

Residual Coulomb Interaction Fluctuations in Chaotic Systems: The Boundary, Random Plane Waves, and Semiclassical Theory

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(Received 30 November 2007; published 25 April 2008)

New fluctuation properties arise in problems where both spatial integration and energy summation are necessary ingredients. The quintessential example is given by the short-range approximation to the first order ground state contribution of the residual Coulomb interaction. The dominant features come from the region near the boundary where there is an interplay between Friedel oscillations and fluctuations in the eigenstates. Quite naturally, the fluctuation scale is significantly enhanced for Neumann boundary conditions as compared to Dirichlet. Elements missing from random plane wave modeling of chaotic eigenstates lead surprisingly to significant errors, which can be corrected within a purely semiclassical approach.

DOI: 10.1103/PhysRevLett.100.164101

PACS numbers: 05.45.Mt, 03.65.Sq, 71.10.Ay, 73.21.La

The characterization of quantum systems with any of a variety of underlying classical dynamics, ranging from diffusive or chaotic to regular, has often demonstrated that the study of their statistical properties is of primary importance. Spectral fluctuations are a principle example as they gave the first support to one of the main results linking classical chaos and random matrix theory [1], the Bohigas-Giannoni-Schmit conjecture [2,3]. Needless to say, the statistical properties of eigenfunctions are also a subject of paramount interest [4–12].

For chaotic systems, a widely accepted starting point for the treatment of eigenfunction fluctuations *locally*, such as the amplitude distribution or the two-point correlation function $c(|\mathbf{r} - \mathbf{r}'|) = \langle \psi(\mathbf{r})\psi(\mathbf{r}') \rangle$ of a given eigenfunction ψ , is a modeling in terms of a random superposition of plane waves (RPW) [4,5]. For two-degrees-of-freedom systems, $c(r)$ can be understood as being given approximately by a Bessel function. For distances $|\mathbf{r} - \mathbf{r}'|$ short compared to the system size, and in the absence of effects related to classical dynamics [8,9,13], this is roughly observed in numerical [7,14,15] and experimental [16] studies. Our interest here is in statistical properties of eigenfunctions going beyond local quantities such as $c(r)$.

One motivation for the introduction of these new statistical measures is to study the interplay between interferences and interactions in low-temperature mesoscopic systems in or near the Coulomb blockade regime. For typical electronic densities, the screening length is close to the Fermi wavelength λ_F , and the screened Coulomb interaction can be approximated by the short-range expression $V_{sc}(\mathbf{r} - \mathbf{r}') = (2\nu)^{-1} F_0^a \delta(\mathbf{r} - \mathbf{r}')$ with 2ν the mean local density of states, including spin degeneracy ($\nu = m/2\pi\hbar^2$ for $d = 2$) and F_0^a a constant of order one.

To this level of approximation, the first order ground state energy contribution of the residual interactions can be expressed in the form $\delta E^{\text{RI}} = (2\nu)^{-1} F_0^a \int d\mathbf{r} N_\uparrow(\mathbf{r}) N_\downarrow(\mathbf{r})$

with N_σ the unperturbed ground state density of particles with spin σ . From this expression, it is seen that the increase of interaction energy associated with the addition of an extra electron is related to

$$S_i = \mathcal{A} \int d\mathbf{r} |\Psi_i(\mathbf{r})|^2 N(\mathbf{r}; E_i^+), \quad (1)$$

with $N(\mathbf{r}; E) \equiv \sum_{i=1}^{\infty} |\Psi_i(\mathbf{r})|^2 \theta(E - E_i)$ ($E_i < E_i^+ < E_{i+1}$). To within small corrections, promotion of an electron from the j th to the i th orbital is proportional to $S_i - S_j$. The local mean behavior of S_i cannot contribute to this difference. However, if the fluctuations of δE^{RI} ($\propto S_i - S_j$) are roughly on the scale of the single particle energy differences or larger, then the residual interactions would lead to altered single particle orbital occupations in some cases, and possibly unusual behavior as external parameters are varied. The fluctuation properties of the S_i (i.e., short-range correlations, standard deviation) are therefore governing whether or not residual interactions play an important role for such systems. Here, we focus on the simpler case of two-dimensional billiards with either Dirichlet or Neumann boundary conditions; for them, \mathcal{A} is the billiard area.

