

## Statistics of Hartree-Fock levels in small disordered systems

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We study the statistics of quasiparticle and quasihole levels in small interacting disordered systems within the Hartree-Fock approximation. The distribution of the inverse compressibility, given according to Koopmans' theorem by the distance between the two levels across the Fermi energy, evolves from a Wigner distribution in the noninteracting limit to a shifted Gaussian for strong interactions. On the other hand, the nature of the distribution of spacings between neighboring levels on the same side of the Fermi energy (corresponding to energy differences between excited states of the system with one missing or one extra electron) is not affected by the interaction and follows Wigner-Dyson statistics. These results are derived analytically by isolating and solving the appropriate Hartree-Fock equations for the two levels. They are substantiated by numerical simulations of the full set of Hartree-Fock equations for a disordered quantum dot with Coulomb interactions. We find enhanced fluctuations of the inverse compressibility compared to the prediction of the random matrix theory, possibly due to the localization of the wave functions around the edge of the dot. The distribution of the inverse compressibility calculated from the discrete second derivative with respect to the number of particles of the Hartree-Fock ground state energy deviates from the distribution of the level spacing across the Fermi energy. The two distributions have similar shapes but are shifted with respect to each other. The deviation increases with the strength of the interaction thus indicating the breakdown of Koopmans' theorem in the strongly interacting limit. [S0163-1829(99)15031-8]

### I. INTRODUCTION

It is universally accepted that the principal signature of quantum chaos is the statistics of the random matrix theory<sup>1,2</sup> (RMT), which is obeyed by the energy levels of chaotic systems. This is supported by semiclassical considerations<sup>3</sup> as well as many numerical<sup>3,4</sup> and analytical<sup>5</sup> examples. However realistic chaotic systems such as quantum dots, small metallic grains, or the so-called yrast levels in rotating nuclei involve interactions between many particles (electrons, nucleons, etc). An interesting problem then arises of how the interactions are expected to modify the RMT predictions. Several recent experimental and theoretical publications have begun to deal with this problem.<sup>6-19</sup>

Applications of RMT to noninteracting chaotic systems, such as quantum dots, are concerned with the statistical properties of single particle quantities. Analogous and experimentally relevant in interacting systems are quantities which characterize quasiparticles. In small disordered systems one can discuss the statistics of their energy levels, lifetimes, and wave functions (real and imaginary parts and the residues of the poles of the single particle Green's function, respectively). Experience gained in nuclear and atomic physics indicates that the Hartree-Fock (HF) method provides a very reasonable approximate description of quasiparticle properties in finite systems. The nondegenerate HF particle-hole excitations form a convenient basis to describe low lying excitations of these systems. In this paper we adopt this description and study statistical properties of the HF levels in small disordered systems. Properties of charged excitations have been probed experimentally by measuring the

Coulomb blockade in disordered quantum dots, cf. Refs. 6-8. The neutral particle-hole excitations can be measured by studying acoustic phonon<sup>20</sup> and microwave absorption.<sup>21</sup>

### II. THE HARTREE-FOCK APPROXIMATION IN WEAKLY DISORDERED SYSTEMS

Interacting electrons in a disordered system are described by the Hamiltonian

$$H = \sum_{\alpha\beta} h_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \quad (1)$$

where  $|\alpha\rangle, |\beta\rangle, \dots$ , denote states of a single particle basis. The noninteracting part of  $H$  is controlled by the one body Hamiltonian  $h_{\alpha\beta}$  representing the disordered system. In this work we are interested in the regime of disorder for which the random matrix  $h_{\alpha\beta}$  can be viewed as described by the rules of RMT. The interaction  $V_{\alpha\beta\gamma\delta}$  is not random and in a quantum dot, for example, represents matrix elements of the Coulomb or screened Coulomb interaction. In our discussion, however, we will regard it as a general matrix and will be able to draw conclusions for wide classes of possible  $V_{\alpha\beta\gamma\delta}$ .

Our main approximation will be to treat the Hamiltonian (1) in the HF approximation. The HF equations are

$$\sum_{\beta} h_{\alpha\beta}^{(\text{HF})} \psi_i(\beta) = \varepsilon_i \psi_i(\alpha) \quad (2)$$

with

$$h_{\alpha\beta}^{(\text{HF})} = h_{\alpha\beta} + \sum_{\alpha'\beta'} V_{\alpha\alpha'\beta\beta'}^A \rho_{\beta'\alpha'} \quad (3)$$

or symbolically  $h^{(\text{HF})} = h + \text{tr}(V^A \rho)$ . Here  $V^A$  is the antisymmetrized interaction matrix  $V_{\alpha\beta\gamma\delta}^A \equiv V_{\alpha\beta\gamma\delta} - V_{\alpha\beta\delta\gamma}$  and the trace is taken over the second pair of the indices of  $V^A$ . The self-consistent density matrix  $\rho$  is given by

$$\rho_{\alpha\beta} = \sum_{h \in \text{holes}} \psi_h(\alpha) \psi_h^*(\beta) \quad (4)$$

Henceforth we will denote by  $h$ ,  $h'$  and  $p$ ,  $p'$ , etc., the hole (occupied) and particle (unoccupied) levels, respectively.

It is common to view the HF approximation as arising from the variational minimization of the total energy of the system. In this interpretation the direct physical meaning of the energies  $\varepsilon_i$  and the wave functions  $\psi_i(\alpha)$  remains obscure and one must use the so-called Koopmans' theorem.<sup>22</sup> We recall however that the HF equations can also be derived from an approximation to the equation of motion for the one particle Green's function

$$\begin{aligned} G(\alpha, \beta; \omega) &= -i \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \Phi_0(N) | T a_{\alpha}(t) a_{\beta}^{\dagger}(0) | \Phi_0(N) \rangle \\ &= - \sum_i \frac{\langle \Phi_0(N) | a_{\alpha} | \Phi_i(N+1) \rangle \langle \Phi_i(N+1) | a_{\beta}^{\dagger} | \Phi_0(N) \rangle}{E_i(N+1) - E_0(N) - \omega - i0} \\ &\quad - \sum_i \frac{\langle \Phi_0(N) | a_{\beta}^{\dagger} | \Phi_i(N-1) \rangle \langle \Phi_i(N-1) | a_{\alpha} | \Phi_0(N) \rangle}{E_0(N) - E_i(N-1) - \omega + i0} \end{aligned} \quad (5)$$

The HF energies  $\varepsilon_p$  and  $\varepsilon_h$  and the corresponding wave functions  $\psi_p(\alpha)$  and  $\psi_h(\alpha)$  are then approximate energies and wave functions of, respectively, quasiparticles and quasiholes,

$$\varepsilon_p \approx E_p(N+1) - E_0(N),$$

$$\varepsilon_h \approx E_0(N) - E_h(N-1),$$

$$\psi_p(\alpha) \approx \langle \Phi_0(N) | a_{\alpha} | \Phi_p(N+1) \rangle,$$

$$\psi_h(\alpha) \approx \langle \Phi_h(N-1) | a_{\alpha} | \Phi_0(N) \rangle.$$

We wish to study the statistical properties of the set  $\varepsilon_i$  and the wave functions  $\psi_i(\alpha)$  which follow from the random nature of  $h_{\alpha\beta}$ . Ideally one would like to be able, starting from the probability distribution  $P(h)$ , to determine the joint probability distribution  $P(\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n, \dots)$  and similar distribution for  $\psi_i(\beta)$  and on its basis to predict various correlation properties of these quantities. In the present paper we address a much simpler problem of the repulsion pattern of neighboring pairs of  $\varepsilon_i$  and its application to the addition spectra of quantum dots. We will present simple analytic approximations and perform numerical investigations to check their validity.

### III. THEORETICAL CONSIDERATIONS

#### A. Constant part of the interaction

The simplest limiting case is a constant interaction  $V(|\mathbf{r} - \mathbf{r}'|) = V_0$  which will serve as a reference point for our discussion. In the following we consider the spinless case. One has for the matrix elements in (1)

$$V_{\alpha\beta\gamma\delta} = V_0 \delta_{\alpha\gamma} \delta_{\beta\delta} \quad (6)$$

This interaction allows for a trivial exact solution which is reproduced by the HF equations. They are solved by the eigenfunctions  $\psi_i^{(0)}(\alpha)$  of the one body Hamiltonian

$$h_{\alpha\beta} \psi_i^{(0)}(\beta) = \varepsilon_i^{(0)} \psi_i^{(0)}(\alpha) \quad (7)$$

and have the following eigenvalues

$$\varepsilon_i = \begin{cases} \varepsilon_i^{(0)} + V_0(N-1), & n_i = 1 \\ \varepsilon_i^{(0)} + V_0 N, & n_i = 0 \end{cases} \quad (8)$$

where  $N$  is the number of particles and  $n_i$  is the occupation number of the  $i$ th level. It is clear that the lowest energy solution is obtained by occupying the lowest  $N$  noninteracting states. The gap which separates the energies of the occupied (hole) and empty (particle) levels for  $V_0 > 0$  results from the absence of the contribution from the exchange term in the latter. In a sense one can say that the empty levels do not create the exchange hole which decreases (increases) the level energy for positive (negative)  $V_0$ .

