution in the form $P(\{\lambda_a\}) = \exp[-\beta H(\{\lambda_a\})]$, where the eigenvalue "Hamiltonian" H is given by

$$H(\{\lambda_a\}) = -\sum_{a<b}^{N} \ln|\lambda_a - \lambda_b| + \sum_{c=1}^{N} V(\lambda_c) \tag{8}$$

and β^{-1} plays the role of "temperature". The logarithmic interaction term is universal, depending only on the symmetries of the transfer matrix. The single particle potential $V(\lambda)$, which confines the eigenvalues is then the only point at which information on system parameters, including dimensionality, enters the approach. This is the classic "Coulomb gas analogy" in random matrix theory in a form adapted to describe transmission. A formal justification for [15] this analogy can be given in the quasi–1d limit only. Our purpose here is to critically test its validity in higher dimensions.

For later convenience we mention an alternative definition [19] of $\{\lambda_a\}$ in terms of a polar decomposition of M. This decomposition is convenient for discussion of the structure of the eigenvectors of X, $t.t^{\dagger}$ and $r.r^{\dagger}$. It requires 4 unitary matrices $u^{(i)}$ and a real diagonal matrix Λ, whose elements are again the eigenvalues $\{\lambda_a\}$ of X.

$$M = \begin{pmatrix} u^{(1)} & 0 \\ 0 & u^{(3)} \end{pmatrix} \begin{pmatrix} \sqrt{1+\Lambda} & \sqrt{\Lambda} \\ \sqrt{\Lambda} & \sqrt{1+\Lambda} \end{pmatrix} \begin{pmatrix} u^{(2)} & 0 \\ 0 & u^{(4)} \end{pmatrix} \tag{9}$$

For time reversal symmetric systems where $\beta = 1$, we have the additional relations:

$$u^{(3)} = (u^{(1)})^{*}, \quad u^{(4)} = (u^{(2)})^{*} \tag{10}$$

The $u^{(i)}$ characterize how the different incoming and outgoing channels are mixed by the sample, while the $\{\lambda_a\}$ describe the decay of the transmission coefficients of the "eigen-channels"

Table I.

L_x	L_y	L_z	E	B	W	N	$< T >$	var(T)
20	1	80	0	0.02	0.85	12	3.36	0.072
20	1	20	0	0.02	2	12	3.45	0.099
6	6	6	1.25	0.1	5.5	12	3.39	0.126

of the disordered conductor. One can easily see that $t.t^\dagger$ is diagonalizable by the unitary transformation $u^{(1)}$.

$$t.t^\dagger u^{(1)} = u^{(1)} \frac{\mathbf{1}}{\mathbf{1}+\Lambda}. \tag{11}$$

The a^{th} column of $u^{(1)}$ contains the projections on the N propagating channels of the non–disordered leads of the eigenvector of $t.t^\dagger$ associated with the eigenvalue $1/(1+\lambda_a)$.

The main limitation of the maximum entropy ansatz is the assumption that the eigenvectors of X are distributed at random and are uncorrelated with the eigenvalues. This means that the distribution of the u–matrices is just given by the invariant Haar measure on the unitary group U(N). Note that an arbitrary constraint on X would correlate eigenvalues and eigenvectors. It is only because we consider here for X a maximum entropy ensemble where only a *spectral* constraint is imposed that we have the Coulomb gas analogy for the eigenvalue statistics with the classical values of β. This is not the most general assumption and an arbitrary constraint need imply not only a single particle potential. In particular it could give rise either to an additional logarithmic interaction [20] over the whole spectrum (changing the effective temperature β^{-1}) or to some more complicated screening of the logarithmic interaction, which would limit our ability to calculate arbitrary n-point correlation functions exactly.

2. Eigenvalue densities and single particle potentials for different system shapes.

To see if there is indeed enough physical information in $\sigma(\lambda)$, particularly concerning the system dimensionality, we have studied this quantity for quasi- 1d, 2d and 3d conductors modelled by microscopic Anderson- Hofstadter Hamiltonians with the parameters given in the table I.
The system transverse dimensions are L_x, L_y and the longitudinal dimension L_z. The energy E is measured from the band centre in units of the nearest neighbour hopping energy. We assume a diagonal disorder with a rectangular distribution of width W measured in the same units. The strength of disorder has been adjusted in order that the three samples are distinguished only by their shape and not by their averaged transmission $< T >$ which in all cases are approximately equal. A magnetic field of strength B, measured in units of flux quanta per lattice cell, is applied in the $+y$ direction. The energy and field have been chosen to ensure that the number of propagating modes N is the same in all cases.

In perturbation theory [1] (assuming a rectangular geometry,) the diffusion modes are characterized by a wave–vector of transverse components q_x and q_y and of longitudinal component q_z. The shape dependence of conductance fluctuations arises through a factor proportional to $\sum_{q_x,q_y,q_z}(q_x^2+q_y^2+q_z^2)^{-2}$. In quasi–1d where $L_z >> L_x, L_y$, the contribution of the $q_x = q_y = 0$ modes dominates and this factor reduces to $\sum_{q_z}(q_z^2)^{-2}$, while it is equal to $\sum_{q_x,q_z}(q_x^2+q_z^2)^{-2}$ for $d = 2$. Substituting continuous integrals to summations, one gets a clear shape dependence of the variance of T (0.296(3d), 0.185(2d), 0.133 (quasi–1d)) in the absence of a magnetic field ($\beta = 1$). The field ($\beta = 2$) halves these values. The numerically generated ensembles of 30,000

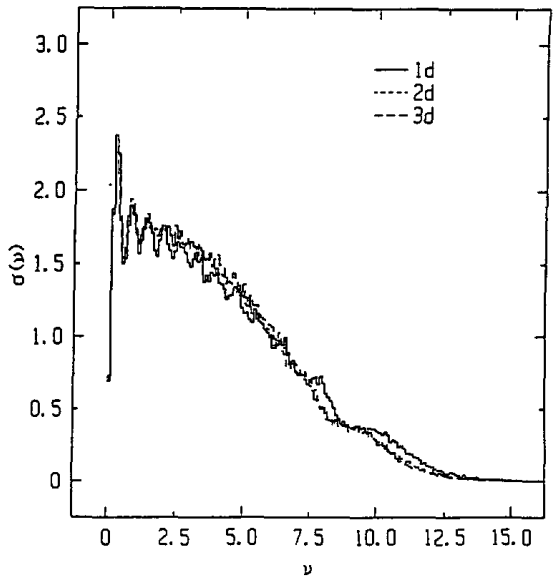

Fig.1. — Shape dependence of the density $\sigma(\nu)$. $20 * 80$ strips (1d), $20 * 20$ squares (2d) and $6 * 6 * 6$ cubes (3d).

