Quantum-Dot Ground-State Energies and Spin Polarizations: Soft versus Hard Chaos

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We consider how the nature of the dynamics affects ground state properties of ballistic quantum dots. We find that "mesoscopic Stoner fluctuations" that arise from the residual screened Coulomb interaction are very sensitive to the degree of chaos. It leads to ground state energies and spin polarizations whose fluctuations strongly increase as a system becomes less chaotic. The crucial features are illustrated with a model that depends on a parameter that tunes the dynamics from nearly integrable to mostly chaotic.

Our interest in this Letter lies in microstructures fabricated using electrostatic gates or etching that pattern a two-dimensional electron gas in a semiconductor heterostructure, for example, GaAs/AlGaAs. Typically, the electronic transport mean free path is significantly larger than the dimensions of the device, and the electrons essentially travel ballistically across the microstructure. Their motion is governed by the shape of a smooth, self-consistent, steep-walled, confining potential which is often conceptualized as a quantum billiard.

For many physical properties, the simplifying assumption that the dots' underlying classical dynamics are fully chaotic (hard chaos) is consistent with the experimental data [1–4]. It has been used to justify various hypotheses from the applicability of random matrix theory (RMT) and random plane wave modeling (RPW) to statistical assumptions applied within semiclassical mechanics [5–7]. Indeed, chaotic systems manifest a large variety of *universal* behaviors. Furthermore, chaotic quantum dots are often very similar to diffusive ones (given a properly defined Thouless energy). Consequently, most techniques, developed much earlier to study disordered metals (diagrammatic approaches [8], nonlinear sigma model [9]) and applied to disordered quantum dots [10–12], are applicable to ballistic quantum dots.

Nevertheless, unlike billiards, there are no known smooth potentials which are fully chaotic. Unless designed otherwise (as was done for the weak localization line shape [13]), an odd-shaped, smooth potential generically exhibits *soft* chaos, i.e., significant contributions of *both* stable and unstable motion. The general assumption of hard chaos is unfounded.

As opposed to a genuine belief that the electrons' dynamics are strongly chaotic, the implicit assumption is that for many properties the distinctions between soft and hard chaos are more subtle than spectacular. This has been shown explicitly, for instance, for the fluctuation properties of Coulomb blockade (CB) peak heights [14] or for their correlations [15]. In such circumstances, using a chaotic model allows for simpler analytic derivations without drastically altering the results.

Our purpose is to demonstrate that even this weaker assumption may not always hold and that for some properties a strong sensitivity to the nature of the dynamics arises. Because the distinction between chaos and integrability becomes most apparent at long (infinite) times, long electron confinement within the dot holds the promise of exposing the dynamics. We therefore consider [zero-temperature] properties of isolated dots and find that ground state energies (whose second differences are probed by CB peak spacings) and spin polarizations are markedly affected by the dynamics. To proceed, we start with a general discussion of why, in principle, chaotic dots should be "atypical," at least for their ground state properties. Then we consider a time-reversal noninvariant coupled quartic oscillator system and show quantitatively the relevance of the underlying dynamics.

We assume that a Fermi-Landau liquid description is valid [10,11,16], and, thus, the ground state energy is due to three terms

$$E_{gr}[N] = \mathcal{E}_{TF} + \mathcal{E}_{1p} + \mathcal{E}_{ri}. \tag{1}$$

$\mathcal{E}_{TF}[N] = (eN)^2/2C$ is an electrostatic energy, $\mathcal{E}_{1p}[N]$ is the sum of the single particle energies (SPE) of N *independent* particles, and $\mathcal{E}_{ri}$ is a residual interaction term. Specifically,

$$\mathcal{E}_{1p}[N] = \sum_{i,\sigma} f_i^{\sigma} \epsilon_i, \tag{2}$$

with $\{\epsilon_i\}$ the SPEs corresponding to an effective potential $V_{eff}(\mathbf{r})$ (that can be determined self-consistently within the electrostaticlike approximation) and $f_i^{\sigma} = 0$ or 1 is the occupation number of orbital i with spin $\sigma = \pm$, ($\sum_{i,\sigma} f_i^{\sigma} = N$). Furthermore, denoting ψ_i the eigenstate associated to ϵ_i,