From the known distribution of  $\varepsilon_i^{(0)}$  it is easy to calculate the statistical properties of the HF levels  $\varepsilon_i$ . Since the spacings of neighboring levels are  $s = \Delta \varepsilon^{(0)}$  for levels below and above  $\varepsilon_f$  their distribution is given by the ordinary Wigner surmise, e.g.,

$$P(s) = P_W(s) = \frac{\pi}{2 \langle s \rangle^2} s \exp \left[ -\pi \left( \frac{s}{2 \langle s \rangle} \right)^2 \right]$$

for GOE. The spacing between the levels lying across the Fermi energy is  $s = V_0 + \Delta \varepsilon^{(0)}$  and therefore its distribution is given by the Wigner surmise shifted by the value  $V_0$ ,

$$P(s) = P_W(s - V_0). \quad (9)$$

The gap in the distribution of the level spacings across the Fermi energy is reflected in the differences of the total ground state energy  $E_0$  of the system as a function of the particle number

$$E_0(N) = \sum_{i=1}^N \varepsilon_i^{(0)} + \frac{V_0}{2} N(N-1), \quad (10)$$

$$E_0(N+1) - E_0(N) = \varepsilon_{N+1}^{(0)} + V_0 N = \varepsilon_{N+1}, \quad (11)$$

$$\begin{aligned} D_2(N) &\equiv E_0(N+1) - 2E_0(N) + E_0(N-1) \\ &= \varepsilon_{N+1}^{(0)} - \varepsilon_N^{(0)} + V_0 = \varepsilon_{N+1} - \varepsilon_N. \end{aligned} \quad (12)$$

Here we defined the quantity  $D_2(N)$  which is essentially the inverse compressibility of the dot. Its distribution has been measured in transport experiment of quantum dots in the Coulomb blockade regime.<sup>6-8</sup> Equation (11) is Koopmans theorem which is exact in this case. It leads directly to the expression (12) of  $D_2$  in terms of the energy difference between the two HF levels across the Fermi energy, a fact which motivates the study of this spacing. The Coulomb gap in  $D_2$  does not fluctuate in the limit of constant interaction. For more realistic interactions the Coulomb blockade gap must undergo fluctuations in addition to the fluctuations of the single particle energies  $\varepsilon_i$ . Study of these fluctuations will be one of our principal goals.

### B. Realistic interaction—repulsion of the Hartree-Fock levels

For small  $s$  ( $s \ll \Delta$ , the mean level spacing) the well known behavior of the distribution  $P(s)$  for random Hamiltonians (i.e., linear for GOE, quadratic for GUE, etc.) can be derived by considering the repulsion of close pairs of levels. In this subsection we generalize this analysis to the case of two close HF levels. The new element in the HF problem, Eq. (2), is the presence of the non linear self-consistent term  $\sum_{\alpha'\beta'} V_{\alpha\alpha'\beta\beta'}^A \rho_{\beta'\alpha'}$  which implicitly depends on the realization of the random part  $h_{\alpha\beta}$ .

Let us assume that for some realization of  $h_{\alpha\beta}$  the HF Hamiltonian  $h_{\alpha\beta}^{(\text{HF})}$  has two closely lying levels,  $\varepsilon_2 > \varepsilon_1$ , so that  $\Delta\varepsilon \equiv \varepsilon_2 - \varepsilon_1 \ll \Delta$ . We wish to investigate how  $\Delta\varepsilon$  reacts when the random  $h$  is varied by  $\delta h$  with  $\Delta \gg |\delta h_{IJ}| \sim \Delta\varepsilon$  for  $I, J = 1, 2$ .

The variation of  $h$  causes a change  $\delta h^{(\text{HF})} = \delta h + \text{tr}(V^A \delta \rho)$  in the HF Hamiltonian where the second term is due to the induced change of the self-consistent density. Without this term one would get for the new spacing the standard result  $s = 2\sqrt{(\Delta\varepsilon + \delta h_{22} - \delta h_{11})^2 + 4|\delta h_{12}|^2}$ , which for future reference we shall rewrite in the form

$$s = 2\sqrt{B_1^2 + B_2^2 + B_3^2} \equiv 2|\mathbf{B}|. \quad (13)$$

The vector  $\mathbf{B}$  is a projection on the Pauli matrices of the  $2 \times 2$  Hamiltonian  $(h + \delta h)_{IJ}$  in the subspace of the two close levels,  $I, J = 1, 2$ ,

$$\mathbf{B} = \frac{1}{2} \text{tr}[\boldsymbol{\sigma}(h + \delta h)], \quad (14)$$

where  $\sigma_i$  are the Pauli matrices. The level repulsion at small spacings is a consequence of the proportionality of  $s$  to

the square root of the sum of squares of real quantities and can be deduced by evaluating, for small  $s$

$$P(s) = \int \delta[s - s(\mathbf{B})] P(\mathbf{B}) d\mathbf{B}. \quad (15)$$

The familiar behavior  $P(s) \sim s$  for GOE and  $P(s) \sim s^2$  for GUE ( $s \ll \Delta$ ) follows then directly for any  $P(\mathbf{B})$  which does not vanish for small  $B = |\mathbf{B}|$ . The (unjustified) evaluation of (15) for all values of  $s$  taking  $P(B)$  to be of a Gaussian form results in the Wigner distribution for the case of real  $h$ .

In the Appendix we discuss how the result (13) is modified by the presence of the self-consistent term  $\text{tr}(V^A \delta \rho)$ . Under the conditions discussed in Sec. III C we show the following:

(1) When the two close levels are both occupied or both empty the distribution of their level spacings for small  $s \ll \Delta$  is  $\sim s$  or  $\sim s^2$  as in the noninteracting case.

(2) When the two levels are on opposite sides of the Fermi level, i.e., one occupied and one empty the expression (13) changes to

$$s = 2|\mathbf{B} - \vec{\mathbf{J}} \cdot \mathbf{m}(\mathbf{B}, \vec{\mathbf{J}})|. \quad (16)$$

Here we use the dyadic notation  $[\vec{\mathbf{J}} \cdot \mathbf{m}]_a = \sum_{b=1}^3 J_{ab} m_b$ . As in the noninteracting case the ‘‘vector’’  $\mathbf{B}$  contains the information about the random part  $h + \delta h$  of the HF Hamiltonian whereas the matrix  $\vec{\mathbf{J}}$  is the projection on the Pauli matrices of the interaction matrix  $\tilde{V}_{IJKL}$ , ( $I, J, K, L = 1, 2$ ) in the subspace of the two close levels  $\psi_1$  and  $\psi_2$  (cf. the Appendix for the precise definition of  $\tilde{V}$ ,  $\mathbf{B}$  and  $\vec{\mathbf{J}}$ ). The vector  $\mathbf{m}(\mathbf{B}, \vec{\mathbf{J}})$  is a unit vector  $|\mathbf{m}| = 1$  and is a solution of the self-consistent HF equations for the two levels

$$\mathbf{m} \times (\mathbf{B} - \vec{\mathbf{J}} \cdot \mathbf{m}) = 0. \quad (17)$$

In this notation the total HF energy is

$$\varepsilon = \mathbf{B} \cdot \mathbf{m} - \frac{1}{2} \mathbf{m} \cdot \vec{\mathbf{J}} \cdot \mathbf{m}. \quad (18)$$

The full investigation of the solutions of the above equations and the expression (16) is found in the Appendix. Here we will concentrate on the simplest case when the matrix of interactions  $J_{ab}$  is degenerate, i.e., has equal eigenvalues. As is shown in the Appendix such a degenerate  $J_{ab}$  matrix corresponds to a complete absence of degeneracy (such as spin) of the close HF levels. We will furthermore restrict ourselves to real Hamiltonians  $h + \delta h$ . Then the vector  $\mathbf{B}$  has only two components  $B_1$  and  $B_3$  and one needs to consider only the corresponding components of  $J_{ab}$  with  $a, b = 1, 3$ . For a degenerate  $J_{ab}$  the vector  $\vec{\mathbf{J}} \cdot \mathbf{m}$  is parallel to  $\mathbf{m}$  and the two level HF equation (17) becomes a simple linear relation  $m_1 B_3 - m_3 B_1 = 0$  without any dependence on the interaction. The level spacing (16) however still contains the interaction term. Using the normalization condition  $m_1^2 + m_3^2 = 1$  one obtains

$$s = 2|B + J|, \quad (19)$$

where  $B = \sqrt{B_1^2 + B_3^2}$  and  $J$  is the degenerate eigenvalue. The explicit expression for  $J$  is

$$J = (V_{1212} - V_{1221})/2. \quad (20)$$

For a positive  $J$  which corresponds to the case of a repulsive interaction the equation for the spacing (19) describes a conical surface separated by a distance  $2J$  from the  $(B_1, B_3)$  plane. This means that the probability for a given  $s$  has a gap of the magnitude  $2J$  above which it must rise linearly

$$P(s; J) = \begin{cases} 0, & s < 2J \\ (s - 2J)f(s), & s \geq 2J \end{cases} \quad (21)$$

where  $f(s)$  is an undefined function which is finite at  $s = 2J$ . For general reasons one should expect that  $f(s)$  vanishes at  $s \rightarrow \infty$ .