samples we have studied exhibit a similar dimensionality dependence. In figure 1 the density $\sigma(\nu)$) of the numerically generated ensembles are shown, where for the sake of clarity we have made a transformation to the variable ν defined as

$$\lambda = \frac{\cosh(\nu) - 1}{2} \tag{12}$$

We immediately see that dimensionality appears only very weakly as a small correction to the density of the larger eigenvalues. This suggests that it is unlikely that the global maximum entropy model can correctly describe the shape dependence of the UCF.

To eliminate the possibility of a deviation of β from the values determined on the symmetry grounds ($\beta = 1$ or 2) we have examined the nearest neighbour spacing distribution and the Δ_3 statistics [21] of the unfolded spectra. Unfolding refers to a transformation of the original highly non- uniform spectrum to a spectrum with a uniform average eigenvalue density. In all dimensions the spacing distribution, which reflects the local eigenvalue repulsion, agrees with the Wigner surmise for $\beta = 1, 2$ without visible deviations. The result for the Δ_3 statistic, which measures the deviation of the eigenvalues of the unfolded spectrum from a regular sequence as a function of the average number of eigenvalues, is shown in figure 2. The random matrix theory is extremely accurate for the quasi–1d samples but there is a slight discrepancy for $d = 2$, which becomes more pronounced for $d = 3$. The integration in the Δ_3 statistics is taken over an interval starting at the origin.

Returning to the analysis of the original unfolded spectra we evaluate directly, rather than by use of (7), the single particle potential $V(\lambda)$ as $< \sum_{a=1}^{N} |\lambda - \lambda_a| >$ .The results are presented in figure 3 where a comparison is also made with a two parameter fit of the form

$$V(\lambda) = a \ln^2(1 + b\lambda). \tag{13}$$

In strictly one dimension, where there is only one eigenvalue and hence no interaction term, such a form leads to a log–normal distribution for large resistances [22]. A similar fit has

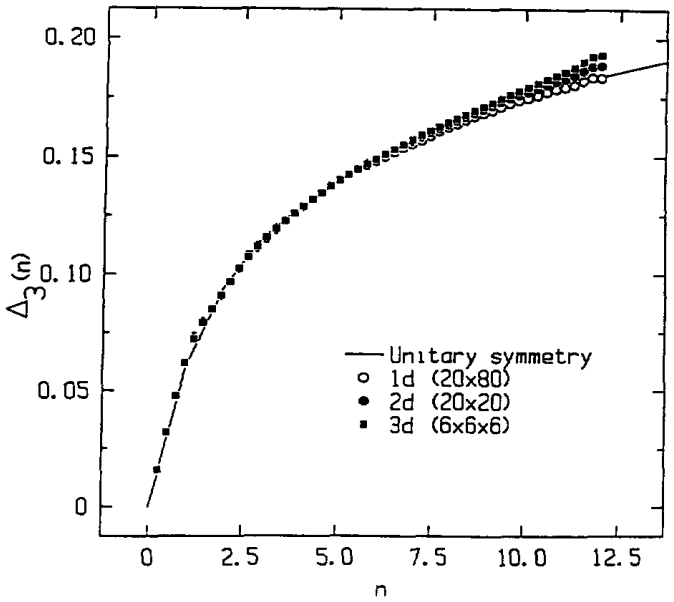

Fig.2. — Δ_3-statistics obtained from unfolded spectra for different dimensions. The solid line is the universal curve for the standard Gaussian Unitary Ensemble.

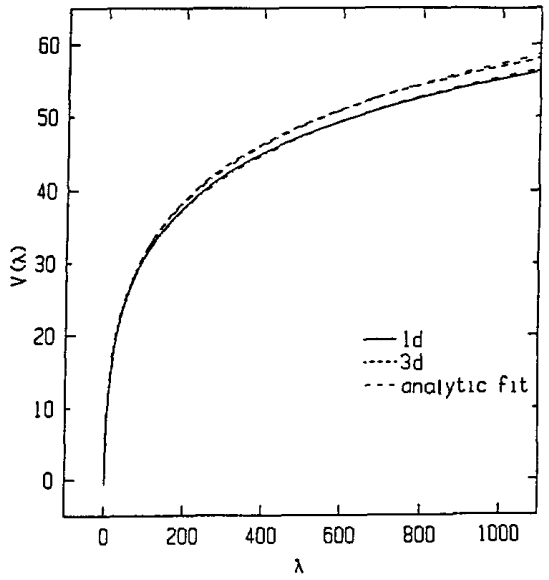

Fig.3. — 3 Potential $V(\lambda)$ evaluated from strips (1d, solid line) and cubes (3d, dashed line) compared to the analytical fit (13) (dot–dasher line). $a = 0.6719(0.72776)$ and $b = 8.877, (7.206)$ for $d = 1(d = 3)$.

also been made to data for 3d random quantum wire networks [13] in the insulating regime, indicating that there is some universality in this form for $V(\lambda)$.

