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

Steven Tomsovic,1,8 Denis Ullmo,2 and Arnd Bäcker3

1Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany
2CNRS; Université Paris-Sud; LPTMS UMR 8626, 91405 Orsay Cedex, France
3Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

(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 \( \psi \), is a modeling in terms of a random superposition of plane waves (RPW) [4,5]. For two-degrees-of-freedom systems, \( c(\mathbf{r}) \) 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 \( c(\mathbf{r}) \).

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 \( \lambda_F \), and the screened Coulomb interaction can be approximated by the short-range expression \( V_{sc}(\mathbf{r} - \mathbf{r}') = (2\nu)^{-1}F_{0}^{2}\delta(\mathbf{r} - \mathbf{r}') \) with \( 2\nu \) the mean local density of states, including spin degeneracy \( (\nu = m/2\pi\hbar^2) \) for \( d = 2 \) and \( F_0^2 \) 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 \( \delta E^{RI} = (2\nu)^{-1}F_{0}^{2}\int d\mathbf{r}N_{\uparrow}(\mathbf{r})N_{\downarrow}(\mathbf{r}) \) with \( N_\sigma \) the unperturbed ground state density of particles with spin \( \sigma \). From this expression, it is seen that the increase of interaction energy associated with the addition of an extra electron is related to

\[
S_I = \mathcal{A} \int d\mathbf{r} |\Psi_{I}(\mathbf{r})|^2 N(\mathbf{r}; E_I^+),
\]

with \( N(\mathbf{r}; E) = \sum_{i=1}^{\infty} |\Psi_{i}(\mathbf{r})|^2 \theta(E_i - E) \) (\( E_i < E_I^+ < E_i+1 \)). 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 \( \delta E^{RI} (\propto S_I - S_{j}) \) 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 \( N_{Friedel}(\mathbf{r}; E) = N_{b}(E) \frac{1}{2\pi} \left[ 1 + J_1(2x) \right] \) [17], with \( x \) the distance from the boundary, the + and – sign corresponding, respectively, to Neumann and Dirichlet boundary conditions, and \( N_{b}(E) \) refers to the leading term of the Weyl formula, \( N_{b}(E) = \nu \mathcal{A} E \). To leading order we can therefore use the approximation

\[
S_I = i \pm i \int d\mathbf{r} \left[ \frac{J_1(2k_F x)}{k_F x} |\Psi_{I}(\mathbf{r})|^2 \right].
\]
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 $\sum_{i} a_i \exp(i \mathbf{k}_i \cdot \mathbf{r})$ with wave vectors of fixed modulus $|\mathbf{k}_i| = k_F$ 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 $\mathbf{k}_i$ [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,

$$\psi_i(\mathbf{r}) = \frac{1}{N_{\text{eff}}} \sum_{l=1}^{N_{\text{eff}}} a_i \cos(\mathbf{k}_j \cdot \hat{\mathbf{x}}) \cos(\mathbf{k}_j \cdot \hat{\mathbf{y}} + \varphi_i),$$

(3)

where $\cos(\cdot)$ is defined for Dirichlet and Neumann boundary conditions. The phase angle $\varphi_i$, the orientation of the wave vector $\mathbf{k}_i$, and the real amplitude $a_i$ with $(a_i a_j^*) = \delta^{ij} c^2$ are all chosen randomly. The variance $\sigma^2$ is fixed by the normalization condition

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

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

$$\text{Var}(S_i) = \frac{i^2}{\mathcal{A}^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \left[ \frac{J_1(2k_F x_1)}{k_F x_1} \frac{J_1(2k_F x_2)}{k_F x_2} \right]$$

\times \left[ (|\Psi_i(\mathbf{r}_1)|^2 |\Psi_i(\mathbf{r}_2)|^2) - (|\Psi_i(\mathbf{r}_1)|^2 |\Psi_i(\mathbf{r}_2)|^2) \right].

