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Spectral correlations: Understanding oscillatory contributions

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We give a different derivation of a relation obtained using a supersymmetric nonlinear sigma model by Andreev and Altshuler [Phys. Rev. Lett. **72**, 902 (1995)], which connects smooth and oscillatory components of spectral correlation functions. We show that their result is not specific to the random matrix theory. Also, we show that despite an apparent contradiction, the results obtained using their formula are consistent with earlier perspectives on random matrix models.

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Spectral correlations of complex quantum systems, such as disordered metals and classically chaotic quantum systems, are known to be nearly universal. For small ranges of energy they are well approximated by the Gaussian invariant ensembles of the random matrix theory (GXE, where X=O, U, or S stands for orthogonal, unitary, and symplectic invariance) [1,2]. Deviations from GXE behavior at larger energy scales may be consistently incorporated using semiclassical or perturbative approaches [3–5]. An interesting development in this field was a paper by Andreev and Altshuler (AA) [6] who introduced a relation that suggests a degree of nonuniversality in short-range spectral correlations. Their calculations are based on the nonlinear sigma model. Our paper will give an alternative derivation of this relation providing additional physical insight.

AA [6] consider the spectral two-point correlation function, defined as

$$R_\beta(\epsilon)=\Delta^2\langle d(E+\epsilon/2)d(E-\epsilon/2)\rangle-1. \tag{1}$$

Here $d(E)=\Sigma_n\delta(E-E_n)$ is the density of states, E_n are the eigenvalues of a Hamiltonian $\hat{H}$, and $\Delta(E)=\langle d(E)\rangle^{-1}$ is the mean level spacing that is assumed to be independent of E in the following. The index $\beta=1,2,4$ distinguishes orthogonal, unitary, or symplectic symmetry classes, respectively.

AA divide Eq. (1) into a smooth and an oscillatory contribution, and propose that (for $\beta=2$) these are related as follows:

$$R_2^{\mathrm{av}}(\epsilon)\simeq-\frac{\Delta^2}{4\pi^2}\frac{\partial^2}{\partial\epsilon^2}\log D(\epsilon), \tag{2}$$

$$R_2^{\mathrm{osc}}(\epsilon)\simeq\frac{1}{2\pi^2}\cos(2\pi\epsilon/\Delta)D(\epsilon). \tag{3}$$

The relation is exact for the GUE with a suitable choice for $D(\epsilon)$ and generalizations are approximately true for the other ensembles. AA propose that Eqs. (2) and (3) are quite general, and should be used to predict the oscillatory component from the average component. The quantity $D(\epsilon)$ is a spectral determinant.

The AA relation contained in Eqs. (2) and (3) has attracted considerable attention (see, for example, [7–9]), partly because of the suggestion that it contains information about "resurgence." This is to be interpreted in terms of Gutzwiller's [10] relationship between periodic orbits and the density of states: periodic orbits with period t_j are associated with oscillations in the density of states of period $\epsilon_j=\hbar/t_j$. One interpretation of the concept of resurgence is that information about long period orbits is encoded in properties of the short orbits. In this context, $R^{\mathrm{av}}(\epsilon)$ may be derived using Gutzwiller's relation from properties of short orbits, and the AA relation then gives information about fluctuations in the spectrum with the wavelength equal to the mean level spacing Δ, corresponding to orbits of a period equal to the "Heisenberg time," $t_{\mathrm{H}}=2\pi\hbar/\Delta$.

In the following we provide an alternative interpretation of the AA results using old ideas of the applicability of the random matrix theory. Dyson [11] introduced a Brownian motion model for the random matrix theory, giving a Langevin equation of motion for the response of energy levels to a stochastic perturbation. Dyson later suggested [12] that this model may give valuable insights into why the random matrix theory applies to generic systems. He considered the dynamics of the energy levels under the effect of a stochastic perturbation, which is large enough to shift energy levels significantly, but which remains small enough to leave other features of the system (such as the classical dynamics) unchanged. Dyson showed that the equations of motion simplify if the discrete Fourier coefficients a_k of the level displacements are used as dynamical variables:

$$a_k=\frac{1}{N}\sum_{n=0}^{N-1}\Delta E_n\exp(-2\pi ikn/N), \tag{4}$$

where $\Delta E_n=E_n-n\Delta$, N is the number of energy levels, and k takes N successive integer values. We will take the maximal k to be int(N/2). The long wavelength modes evolve almost independently, with a long relaxation time, which scales as k^{-1} [12,4]. The short wavelength modes remain strongly coupled. The stochastic perturbation will bring the short wavelength modes into equilibrium, giving statistics of the a_k, which are identical to the random matrix ensemble for sufficiently large k.