3. The method of orthogonal polynomials for non–polynomial $V(\lambda)$..

Given an explicit potential $V(\lambda)$, the maximum entropy model yields for the joint probability distribution of the N eigenvalues $\{\lambda_a\}$:

$$P_N(\{\lambda_a\}) = Z_N^{-1}\Delta_N^{\beta}\exp[-\beta\sum_{a=1}^{N}V(\lambda_a)] \tag{14}$$

where Z_N is the partition function and $\Delta_N = \prod_{a<b}^{N}|\lambda_a - \lambda_b|$ is a Vandermonde determinant. An arbitrary n-point correlation function for this distribution can be calculated exactly for any given N and for $\beta = 1, 2, 4$. The method [23] is simpler for $\beta = 2$, which is the reason why we consider systems under applied magnetic fields (unitary case,) and is based on the use of orthogonal polynomials. We define a family of orthogonal polynomials $p_n(\lambda)$, with a given weight $e^{-2V(\lambda)}$, such that

$$\int_0^{\infty} d\lambda e^{-2V(\lambda)}p_n(\lambda)p_m(\lambda) = \delta_{n,m}h_n. \tag{15}$$

We choose the normalisation h_n such that the coefficient of λ^n in $p_n(\lambda)$ is unity. In terms of these polynomials, we define a function

$$K_N(\lambda,\lambda') = e^{-(V(\lambda)+V(\lambda'))}\sum_{n=0}^{N-1}\frac{1}{h_n}p_n(\lambda)p_n(\lambda') \tag{16}$$

which determines uniquely the correlation functions of all orders. The method follows from writing for $\beta = 2$ the distribution $P_N(\{\lambda_a\})$ as the determinant of a matrix of order N

$$P_N(\{\lambda_a\}) = \det|K_N(\lambda_a,\lambda_b)| \tag{17}$$

where $(a, b = 1, . \quad , N)$. For $\beta = 1$ and 4 $P_N(\{\lambda_a\}$ can be written as a quaternion determinant, and the method is then based on the use of skew- orthogonal polynomials. Using relation (16) the integral of $P(\{\lambda_a\})$ over $N - n$ variables λ_a $(a = N - n + 1, . \quad , N)$ can be expressed in terms of the determinant of the matrix with the same elements $K_N(\lambda_a, \lambda_b)$ truncated at the order n $(a, b = 1, . \ . , n)$. In particular, the level density $\sigma_N(\lambda)$ and the two- level correlation function $R_2(\lambda, \lambda')$, defined respectively as

$$\sigma_N(\lambda) = N\int_0^{\infty}P(\lambda,\lambda_2, . \quad ,\lambda_N)d\lambda_2 . \quad d\lambda_N \tag{18}$$

and

$$R_2(\lambda,\lambda') = N(N-1)\int_0^{\infty}P(\lambda,\lambda',\lambda_3, . \quad ,\lambda_N)d\lambda_3 . \quad d\lambda_N, \tag{19}$$

are given by

$$\sigma_N(\lambda) = K_N(\lambda,\lambda) \tag{20}$$

and

$$R_2(\lambda,\lambda') = K_N(\lambda,\lambda)K_N(\lambda',\lambda') - (K_N(\lambda,\lambda'))^2. \tag{21}$$

To determine the polynomials defined in equation (15) needed to evaluate $K_N(\lambda, \lambda')$, we use the fact that they satisfy a three term recursion relation [24] for arbitrary $V(\lambda)$

$$\lambda p_n(\lambda) = p_{n+1}(\lambda) + S_n p_n(\lambda) + R_n p_{n-1}(\lambda) \tag{22}$$

The coefficients R_n are related to the normalization constants h_n by $h_{n+1} = R_{n+1}h_n$. Unfortunately since the potential is not a simple polynomial, we were not able to obtain explicit expressions for R_n and S_n using the standard method [25]. We therefore develop a procedure suitable for an arbitrary potential. We define

$$Q_{n,m} = \int_0^\infty \lambda^m \mathrm{e}^{-2V(\lambda)} p_n(\lambda) \mathrm{d}\lambda \tag{23}$$

Since $\lambda^n = p_n(\lambda) + \sum_{k=0}^{n-1} a_k p_k(\lambda)$ where all the $p_k(\lambda)$ are orthogonal to $p_n(\lambda)$ and using (23), one gets:

$$Q_{n,n} = h_n \tag{24}$$

$$Q_{n,n+1} = h_n \sum_{k=0}^{n} S_k \tag{25}$$

and

$$Q_{n,m} = Q_{n-1,m+1} - S_{n-1}Q_{n-1,m} - R_{n-1}Q_{n-2,m}. \tag{26}$$

The determination of the R_n and S_n necessary to calculate the polynomials of degree $n \leq N-1$ requires only the knowledge of the $2N+1$ integrals

$$Q_{0,m} = \int_0^\infty \lambda^m \mathrm{e}^{-2V(\lambda)} \mathrm{d}\lambda \tag{27}$$

for $m = 0, \ldots, 2N$. Taking for $V(\lambda)$ the analytical fit (13), making the change of variable $X = 1 + b\lambda$, we can calculate the $K_N(X, X')$ from the polynomials $p_N(X)$ orthogonal on the interval $[1, \infty]$. The $2N$ moments

$$Q_{0,m} = \int_1^\infty X^m \mathrm{e}^{-2a \ln^2(X)} \mathrm{d}X \tag{28}$$

are given in terms of the error function

$$Q_{0,m} = \frac{1}{\sqrt{2a}} \exp\left(\frac{(n+1)^2}{8a}\right) \frac{\sqrt{\pi}}{2} \left(1 + erf\left(-\frac{n+1}{2\sqrt{2a}}\right)\right). \tag{29}$$

In order to eliminate any possibility of an error arising from a possible inaccuracy of the fit (13) we also calculate the moments (23) directly using a precise cubic spline fit to $V(\lambda)$ on $[0, \infty]$.

4. Correlation functions in the bulk and at the edges of the spectrum.

In order to study the validity of the two point correlation functions calculated from the maximum entropy ansatz we solve the microscopic Anderson model, numerically obtaining a spectrum for each realization of randomness. We then proceed in two independent ways. Firstly we obtain the potential $V(\lambda)$ by evaluating the ensemble averaged quantity $< \sum_{a=1}^{N} \ln|\lambda - \lambda_a| >$. We fit the potential, calculate the necessary polynomials and evaluate the correlation function implied by the maximum entropy ansatz. Secondly we use the $\{\lambda_a\}$ directly to evaluate the same correlation function without any reference to random matrix theory. A detailed comparison is possible because the polynomial method is valid for any N. This permits a critical examination of the validity of the assumptions in the maximum entropy model.