The result (21) implies that the distribution  $P(s; J)$  is qualitatively the same as the shifted Wigner distribution

$$P(s; J) = \begin{cases} 0, & s < 2J \\ \frac{\pi}{2\Delta^2} (s - 2J) e^{-\pi/4[(s - 2J)/\Delta]^2}, & s \geq 2J, \end{cases} \quad (22)$$

similar to what was found in the case of the constant interaction, Eq. (9). There is however a crucial difference which we will now try to elucidate.

As is seen from Eq. (20) the degenerate eigenvalue  $J$  is invariant under unitary transformations in the subspace spanned by the two given close states  $\psi_1$  and  $\psi_2$ . As long as one examines realizations of the random  $h$  for which these two particular states stay close in energy they mix strongly only between themselves and  $J$  stays the same. The distribution of the level spacings for such selection of  $h$ 's is given by (21) with a fixed  $J$  as in the constant interaction case. However variations of  $h$  may bring another pair of levels, say,  $\psi_1$  and  $\psi_3$  at close distance on both sides of  $\varepsilon_f$ . For such levels the value of  $J$  may be completely different and given by the corresponding matrix elements  $(V_{1313} - V_{1331})/2$ . In calculations of the overall  $P(s)$  for small  $s$  one should therefore average over the distribution  $P(J)$  of all  $J$ 's

$$P(s) = \int P(J) P(s; J) dJ. \quad (23)$$

For a constant interaction  $J = V_0$  for any pair of states  $\psi_i$ ,  $\psi_j$  and therefore  $P(J)$  is a  $\delta$  function centered at  $V_0$ . For an extreme short range interaction  $V(|\mathbf{r} - \mathbf{r}'|) = V_0 \delta(\mathbf{r} - \mathbf{r}')$  all values of  $J$  are zero and do not fluctuate. One expects therefore that for a general interaction the average value of  $J$  is coming mainly from the very long range component while its fluctuations reflect the middle range components of  $V$ .

The main feature of matrix elements (6) of a constant interaction is that they have the same form in any (orthonormal) basis of the single particle states  $\psi_\alpha$  which are used to calculate  $V_{\alpha\beta\gamma\delta}$ . In other words for a constant interaction the matrix elements  $V_{\alpha\beta\gamma\delta}$  are invariant under the unitary group  $U(M)$  of all transformations in the entire single particle Hilbert space of the problem. Here  $M$  is the dimensionality of this space (typically  $M \rightarrow \infty$ ). This invariance of  $V_{\alpha\beta\gamma\delta}$  for a constant interaction is the reason that  $P(J)$  is a  $\delta$  function in this case. In order to develop a theory of  $P(J)$  for a general interaction one must understand the statistical properties of the single particle wave functions—solutions of the HF prob-

lem. The matrix elements in (20) are defined with respect to such wave functions. Although we do not have an analytic theory of  $P(J)$  we will present below numerical investigation of this function and the validity of the expression of the type (23). Numerically we find that the distribution of  $J$  is approximately Gaussian. Adopting this finding into expression (23) and assuming the form (22) for  $P(s; J)$  one obtains

$$P(s) = \beta \left( \frac{\alpha}{\alpha + \beta} \right)^{1/2} e^{-[\alpha\beta/(\alpha + \beta)](s - 2J_0)^2} \times \left\{ \frac{\alpha}{\alpha + \beta} \operatorname{erfc} \left[ -\frac{\alpha}{\sqrt{\alpha + \beta}} (s - 2J_0) \right] + \frac{1}{\sqrt{\pi(\alpha + \beta)}} e^{-[\alpha^2/(\alpha + \beta)](s - 2J_0)^2} \right\}, \quad (24)$$

where  $\alpha = (8\sigma_J^2)^{-1}$  and  $\beta = \pi/(2\bar{\Delta})^2$  with  $\bar{\Delta}$  being the mean level spacing at the vicinity of the Fermi energy.  $J_0$  and  $\sigma_J$  are the mean and standard deviation of  $P(J)$ , respectively.

### C. Validity of the two level treatment— why only the statistics of spacings across the Fermi level is effected by the interaction

The above results are valid as long as the spacing between the given two levels is much smaller than the distance to other levels. This restriction is needed in order to be able to isolate the two levels from the rest. For repulsive interactions the distance between the pair of levels on different sides of the Fermi energy is determined by the matrix element  $J$  [cf., Eq. (19)]. Therefore the condition of the validity of our treatment for such levels is  $J \ll \Delta$ . As we will see below numerical evidence indicates that at least qualitatively the expression (23) remains correct also for a much larger  $J \sim \Delta$ . For an even stronger interaction the two level treatment ceases to be valid and one must account for the reaction of distant levels to the changes of the self-consistent potential  $\operatorname{tr}(V^A \delta\rho)$ .

Here we wish to add the following remark. For a constant interaction our result is trivially valid for any strength. On the other hand for any given interaction one can extract a constant part, i.e.,  $V_{\alpha\beta\gamma\delta} = V_0 \delta_{\alpha\gamma} \delta_{\beta\delta} + U_{\alpha\beta\gamma\delta}$ , where  $U_{\alpha\beta\gamma\delta} = V_{\alpha\beta\gamma\delta} - V_0 \delta_{\alpha\gamma} \delta_{\beta\delta}$ . Since the HF wave functions are independent of  $V_0$  one may try to solve the problem using  $U$  first and then add  $V_0$ . This procedure is not unambiguous and must be dictated by the physics of the problem. If  $P(J)$  vanishes for  $J < J_c$ , i.e., in the presence of a hard gap (like in a quantum dot with Coulomb interaction), it is natural to take  $V_0 = J_c$ . The condition of validity is then  $J_r \ll \Delta$  where  $J_r$  is the typical gap due to the residual interaction  $U$ .

When there is no minimal value for  $J$  any subtraction is bound to produce  $U$  which has both attractive and repulsive components. This fact may introduce fundamental differences between the solutions to the HF problem obtained using the interaction  $V$  and the one derived in the manner indicated above. Most notably using the latter procedure one will find cases for which there exists enhanced probability for the two levels across  $\varepsilon_f$  to be close to each other [or at distance  $V_0$  after the addition of the constant part, see result

(A15) of the Appendix]. However if the width  $\sigma_J$  of  $P(J)$  is much smaller than its mean  $J_0$  the use of  $V_0 = J_0 - \sigma_J$  will cause  $U$  to change sign only in a small number of cases. Consequently we may use in such a case  $\sigma_J \ll \Delta$  as our criterion for the validity of the two level treatment.

For pairs of neighboring levels which lie on the same side of the Fermi energy the change in the density matrix  $\delta\rho$  vanishes as long as only the two level subspace is considered. Consequently there is no self-consistent term  $V^A \delta\rho$  present and one recovers the results of the non-interacting case. There are two types of corrections to this two level treatment which must be considered. One is the nonzero contribution of the distant levels to  $\delta\rho$ . Another is the correction to the energies of the two close levels due to virtual transition to distant levels.

