Long-Range Spatial Correlations of Eigenfunctions in Quantum Disordered Systems

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This paper is devoted to the statistics of the quantum eigenfunctions in an ensemble of metallic grains. We focus on moments of inverse participation ratio. In the universal limit that corresponds to the infinite conductance of the grains, these moments are self-averaging quantities. At large but finite conductance the moments do fluctuate due to the long-range correlations in the eigenfunctions. We evaluate the distributions of fluctuations at given conductance and geometry of the grains and express them through the spectrum of the diffusion operator in the grain. [S0031-9007(98)05328-9]

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Weakly disordered metallic grains make an excellent laboratory to study the phenomenon of quantum chaos (for a general discussion, see, e.g., Ref. [1]). Provided electrons within a grain interact weakly, one can describe properties of this system through one particle quantum spectrum and eigenfunctions. The problem is reduced to a Shrödinger equation for a particle subject to a potential that consists of two components: a regular potential that confines electrons within the grain and some random potential due to disorder. Given the distribution of the random potential we get an ensemble of disordered grains and can consider various statistics of the spectra and eigenfunctions.

Classical motion in a random potential is diffusive (provided the grain size *R* exceeds the mean free path) with a diffusion constant *D*. Ensembles of weakly disordered metallic grains can be characterized by the "dimensionless conductance" *g* determined as a ratio $g = t_H/t_T$ of Heisenberg time $t_H = \hbar/\Delta$ and Thouless time of the diffusion through the grain $t_T = R^2/D$, where Δ is the mean energy level spacing. A grain would be called weakly disordered provided $g \gg 1$.

The spectral statistics for the ensembles of grains in the limit $g \to \infty$ are proven [2,3] to coincide with those for the corresponding ensembles of random matrices [4]. These statistics would be called *universal*. The field theoretical way of evaluating statistics in ensembles of disordered grains is based on the supersymmetric σ model [2]. When $g \to \infty$ the zero-dimensional σ model can be used for straightforward evaluation of universal statistics of both spectra and eigenfunction [5].

Finite g corrections to the universal properties of quantum systems recently attracted substantial interest. The smooth part of the spectral correlation function was evaluated in Ref. [6]. The first order in 1/g correction to the spectral correlation function was evaluated by Kravtsov and Mirlin [7]. Nonperturbative analysis of the problem [8] pointed out a qualitative change of the behavior at finite g—washing out the oscillations in the two-point correlation function, and, hence, smoothing of

the singularities [9] in the quantum dynamics at times close to t_H . A remarkable feature of the spectral statistics at finite g is that both their smooth [6] and their oscillating parts [8] can be presented through the spectral determinant of the classical diffusion operator $D\nabla^2$. This paper is devoted to the connection of this spectral determinant to the long-range correlations in the eigenfunctions.

In this paper we concentrate on the moments [10]

$$I_{\alpha}(n) = V^{n-1} \int |\psi_{\alpha}(\mathbf{r})|^{2n} d\mathbf{r}, \qquad (1)$$

where $\psi_{\alpha}(\mathbf{r})$ is an eigenfunction of the system which corresponds to an eigenenergy ϵ_{α} , and V is the volume of the grain (for a *d*-dimensional cube $V = L^d$). The n = 2 moment, known as the inverse participation ratio, is related to the level-velocity distribution [11] or to Hubbard-like interaction of two particles on the same quantum state. In general, the moments (1) describe the fluctuations of wave functions which occupy an appreciable fraction of dot volume.