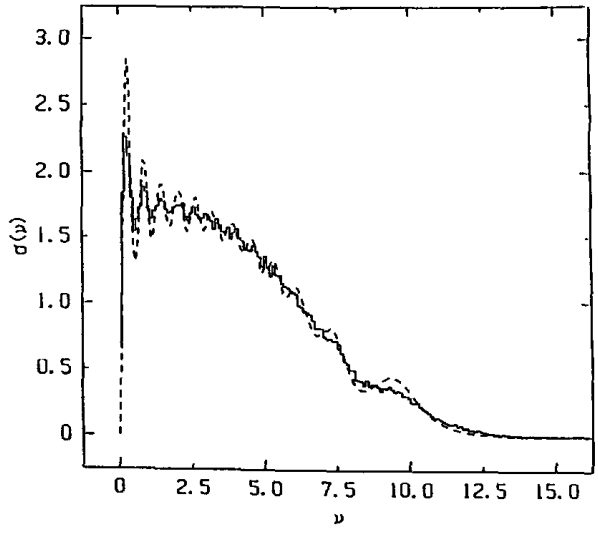

Fig.4. — 3d–density $\sigma(\nu)$ directly evaluated (solid line) and calculated from $K(\lambda,\lambda)$ (dashed line).

In figure 4 we compare the original density $\sigma(\lambda)$ with $K_N(\lambda,\lambda)$ calculated from a cubic spline fit to $V(\lambda)$ in order to verify the self consistency of our calculations. The results shown are for $d = 3$, a similar agreement is obtained for $d = 1, 2$. We have verified that the average of any quantity calculated from the $K(\lambda,\lambda)$ given by the orthogonal polynomials is always in agreement with the value calculated directly from the spectrum.

To study the correlations we introduce a function

$$Y(\lambda,\lambda') = \frac{(K(\lambda,\lambda'))^2}{K(\lambda,\lambda)K(\lambda',\lambda')} \tag{30}$$

which determines with the density the two–point correlation function $R_2(\lambda,\lambda')$ of (21). Figures 5 show this correlation function $Y(\nu,\nu')$ as the function of the variable ν (see (12)) for various values of ν' chosen in the bulk and at the edges of the spectrum. We compare the correlation functions implied by the maximum entropy model (dashed line) to the histogram of the actual correlation function (solid line) directly calculated from microscopic Anderson models. Results for $d = 3$ are presented in figures 5a, b, c, d while figure 5e is for quasi-1d. The quality of the agreement between the microscopic model and the maximum entropy ansatz is not noticeably different in different dimensions, at least in the metallic regime we consider and for the ensemble size of 3.10^4 samples used here. We conclude that the maximum entropy ansatz is a good approximation in all dimensions. Note that although $\beta = 2$, the correlations are not those of the standard Gaussian Unitary Ensemble (GUE) [23], as can be seen from the asymmetry of $Y(\nu,\nu')$ when ν' is small or large. This is not in contradiction with maximum entropy ansatz and is a consequence of the restriction on the $\{\lambda_a\}$ to be strictly positive [14].

In order to demonstrate a discrepancy between the maximum entropy model and the microscopic model it is necessary to calculate an integrated quantity such as the variance of T or R. We consider this in the next section.