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

$$\text{Var}(S_i) = \frac{8i}{\mathcal{A}^2} \frac{1}{N_{\text{eff}}^2} \sum_{l=1}^{N_{\text{eff}}} \int d\mathbf{r}_1 d\mathbf{r}_2 \left[ \frac{J_1(2k_F x_1)}{k_F x_1} \frac{J_1(2k_F x_2)}{k_F x_2} \right]$$

$$\cos(\mathbf{k}_j \cdot \mathbf{x}_1) \cos(\mathbf{k}_j \cdot \mathbf{x}_2) \cos(\mathbf{k}_m \cdot \mathbf{x}_1) \cos(\mathbf{k}_m \cdot \mathbf{x}_2)$$

$$\cos(\mathbf{k}_j \cdot (\mathbf{y}_1 - \mathbf{y}_2)) \cos(\mathbf{k}_m \cdot (\mathbf{y}_1 - \mathbf{y}_2)). \quad (5)$$

Performing the integration gives

$$\text{Var}(S_i) = \frac{k_F L}{4 \pi^2} \langle \lambda^2(\theta) \rangle_\theta$$

(6)

with $L$ the perimeter, $\lambda(\theta) = [1 \pm |\sin(\theta)|] |\cos(\theta)|$, and the expression for $\langle \lambda^2(\theta) \rangle_\theta = \int_0^\pi d\theta (\sin(\theta))^2 \lambda^2(\theta)$ is given ahead in Eq. (15).

In Fig. 1, the variance of $S_i$ as a function of $i$ is represented for a chaotic system, the cardioid billiard 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 $S_i$ 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,

$$\langle S_i \rangle_{\Delta N} = \frac{1}{\Delta N} \sum_{E-(\Delta E)/2 < E < E+(\Delta E)/2} S_i,$$

(7)

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

$$\text{Var}[\langle S_i \rangle_{\Delta N}] \equiv \langle (S_i)_{\Delta N} - \langle S_i \rangle_{\Delta N} \rangle^2$$

$$= \frac{1}{\Delta N} \text{Var}[S_i] + \left(1 - \frac{1}{\Delta N}\right) \text{Covar}[S_i S_{i+j}]. \quad (8)$$

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

Our starting point for this calculation is

$$\mathcal{A} \langle |\Psi_i(\mathbf{r})|^2 \rangle_{\Delta N} = 1 \pm J_0(2k_F x) - \frac{1}{\nu} \text{Im}(\hat{G}^{\text{osc}}(\mathbf{r}, E))_{\Delta E}$$

$$- \frac{1}{\mathcal{A} \nu} \langle \rho^{\text{osc}} \rangle_{\Delta E}. \quad (9)$$

FIG. 1. Variance of $S_i$ 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).
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 $\rho^{osc}$ is the oscillating part of the density of states, given semiclassically as a sum over periodic orbits

$$
\rho^{osc}(E) = \frac{1}{\pi \hbar} \sum_{\gamma \neq p.o.} \tau \frac{\cos(S_\gamma(E)/\hbar - \sigma_\gamma \pi)}{|\text{Det}(M_\gamma - 1)|^{1/2}}. 
$$

(10)

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

$$
G^{osc}(r, r, E) \approx \frac{1}{i \hbar} \frac{1}{2\pi m_{12}} \sum_{\mu, \nu} \frac{1}{\sqrt{|\text{det}(M_{12, \mu})|}} \times \exp \left[ \frac{i}{\hbar} S_{\mu}(r, r, E) - i \frac{\pi}{2} \eta_{\mu} \right]. 
$$

(11)

In the above expressions, $S$ is the action integral along the orbit, $\tau$ the period, $m_{12} \equiv \partial y^{\text{final}} / \partial p^{\text{initial}}$, $M_\gamma$ the monodromy matrix, and $\sigma_\gamma$, $\eta_\mu$ are Maslov indices. The tilde on $S$ denotes the oscillating part of the density of states, given semiclassically as a sum over periodic orbits. It implies that the range of integration in the direction perpendicular to the boundary is important to note. The range of integration in the direction perpendicular to the boundary is

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

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

$$
\langle (S)_{\Delta N} - \bar{S} \rangle^2 = \frac{k_F L}{2\pi^2} \left[ \langle \lambda(\theta) - \langle \lambda \rangle \rangle^2 \right]_{\theta} \frac{1}{\Delta N}.
$$

(13)

As before, angle average $\langle \gamma \rangle_\theta$ 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

$$
\text{Var}(S) = \frac{k_F L}{2\pi^2} \left[ \langle \lambda(\theta) - \langle \lambda \rangle \rangle^2 \right]_{\theta},
$$