In the universal regime $g \to \infty$ each wave function is extended over the whole volume; however, only very short-range correlations persist: $\psi_{\alpha}(\mathbf{r}_1)$ and $\psi_{\alpha}(\mathbf{r}_2)$ are uncorrelated provided $r = |\mathbf{r}_1 - \mathbf{r}_2|$ is not much bigger than the particle wavelength [5,12–14]. As a result, the integration in Eq. (1) provides self-averaging, and $I_{\alpha}(n)$ do not fluctuate in the universal regime. They coincide with the moments b_n of the Porter-Thomas distribution [4] for the intensity fluctuations $|\psi_{\alpha}(\mathbf{r})|^2$. For unitary (*u*) and orthogonal (*o*) symmetries $I_{\alpha}(n) = b_n$, where

$$b_n^{(u)} = \Gamma(n+1), \qquad b_n^{(o)} = 2^n \Gamma(n+1/2) / \Gamma(1/2).$$
(2)

The most striking difference of finite g case from the universal situation is the existence of spatial correlations of wave function density even at r comparable with the size of the system. As a result $I_{\alpha}(n)$ demonstrates finite fluctuations from state to state and from sample to sample [11]. $I_{\alpha}(n)$ are characterized by their *distribution*

functions. Let us consider the distribution $P_n(u)$ of relative deviations of $I_{\alpha}(n)$ from b_n :

$$u_{\alpha}(n) = I_{\alpha}(n)/b_n - 1, \qquad P_n(u) = \langle \delta(u - u_{\alpha}(n)) \rangle,$$
(3)

where $\langle \cdots \rangle$ stands for ensemble averaging.

As we show below the Laplace transforms $\tilde{P}_n(s) = \langle \exp[-su_\alpha(n)] \rangle$ of the distribution $P_n(u)$ for large but finite g can be written as

$$\tilde{P}_{n}(s) = \prod_{\mu \neq 0} \left[1 + (n^{2} - n) \frac{2s\Delta}{\pi\beta\omega_{\mu}} \right]^{-1/2}$$
$$\equiv \sqrt{\tilde{Z} \left[(n - n^{2}) \frac{2s\Delta}{\pi\beta} \right]}.$$
(4)

 β is different for *T* invariant and not *T*-invariant systems: $\beta^{(o)} = 1, \beta^{(u)} = 2. \omega_{\mu}$ is the spectrum of the diffusion equation with Neumann boundary conditions on the grain boundary *B*:

$$D\nabla^2 \phi_\mu(\mathbf{r}) = -\omega_\mu \phi_\mu(\mathbf{r}), \qquad \nabla \phi|_B = 0.$$
 (5)

 ω_{μ} are not universal: this spectrum is determined by both g and the shape of the grain. (We take $g = \beta \omega_1/2\Delta$ as a definition of g, since this ratio is proportional to the dimensionless conductance for a rectangular grain.) However, the ground state of the problem is spatially uniform, and corresponds to $\omega_0 = 0$. All universal statistics become applicable to disordered grains when $\omega_{\mu} \rightarrow \infty$ for all μ except $\mu = 0$. In this limit, known as zero mode approximation, $P_n(u) = \delta(u)$ since Eq. (4) gives $\tilde{P}_n(s) = \text{const.}$ Therefore $I_{\alpha}(n)$ does not fluctuate in the universal regime.

In Eq. (4) we introduced the function

$$1/\tilde{Z}(z) = \prod_{\mu \neq 0} [1 - z/\omega_{\mu}] = z/Z(z), \qquad (6)$$

where Z(z) is the dynamical Ruelle zeta function [15], associated with the diffusion operator in Eq. (5). As is shown in Ref. [16] the pair spectral correlation function for an ensemble of disordered grains also can be expressed through $\tilde{Z}(z)$ function. However the spectral statistics are determined by $|\tilde{Z}(iz)|^2$, while for the distributions $P_n(u)$ one has to evaluate Z(z) at real negative z or to determine both modulus and phase of Z(iz). An interesting feature of the distributions $P_n(u)$ is that, in contrast with other statistics of the quantum eigenfunctions, they are independent on the diffusion operator eigenfunctions ϕ_{μ} , and are determined solely by the spectrum of Eq. (5).