The dominant contributions to S_i (and its fluctuations) originate from the Friedel oscillations of the density of particles near the boundary. For billiards systems, they can be expressed as $N_{\text{Friedel}}(\mathbf{r}; E) = \frac{N_w(E)}{\mathcal{A}} [1 \pm \frac{J_1(2kx)}{kx}]$ [17], with x the distance from the boundary, the $+$ and $-$ sign corresponding, respectively, to Neumann and Dirichlet boundary conditions, and $N_w(E)$ refers to the leading term of the Weyl formula, $N_w(E) = \nu \mathcal{A} E$. To leading order we can therefore use the approximation

$$S_i = i \pm i \int d\mathbf{r} \left[\frac{J_1(2k_F x)}{k_F x} |\Psi_i(\mathbf{r})|^2 \right]. \quad (2)$$

To proceed, a description of the fluctuations of $|\Psi_i(\mathbf{r})|^2$ is also required. These are obtained ahead using a semiclassical approach closely related to the Gutzwiller trace formula. However, it is useful first to consider the oft-employed RPW description, which very interestingly turns out to lack a couple of crucial ingredients. Nevertheless, it sheds light on the mechanism governing the fluctuations under study.

Within RPW [4,5] eigenstates are represented, in the absence of any symmetry, by a random superposition of plane waves $\sum_l a_l \exp(i\mathbf{k}_l \cdot \mathbf{r})$ with wave vectors of fixed modulus $|\mathbf{k}_l| = k_F$ distributed isotropically. Time reversal invariance introduces a correlation between time reversed plane waves such that the eigenfunctions are real. Similarly, the presence of a planar boundary imposes a constraint between the coefficients of plane waves related by a sign change of the normal component of the wave vector \mathbf{k}_l [18,19]. Near a boundary, and using a system of coordinates $\mathbf{r} = \hat{\mathbf{x}} + \hat{\mathbf{y}}$ with $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ the vectors, respectively, perpendicular and parallel to the boundary, eigenfunctions are mimicked statistically by a superposition,

$$\psi_i(\mathbf{r}) = \frac{1}{N_{\text{eff}}} \sum_{l=1}^{N_{\text{eff}}} a_l \mathbf{cs}(\mathbf{k}_l \cdot \hat{\mathbf{x}}) \cos(\mathbf{k}_l \cdot \hat{\mathbf{y}} + \varphi_l), \quad (3)$$

where $\mathbf{cs}(\cdot) \stackrel{\text{def}}{=} \sin(\cdot)$ for Dirichlet and $\cos(\cdot)$ for Neumann boundary conditions. The phase angle φ_l , the orientation of the wave vector \mathbf{k}_l , and the real amplitude a_l with $\langle a_l a_{l'} \rangle = \delta_{ll'} \sigma^2$ are all chosen randomly. The variance σ^2 is fixed by the normalization condition

$$1 = \int d\mathbf{r} \langle |\psi_i(\mathbf{r})|^2 \rangle \simeq \frac{\mathcal{A} \sigma^2}{4N_{\text{eff}}}. \quad (4)$$

The variance is a natural measure of the fluctuations. To leading order

$$\text{Var}(\mathcal{S}_i) = \frac{i^2}{\mathcal{A}^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{J_1(2k_F x_1)}{k_F x_1} \frac{J_1(2k_F x_2)}{k_F x_2} \times [\langle |\Psi_i(\mathbf{r}_1)|^2 |\Psi_i(\mathbf{r}_2)|^2 \rangle - \langle |\Psi_i(\mathbf{r}_1)|^2 \rangle \langle |\Psi_i(\mathbf{r}_2)|^2 \rangle].$$