(14)

where

$$
\langle \lambda(\theta) - \langle \lambda \rangle \rangle^2_{\theta} = \begin{cases} 
(2 \ln 2 - 1 - (\ell - 1)^2) & \approx 0.06 \quad \text{Dirichlet} \\
(2 \ln 2 - 1 - (\ell - 1)^2 + 4 \ln \left( \frac{\pi k_F A}{2 \xi} \right) - \ell) & \text{Neumann}.
\end{cases}
$$

(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 $\langle \lambda^2(\theta) \rangle_g$ has been replaced by the variance of $\lambda(\theta)$, giving now a much better agreement with the numerically evaluated $S_i$ (see Fig. 1).

In Eq. (12), the term proportional to $\lambda(\theta)$ can be seen to arise from $G^{\text{osc}}$ in Eq. (9), while the one proportional to $\tilde{\lambda}$ originates from $\rho^{\text{osc}}$. The random plane wave result is thus, in some sense, ignoring the latter contribution. As $\rho^{\text{osc}}$ 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 individual state normalization leads to a significant factor of 2 in the prefactor can be traced to dynamical effects 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.

*Permanent address: Department of Physics and Astronomy, Washington State University, Pullman, WA 99164-2814, USA.

[1] M. L. Mehta, Random Matrices (Elsevier, Amsterdam, 2004), 3rd ed.

[2] O. Bohigas, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. 52, 1 (1984).

[3] O. Bohigas, in Chaos and Quantum Physics, edited by M. J. Giannoni, A. Voros, and J. Jinn-Justin (North-Holland, Amsterdam, 1991), pp. 87–199.

[4] M. V. Berry, J. Phys. A 10, 2083 (1977).

[5] A. Voros, in Stochastic Behaviour in Classical and Quantum Hamiltonian Systems, edited by G. Casati and G. Ford (Springer-Verlag, Berlin, 1979), p. 334.

[6] S. W. McDonald and A. N. Kaufman, Phys. Rev. Lett. 42, 1189 (1979).

[7] S. W. McDonald, Ph.D. thesis, University of California, 1983 [Lawrence Berkeley Laboratory Report No. LBL-148377].

[8] E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984).

[9] R. Heller, in Chaos and Quantum Physics (Ref. [3]).

[10] M. Srednicki, Phys. Rev. E 54, 954 (1996).

[11] S. Hortikar and M. Srednicki, Phys. Rev. Lett. 80, 1646 (1998).

[12] A. D. Mirlin, Phys. Rep. 326, 259 (2000).

[13] O. Bohigas, S. Tomsovic, and D. Ullmo, Phys. Rep. 223, 43 (1993).

[14] S. W. McDonald and A. N. Kaufman, Phys. Rev. A 37, 3067 (1988).

[15] A. Bäcker and R. Schubert, J. Phys. A 35, 539 (2002).

[16] Y.-H. Kim, M. Barth, U. Kuhl, and H.-J. Stöckmann, Prog. Theor. Phys. Suppl. 150, 105 (2003).

[17] A. Bäcker, R. Schubert, and P. Stöferle, Phys. Rev. E 57, 5425 (1998); 58, 5192(E) (1998).

[18] M. V. Berry, J. Phys. A 35, 3025 (2002).

[19] J. D. Urbina and K. Richter, Phys. Rev. E 70, 015201(R) (2004).

[20] M. Robnik, J. Phys. A 17, 1049 (1984).

[21] A. Bäcker, F. Steiner, and P. Stöferle, Phys. Rev. E 52, 2463 (1995).

[22] E. Bogomolny, Physica (Amsterdam) 31D, 169 (1988).

[23] A. M. Ozorio de Almeida, Hamiltonian Systems: Chaos and Quantization (Cambridge University Press, Cambridge, 1988).

[24] D. Ullmo, S. Tomsovic, and A. Bäcker (to be published).

[25] J. D. Urbina and K. Richter, Eur. J. Phys. Special Topics 145, 255 (2007).

[26] L. Kaplan, report arXiv:0712.4095v1; L. Kaplan and Y. Alhassid, arXiv:0802.2410v1.

[27] D. Ullmo, T. Nagano, and S. Tomsovic, Phys. Rev. Lett. 90, 176801 (2003).