To estimate the first correction we use the first order result

$$\delta\rho_{\alpha\beta} = \sum_{ph} \left[ \frac{\langle p | \delta h + V^A \delta\rho | h \rangle}{\varepsilon_h - \varepsilon_p} \psi_p(\alpha) \psi_h^*(\beta) + \text{H.c.} \right], \quad (25)$$

which can be solved to obtain the RPA expression

$$\delta\rho_{\alpha\beta} = \sum_{\alpha'\beta'} \left[ - \sum_{p'h'} \left( \frac{\langle p' | V^A | h' \rangle}{\varepsilon_{h'} - \varepsilon_{p'}} \psi_{p'} \psi_{h'}^* + \text{H.c.} \right) \right]_{\alpha\beta, \alpha'\beta'}^{-1} \\ \times \sum_{ph} \left[ \frac{\langle p | \delta h | h \rangle}{\varepsilon_h - \varepsilon_p} \psi_p(\alpha') \psi_h^*(\beta') + \text{H.c.} \right]. \quad (26)$$

Thus we find

$$\delta\rho \sim \frac{\delta h}{\Delta + V}, \quad (27)$$

where here  $V \sim \sum_{p',h'} V_{pp'h'h'}$ . The contribution to  $\delta h^{(\text{HF})}$  is therefore not just  $\delta h$  but  $\delta h^{(\text{HF})} \sim \delta h [1 + V/(V + \Delta)]$ . However this still means that for such levels  $\delta h^{(\text{HF})} \sim \delta h$  for any strength of interaction  $V$ , the sole role of which is to renormalize the random part  $\delta h$ .

The corrections to the energies of the close levels due to transitions to distant levels are

$$E_I = \varepsilon_I + \sum_{i \neq 1,2} \frac{|\delta h_{li}^{(\text{HF})}|^2}{\varepsilon_I - \varepsilon_i}, \quad I = 1,2 \quad (28)$$

where the  $\varepsilon_I$ 's are the energies obtained in the two level treatment. But we have just shown that  $\delta h^{(\text{HF})} \sim \delta h$ . Therefore the correction term in expression (28) is of order  $(\delta h)^2/\Delta \ll \delta h$  and can be disregarded for any  $V$ . Thus we expect that the two level treatment for a couple of occupied or empty levels gives correctly the small  $s$  behavior of  $P(s)$  for any interaction strength. To stress, the difference between this case and the case of two levels on both sides of  $\varepsilon_f$  is that there  $\delta\rho$  also included a ‘‘nonperturbative’’ zero order term coming from the mixing of the wave functions of the occupied and the empty states.

#### D. Addition spectrum vs excitation spectrum

The HF energies are interpreted as energies of quasiparticles (for  $\varepsilon_i > \varepsilon_f$ ) or quasiholes ( $\varepsilon_i < \varepsilon_f$ ). They are excitations of a system with one added or one subtracted particle, i.e.,

$E_i(N \pm 1) - E_0(N) = \pm \varepsilon_i$ . The excitations with the same particle number  $E_i(N) - E_0(N)$  are described in the HF approximation by solutions representing determinants with the same particle number  $N$  which are orthogonal to the HF ground state determinant. In the case of a constant interaction such excitations are simply particle-hole excitations of the noninteracting problem. The distribution of their spacings does not show any Fermi energy related gap and coincides with the non shifted Wigner distribution. This is also true in the two level HF model, Eq. (17). Let us demonstrate this in the simple case of the degenerate  $\vec{J}$ . The HF equation (17) in this case is  $m_1 B_3 - m_3 B_1 = 0$  which together with the normalization condition  $m_1^2 + m_3^2 = 1$  produce two solutions with different total HF energies, Eq. (18),  $\mathcal{E} = \pm B - J/2$ . These solutions represent the ground and excited states of this model which have the same number of particle. The linear dependence of the difference  $\Delta\mathcal{E} = 2B$  indicates that at least as long as the two level treatment of the level repulsion is valid the HF energy spacing distribution between such states obeys  $P(\Delta\mathcal{E}) \sim \Delta\mathcal{E}$  for small  $\Delta\mathcal{E}$  without any gap, as in the noninteracting systems.

Yet another way to obtain this result is to consider the spacings between neighboring particle or hole levels. They correspond, within the HF approximation, to the distances between adjacent excited states of the system with  $N+1$  and  $N-1$  electrons respectively. By the arguments given in the preceding subsection these spacings follow the Wigner-Dyson statistics.

#### E. A schematic model—Keeping only the average interaction matrix elements

For a given realization of the random  $h_{\alpha\beta}$  let us consider the Hamiltonian in the eigenbasis of  $h$ , for which  $h_{\alpha\beta} = \varepsilon_\alpha^{(0)} \delta_{\alpha\beta}$ . In this random basis also the matrix elements of the interaction  $V_{\alpha\beta\gamma\delta}$  are random. Their statistical properties are known, cf., Refs. 24 and are as follows. Only the matrix elements  $V_{\alpha\beta\alpha\beta}$  and  $V_{\alpha\beta\beta\alpha}$  have nonzero averages. Their distributions are narrow with the width behaving like  $1/M$  in the random matrix theory ( $M$  is the size of the single particle space) and like  $1/g$  in the random potential theory ( $g$  is the dimensionless conductance). Based on these properties one is tempted to approximate the interaction by retaining only the matrix elements with non zero averages, i.e., to assume that

$$V_{\alpha\beta\gamma\delta} = \delta_{\alpha\gamma} \delta_{\beta\delta} V_1^{(\alpha\beta)} + \delta_{\alpha\delta} \delta_{\beta\gamma} V_2^{(\alpha\beta)}, \quad (29)$$

with  $V_1^{(\alpha\alpha)} = V_2^{(\alpha\alpha)}$ . Such a model has an easy exact solution. The Hamiltonian

$$H = \sum_{\alpha} \varepsilon_{\alpha}^{(0)} \hat{n}_{\alpha} + \frac{1}{2} \sum_{\alpha,\beta} J_{\alpha\beta} \hat{n}_{\alpha} \hat{n}_{\beta}, \quad (30)$$

where  $J_{\alpha\beta} = V_1^{(\alpha\beta)} - V_2^{(\alpha\beta)}$  has exact eigenstates given by the eigenfunctions of the occupation operators  $\hat{n}_{\alpha}$

$$\psi = |n_1, n_2, \dots, n_k, \dots\rangle, \quad (31)$$

with the corresponding eigenenergies

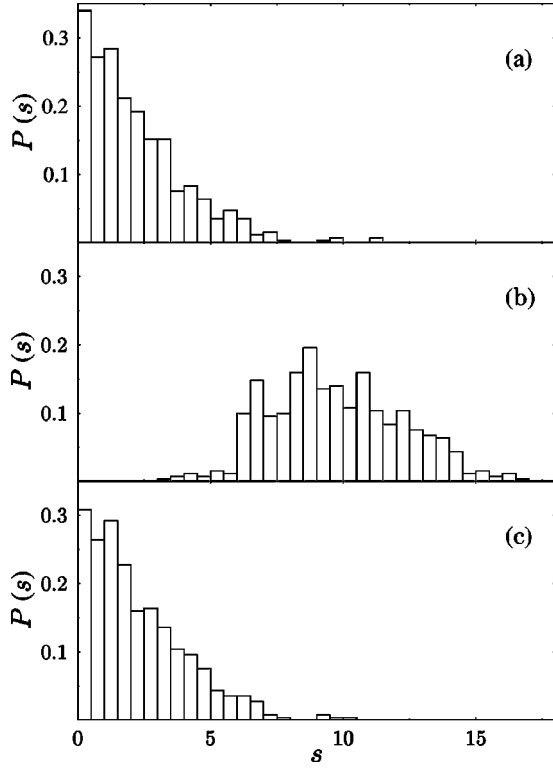


FIG. 1. Probability density distributions of the spacings between (a) the last two hole levels below  $\varepsilon_f$ , (b) the two levels across  $\varepsilon_f$ , and (c) the first two particle levels above  $\varepsilon_f$ . The results were derived by solving the HF equations of the schematic model Eq. (30).  $\varepsilon_\alpha^{(0)}$  and  $J_{\alpha\beta}$  were generated by the random potential model with Coulomb interaction, described in Sec. IV, for a dot with 15 electrons,  $W/t=1.2$ , and  $U/t=1.2$ . We also included a constant interaction part of strength  $V_0=6\Delta_0$ . The spacings are measured in terms of the noninteracting mean level spacing  $\Delta_0$ .

$$E(\{n_i\}) = \sum_i \varepsilon_i^{(0)} n_i + \frac{1}{2} \sum_{i,j} J_{ij} n_i n_j. \quad (32)$$

Like in the case of the constant interaction the exact results are reproduced by the HF approximation. The HF equations are

$$\left[ \varepsilon_\alpha^{(0)} + \sum_\beta J_{\alpha\beta} \rho_{\beta\beta} \right] \phi_i(\alpha) - \sum_\beta J_{\alpha\beta} \rho_{\alpha\beta} \phi_i(\beta) = \varepsilon_i \phi_i(\alpha), \quad (33)$$

and are solved by  $\phi_i(\alpha) = \delta_{i\alpha}$ . Therefore

$$\varepsilon_i = \varepsilon_i^{(0)} + \sum_h J_{ih}, \quad (34)$$

where the sum is over the occupied levels.