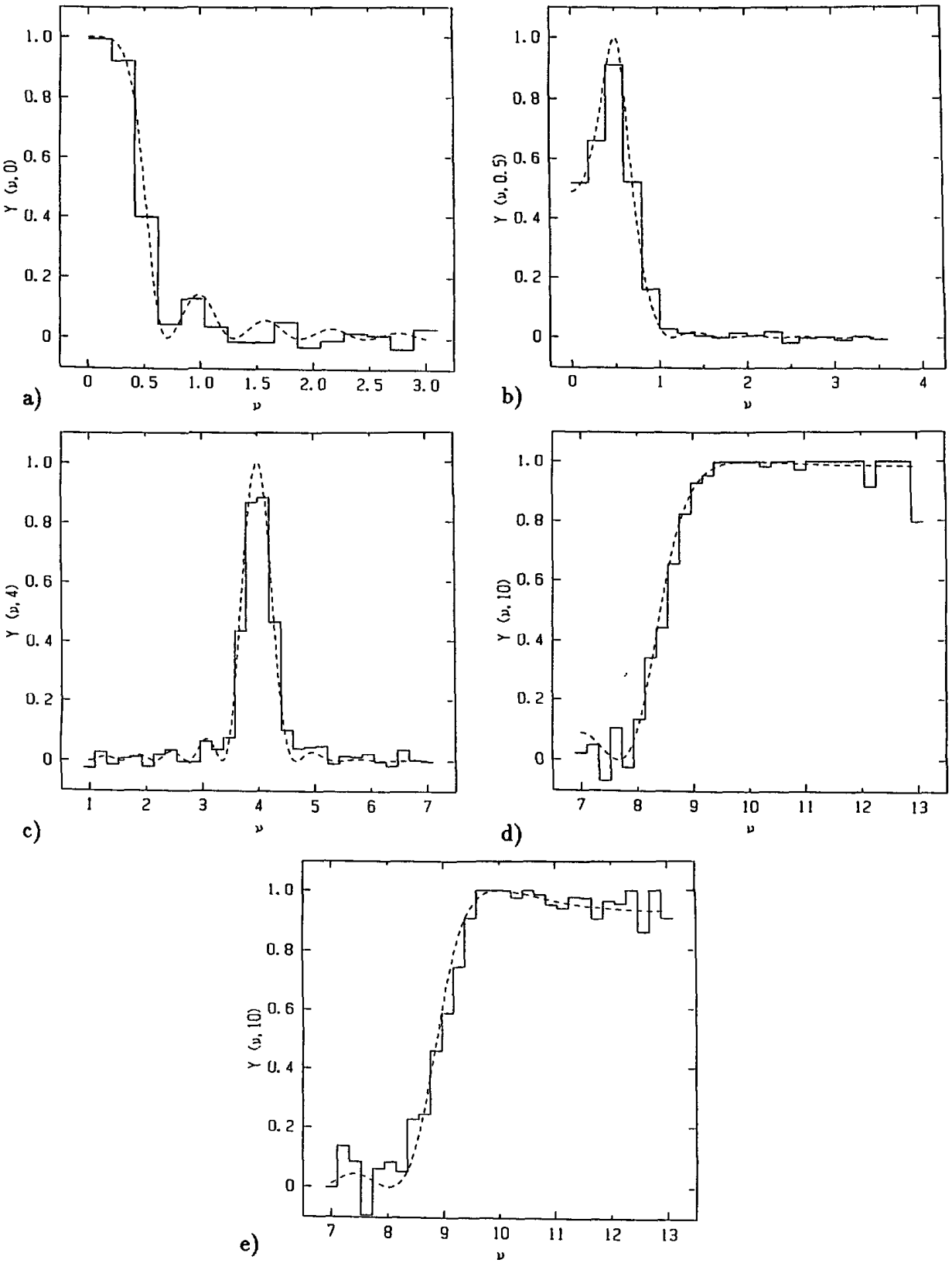

Fig.5. — a) Correlation function $Y(\nu, 0)$ (lower edge of the 3d spectrum). histogram of the Anderson model (solid line) and ansatz (6) (dashed line). b) $Y(\nu, 0.5)$ near the lower edge of the 3d spectrum. c) $Y(\nu, 4)$ in the bulk of the 3d–spectrum. d) $Y(\nu, 10)$ at the upper edge of the 3d–spectrum. e) $Y(\nu, 10)$ at the upper edge of the quasi–1d spectrum.

5. Universal conductance fluctuations and dimensionality effects.

A function $F = \sum_{a=1}^{N} f(\lambda_a)$ defines a linear statistic [21] of the spectrum. Its variance is given by the difference between a simple integral I_1 and a double integral I_2:

$$\mathrm{var}(F) = I_1 - I_2 \tag{31}$$

$$I_1 = \int_0^\infty K_N(\lambda,\lambda) f^2(\lambda) \mathrm{d}\lambda \tag{32}$$

$$I_2 = \int_0^\infty \int_0^\infty K_N^2(\lambda,\lambda') f(\lambda) f(\lambda') \mathrm{d}\lambda \mathrm{d}\lambda'. \tag{33}$$

To calculate the variance of the total transmission T we take $f(\lambda) = 1/(1+\lambda)$, while for the total reflection R we take $f(\lambda) = \lambda/(1+\lambda)$. These two functions probe the correlations at the lower and upper edges of the spectrum respectively.

Fitting $V(\lambda)$ with cubic splines we can calculate the variances of T and R implied by the maximum entropy ansatz and compare them with the same statistics calculated directly from the spectrum. Surprisingly we find that we obtain agreement only for the quasi-1d system. The ansatz does not reproduce the shape dependence of the variances of T and R but gives in all cases something close to the the quasi-1d value. Since the density $\sigma(\lambda) = K_N(\lambda,\lambda)$ enters as a constraint the maximum entropy ansatz (the self consistency of $V(\lambda)$ and $\sigma(\lambda)$ has already been checked in Sect. 3; see Fig. 4) it is clear that the error arises only in the second integral I_2. This result is surprising since it appears to be in contradiction with the results of section 4 where the agreement between the two point correlations of the ansatz and the data was not noticeably different in different dimensions.

In an attempt to resolve this apparent contradiction we have studied the variances of:

$$F(\lambda_{\max}) = \sum_{\lambda_a < \lambda_{\max}} f(\lambda_a), \tag{34}$$

both for transmission and reflection, as a function of the cut- off $\lambda_{\max}$. Figure 6 shows a comparison between the variances of $T(\lambda_{\max})$ and $R(\lambda_{\max})$ obtained directly from the numerical data and implied by the ansatz. For clarity of presentation the abcissa is given in terms of ν. It is clear that the ansatz is more accurate for systems closer to the quasi- 1d limit (aspect ratio $L_z/L_x = 4$, figure 6a) than for 3d cubes (Fig. 6b). In 3d the transmission fluctuations are well described by the ansatz when ν_{max} is small, confirming that the short range correlations are correctly described at the origin. For larger $\nu_{\max}$ we see that the ansatz underestimates the variance indicating that the correlations between the lower edge and the bulk of the spectrum are less rigid in three dimensions than assumed in the ansatz. Above $\nu_{\max} \approx 4$, the variance of T saturates at the expected 3d UCF-value for the data while the variance calculated on the basis of the ansatz saturates close to the quasi- 1d value. Considering the variance of the reflection, which is not sensitive to the correlation function at the lower edge of the spectrum, a disagreement appears only when $\nu_{\max}$ approaches the upper edge of the spectrum. This indicates that the correlations in the bulk of the spectrum are correctly described by the ansatz. The ansatz seems to overestimate the correlations between the bulk and the upper edge of the spectrum.

In order to be more precise we now consider the variance of the number $N(\nu_0, \Delta\nu)$ of eigenvalues inside an interval of width $\Delta\nu$ centered at ν_0 . This corresponds to $f(\lambda) = 1$ in the relevant interval $f = 0$ otherwise. The ansatz is satisfactory in 3d (see Fig. 7) when the interval width is small ($\Delta\nu < 0.5$) but becomes less accurate for larger intervals (e.g: when