Let us describe the main features of the distributions $P_n(u)$. It is clear that long-scale correlations increase the mean value $\langle I(n) \rangle = b_n [1 + \langle u \rangle]$ of $I_\alpha(n)$ as compared with Eq. (2). According to Eq. (4)

$$P_n(u) = \frac{1}{(n^2 - n)} P(w), \qquad w = u_n / (n^2 - n), \quad (7)$$

and for $\langle u \rangle = \int u P_n(u) \, du$ we obtain

$$\frac{\langle u \rangle}{n^2 - n} = \bar{w} = \frac{-1}{n^2 - n} \frac{d}{ds} \tilde{P}_n(s)|_{s=0} = \frac{\Delta}{\beta \pi} \sum_{\mu \neq 0} \frac{1}{\omega_\mu}$$

In terms of the $\tilde{Z}(z)$ function \bar{w} can be rewritten as

$$\langle w \rangle = \frac{1}{2} \mathcal{G}_1(0), \qquad \mathcal{G}_m(z) \equiv \left(\frac{2\Delta}{\pi\beta}\right)^m \frac{d^m \ln \tilde{Z}(z)}{dz^m}.$$
 (8)

Behavior of P(w) at small w can be evaluated by making a saddle-point approximation in the inverse Laplace transformation of Eq. (4)

$$P(w) = \tilde{Z}^{1/2}(z_c) \left[\pi G_2(z_c) \right]^{-1/2} \exp \left[-\frac{\pi \beta}{2\Delta} w z_c \right], \quad (9)$$

provided $z_c(w)$ determined by the equation $G_1(z_c) = 2w$ is large, $|z_c| \gg \omega_1$.

It follows from Eq. (4) that the probability for w to be much bigger than $\langle w \rangle$ is exponentially small:

$$P(w) = C \sqrt{g/(4w)} \exp[-\pi gw],$$

$$C = \prod_{\mu \neq 0,1} \sqrt{1 - \omega_1/\omega_\mu}$$

$$= [\tilde{Z}(z) (1 - z/\omega_1)]^{-1/2}|_{z \to \omega_1}.$$
(10)

Consider a disordered two-dimensional grain with a particle mean free path l. From Eq. (5) it follows

$$\mathcal{G}_1(z) = \frac{1}{g} \ln \left[1 + \frac{\omega_1}{\omega_1 - z} \frac{R^2}{l^2} \right], \qquad \langle w \rangle = \frac{\ln(R/l)}{g}.$$
(11)

Therefore in the weak localization regime [17] when all quantum states are extended $\bar{w} \ll 1$. Equation (11) for \bar{w} is in agreement with the perturbation theory calculation [11]. For $1/g \ll w \ll \bar{w}$ Equation (9) gives

$$P(w) = \frac{g}{2} \exp \left[g(\bar{w} - w) - \frac{\pi}{2} e^{2g(\bar{w} - w)} \right],$$

where \bar{w} is determined by Eq. (11). For $gw \leq 1$

$$P(w) = \frac{g^{3/2}}{\sqrt{2w}} \exp\left[g\bar{w} - \frac{\pi}{4gw}e^{2g\bar{w}}\right]$$

According to Eq. (10) $\ln C = \pi g \bar{w}$, and at $\bar{w} \leq w \ll 1$

$$P(w) = \sqrt{g/4w} \exp[-\pi g(w - \bar{w})].$$
 (12)

It should be mentioned that Eqs. (4)–(12) are valid only for $u \ll 1$. According to Eq. (7) this means that Eqs. (4)–(12) describe the main body of the distribution $P_n(u)$ which never takes a Gaussian form. Therefore, the first two moments (the average and variance) are not sufficient to describe the whole distribution.