We are interested in the ground state of the Hamiltonian (30). A general argument due to Ref. 23 guarantees that at least for positive definite (repulsive) interactions, which we assume below, the HF ground state must be comprised of the  $N$  lowest energy single particle HF levels  $\phi_1, \dots, \phi_N$ . While the ground state of the constant interaction model is obtained by filling the  $N$  lowest noninteracting states this need not be the case for the present model. Consider

$$\begin{aligned} \varepsilon_{N+1} - \varepsilon_N &= \varepsilon_{N+1}^{(0)} - \varepsilon_N^{(0)} \\ &+ J_{N+1,N} + \sum_{k=1}^{N-1} (J_{N+1,k} - J_{N,k}). \end{aligned} \quad (35)$$

Although  $\varepsilon_{N+1}^{(0)} - \varepsilon_N^{(0)} + J_{N+1,N}$  is positive definite the sum in (35) is over  $2N-2$  random variables and can be large and negative. Consequently it may happen that  $\varepsilon_{N+1} < \varepsilon_N$  in variance with the above condition on the ground state. In such a case a different occupation pattern must be sought (we note that even if the condition is not violated there may exist other solutions that are consistent with it and which have lower energies). We expect such crossings of levels across the Fermi energy to take place when  $\Delta + J_0 \approx \sqrt{2N}\sigma_J$ , where  $J_0$  and  $\sigma_J$  are the mean and standard deviation of  $J_{\alpha\beta}$ , respectively.

Similar crossings may occur for levels below or above  $\varepsilon_f$  when  $\Delta \approx \sqrt{2N}\sigma_J$  since for them

$$\varepsilon_j - \varepsilon_{j-1} = \varepsilon_j^{(0)} - \varepsilon_{j-1}^{(0)} + \sum_{k=1}^N (J_{jk} - J_{j-1,k}). \quad (36)$$

This shuffling of levels tends to reduce the correlation between the energies of neighboring states. In particular one expects to find weaker level repulsion when either  $N$  or the interaction strength ( $\sigma_J$ ) are increased.

To verify the above discussion we have calculated the HF energies (34) using numerical values for  $\varepsilon_\alpha^{(0)}$  and  $J_{\alpha\beta}$  generated by the random potential model described in the next section. We took care to choose the lowest energy solution. The results for  $P(s)$  below, across and above  $\varepsilon_f$  are shown in Fig. 1. These distributions differ significantly from the exact HF distributions calculated while retaining the off-diagonal elements of  $V$ , cf., Figs. 2,3,6. The most prominent incorrect feature is the absence of level repulsion in  $P(s)$  for the levels below or above  $\varepsilon_f$ . One can attempt to correct this feature by using the average rather than the exact matrix elements which enter  $J_{\alpha\beta}$ . As it follows from the random potential model,<sup>24</sup> such average matrix elements are functions of the corresponding eigenenergies, i.e.,  $J_{\alpha\beta} = j(|\varepsilon_\alpha - \varepsilon_\beta|)$  with  $j(x)$  a known function which is approximately  $-\ln x$  in two dimensions. Although this model reproduces the density of states in the vicinity of the Fermi energy it is not expected to account for the correct correlations between neighboring levels as manifested in  $P(s)$ .

#### IV. COMPARISON WITH NUMERICAL RESULTS

In order to substantiate the results of our analytical two level treatment we have numerically solved the complete set of HF equations (2) derived from a tight-binding Hamiltonian for a disordered two dimensional quantum dot. With the labeling of the sites by a double index  $(i,j)$  the one-body Hamiltonian is given by

$$\begin{aligned} h &= \sum_{i,j} \varepsilon_{i,j} a_{i,j}^\dagger a_{i,j} \\ &- t \sum_{i,j} (a_{i+1,j}^\dagger a_{i,j} + a_{i,j+1}^\dagger a_{i,j} + \text{H.c.}), \end{aligned} \quad (37)$$

where  $\varepsilon_{i,j}$  is the energy of the site  $(i,j)$  and  $t$  is a constant hopping matrix element. Each of the energies  $\varepsilon_{i,j}$  is chosen

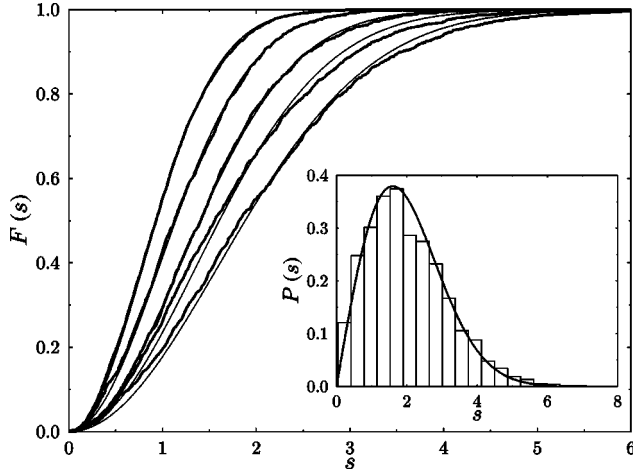


FIG. 2. Probability distributions  $F(s) = \int_0^s P(s') ds'$  of spacings between the last two hole levels just below  $\varepsilon_f$ . The heavy lines depict from top to bottom the numerical results for  $U/t = 0, 0.4, 0.8, 1.2$ , and  $1.6$ . The solid curves present the best fit to the data assuming a Wigner function with renormalized mean level spacing  $\bar{\Delta}$ . The inset contains  $P(s)$  for  $U/t = 1.6$  (histogram) together with its best fit to a Wigner function.

randomly from a Gaussian distribution with the standard deviation  $W/2$ . We assume repulsive  $1/r$  interaction

$$V = U \sum_{i,j,k,l} \frac{a_{i,j}^\dagger a_{k,l}^\dagger a_{k,l} a_{i,j}}{|\mathbf{r}_{i,j} - \mathbf{r}_{k,l}|/b}, \quad (38)$$

where  $b$  is the lattice constant and  $U = e^2/b$ .

The dot was approximated by a grid of  $M = 20 \times 20 = 400$  sites with hard wall boundary conditions. Most of the numerical data was obtained for a dot filled with  $N = 15 - 17$  spinless electrons and a disorder strength  $W = 1.2t$ . Under such conditions the dot was in the diffusive regime and the levels in the vicinity of  $\varepsilon_f$  exhibited RMT statistics in the noninteracting limit. For the low filling that we used the energy band was approximately parabolic and the Fermi energy for a clean noninteracting system was  $\varepsilon_f = 4\pi tN/M$ . A

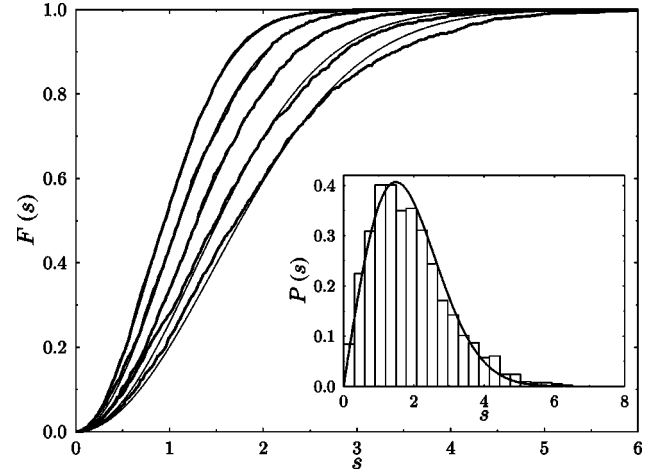


FIG. 3. Same as Fig. 2 but for the spacing between the first two particle levels just above the Fermi energy.

convenient dimensionless measure of the strength of the interaction is  $r_s = (e^2/a)/\varepsilon_f$  where  $a = \sqrt{M/\pi N}b$  is the average interparticle distance. In our case  $r_s = (U/t)\sqrt{M/16\pi N} \approx 0.7U/t$ . Below we describe our results for  $U/t = 0.2 - 1.6$ . Henceforth energy is quoted in units of the observed noninteracting mean level spacing at the Fermi energy  $\Delta_0$  which was found to be larger by 7% than the clean value  $4\pi t/M$ .