$$\mathcal{E}_{ri} = \frac{1}{2} \sum_{i,j,\sigma,\sigma'} f_i^{\sigma} f_j^{\sigma'} \Bigg[\int d\mathbf{r} d\mathbf{r}' |\psi_i(\mathbf{r})|^2 V_{sc}(\mathbf{r} - \mathbf{r}') |\psi_j(\mathbf{r}')|^2$$
$$- \delta_{\sigma,\sigma'} \int d\mathbf{r} d\mathbf{r}' \psi_i(\mathbf{r}) \psi_j^*(\mathbf{r}) V_{sc}(\mathbf{r} - \mathbf{r}')$$
$$\times \psi_j(\mathbf{r}') \psi_i^*(\mathbf{r}') \Bigg]$$

is the direct-plus-exchange, first order perturbation contribution in terms of the weak screened Coulomb interaction V_{sc}. For the experimentally relevant electronic densities, V_{sc} is a short range function, and we model it as

$$V_{sc} = \frac{\zeta}{\nu} \delta(\mathbf{r} - \mathbf{r}'), \quad (3)$$

with ν the total density of states (including the spin degeneracy, $g_s = 2$) and $\zeta \in [0, 1]$, which can be related to the electron density (i.e., the electron gas parameter r_s) and is typically in the range $[0.5, 0.8]$. To this zero range approximation, the residual interaction contributions read

$$\mathcal{E}_{ri} = \zeta \frac{\Delta}{g_s} \sum_{i,j} f_i^{(+)} f_j^{(-)} M_{ij}, \quad (4)$$

with Δ the (local) mean SPE spacing and

$$M_{ij} = A \int d\mathbf{r} |\psi_i(\mathbf{r})|^2 |\psi_j(\mathbf{r})|^2. \quad (5)$$

A is the dot area, the M_{ij} are dimensionless, and semiclassical reasoning gives their mean ($i \neq j$) to be unity.

It is crucial that in Eq. (4) only electrons with opposite spins contribute. Aligning two spins decreases the residual interaction by a quantity of $O(\Delta)$. There is thus a competition between the SPE term, which favors the occupation of the lowest orbitals, and the residual interaction term, which tends to align the electron spins. The relative strength of these two effects is governed by the dimensionless parameter ζ. If $\zeta > 2$, the ground state is completely polarized. This is the well known Stoner instability [17].

Here ζ is just less than one. Although full polarization is excluded, the proximity of the Stoner instability makes the ground state spin very sensitive to the fluctuations of the M_{ij} and ϵ_i, which affects the fluctuation properties of the ground state [7,10,11,18]. This is sometimes referred to as the "mesoscopic Stoner fluctuation."

Now consider the diagonal term

$$M_{ii} = A \int d\mathbf{r} |\psi_i(\mathbf{r})|^4. \quad (6)$$

M_{ii} is the inverse participation ratio (IPR) in position representation of the state ψ_i, which measures its extent of localization. Hard chaotic systems possess eigenfunctions that are the least localized in the sense that their Wigner transforms uniformly cover the energy surface [19]. However, mixed systems are known to display *phase space localization* by various mechanisms [20]. The most familiar one is associated with torus quantization (WKB). It may affect only a few states, yet localize them very strongly. Another mechanism is associated with the presence of partial transport barriers in phase space [20], which are quite typical in mixed systems. Such partial barriers, if they are effective, should affect almost all eigenstates, but produce a lesser degree of localization.

Similarly, it can be shown that the mean of the off-diagonal terms $M_{i,j \neq i}$ is independent of the dynamics, and their fluctuations are extremely small for chaotic systems (vanishing in the semiclassical limit [7]). However, they would be of $O(\Delta)$ if significant phase space localization were present. Thus, chaotic systems, rather than behaving *typically*, are the limiting class of systems for which the interaction is the *least* effective.