When $u \gg 1$, the distributions $P_n(u)$ are determined by both ω_{μ} and ϕ_{μ} . This asymptotic of $P_n(u)$ can be found by the method of optimal fluctuation. For a spherical grain of arbitrary dimension *d* and radius *R*

$$P_n(u \gg 1) \approx \exp[-a_n g u^{1/(n-1)}],$$
 (13)

where $g = \pi \beta D / 4R^2 \Delta$ and

$$a_n = \frac{d^2}{\pi n(n-1)} \Gamma^2 \left(\frac{1}{2n-2}\right) \Gamma^{-2} \left(\frac{n}{2n-2}\right) n^{1/(n-1)}.$$
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Equation (13) is valid as long as $1 \ll u \ll (a_n R/l)^{n-1}$. At large *u* the σ model approach fails [18].

In order to derive Eq. (4) we consider mutual distribution of $v_1 = V |\psi_{\alpha}(\mathbf{r}_1)|^2$ and $v_2 = V |\psi_{\alpha}(\mathbf{r}_2)|^2$ densities of a quantum eigenfunction $\psi_{\alpha}(\mathbf{r})$. This distribution can be reconstructed through its moments $M_{pq} = V^{p+q} \langle |\psi_{\alpha}(\mathbf{r}_1)|^{2p} |\psi_{\alpha}(\mathbf{r}_2)|^{2q} \rangle$. The latter can be calculated for a disordered grain by analyzing moments of one-electron Green functions using the supersymmetric σ -model technique in a way similar to how one-point moments M_{p0} were calculated by Muzykantskii and Khmelnitskii [19], and by Fal'ko and Efetov [20].

The ratio of M_{pq} and its universal $(g \rightarrow \infty)$ value $M_{pq}^{(un)}$ can be written as the functional integral

$$\frac{M_{pq}}{M_{pq}^{(un)}} = \frac{1}{\Xi} \int \mathcal{D}\theta(\mathbf{r}) e^{-F + p(\theta_1 - \Omega) + q(\theta_2 - \Omega)}, \quad (14)$$

where $\theta_{1,2} = \theta(\mathbf{r}_{1,2})$ and $\Xi = \int \mathcal{D}\theta(\mathbf{r})e^{-F}$. Note that while M_{pq}^{un} is determined by the zero mode of the diffusion operator, the ratio Eq. (14) does not include the integration over this mode. As a result the functional integral in Eq. (14) is over all functions $\theta(\mathbf{r})$ that satisfy the condition $\int d\mathbf{r} \theta = 0$, and

$$F[\theta] = \frac{\pi\beta D}{4\Delta} \int (\nabla\theta)^2 \frac{d\mathbf{r}}{V}, \qquad \Omega[\theta] = \ln\left(\int e^{\theta} \frac{d\mathbf{r}}{V}\right).$$
(15)

Equation (14) enables us to express the two-points mutual distribution function $P(v_1, v_2)$ at finite g through the

universal one $P_{un}(v_1, v_2)$

$$P(v_1, v_2) = \frac{1}{\Xi} \int \mathcal{D}\theta(\mathbf{r}) e^{-F + 2\Omega - \theta_1 - \theta_2} \\ \times P_{\mathrm{un}}(v_1 e^{\Omega - \theta_1}, v_2 e^{\Omega - \theta_2}).$$
(16)

The universal two-point distribution functions $P_{un}(v_1, v_2)$ for unitary and orthogonal symmetries were determined earlier [5,14]:

$$\begin{split} P_{\rm un}^{(u)}(v_1,v_2) &= \frac{\exp(-\frac{v_1+v_2}{1-f^2})}{1-f^2} I_0\left(\frac{2f\sqrt{v_1v_2}}{1-f^2}\right),\\ P_{\rm un}^{(o)}(v_1,v_2) &= \frac{\exp[-\frac{v_1+v_2}{2(1-f^2)}]}{2\pi\sqrt{(1-f^2)v_1v_2}}\cosh\left(\frac{f\sqrt{v_1v_2}}{1-f^2}\right), \end{split}$$

where *f* is the Friedel function of $r = |\mathbf{r}_1 - \mathbf{r}_2|$

$$f(r) = \Gamma(d/2) \left(\frac{2}{kr}\right)^{d/2-1} J_{d/2-1}(kr) e^{-r/(2l)}.$$

Above $J_p(x)$ and $I_0(x)$ are Bessel and modified Bessel functions, respectively; k is the wave number.