Inserting (3) and pairwise correlating the random plane wave coefficients a_n one obtains

$$\text{Var}[\mathcal{S}_i] = \frac{8i^2}{\mathcal{A}^2} \frac{1}{N_{\text{eff}}^2} \sum_{l,m=1}^{N_{\text{eff}}} \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{J_1(2k_F x_1)}{k_F x_1} \frac{J_1(2k_F x_2)}{k_F x_2} \mathbf{cs}(\mathbf{k}_l \cdot \mathbf{x}_1) \mathbf{cs}(\mathbf{k}_l \cdot \mathbf{x}_2) \mathbf{cs}(\mathbf{k}_m \cdot \mathbf{x}_1) \mathbf{cs}(\mathbf{k}_m \cdot \mathbf{x}_2) \cos[\mathbf{k}_l \cdot (\mathbf{y}_1 - \mathbf{y}_2)] \cos[\mathbf{k}_m \cdot (\mathbf{y}_1 - \mathbf{y}_2)]. \quad (5)$$

Performing the integration gives

$$\text{Var}[\mathcal{S}_i] = \frac{k_F \mathcal{L}}{4\pi^3} \langle \lambda^2(\theta) \rangle_\theta \quad (6)$$

with \mathcal{L} the perimeter, $\lambda(\theta) \stackrel{\text{def}}{=} [1 \pm |\sin(\theta)|] / |\cos(\theta)|$, and the expression for $\langle \lambda^2(\theta) \rangle_\theta \equiv \int_0^1 d(\sin\theta) \lambda^2(\theta)$ is given ahead in Eq. (15).

In Fig. 1, the variance of \mathcal{S}_i as a function of i is represented for a chaotic system, the cardioid billiard

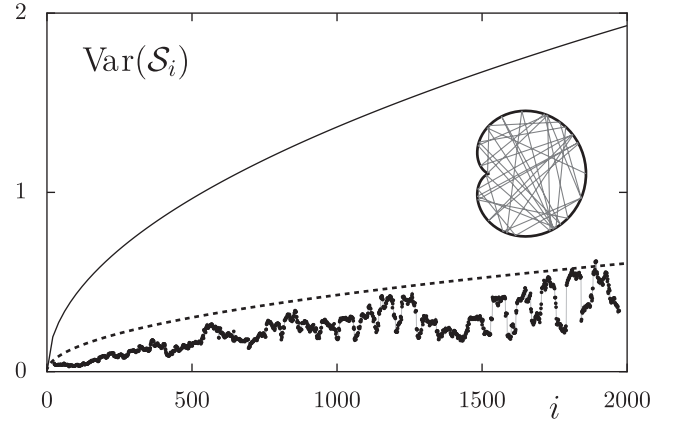


FIG. 1. Variance of \mathcal{S}_i for the cardioid billiard with Dirichlet boundary conditions. The solid line is the RPW expression, Eq. (6), the dashed line is the semiclassical prediction, Eq. (14), and the discrete points are for the cardioid billiard (shown in inset).

with Dirichlet boundary conditions [20,21]. In this case, quite surprisingly given the history of modeling chaotic eigenstates within the RPW framework, its predictions significantly overestimate the fluctuations. In fact, two important elements are missing from this approach, both of which are addressed properly within a purely semiclassical approach.