To explore the effects of soft chaos on the ground state properties, let the effective Hamiltonian $\hat{H}_{eff}$ resulting from the lowest order, electrostaticlike, self-consistent calculation be [$\mathbf{r} = (x, y)$, $r = |\mathbf{r}|$]

$$\hat{H}_{eff} = \frac{[\mathbf{p} - \kappa \sqrt{a(\lambda)} x^2 \frac{\mathbf{r}}{r}]^2}{2} + a(\lambda)\left(\frac{x^4}{b} + by^4 + 2\lambda x^2 y^2\right). \quad (7)$$

Weyl operator ordering is assumed for the quantized version. To have the symmetry of the rectangle instead of the square, b is set to $\pi/4$. For convenience, $a(\lambda)$ is set so that the mean number of states to energy E is given by $N(E) = E^{3/2}$, regardless of the choice of λ or κ. λ gives the oscillator coupling. Finally, κ breaks time-reversal invariance (TRI). Note that for TRI systems, higher order terms in the ground state energy expansion, in particular, the Cooper series, should be taken into account. So κ is chosen to break TRI completely; the form of the TRI breaking term has been chosen to ensure that the phase space portrait of the dynamics is energy independent. We consider the following dynamical regimes: $(\lambda, \kappa) = (+0.20, 1.00)$ [nearly integrable], $(-0.20, 1.00)$ [mixed], and $(-0.80, 1.00)$ [mostly chaotic]. Because of the TRI breaking term somewhat stabilizing the dynamics, the motion in the chaotic case is still not quite fully chaotic.

The reflection symmetries lead to four irreducible representations, which we take as independent quantum dots with the same dynamics. We consider the four systems as an ensemble; in fact, the ensemble size is increased by allowing λ to vary ± 0.02, which is enough to get nearly independent quantum eigenproperties, but small enough that the structure of the dynamics is essentially unchanged. Each statistical measure calculated within a given dynamical regime is thus the result of averaging over an ensemble of 12 similar quantum dots.

For each parameter set and symmetry class, we compute the eigenvalues ϵ_i and eigenvectors ψ_i, from which the residual interaction terms can be deduced [Eqs. (4) and (5), see [21] for the numerical details]. We begin with a few interesting statistical properties of the $\{M_{ij}\}$ and afterward see how the spin distribution and ground state energy fluctuations are affected.

In Fig. 1, values of sets of diagonal terms M_{ii} are represented for the symmetry class $(+, +)$ in the various dynamical regimes. The presence of very localized states in the nearly integrable and mixed regimes is immediately apparent. Curiously enough, it turns out that for all dynamical regimes, the IPR M_{ii} is not very far from 2 for
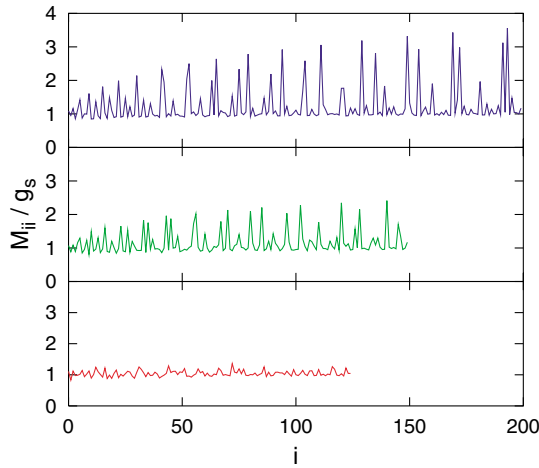
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FIG. 1 (color online).   Inverse participation ratio as a function of the orbital index for $(+, +)$. From top down: $(\lambda, \kappa) = (+0.20, 1.00)$ [nearly integrable], $(-0.20, 1.00)$ [mixed], and $(-0.80, 1.00)$ [mostly chaotic].