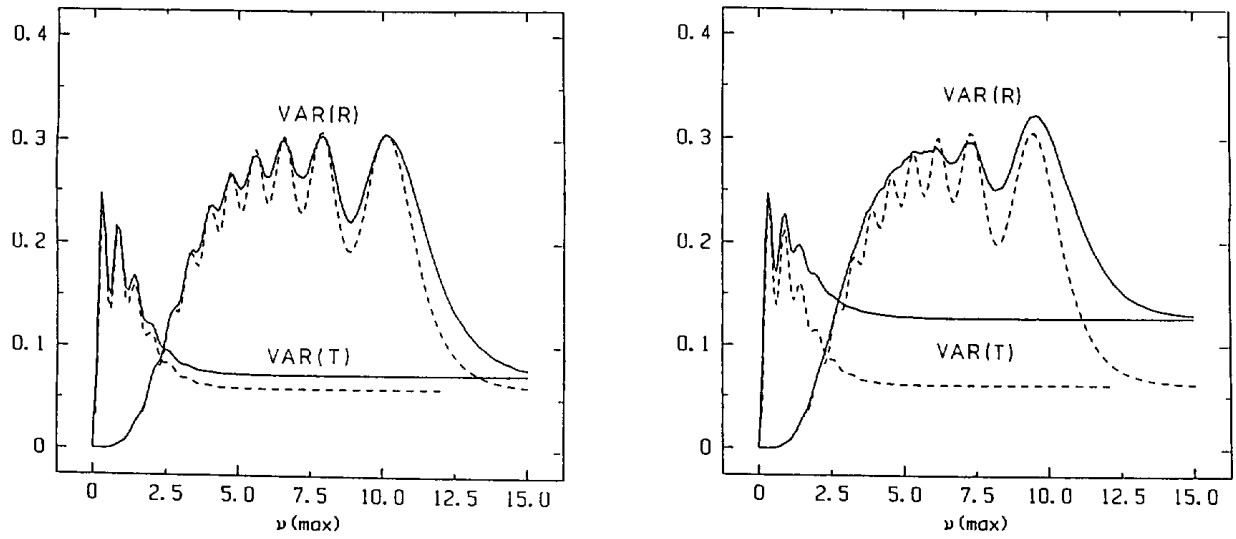

Fig.6. — a) var($T(\nu_{\max})$) and var($R(\nu_{\max})$) as a function of $\nu_{\max}$. Anderson model on quasi–1d strips (solid line) and ansatz (dashed line). b) Anderson model on 3d–cubes (solid line) and ansatz (dashed line)

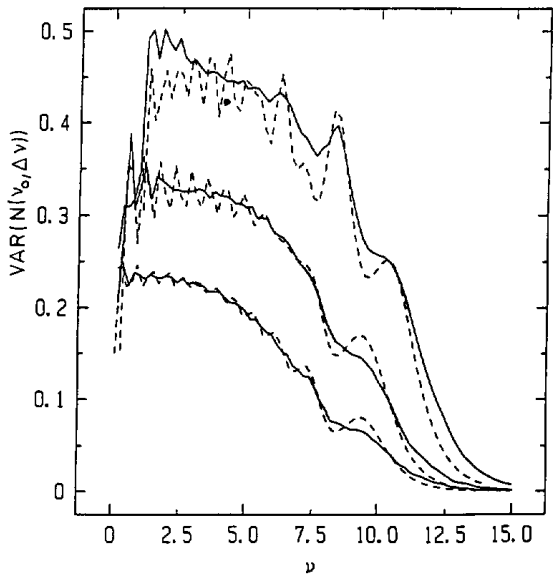

Fig.7. — var($N(\nu_0, \Delta\nu)$ as a function of ν_0, for $\Delta\nu = 0.2$ (lower curves), 0.5 (middle curves) and 2 (upper curves) for 3d–cubes. Anderson model (solid line) and ansatz (dashed line).

$\Delta\nu = 2$, for $\nu_0 \approx 2$ and $\nu_0 > 10$). The error is dependent not only on the width $\Delta\nu$ of the interval, but also on the position of the interval ν_0. This can be seen in figure 8 where the error is plotted as a function of the mean number $< N(\nu_0, \Delta\nu) >$ of eigenvalues in the interval. In 3d the ansatz is accurate up to $< N > \approx 10$ provided that the interval is centered in the bulk of the spectrum ($\nu_0 = 5; \Delta(\mathrm{var}(N)) < 5 \times 10^{-2}$) , while a clear discrepancy occurs at the edges of the spectrum ($\Delta(\mathrm{var}(N)) > 5 \times 10^{-2}$ for $< N > \approx 3$ if $\nu_0 < 1$ or > 7). In the quasi 1d limit the results are qualitatively similar but the magnitude of the error is considerably reduced (by

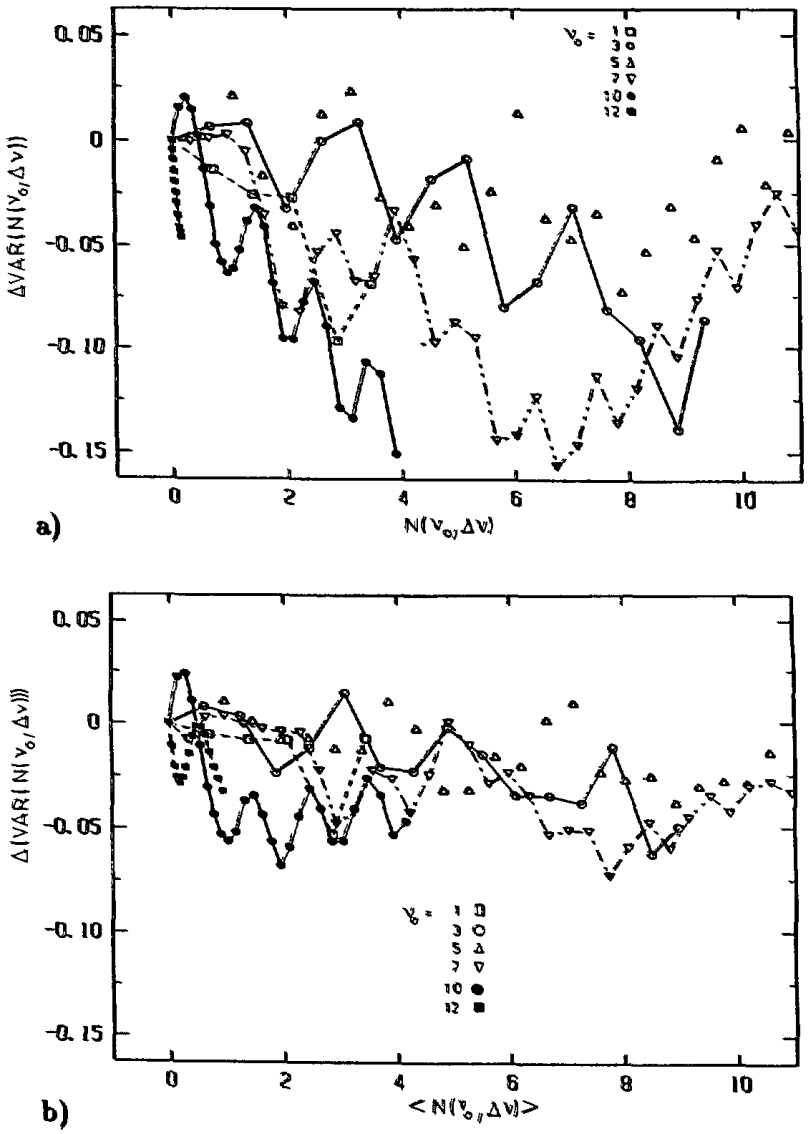

Fig.8. — $\Delta(\mathrm{var}(N(\nu_0, \Delta\nu))$ as a function of the mean number of levels in $\Delta\nu$ for $\nu_0 = 1, 3, 5, 7, 10$ and 12. a) 3d-cubes. b) quasi-1d strips.

a factor of order three in the case we consider.)