One difficulty immediately encountered with a semiclassical treatment of the \mathcal{S}_i is that their computation implies addressing the fluctuations of individual wave functions, whereas the semiclassical approximations valid for chaotic systems of use here converge only for (locally) smoothed quantities. This difficulty may be overcome by following the spirit of Bogomolny's calculation [22] and introducing a local energy averaging,

$$\langle \mathcal{S} \rangle_{\Delta N} \stackrel{\text{def}}{=} \frac{1}{\Delta N} \sum_{E - (\Delta E/2) < E_i < E + (\Delta E/2)} \mathcal{S}_i \quad (7)$$

with $\Delta N \stackrel{\text{def}}{=} N(E + \frac{\Delta E}{2}) - N(E - \frac{\Delta E}{2})$. Assuming that there is translational invariance (smooth, uniform behavior) locally in indices (i, j) one obtains the relation

$$\begin{aligned} \text{Var}[\langle \mathcal{S} \rangle_{\Delta N}] &\stackrel{\text{def}}{=} \overline{(\langle \mathcal{S} \rangle_{\Delta N} - \bar{\mathcal{S}})^2} \\ &= \frac{1}{\Delta N} \text{Var}[\mathcal{S}_i] + \left(1 - \frac{1}{\Delta N}\right) \text{Covar}[\mathcal{S}_i \mathcal{S}_{i+j}]. \end{aligned} \quad (8)$$

Computing the smoothed quantity $\langle \mathcal{S} \rangle_{\Delta N}$, for which semiclassical approximations are convergent, one can therefore extract the variance of the \mathcal{S}_i from the scaling in ΔN of $\text{Var}[\langle \mathcal{S} \rangle_{\Delta N}]$.

Our starting point for this calculation is

$$\begin{aligned} \mathcal{A} \langle |\Psi_i(\mathbf{r})|^2 \rangle_{\Delta N} &= 1 \pm J_0(2k_F x) - \frac{1}{\nu} \frac{1}{\pi} \text{Im} \langle \tilde{G}^{\text{osc}}(\mathbf{r}, \mathbf{r}, E) \rangle_{\Delta E} \\ &\quad - \frac{1 \pm J_0(2k_F x)}{\mathcal{A} \nu} \langle \rho^{\text{osc}} \rangle_{\Delta E}, \end{aligned} \quad (9)$$

valid near the boundary, which differs from the expression given by Bogomolny [22] only through the inclusion of the Bessel function $J_0(2k_F x)$ accounting for the Friedel oscillations. Here, the energy smoothing indicated is similar to that above except normalized by the energy range, and ρ^{osc} is the oscillating part of the density of states, given semiclassically as a sum over periodic orbits

$$\rho^{\text{osc}}(E) = \frac{1}{\pi\hbar} \sum_{\gamma=\text{p.o.}} \tau_\gamma \frac{\cos(\frac{S_\gamma(E_\gamma^+)}{\hbar} - \sigma_\gamma \frac{\pi}{2})}{|\text{Det}(M_\gamma - \mathbf{1})|^{1/2}}. \quad (10)$$

Similarly, the diagonal part of the Green's function $G^R(\mathbf{r}, \mathbf{r}, E)$ is expressed as a sum over closed (not necessarily periodic) orbits

$$G^{\text{osc}}(\mathbf{r}, \mathbf{r}, E) \simeq \frac{1}{i\hbar} \frac{1}{\sqrt{2i\pi\hbar}} \sum_{\mu: \mathbf{r} \rightarrow \mathbf{r}} \frac{1}{\sqrt{|\dot{x}\dot{x}' m_{12, \mu}|}} \times \exp\left[\frac{i}{\hbar} S_\mu(\mathbf{r}, \mathbf{r}, E) - i\frac{\pi}{2} \eta_\mu\right]. \quad (11)$$

In the above expressions, S is the action integral along the orbit, τ the period, $m_{12} \equiv \partial y^{\text{final}} / \partial p_y^{\text{initial}}$, M_γ the monodromy matrix, and σ_γ, η_μ are Maslov indices. The tilde on the Green's function in Eq. (9) furthermore indicates that the short orbit giving rise to Friedel oscillations, namely, the one bouncing off the boundary and returning directly to its initial location, is excluded from the semiclassical sum [as in Eq. (9) it is already taken into account by the Bessel function].