most states, but the distribution has a very long tail if the dynamics are not sufficiently chaotic. Consequently, it is reasonable to assume that the localization mechanism at work here is associated with stable periodic orbits or tori. A more detailed analysis of the classical dynamics reveals that partial barriers are actually present in $(\lambda, \kappa) = (-0.20, 1.00)$, but that their position with respect to the symmetry lines of the system make them ineffective in changing the statistics of the M_{ii}. Furthermore, and as can be seen in Table I, the off-diagonal terms M_{ij} $(i \neq j)$ are also affected by eigenstate localization as their variance is significantly larger if the state i is localized.

The difference between the distribution of M_{ij} observed for the quartic oscillator system and that predicted for a chaotic system is essentially that a non-negligible number of very localized states ψ_i gives much larger diagonal terms and much larger variation of the corresponding off-diagonal terms. The question is how this affects the ground state properties. The answer for given (λ, κ) and number of electrons in the dot N follows from the ϵ_i and M_{ij}. To compute the energy $E[\{f_i^\sigma\}]$, we use Eqs. (1), (2), and (4) for the various occupations $\{f_i^\sigma\}$ such that $\sum_{i\sigma} f_i^\sigma = N$. The ground state follows by selecting the occupation sequence minimizing this energy. Varying

TABLE I.   Conditional variance of the interaction terms M_{ij} with $0 < |i - j| \leq 10$, $i \geq 51$. Rows top down: (i) dynamical case, (ii) superior limit, (iii) inferior limit, (iv) conditional variance with localized orbitals, and (v) conditional variance with delocalized orbitals.

λ	+0.20	−0.20	−0.80
I^{sup}	2.0	1.8	1.2
I^{inf}	1.2	1.2	1.0
$M_{ii}/g_s > I^{\text{sup}}$	0.097	0.108	0.070
$M_{ii}/g_s < I^{\text{inf}}$	0.024	0.023	0.009

N in the range $[100, 200]$ for each parameter set, one constructs a distribution of total spins and second differences in the ground state energy $\xi[N] = E_{\text{gr}}[N + 1] + E_{\text{gr}}[N - 1] - 2E_{\text{gr}}[N]$. $\xi[N]$ is experimentally accessible by measuring CB peak spacings, and we therefore refer to it as a "peak spacing." The various dynamical regimes' peak spacing distributions are shown in Fig. 2.

We see that the observed distributions are strikingly different from the RMT/RPW predictions (shown on the same plot) that should apply for fully chaotic systems. Even our most chaotic case shows significant deviations, and this increases considerably as the system moves away from hard chaos. The peak spacings fluctuate much more, and very large spacings appear for the mixed and nearly integrable regimes. Moreover, as shown in Table II, larger spins become significantly more probable.

We next ask how such a drastic change is made possible by the presence of a moderate number of very localized states. Let us consider one example in detail. Figure 3 shows the succession of orbital fillings for a range of N. Here two of the single particle states $(i = 64, 66)$ are highly localized. Since the system is not chaotic, there is also less level repulsion, which allows for the clustering of levels around ϵ_{64} or ϵ_{69} that would otherwise be improbable. We see that none of the orbital occupations follow the simple "up/down" scenario characteristic of noninteracting systems. As would seem natural, the very localized orbitals $i = 64, 66$ remain singly occupied across many values of N. There is an additional non-intuitive feature, namely, that the other orbitals also prefer single occupancy despite not being particularly localized.