We conclude that the maximum entropy ansatz overestimates the correlations between the best transmitting (reflecting) channels and the other channels outside the quasi- 1d limit, though otherwise providing a good approximation. This reconciles two apparently contradictory observations : the relevance in all dimensions of the random matrix description demonstrated in section 4 and its failure to reproduce the weak dimensional dependence of the UCF-values.

6. Concluding remarks and memory effect for high transmission and reflection.

We conclude by discussing how our understanding of the correlations in high dimensions could be improved. In addition, we report a memory effect which we have observed, though its

relevance for the discussed issue is unclear, since it is not strongly dependent on the shape of the system.

We begin by recalling the limitations of the random matrix description of the Hamiltonian. As first shown by Efetov [26], the spectra of small metallic particles have Wigner–Dyson correlations. However, using either standard perturbation theory [27] or semi–classical methods [28] starting from Gutzwiller trace formula, one can see from the dynamics of the electronic trajectories how dimensionality enters the level correlations, limiting the validity of Efetov's result. The physical origin of these corrections is related to the diffusive nature of the classical periodic orbits which matter in a semi–classical approximation. If τ_d is the time for the electron to diffuse through the entire system, the probability to return after a time t to the same point is proportional to $1/(Dt)^{d/2}$ for $t < \tau_d$ and is independent of dimension when $t > \tau_d$. From this, the Gutzwiller trace formula and Berry's diagonal approximation it can be shown that Efetov's result is restricted to energy intervals ΔE smaller than the Thouless energy $E_c = \hbar/\tau_d$. On larger energy intervals the spectrum is less rigid than predicted by the random matrix theory. In a loose way we can say that the Hamiltonian random matrix theory is "zero–dimensional" since it applies only to energy intervals $\Delta E < E_c$ corresponding to time scales on which the electron can diffuse throughout the whole system. Correlations on larger energy intervals $\Delta E > E_c$ are not described by standard Wigner–Dyson correlations since the diffusion at a time scale $t < \tau_d$ depends on dimensionality.

Is there an analogue of E_c for the transmission spectrum? The success of the random matrix description for quasi–1d systems, even in the localised limit [10, 29] seems to indicate that the relevant time scales are associated with transverse diffusion, and not longitudinal diffusion or localisation. By analogy we might suppose that the random matrix theory should apply on time scales on which the *transverse* motion is "zero–dimensional". Our results indicate that the equivalent of E_c for transmission is some function $\lambda_c(\lambda)$ which is larger in the bulk of the spectrum than near its edges. Further progress may be achieved by an analysis of the characteristic time scales associated with the different transmission modes. Such time scales could be calculated from an appropriate delay time matrix [30] defining the interaction times of the different transmission modes with the sample and which should be compared to the transverse diffusion time. We speculate that for systems far from the quasi- 1d limit electronic trajectories which do not involve numerous reflections by the transverse boundaries are responsible for the presence of dimensionality dependent corrections to the random matrix description. A semi-.classical approach may clarify this point.

To obtain the full distribution of the $\{\lambda_a\}$ another approach may be more appropriate. We have shown that the assumption that all parameter dependence including dimensionality enters via a single constraint, the single particle potential $V(\lambda)$, correctly describes the quasi-1d limit. We have also shown that while qualitatively correct this assumption is not quantitatively exact in higher dimensions. We speculate that the introduction of a d dependent screening of the usual logarithmic interaction between the eigenvalues above a characteristic scale $\lambda_c(\lambda)$ may be sufficient to recover the shape dependence of the UCF. To understand how such a screening may come about it is helpful to consider two extreme cases. As was pointed out by Balian [31] maximising the entropy subject to the constraint of fixed eigenvectors yields an uncorrelated eigenvalue spectrum. We have already seen that assuming the eigenvectors to be completely random yields the standard infinite range logarithmic interaction between the eigenvalues. This suggests that the introduction of some constraint on the eigenvectors may be necessary in higher dimensions. Similar suggestions have been made in the context of the statistical theory of nuclear reactions [32] and also recently in quantum transport theory [17, 33].

In an attempt to identify a more appropriate constraint in higher dimensions we studied the dimensionality dependence of the eigenvectors distribution. Referring to (11) we can see

that the eigenvectors of $t^{\dagger}t$ are contained in the matrix $u^{(1)}$ Maximising the entropy subject to only a spectral constraint clearly implies that $u^{(1)}$ is isotropic, the probability distribution is just given by the invariant measure for the unitary group. An obvious consequence is that components of the eigenvectors are uniformly distributed across the modes of the attached leads so that after averaging