The distribution functions  $F(s) = \int_0^s P(s') ds'$  of the spacings between the last two occupied (hole) levels and between the first two empty (particle) levels are shown in Figs. 2 and 3. They are compared with the best fit to an integrated Wigner function with a renormalized mean level spacing  $\bar{\Delta}$ . These and the following results were obtained by averaging the HF spectrum of 15, 16, and 17 electrons over 450–500 realizations of the disorder. While the distributions vanish quadratically for small spacings increasing deviations from the Wigner function are observed when the interaction becomes stronger. We find enhanced probability for the occurrence of spacings smaller and much larger than  $\bar{\Delta}$  for large values of  $U/t$ . The renormalized mean level spacing  $\bar{\Delta}$  also

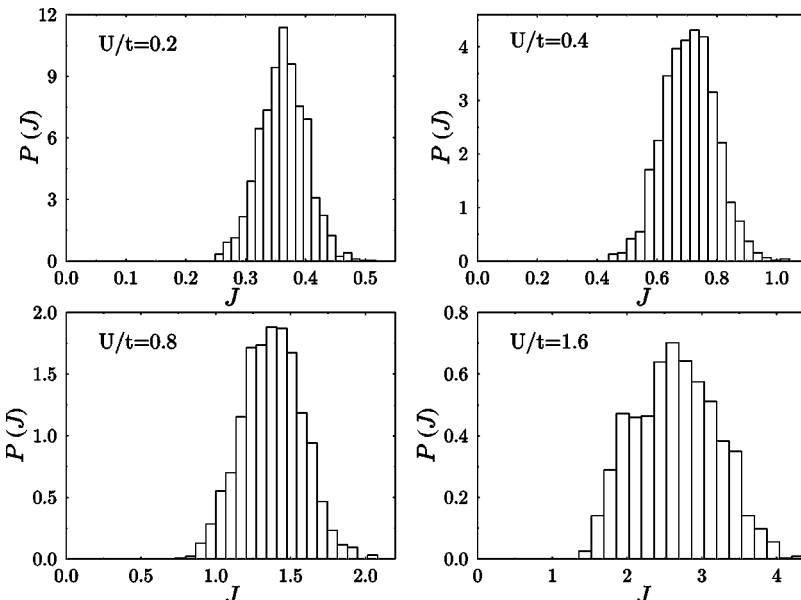


FIG. 4. Probability density distributions of the parameter  $J$  for various interaction strengths.

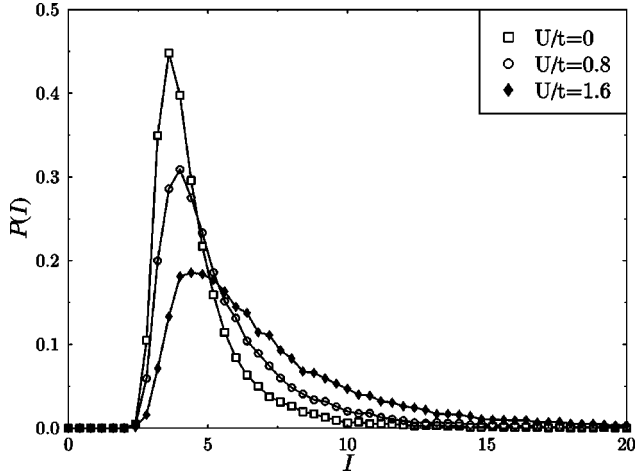


FIG. 5. Probability density distributions of the inverse participation ratio of the 10 hole and 10 particle levels around  $\epsilon_f$  for various interaction strengths.

increases with the strength of the interaction. The width of the fitted Wigner function  $\sigma(P_W) = 0.52 \bar{\Delta}$  is presented in Fig. 7. It grows approximately linearly with  $U/t$ . The mean level spacing between adjacent levels further away from the Fermi energy decreases with the distance from  $\epsilon_f$  and approaches 1.

The distributions of the quantity  $J$  defined in Eq. (20) are depicted in Fig. 4. They are approximately Gaussian for

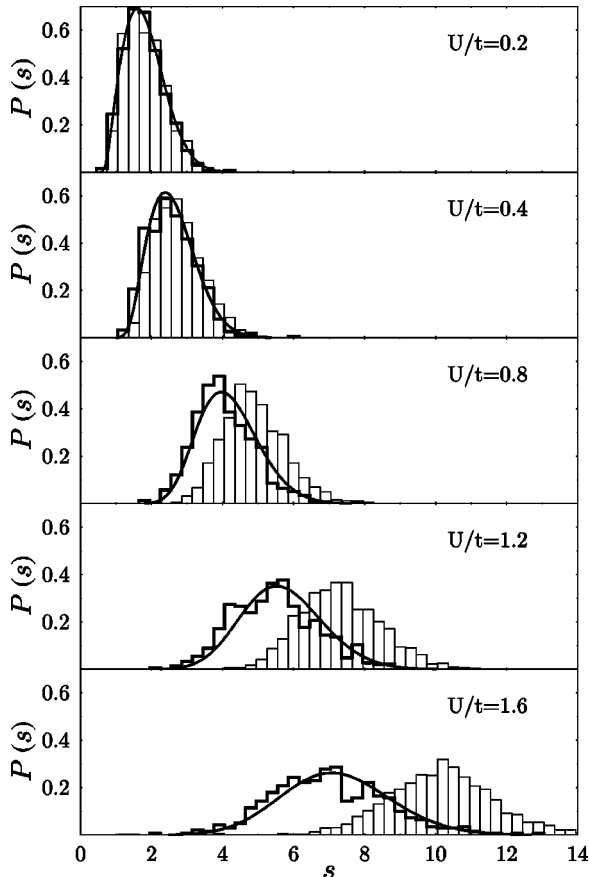


FIG. 6. Probability density distributions of the spacing between the levels across  $\epsilon_f$  (histograms) and of  $D_2(16)$  (broken lines). The solid curves correspond to the estimate (24).

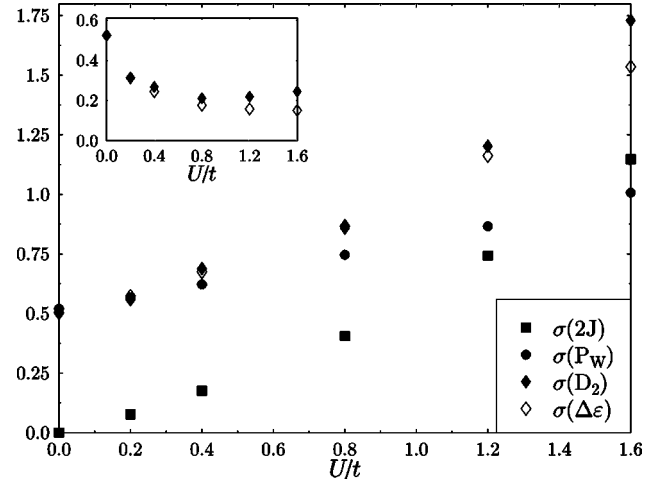


FIG. 7. The standard deviations of  $2J$ ,  $P_W$ —the Wigner distribution that fits best the distribution of spacings in the vicinity of  $\epsilon_f$ ,  $D_2(16)$  and  $\Delta\epsilon$ —the spacing between the two levels across the Fermi energy. The inset depicts the normalized fluctuations  $\sigma(D_2)/\langle D_2 \rangle$  (full diamonds) and  $\sigma(\Delta\epsilon)/\langle \Delta\epsilon \rangle$  (empty diamonds). The results are for a dot with 15–17 electrons and disorder strength  $W = 1.2t$ .

small values of the interaction strength but develop asymmetry towards the high  $J$  end when  $U/t$  is increased. The mean of the distribution scales with the interaction as  $\langle J \rangle \approx 1.7 U/t$ . For the width  $\sigma(J) = \sqrt{\langle J^2 \rangle - \langle J \rangle^2}$  we find  $\sigma(J) \approx 0.16U/t + 0.13(U/t)^2$  over the range of parameters studied (see Fig. 7). These fluctuations are responsible for the smearing of the distribution of spacings across  $\epsilon_f$  as will be shown below. A lengthy calculation using the random vector model (RVM) gives for our system  $\langle J \rangle = 2.1U/t$  and  $\sigma(J) = 0.032U/t$ . The fact that the RVM result for  $\langle J \rangle$  is larger than the observed one reflects the tendency of the system to prefer a nonuniform density distribution that reduces the Coulomb energy. We believe that this is also the reason for at least part of the enhancement of the actual fluctuations relative to the RVM predictions. Typically we found the HF eigenfunctions (both particles and holes) to have large amplitude along the periphery of the dot, as expected from simple electrostatic considerations. The localizing effect of the interaction is evident from Fig. 5 where we present the distribution of the inverse participation ratio  $I = Mb^4 \sum_{i,j} \psi^4(i,j)$  averaged over the 10 particle and 10 hole levels around  $\epsilon_f$ .