Inserting Eq. (9) into Eq. (2) and performing the integral over space, it is important to note that the range of integration in the direction perpendicular to the boundary is short, even on the quantum scale, and that therefore a stationary phase condition should be imposed only on the parallel direction. Gathering, however, the four orbits shown in Fig. 2, and labeling their total contribution with the index γ of the periodic orbit to which they converge as $x \rightarrow 0$, one obtains, following the usual steps of the derivation of the Gutzwiller trace formula,

$$\langle S \rangle_{\Delta N} - \bar{S} = \pm \frac{1}{\pi} \sum_{\gamma=\text{p.o.}} \frac{\cos[\frac{S_\gamma(E)}{\hbar} - \bar{\nu}_\gamma \frac{\pi}{2}]}{\sqrt{|\text{Det}(M_\gamma - \mathbf{1})|}} \times \text{sinc}\left(\frac{\tau_\gamma \Delta E}{2\hbar}\right) \sum_{l \in \gamma} [\lambda(\theta_l) - \tilde{\lambda}_\gamma], \quad (12)$$

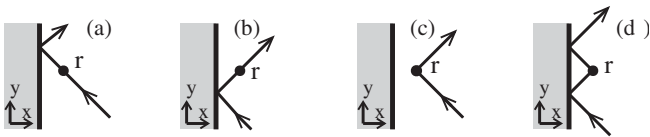


FIG. 2. In the semiclassical sums, the four orbits that, as $x \rightarrow 0$, coalesce into the same (nearly) periodic orbit, need to be aggregated. (a),(b) Two (nearly) periodic orbits. (c),(d) Two nonperiodic orbits ($p'_x = -p_x$).

where $\lambda(\theta_l)$ is the function introduced in Eq. (6) evaluated at the angle at which the periodic orbit γ strikes the boundary on the l th bounce, and $\tilde{\lambda}_\gamma \stackrel{\text{def}}{=} \frac{\mathcal{L} \ell_\gamma}{2\mathcal{A} n_\gamma} (1 \pm \frac{\Delta}{\pi})$, with ℓ_γ the total length and n_γ the number of bounces of the orbit γ .

Equation (12) can be used directly to compute the Fourier transform of \mathcal{S}_i , yielding a structure very similar to that of the density of states Eq. (10). Both Fourier transforms can be done so as to have peaks with the same shape and positions, but different amplitudes. Equation (12) can furthermore be used to compute the variance of $\langle S \rangle_{\Delta N}$. To begin, square Eq. (10), use the diagonal approximation in which orbits are paired only with themselves or their time reverse symmetric partner, and apply the Hannay–Ozorio de Almeida sum rule [23]

$$\sum_{\gamma=\text{p.o.}} \frac{n}{|\text{Det}(M_l - \mathbf{1})|} = 1,$$

where only periodic orbits of n bounces from the boundary are included. Then for the long orbits relevant here, replace the mean length ℓ_γ/n_γ between two successive bounces for a specific orbit γ by $\bar{d} = \pi\mathcal{A}/\mathcal{L}$, the mean length between bounces averaged for all initial conditions on the boundary. Noting $\langle \lambda(\theta) - \tilde{\lambda} \rangle = 0$, this gives

$$\overline{(\langle S \rangle_{\Delta N} - \bar{S})^2} = \frac{k_F \mathcal{L}}{2\pi^3} \langle [\lambda(\theta) - \tilde{\lambda}]^2 \rangle_\theta \frac{1}{\Delta N}. \quad (13)$$

As before, angle average $\langle \cdot \rangle_\theta$ is over the measure $d \sin \theta$.

The structure of this result is quite interesting. The surviving contribution comes from what may be called the “diagonal-diagonal” terms, i.e., pairing not only of the same orbit but of the same bounce from the boundary. This term contributes only to the variance as it scales as $1/\Delta N$; see Eq. (8). The terms that would be called “diagonal-off-diagonal” give a vanishing contribution. In addition, note the absence of a constant term. It implies that the covariance vanishes, which is consistent with our cardioid billiard calculations (not shown here).