This behavior derives from the following mechanism. Consider a singly occupied orbital i^*. Particles in other orbitals i interact with this later only if their spin antialigns with the one on i^*. This typically increases the energy cost of occupying an orbital with antiparallel spin a quantity $(\zeta\Delta/g_s)$. Assuming N_l such singly occupied orbitals already exist, and adding the intra-orbital term, on average the residual interaction energy cost of doubly occupying some orbital i is $[(N_l + 2)\zeta\Delta/g_s]$ even for a nonlocalized state. For typical values of ζ, this is larger
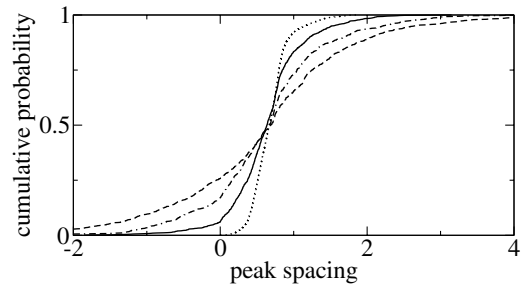

FIG. 2.   Integrated peak spacing distribution with $\zeta = 0.8$ for RMT/RPW prediction [7] (dotted line), mostly chaotic (solid line), mixed (dash-dotted line), and nearly integrable (dashed line) regimes.

TABLE II. Probabilities $P(s = 2)$, $P(s = 5/2)$ to find a spin two (even N) or five halves (odd N) ground state, and average value $\langle \delta s \rangle$ of the ground state spin augmentation [$\delta s = s$ or $(s - 1/2)$ for even or odd number of particles, respectively], for the various dynamical regimes (values of λ) with $\kappa = 1.0$ and $\zeta = 0.8$. The last column is the RMT/RPW prediction [7].

λ	$+0.20$	-0.20	-0.80	RMT/RPW
$P(s = 2)$	0.13	0.16	0.07	0.01
$P(s = 5/2)$	0.08	0.10	0.02	0.00
$\langle \delta s \rangle$	0.51	0.54	0.38	0.23

than a mean spacing as soon as $N_l \geq 1$. Consequently, as illustrated by Fig. 3, the localized orbitals will not only remain singly occupied, but also have a tendency to polarize the electrons in the other nearby orbitals. Lack of level repulsion and larger fluctuations of the M_{ij} will further enhance such effects.

To conclude, we have shown that for the non-TRI quartic oscillators the eigenfunction statistics behave differently than those from a RMT/RPW approach. The significance is correlated with the degree of chaos (or lack thereof) in the underlying classical dynamics. Because of the proximity of the Stoner instability, strong effects arise in ground state spin polarizations, occupancies, and energies of the corresponding "model" quantum dot. The quartic oscillators more fairly represent a generic experimental dot than the hard chaos assumption. The hard chaos assumption leads to predictions that are qualitatively and quantitatively incorrect.

Finally, such considerations should affect the understanding of realized dots, which needs to be discussed on a case-by-case basis. For instance, the dots used in Ref. [22] are certainly far from chaotic. They should show a large degree of phase space localization in their single particle properties, whereas this point is debatable with respect to the dots of Ref. [4]. However, it may be more interesting to address this question from the opposite point of view. Since creating dots away from the hard chaos limit leads to behaviors that are qualitatively differ-
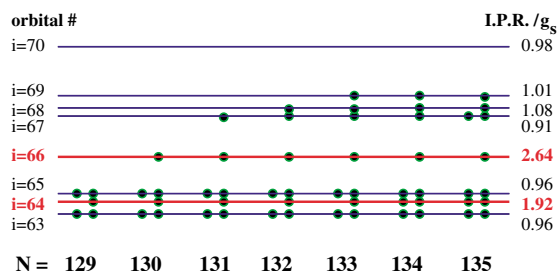
ent from those predicted using chaotic or diffusive modeling, if the interest is in devising a dot to perform some particular function, such as spin manipulation, for instance, it is in the soft chaos regime that richer behavior involving large fluctuations of ground state energies and spins will be found.

FIG. 3 (color online).   Successive filling of the $(+, +)$ orbitals $i = 63$ to 69 as the number of particles in the dot goes from $N = 129$ to 135 for $(\lambda, \kappa) = (+0.20, 1.00)$ and $\zeta = 0.8$. The spacing between the horizontal lines is proportional to the actual level spacings. The numbers in the right column are the corresponding IPRs.

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