These arguments were later supported and extended with the aid of semiclassical estimates of matrix elements [4]. The argument in [12] assumes that the matrix elements of the perturbation are uncorrelated. It was shown that semiclassical estimates are consistent with this hypothesis when considering the stochastic force driving the large k modes. The forces driving the small k modes are modified by the classical dynamics of the system. The resulting picture is that long wavelength fluctuations are nonuniversal, but that at short wavelengths the excitations of the modes are precisely the same as for the appropriate GXE. In particular, there is no modification of the statistics of the Fourier coefficients a_k unless $|k|/N$ is small.

These observations appear to contradict the AA relations. A nonuniversal form for $R_2^{\rm av}(\epsilon)$ will be reflected in nonuniversal statistics of the a_k for small k. The AA relations suggest that there will be corresponding nonuniversal statistics for large k, determining $R_2^{\rm osc}(\epsilon)$. This apparent contradiction has two possible resolutions. Either there are previously unsuspected nonuniversal modifications of the a_k for large k, which are not captured by the semiclassical approximations in [4], or it must be possible to derive the AA relations from the Brownian motion model described in [4] without such modifications at large times. In the following we show that the latter is the case.

The remainder of this article is organized as follows. We will first describe a simple derivation of the AA result, and comment on its applicability. We will then describe the Brownian motion model and use it to derive the correlation function $R_\beta(\epsilon)$ for the case of a system with diffusive electron motion. In this calculation we assume that the statistics of the Fourier coefficients are unchanged for large $|k|$. The fact that we reproduce existing results for $R_\beta(\epsilon)$ verifies that corrections to the Brownian motion model with a large wave number are not required. Finally, we will comment on the correlation function for classically chaotic systems.

Our starting point is the following general expression for the correlation function $R_\beta(\epsilon)$:

$$R_\beta(\epsilon) = -1 + \Delta \sum_{n=-\infty}^{\infty} p_\beta(n,\epsilon), \tag{5}$$

where $p_\beta(n,\epsilon)d\epsilon$ denotes the probability of finding that the difference between E_0 and E_n is in the interval $[\epsilon, \epsilon + {\rm d}\epsilon]$. We will show below that in many cases, the $p_\beta(n,\epsilon)$ are well approximated for a large n by Gaussians, with variance $\sigma_\beta^2(n)$.

First, however, we show how relations (2) and (3) can be derived from Eq. (5). We write

$$R_\beta(\epsilon) = R_\beta^{\rm av}(\epsilon) + R_\beta^{\rm osc}(\epsilon). \tag{6}$$

Here $R_\beta^{\rm av}(\epsilon)$ is defined as

$$R_\beta^{\rm av}(\epsilon) = \int_{-\infty}^{\infty} d\epsilon' w(\epsilon - \epsilon') R_\beta(\epsilon'), \tag{7}$$

where $w(\epsilon)$ is a suitable window function (which could be a Gaussian centered around zero with a variance much larger than $\sigma_\beta^2(n)$ and normalized to Δ^{-1}). $R_\beta^{\rm osc}(\epsilon)$ is the remaining oscillatory contribution. Using Eq. (5) we have, upon expanding the slowly varying window function in Eq. (7),

$$\begin{aligned} R_\beta^{\rm av}(\epsilon) &= -1 + \Delta \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\epsilon' w(\epsilon - \epsilon') p_\beta(n,\epsilon') \\ &\simeq -1 + \Delta \sum_{n=-\infty}^{\infty} \left[w(\epsilon - n\Delta) + \frac{1}{2} w''(\epsilon - n\Delta)\sigma_\beta^2(n) \right]. \end{aligned} \tag{8}$$

Assuming that $\sigma_\beta^2(n)$ is a slowly varying function of n, we may approximate the sum over n as an integral and obtain

$$R_\beta^{\rm av}(\epsilon) \simeq \frac{1}{2\Delta^2} \frac{\partial^2}{\partial n^2} \sigma_\beta^2(n), \quad \epsilon = n\Delta. \tag{9}$$

Consider now the oscillatory contribution $R_\beta^{\rm osc}(\epsilon)$. Assuming that $\sigma_\beta^2(n)$ is slowly varying, these can be evaluated from Eq. (5). Using a Poisson summation, and assuming the $p_\beta(n,\epsilon)$ are Gaussian,

$$R_\beta^{\rm osc}(\epsilon) \simeq \sum_{\mu=1}^{\infty} 2\cos(2\pi\mu n) e^{-(2\pi\mu)^2 \sigma_\beta^2(n)/2\Delta^2}. \tag{10}$$