Thus, from Eq. (8) and the above considerations

$$\text{Var}(\mathcal{S}_i) = \frac{k_F \mathcal{L}}{2\pi^3} \langle [\lambda(\theta) - \langle \lambda \rangle_\theta]^2 \rangle_\theta, \quad (14)$$

where

$$\begin{aligned} & \langle [\lambda(\theta) - \langle \lambda \rangle_\theta]^2 \rangle_\theta \\ &= \begin{cases} (2 \ln 2 - 1) - (\frac{\pi}{2} - 1)^2 \simeq 0.06 & \text{Dirichlet} \\ (2 \ln 2 - 1) - (\frac{\pi}{2} - 1)^2 + 4(\ln \frac{\pi k_F \mathcal{A}}{2\mathcal{L}} - \frac{\pi}{2}) & \text{Neumann} \end{cases} \end{aligned} \quad (15)$$

Comparing this expression with Eq. (6), we see that the semiclassical approach and the random plane wave model

lead to the same result, except for two differences. First, a factor of 2 in the prefactor can be traced to dynamical correlations missed by RPW [24]. Second, the mean square $\langle \lambda^2(\theta) \rangle_\theta$ has been replaced by the variance of $\lambda(\theta)$, giving now a much better agreement with the numerically evaluated \mathcal{S}_i (see Fig. 1).

In Eq. (12), the term proportional to $\lambda(\theta_\gamma)$ can be seen to arise from G^{osc} in Eq. (9), while the one proportional to $\tilde{\lambda}_\gamma$ originates from ρ^{osc} . The random plane wave result is thus, in some sense, ignoring the latter contribution. As ρ^{osc} has no spatial dependence, its role is not to describe the variations of the wave function, but rather to ensure their normalization [as can be seen readily by integrating Eq. (9) over space]. Therefore the main reason of the failure of the RPW approach is due to the lack of individually normalized wave functions, and more precisely to the fact that Eq. (4) imposes the normalization of the wave functions only on average [25,26].

Equation (14) emphasizes the importance of the boundary conditions. Indeed, the variance of $\lambda(\theta)$ is extremely small for Dirichlet boundary conditions, which has to be expected since the wave functions are zero near the boundary. As a consequence, and as seen in Fig. 1, the fluctuations remain smaller than 1 even for a relatively large number of particles, in spite of the linear ($k_F \mathcal{L}$) dependence of the variance. On the other hand, Neumann boundary conditions yield a logarithmic divergence that can be considered in practice as a constant somewhat larger than 1. Fluctuations in this case are greatly enhanced relative to the Dirichlet case. For quantum dots, this should imply, in particular, that residual interaction effects on ground state electronic properties should be significantly larger for Neumann than for Dirichlet boundary conditions.

To conclude, “integrated” wave function statistics are introduced, in part motivated by the need to understand the effect of interactions on ground state properties in quantum dots. A significant part of their fluctuation properties can be understood with basic RPW modeling. However, a semiclassical framework is developed here, which indicates missing ingredients of RPW, and, in particular, that lack of individual state normalization leads to a significant overestimate of the fluctuations. It turns out, furthermore, that boundary conditions, which are often not discussed in the context of residual interaction effects in mesoscopic systems, play an important role.

We stress finally that only the extreme limit of strongly chaotic systems has been treated here. For less developed chaos, or systems with some regular dynamics, where some eigenstate localization exists, there may be significant enhancements in the fluctuations and correspondingly greater effects on ground state properties [27]. The consequences for experimentally realizable systems and for such systems with some form of eigenstate localization is left for future study.

One of us (S.T.) gratefully acknowledges support from U.S. National Science Foundation Grant No. PHY-0555301.

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