$$< |u_{ia}|^2 >= \frac{1}{N} \tag{35}$$

In figure 9a the results of a calculation for 2d square systems with $N = 20$ are presented. In order to simplify the interpretation we first consider the case of zero magnetic field. The $1/N$–behaviour is roughly observed for the eigenvectors associated with eigenvalues in the bulk of the spectrum (ν_{10}). However deviations from (35) are clearly visible for the eigenvectors corresponding to the edges of the spectrum. The eigenvector associated with the smallest eigenvalue ν_1 (best transmission) has a greater projection on the incoming channels of the leads characterised by small transverse kinetic energy (the transverse wave vector is $k_i = \pi i/(L_x + 1)$ where $i \approx 10$, $L_x = 20$ and the transverse kinetic energy is $E_i = 2\cos(k_i)$) On the contrary, the eigenvector associated with the largest eigenvalue (best reflection) is preferentially projected on the modes of the leads with large transverse kinetic energy. This has also been predicted by Mello and Tomsovic [17] on the basis of a diffusion equation for the transfer matrix which does not assume isotropy. In simple terms this tell us that even in a diffusive sample, good transmission remains correlated with incoming electrons "shot" perpendicularly to the disordered square, while good reflection is correlated with electrons "shot" tangentially to the sample. This is a statistical "*memory effect*" which depends on transverse section dimensionality. The results are unchanged when the disorder parameter is varied over a large range ($W = 2 \rightarrow 8$), indicating that the distribution of these average amplitudes depend essentially on the geometry of the sample. Note that this effect can be seen only after ensemble averaging, the sample to sample fluctuations being extremely large. When a magnetic field is applied, a better randomization of the eigenvectors is achieved, as shown in figure 9b. The electronic trajectories are curved by the magnetic field in the absence of elastic scattering; good (bad) transmission then corresponds to incoming fluxes entering the sample with angles dependent on the precise value of the field. Elastic scattering does not entirely destroy this correlation. However, from figures 9c and 9d, one can see that the increase of the length ($L_x = 20 \rightarrow 80$) does not change the $< |u_{i,a}|^2 >$, raising doubt that the missing relevant information on the eigenvector distribution reduces to this phenomenon.

In conclusion, both a better understanding of the dynamics of the trajectories associated with the different transmission modes and a more extensive investigation of the distributions of the $u_{i,a}$ (including *the phases* as well as the amplitudes) may be useful for extending the maximum entropy approach.

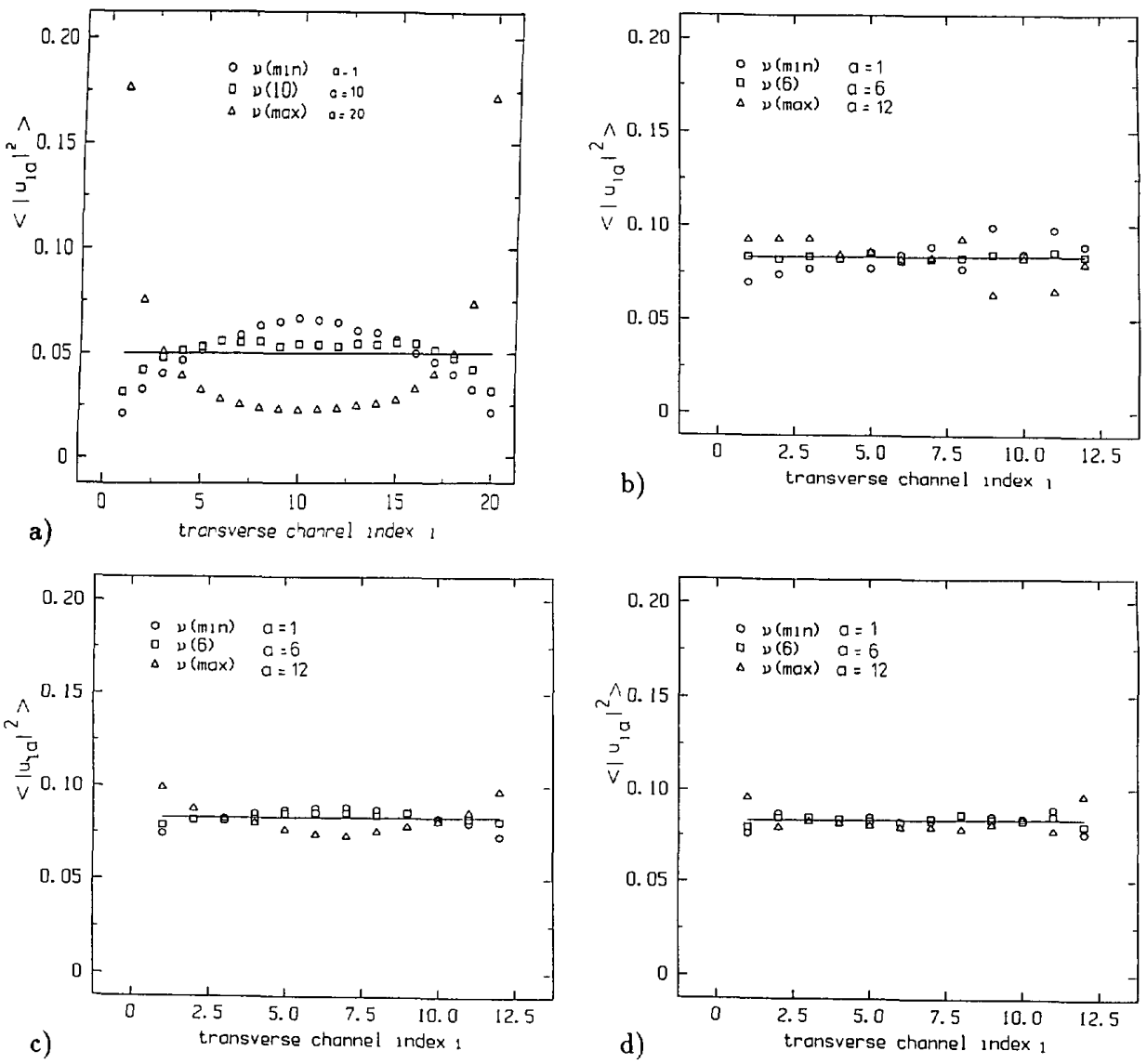

Fig.9. — N averaged amplitudes projections $< |u_i a|^2 >$ of 3 eigenvectors of $t.t^\dagger$ over the propagating channels of the leads as a function of the index i of the transverse wave- vector $k_i = i \times (\pi/(L_x + 1)$ of the channel. Assumption of the ansatz: solid line. Circle: best transmitting mode, square: bulk of the spectrum, triangle: best reflecting mode). a) 2d- squares without applied magnetic field, ($N = 20$). b) 3d-cubes with applied magnetic field, ($N = 12$). c) 2d-squares, ($B = 0.02$, $N = 12$). d) quasi-1d strips, ($B = 0.02$, $N = 12$).

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