This sum is dominated by the $\mu = 1$ term when $\sigma_\beta^2(n)$ is sufficiently large. Defining $D(\epsilon) = 4\pi^2 \exp[-2\pi^2\sigma^2(n)/\Delta^2]$ we obtain relations (2) and (3). We remark that these formulas are valid for any correlation function that can be approximated as a sum of Gaussians, in regions where the variance satisfies $\sigma^2 \gg \Delta^2$, and where σ^2 varies sufficiently slowly as a function of n. Relating $D(\epsilon)$ to $\sigma^2(n)$ gives a clear insight into its meaning. Relations (2) and (3) may be easily extended by considering higher-order derivatives in Eq. (2) and higher Fourier components in Eq. (3). Extensions to non-Gaussian spacing distributions are possible. Also, we emphasize that these relations are not specific to spectral correlation functions. For example, they are applicable to density correlations in solids: for thermal excitation of phonons the corresponding two-point function is a sum of Gaussians, and $\sigma^2(n) \sim \log n$ in $d = 2$ dimensions [13].

Next we consider the calculation of $p_\beta(n,\epsilon)$ and $\sigma_\beta^2(n)$ using Dyson's Brownian motion model [11]. Here the matrix elements of the Hamiltonian $\hat{H}$ undergo a diffusive evolution as a function of a fictitious time variable τ. We denote the infinitesimal change of $\hat{H}$ by $\delta\hat{H}$. In the GOE case, we have for $n > m$ and $n' > m'$,

$$\langle \delta H_{mn} \rangle = 0, \quad \langle \delta H_{mn} \delta H_{m'n'} \rangle = C_{mn}^{\rm off} \delta\tau \delta_{nn'} \delta_{mm'} \tag{11}$$

(extensions for GUE and GSE are given in [11]). The diagonal elements obey

$$\langle \delta H_{nn} \rangle = 0, \quad \langle \delta H_{mm} \delta H_{nn} \rangle = 2\delta\tau \beta^{-1} C_{mn}^{\rm diag}. \tag{12}$$

Dyson [11] originally discussed the case where $C_{mn}^{\rm diag} = \delta_{mn}$ and $C_{mn}^{\rm off} = 1$, for which the statistics of the E_n are the same as for the GXE. We will argue below that nonuniversal deviations from the GXE are encoded in $C^{\rm diag}_{mn}=C^{\rm diag}_{m-n}$ (and $C^{\rm off}_{mn}=C^{\rm off}_{m-n}$). Using the second order perturbation theory leads to a Langevin equation

$$\delta E_n=\sum_{m\neq n}\frac{|\delta H_{mn}|^2}{E_n-E_m}+\delta H_{nn} \tag{13}$$

for the energy level shifts δE_n. Thus,

$$\langle\delta E_n\rangle=\delta\tau\sum_{m\neq n}\frac{C^{\rm off}_{m-n}}{E_m-E_n}, \tag{14}$$

$$\langle\delta E_m\delta E_n\rangle=2\,\delta\tau\beta^{-1}C^{\rm diag}_{m-n}. \tag{15}$$

Semiclassical estimates [14] indicate that the $C^{\rm off}_n$ decrease for large values of n, i.e., the repulsive interaction is screened at long range. This effect was considered in [15]; for our purposes it is not significant, and we will set $C^{\rm off}_n=1$ throughout. We now use Eq. (4) to obtain the same equations of motion in terms of the Fourier variables a_k. Using $\delta\Delta E_n=\delta E_n$, we have

$$\langle\delta a_k\delta a^*_l\rangle=2\,\delta\tau\beta^{-1}I_k\delta_{kl}, \tag{16}$$

where $I_k=N^{-1}\Sigma_n C^{\rm diag}_n\exp(-2\pi ikn/N)$. The transformation of the drift term is less straightforward. In general $\langle\delta a_k\rangle$ is a complicated function of all of the a_k, but in the limit $|k|/N\to 0$ the equations decouple and obey [12,4]

$$\langle\delta a_k\rangle=-\frac{2\pi^2k}{N\Delta^2}a_k\delta\tau. \tag{17}$$

By solving a Fokker-Planck equation for the real and imaginary parts of a_k, these are found to have a steady state distribution that is Gaussian. The value of $\langle|a_k|^2\rangle$ can be deduced by requiring that $\langle|a_k(\tau+\delta\tau)|^2\rangle=\langle|a_k(\tau)|^2\rangle$. Writing $a_k(\tau+\delta\tau)=a_k(\tau)+\delta a_k$ and using Eqs. (16) and (17) we find, provided $|k|/N\ll 1$,