In Fig. 6 we present the distribution for the spacing  $\Delta\epsilon$  between the HF levels across the Fermi energy together with the distribution of  $D_2(16)$  calculated according to its definition (12) and using the HF many body ground state energies for 15, 16, and 17 electrons. We also compare them to the analytic estimate (24). For its evaluation we used  $\bar{\Delta}$  that interpolates between the values found from the Wigner functions fitting  $P(s)$  below and above  $\epsilon_f$  and the numerical results for  $\langle J \rangle$  and  $\sigma(J)$ . The two distributions evolve from shifted Wigner functions at small values of  $U/t$  to an approximate Gaussian distributions as the interaction strength is increased. The crossover occurs when  $r_s \sim U/t \sim 1$ . Around this point the fluctuations of the Coulomb gap  $\sigma(2J)$  are comparable to the width of the Wigner function describing  $P(s)$  at the vicinity of the Fermi energy (see Fig. 7). Conse-



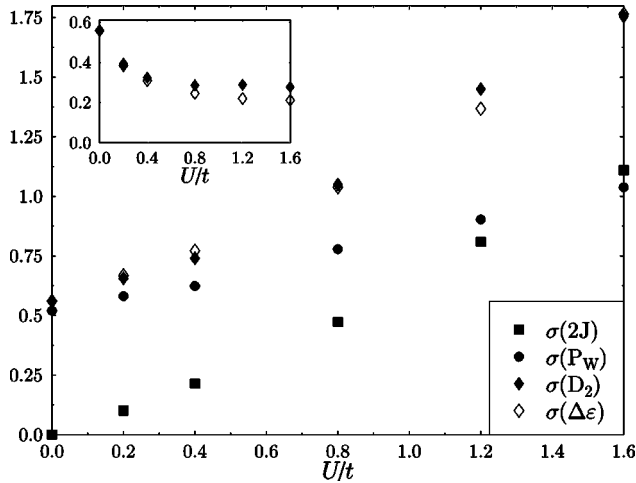


FIG. 8. Same as Fig. 7 but for a dot filled with 10–12 electrons and disorder strength  $W=1.6t$ .

quently the latter is smeared into a new more symmetric and broader distribution. It is evident from Fig. 6 that Koopmans' theorem breaks down for strong interactions, i.e.,  $P(\Delta\varepsilon) \neq P(D_2)$ . However it seems that the two distributions may be viewed as shifted versions of each other having similar shapes but somewhat different widths (see Fig. 7). The shift of  $P(D_2)$  towards lower values is expected and is due to the change of the occupied levels in response to the additional electron. This rearrangements, which is neglected by Koopmans' theorem, tends to lower the electrostatic charging energy. For reasons that are not clear to us our analytic estimate for  $P(\Delta\varepsilon)$  fits rather well  $P(D_2)$ .

We repeated the numerical calculations for the same dot but with stronger disorder  $W/2=1.6t$  and fewer (10–12) electrons. All of the effects reported above have been observed for this case as well. The deviation of  $P(s)$  above or below  $\varepsilon_f$  from the Wigner function were more pronounced. The fluctuations of  $J$  also increased and we found  $\sigma(J) \approx 0.25 U/t + 0.06(U/t)^2$  with enhanced asymmetry in the shape of the distribution for strong interactions. The discrepancy between  $P(\Delta\varepsilon)$  and  $P(D_2)$  at large  $r_s$  persisted although the shapes of the two distributions and particularly their width were closer for this dot then for the one described above. Figure 8 summarizes the dependence of the fluctuations of the different quantities on the strength of the interaction.

Our calculations were done for a fixed number of particles. In order to facilitate comparison with a fixed chemical potential ensemble the Fermi energy of each spectrum in the ensemble was shifted to zero. The resulting density of states is plotted in Fig. 9.

## V. CONCLUSION

The statistics of energy levels and wave functions in non-interacting disordered systems is well established and follows the predictions of RMT. The effects of interactions in this context are relatively unexplored. The strategy adopted by us here was to include interactions within the HF approximation. While being the crudest of approximations it is known to yield a reasonable description of the quasiparticles properties in small systems. It also allows for a natural ex-

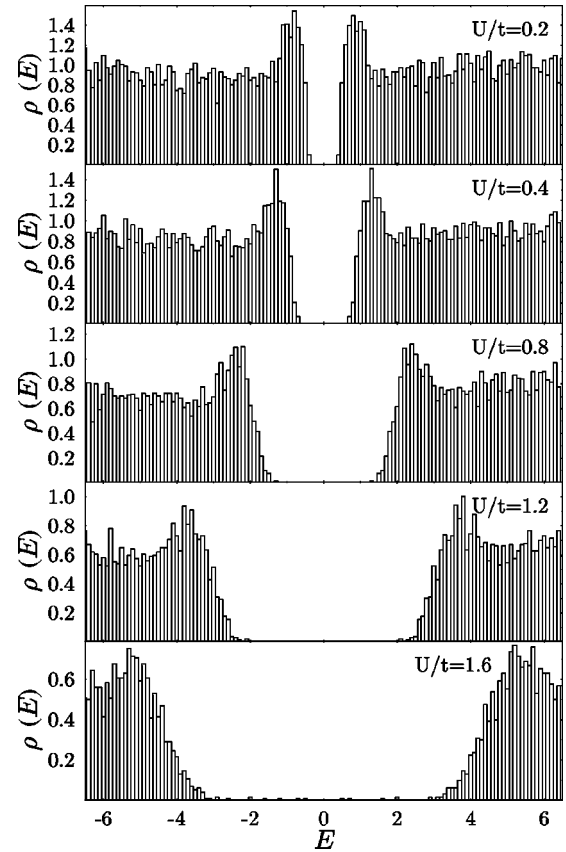


FIG. 9. The density of states near  $\varepsilon_f$ . The results are for a dot filled with 15–17 electrons and disorder strength  $W=1.2t$ .

tension of the concept of single particle level statistics by replacing the non-interacting levels with their HF counterparts. Accordingly it is of interest to generalize the RMT program to study HF Hamiltonians of random systems. This is a difficult task due to the self-consistent nature of the HF problem. As a first step we extended the treatment of Wigner for the statistics of spacings between neighboring levels. We were able to make rigorous statements about the probability to find two levels close to each other and speculated on the nature of the distribution for arbitrary spacing (just as in the noninteracting case). Our analytical considerations and numerical simulations indicate that while the spacing statistics between hole (occupied) or particle (unoccupied) levels is qualitatively unaffected by the interactions they have a dramatic effect on the spacing across the Fermi energy. The probability distribution for this spacing evolves from the Wigner function in the noninteracting limit to a much broader Gaussian-like distribution as the interaction strength is increased. This crossover is driven by increasing fluctuations of the charging energy of the system.

Since the spacings between hole or particle HF levels are related to the neutral excitations of the system and the spacing across the Fermi energy reflects its addition spectrum their statistics have experimental consequences. However, a direct comparison between our results and the recent experimental data on addition spectra of quantum dots<sup>6–8</sup> (which agrees in its general characteristics with our findings) is impaired by the limitation of our treatment to spinless electrons. The inclusion of spin is desirable both on theoretical

grounds and in order to explain the lack of any spin signature in the above mentioned experimental data.

### ACKNOWLEDGMENTS

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### APPENDIX: THE TWO LEVEL HARTREE-FOCK PROBLEM

In Sec. III C we outlined the way in which the density matrix  $\rho$  changes under a variation  $\delta h$  of the random part of the HF Hamiltonian. We argued that while in the case of two close levels that are both occupied or empty the term  $\text{tr}(V^A \delta \rho)$  does not alter the small  $s$  behavior of  $P(s)$  it must be included in a self-consistent manner for a couple of close level residing on both sides of  $\varepsilon_f$ . In this Appendix we will concentrate on the latter scenario assuming  $V \ll \Delta$ .