A usual way to calculate the functional integral like Eq. (16) is to present $\theta(\mathbf{r})$ as a sum $\sum_{\mu} \theta_{\mu} \phi_{\mu}(\mathbf{r})$ (there is no contribution with $\mu = 0$ since $\int d\mathbf{r} \theta = 0$) over the eigenfunctions of the problem Eq. (5) thus reducing the calculation of the functional integral to a sequence of definite integrals over θ_{μ} .

Expansion of the exponent in Eq. (16) up to the second order in θ_{μ} leads to a Gaussian integral that can be evaluated explicitly

$$P(v_1, v_2) = \int_0^\infty \int_0^\infty \frac{ds_1 \, ds_2}{2\pi} \frac{P_{\rm un}(v_1 s_1, v_2 s_2)}{\sqrt{\Pi_{11} \Pi_{22} - \Pi_{12}^2}} \exp\left[-\sum_{\kappa=\pm 1} \frac{(\sqrt{\Pi_{11}} \ln s_2 + \kappa \sqrt{\Pi_{22}} \ln s_1)^2}{\Pi_{11} \Pi_{22} + \kappa \Pi_{12} \sqrt{\Pi_{11} \Pi_{22}}}\right],\tag{17}$$

where Π_{ij} is the Green function of Eq. (5)

$$\Pi_{ij} = \frac{2\Delta}{\pi\beta} \sum_{\mu\neq 0} \frac{\phi_{\mu}(\mathbf{r}_i)\phi_{\mu}(\mathbf{r}_j)}{\omega_{\mu}}.$$
(18)

For $\mathbf{r}_1 \rightarrow \mathbf{r}_2$ Eq. (17) reproduces the result for one-point fluctuations [20].

From Eq. (16) we can guess the probability density of a given realization $\psi(\mathbf{r})$ of an eigenfunction in the form of a functional integral. Instead of the Gaussian distribution that is valid in the universal limit [13,14] we obtain

$$P[\psi]\mathcal{D}\psi = \mathcal{D}\psi\frac{1}{\Xi}\int \mathcal{D}\theta(\mathbf{r})e^{-F}(\beta^{-1}\det\hat{K})^{-\beta/2}\exp\left[-\frac{\beta}{2}\int d\mathbf{r}_{1}\int d\mathbf{r}_{2}\psi^{*}(\mathbf{r}_{1})\hat{K}^{-1}\psi(\mathbf{r}_{2})\right].$$
 (19)

The matrix elements of the operator \hat{K} in the coordinate representation $K_{12} \equiv \langle \mathbf{r}_1 | \hat{K} | \mathbf{r}_2 \rangle$ equal to

$$K_{12} = f(|\mathbf{r}_1 - \mathbf{r}_2|) \exp\left[\frac{\theta_1 + \theta_2}{2} - \Omega\right].$$
(20)

Equation (19) enables us to present $\tilde{P}_n(s)$ in the form

$$\tilde{P}_n(s) = \int \frac{\mathcal{D}\theta(\mathbf{r})}{\Xi} e^{-F} \exp\left[-\frac{s}{V} \int \left(e^{n(\theta-\Omega)} - 1\right) d\mathbf{r}\right].$$
(21)

Using in Eq. (21) the harmonic approximation that is valid for small fluctuations $u \ll 1$, we obtain Eq. (4).