$$\langle|a_k|^2\rangle=\frac{N\Delta^2I_k}{2\pi^2\beta k}. \tag{18}$$

We cannot determine $\langle|a_k|^2\rangle$ for larger values of $|k|$ from this approach. We now make our key assumption, that there are no short-range correlations between the diagonal matrix elements, i.e., $C^{\rm diag}_{n-m}\sim\delta_{nm}$. Semiclassical arguments that support, but do not prove, this assumption are given in [4]. (The existence of short-range correlations would represent a type of ‘‘resurgence,’’ in the sense discussed earlier). Under this assumption, the equations of motion of the a_k are identical to those for the Brownian motion model describing Gaussian invariant ensembles. We therefore conclude that when $|k|/N$ is not small, the mode intensities $\langle|a_k|^2\rangle$ are identical to those of the Gaussian invariant ensembles.

For large n, the level spacings E_n-E_0 are seen to be a sum of many independent random variables and are thus Gaussian distributed,

$$p_\beta(n,\epsilon)=[2\pi\sigma^2_\beta(n)]^{-1/2}e^{-(\epsilon-n\Delta)^2/2\sigma^2_\beta(n)}. \tag{19}$$

The variance $\sigma^2_\beta(n)$ may be calculated in terms of $\langle a^*_k a_{k'}\rangle$, with summation over k, k'. We use the fact that the amplitudes are uncorrelated when $|k|/N\ll 1$, with intensity given by Eq. (18), and the assumption that they are universal when $|k|$ is comparable to N. The resulting expression may be written as a single sum over k, and approximated by an integral. Writing $t=t_{\rm H}k/N$, and $NI_k=I(t)$,

$$\sigma^2_\beta(n)=\frac{4\Delta^2}{\beta\pi^2}\int_0^{t_{\rm H}/2}\frac{dt}{t}J_\beta(t)\sin^2\!\left(\frac{nt\Delta}{2\hbar}\right), \tag{20}$$

where $J_\beta(t)=I(t)$ for $t\ll 1$, and $J_\beta(t)$ takes a universal (but to us, unknown) form when t is not small. For the Gaussian invariant ensembles [where $I(t)=1$], the variances grow logarithmically with n: for $n\gg 1$,

$$\sigma^2_\beta(n)\simeq\frac{2\Delta^2}{\beta\pi^2}[\log(2\pi n)+C_\beta]. \tag{21}$$

Setting $C_1=-\log\sqrt{2}$, $C_2=0$, and $C_4=\log(4/\pi)$, and using this expression in Eqs. (2) and (3) gives the correct leading order contributions to $R^{\rm av}_\beta(\epsilon)$ and $R^{\rm osc}_\beta(\epsilon)$ in the limit $\epsilon/\Delta\to\infty$ (c.f. Ref. [2]).

Next we consider how the function $I(t)$ must be modified at small t to take account of classical dynamics. For small values of $|k|$, the amplitude δa_k can be estimated semiclassically [4],

$$\delta a_k\sim\frac{1}{N}{\rm tr}[\delta\hat H\hat U(t)],\quad t=\frac{2\pi\hbar}{\Delta}\frac{k}{N}=t_{\rm H}\frac{k}{N}, \tag{22}$$

where $\hat U(t)=\exp(-i\hat Ht)$ is the evolution operator. We first consider diffusive systems (electrons in disordered metals), then systems with a chaotic classical limit.

Diffusive systems. In this case we may consider the perturbation $\delta\hat H$ to be uncorrelated random changes of the site energies $V_{\mathbf n}$ in an Anderson tight-binding model [15]

$$\delta\hat H=\sum_{\mathbf n}\delta V_{\mathbf n}\hat P_{\mathbf n},\quad\langle\delta V_{\mathbf n}\delta V_{\mathbf n'}\rangle=\delta_{\mathbf n,\mathbf n'}, \tag{23}$$

where $\hat P_{\mathbf n}$ is the projection for locating an electron on lattice site $\mathbf n$. Using a semiclassical approximation of Eq. (22), $I(t)$ is seen to to be proportional to the probability of returning to the original site after time t. Normalizing so that $I(t)$ approaches unity for large t, we have

$$I(t)=\sum_{\nu=0}^{\infty}e^{-Dk^2_\nu t}, \tag{24}$$

where the sum is over the eigenmodes of the Helmholtz equation $(\nabla^2+k^2_\nu)\psi_\nu(\mathbf r)=0$ with Neumann boundary conditions. In a quasi-one-dimensional system, $k_\nu=\pi\nu/L$. In this case we obtain from Eq. (20)

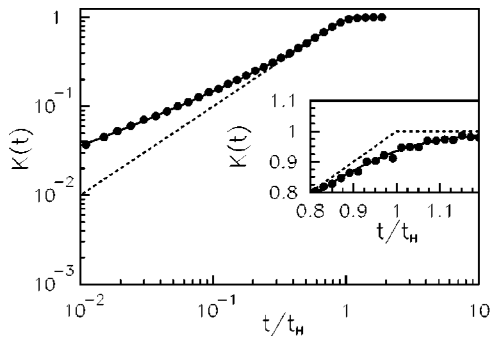

FIG. 1. The form factor $K(t)$ for a quasi-one-dimensional diffusive system. Numerical simulations for banded random matrices (•), are compared with theoretical results (——) according to Eqs. (9), (10), and (25). The GUE result is also shown (- - -).

$$\sigma_\beta^2(n) = \frac{2\Delta^2}{\beta\pi^2}\left[\log(2\pi n) + C_\beta + \frac{1}{2}\sum_{\nu=1}^{\infty}\log\left(1+\frac{n^2}{g^2\nu^4}\right)\right], \tag{25}$$

where $g = \pi^2\hbar D/L^2\Delta$ is a dimensionless conductance.

The ''form factor'' $K(t)$ is the Fourier transform of $R_\beta(\epsilon)$. As discussed by AA, Eq. (3) gives rise to nonuniversal structures in the form factor at the Heisenberg time t_H. We have verified their existence in numerical simulations: we used an ensemble of complex Hermitian banded random matrices (of dimension $N = 1000$ and bandwidth $b = 35$) modeling a quasi-one-dimensional diffusive system [16]. We fitted the dimensionless conductance, using states from the center of the spectrum (obtaining $g \simeq 2.0$). The results are shown in Fig. 1 and are in good agreement with the theoretical predictions, Eqs. (9), (10), and (25). They are precisely equivalent to the AA results (7) and (14) in [6]. We have thus shown that their results are consistent with the approach to justifying the random matrix theory discussed in [4].

Classically chaotic systems. Consider expression (22) for the fluctuation δa_k of the Fourier coefficients. If the system has a smooth classical Hamiltonian, this expression will clearly be negligible unless t corresponds approximately with the period of a periodic orbit. Moreover, it was shown in Ref. [4] that when the motion is chaotic, the δa_k have statistics corresponding to random matrix theory for large t. A simple model capturing the essential features of this case is to replace the lower limit of the integral in Eq. (20) with the period t_0 of the shortest periodic orbit. This gives

$$\sigma_\beta^2(n) \simeq \frac{2\Delta^2}{\beta\pi^2}\left[\mathrm{Ci}\left(\frac{2\pi n t_0}{t_H}\right) - \log\left(\frac{t_0}{t_\mathrm{H}}\right) - \gamma + C_\beta\right]. \tag{26}$$

This model has the feature that $\sigma_\beta^2(n)$ is finite in the limit $n\to\infty$, corresponding to the behavior of Dyson's Δ_3 statistic for systems with a smooth classical limit [3]. We note that this implies [using Eqs. (2) and (3)] that the oscillatory part of the correlation function does not decay to zero. The form factor is seen to have a δ-function at the Heisenberg time t_H, with a magnitude proportional to $(t_0/t_\mathrm{H})^{4/\beta}$. This feature has not been remarked upon in earlier papers that have discussed the form factor for chaotic systems [7–9], although it is implicit in the model discussed in Ref. [17].

A more precise estimate of $\sigma_\beta^2(n)$ for specific systems can be obtained using the periodic orbit theory, following the approach used in Ref. [3]. The conclusions are unchanged: $\sigma_\beta^2(n)$ remains finite as $n\to\infty$, and there must exist oscillations in the correlation function that do not decay. In general, however, the $p_\beta(n,\epsilon)$ are not precisely Gaussian. Moreover, small deviations from a Gaussian distribution can have a large effect on the Fourier transform, which determines the magnitude of the oscillations in Eq. (10). We infer that the AA relations must be treated with caution when applied to the spectra of systems with a smooth classical limit.

In conclusion, we have shown that the AA relations have a simple interpretation, independent of quantum mechanics. Also, we have shown that despite an apparent contradiction, they are consistent with the Brownian motion model for spectral statistics described in Ref. [4].

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