At $u \gg 1$ we can apply the method of optimal fluctuation to Eq. (21). For a spherical dot of the radius *R* the

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saddle-point equations can be written as

$$\tilde{P}_n(s) \approx \exp\left\{s - gd \int_0^1 \left[\dot{\theta}_c^2 + \frac{\Phi(\theta_c)}{n-1}\right] t^{d-1} dt\right\}, \quad (22)$$

where t = r/R, a dot stands for t derivatives, and $\theta_c(t)$ obeys the equation

$$\ddot{\theta}_{c} + \frac{d-1}{t}\dot{\theta}_{c} = -\frac{1}{2}\frac{\delta\Phi}{\delta\theta_{c}},$$

$$\Phi(\theta) = p(e^{n\theta} - ne^{\theta}),$$
(23)

supplied by the condition $\hat{\theta}_c(0) = \hat{\theta}_c(1) = 0$. *p* in Eq. (23) should be determined from the self-consistency

condition

$$p = \frac{d}{1-n} \left(\frac{pg}{-s}\right)^{1/n} \int_0^1 \Phi(\theta_c) t^{d-1} dt.$$

Let us note that the potential $\Phi(\theta)$ has a minimum at $\theta = 0$. At $u \gg 1$ or $s \ll g$ the essential contribution to Eq. (22) is given by the trajectories of $\theta_c(t)$, which starts with $\theta_c(0) \sim -\frac{2}{n-2} \ln |g/s| \rightarrow -\infty$ and ends somewhere near the minimum of potential $\Phi(\theta)$. They correspond to the optimal wave functions that in the center of a dot is small like $|s/g|^{2/(n-2)}$ and increases when approaching the boundary. Such a trajectory leads to the asymptotic Eq. (13) for the distribution function $P_n(u)$.

To summarize, we have calculated the distributions for generalized moments of inverse participation ratio Eq. (1) in an ensemble of disordered metallic grains with a given dimensionless conductance g. In the universal limit $g \rightarrow \infty$ these moments do not fluctuate due to selfaveraging and thus have definite values Eq. (2). The fluctuations appear only at finite g together with longrange correlations in densities of wave functions. Indeed, in the universal limit, when only short-range correlations persist, the fluctuations vanish when the grain volume (the rank of random matrices) tends to infinity. Contrarily, at finite g they appear small (as 1/g) but long-range correlations [see Eq. (18)] controlled entirely by the eigenfunctions of the diffusion operator Eq. (5). These correlations give rise to the fluctuations of the moments.

We have found that there is the universal tail of the distribution in the region of large fluctuations ($\langle u \rangle \ll$ $u \ll 1$). The probability of such a fluctuation decays exponentially with a rate equal to the conductance g. Analyzing the distribution in terms of diffusion modes, we concluded that this exponential decay is due to the large spatial scale fluctuations corresponding to the first diffusion mode. It is in contrast to what is known for local fluctuations of eigenfunctions where the modes of increasingly smaller scale give rise to the logarithmically normal distribution. In the region of very large fluctuations $(u \gg 1)$ the distribution $P_n(u)$ turns out to be a stretched exponent [see Eq. (13)] with the power determined by the order of the moment. The nonlinear equation that describes the shape of optimal fluctuation includes now a potential with a minimum. As a result, a new type of instanton solution appears in the problem.

The explicit form of the central body of the distribution depends on the conductance as well as the shape of a dot. It is amazing, however, that at $g \gg 1$ and for $n \ll \sqrt{g}$ the main part [Eqs. (7), (8), (10)–(12)] can be expressed through the spectrum of the diffusion operator ω_{μ} and do not depend on the eigenfunctions ϕ_{μ} . This fact suggests generalization of these statistics of eigenfunctions from disordered to generic chaotic systems, by making use of the Ruelle (dynamical) zeta function [Eqs. (4) and (6)], in a way similar to what was done in Ref. [16] for spectral statistics. Substitution of the spectral determinant of the diffusion operator by the Ruelle zeta function for

spectral statistics in the generic case was supported by the calculations in the framework of a nonlinear σ model [21]. The analysis of Bogomolny and Keating [22] based on the periodic orbit theory led to similar but different results. We hope that further analytical development of results on the eigenfunction statistics together with numerical evaluations will clarify the relation between quantum statistics and classical dynamics including the phenomenon of scarring [23].

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