Let us denote by  $\psi_i$  the eigenfunctions of  $h^{(HF)}$  and by  $\phi_i$  the eigenfunctions of  $h^{(HF)} + \delta h^{(HF)}$ . Then in the basis of  $\psi_1$  and  $\psi_2$  the HF problem for two close levels on both sides of  $\varepsilon_f$  is

$$\begin{aligned} & \left( \varepsilon_1^{(0)} + \delta h_{11} + \sum_{I,J=1,2} \tilde{V}_{11IJ} \delta \rho_{JI} \right) a \\ & + \left( \delta h_{12} + \sum_{I,J=1,2} \tilde{V}_{112J} \delta \rho_{JI} \right) b = \varepsilon a, \\ & \left( \delta h_{12}^* + \sum_{I,J=1,2} \tilde{V}_{21IJ} \delta \rho_{JI} \right) a \\ & + \left( \varepsilon_2^{(0)} + \delta h_{22} + \sum_{I,J=1,2} \tilde{V}_{212J} \delta \rho_{JI} \right) b = \varepsilon b, \end{aligned} \quad (\text{A1})$$

with  $\delta \rho_{JI}$  the  $2 \times 2$  matrix

$$\delta \rho = \phi_1 \phi_1^+ - \psi_1 \psi_1^+ = \begin{pmatrix} |a|^2 - 1 & ab^* \\ a^* b & |b|^2 \end{pmatrix}, \quad (\text{A2})$$

and the normalization condition  $|a|^2 + |b|^2 = 1$ . The relation between the matrix  $\tilde{V}_{IJKL}$ ,  $I=1,2$ , etc., and the original  $V_{\alpha\beta\gamma\delta}$  will be discussed below. We will also need the part of the HF energy the minimization of which, with respect to  $\phi_1$ , gives (A1)

$$\begin{aligned} E_{\text{HF}}[\phi_1] &= \text{tr}\{[h + \text{tr}(\tilde{V}\rho) + \delta h] \phi_1 \phi_1^+ \\ &+ \frac{1}{2} \text{tr}[\tilde{V}(\phi_1 \phi_1^+ - 2\psi_1 \psi_1^+)] \phi_1 \phi_1^+\}. \end{aligned} \quad (\text{A3})$$

The solution of the set of algebraic equations (A1) is particularly simple if one uses the expansion in terms of Pauli matrices,

$$\begin{aligned} \phi_1 \phi_1^+ &= \frac{1}{2} (1 + \mathbf{m} \cdot \boldsymbol{\sigma}), \\ \psi_1 \psi_1^+ &= \frac{1}{2} (1 + \mathbf{m}_0 \cdot \boldsymbol{\sigma}), \end{aligned} \quad (\text{A4})$$

with the ‘‘pure state’’ conditions  $|\mathbf{m}| = |\mathbf{m}_0| = 1$ . Inserting this into (A3) and transferring to the left all terms which do not depend on  $\mathbf{m}$  one obtains

$$\mathcal{E} = \mathbf{B} \cdot \mathbf{m} - \frac{1}{2} \mathbf{m} \cdot \vec{\mathbf{J}} \cdot \mathbf{m}. \quad (\text{A5})$$

The notation in (A5) stands for

$$\begin{aligned} \mathcal{E} &= E_{\text{HF}} - \frac{1}{2} \text{tr}[h + \text{tr}(\tilde{V}\rho) + \delta h] \\ &+ \frac{1}{4} \text{tr}\{\text{tr}[\tilde{V}(\mathbf{m}_0 \cdot \boldsymbol{\sigma})]\} \\ &+ \frac{1}{8} \text{tr}[\text{tr}(\tilde{V})], \\ \mathbf{B} &= \frac{1}{2} \text{tr}\{\boldsymbol{\sigma}[h + \text{tr}(\tilde{V}\rho) + \delta h]\} \\ &- \frac{1}{4} \text{tr}\{\text{tr}[\boldsymbol{\sigma}\tilde{V}(\mathbf{m}_0 \cdot \boldsymbol{\sigma})]\}, \\ J_{ab} &= -\frac{1}{4} \text{tr}[\boldsymbol{\sigma}^a \text{tr}(\tilde{V}\boldsymbol{\sigma}^b)], \end{aligned} \quad (\text{A6})$$

and  $\mathbf{m} \cdot \vec{\mathbf{J}} \cdot \mathbf{m} = \sum_{a,b=1}^3 J_{ab} m_a m_b$ . Varying  $\mathcal{E}$  with respect to  $\mathbf{m}$  under the condition  $|\mathbf{m}| = 1$  one obtains

$$\mathbf{m} \times (\mathbf{B} - \vec{\mathbf{J}} \cdot \mathbf{m}) = 0. \quad (\text{A7})$$

This is a ‘‘magnetic form’’ of the equations (A1). Of course it could also be obtained by the direct substitution of (A4). The ‘‘magnetic field’’  $\mathbf{B}$  contains the information about the random part  $h + \delta h$  of the HF Hamiltonian whereas the matrix  $\vec{\mathbf{J}}$  is the projection on the Pauli matrices of the interaction matrix  $\tilde{V}_{IJKL}$  taken in the subspace of the two states  $\psi_1$  and  $\psi_2$ . For our general discussion we can diagonalize  $\vec{\mathbf{J}}$ . This will reshuffle the components of  $\mathbf{B}$  which are random anyway.

The distance  $\Delta\varepsilon$  between the eigenvalues of (A1) is  $\Delta\varepsilon = \text{tr}[(\phi_2 \phi_2^+ - \phi_1 \phi_1^+)(h + \delta h)^{\text{HF}}]$  where due to orthogonality  $\phi_2 \phi_2^+ = (1 - \mathbf{m} \cdot \boldsymbol{\sigma})/2$ . Therefore

$$\Delta\varepsilon(\mathbf{B}, \vec{\mathbf{J}}) = 2|\mathbf{B} - \vec{\mathbf{J}} \cdot \mathbf{m}(\mathbf{B}, \vec{\mathbf{J}})|, \quad (\text{A8})$$

where  $\mathbf{m}(\mathbf{B}, \vec{\mathbf{J}})$  is a solution of (A7).

The equations are especially simple in the case when the Hamiltonian and the wavefunctions are real. This corresponds to the orthogonal ensemble in the terminology of RMT. Only the projections on  $\sigma_1$  and  $\sigma_3$  remain in this case. The HF energy and the HF equation are, respectively,

$$\mathcal{E} = B_1 m_1 + B_3 m_3 - \frac{1}{2} (J_1 m_1^2 + J_3 m_3^2), \quad (\text{A9})$$

$$m_1 B_3 - m_3 B_1 + (J_1 - J_3) m_1 m_3 = 0, \quad (\text{A10})$$

with the constraint  $m_1^2 + m_3^2 = 1$ . In the above  $J_1$  and  $J_3$  are the eigenvalues of  $\vec{\mathbf{J}}$ . The solution of (A10) are roots of a fourth order equation. Real roots are the extrema of the curve defined by the intersection of the surface (A9) and the constraint cylinder  $m_1^2 + m_3^2 = 1$ . Only one real root must be selected – that which minimizes  $\mathcal{E}$ .

Let us examine the energy spacing  $\Delta\varepsilon$

$$\Delta\varepsilon = 2\sqrt{(B_1 - J_1 m_1)^2 + (B_3 - J_3 m_3)^2} \quad (\text{A11})$$

and determine when and how level crossings occur. In the absence of the interaction ( $J_1=J_3=0$ )  $\Delta\varepsilon=0$  at  $B_1=B_3=0$ , reproducing the standard result. In the presence of the interaction the level crossing  $\Delta\varepsilon=0$  occurs when

$$m_1=B_1/J_1, \quad m_3=B_3/J_3. \quad (\text{A12})$$

Due to the normalization constraint this can be fulfilled only on an ellipse

$$\frac{B_1^2}{J_1^2} + \frac{B_3^2}{J_3^2} = 1. \quad (\text{A13})$$

It is therefore sufficient to examine the minimum energy solution on the ellipse. We note that the conditions (A12) are consistent with equation (A10), i.e., level crossings must occur at least for one of the solutions. However there is no guarantee that this is also the minimum energy solution. In fact a detailed analysis reveals that the occurrence of level crossing for the minimum energy solution depends on the signs of the eigenvalues  $J_1$  and  $J_3$  as follows: (i) when both signs are positive there are four real solutions (two minima and two maxima) on the ellipse (A13) provided  $J_3 > 2J_1$  or  $J_1 > 2J_3$ . Otherwise there are only two real solutions (one maximum and one minimum). The solution with  $\Delta\varepsilon=0$  is always the (highest) maximum. (ii) when one of the eigenvalues is negative and another positive there are four real solutions on the ellipse (two minima and two maxima). The solution with  $\Delta\varepsilon=0$  is either a metastable minimum or a maximum. (iii) only when both eigenvalues are negative the solution with  $\Delta\varepsilon=0$  coincides with the absolute minimum of the HF energy.

In the first two cases the minimum energy solution always has a nonzero level spacing. Consequently for such  $J_1$  and  $J_3$

the two HF levels *never cross* and one expects a *gap* in the probability distribution of  $\Delta\varepsilon$ . In the last case of two positive eigenvalues the level spacing distribution in the vicinity of  $\Delta\varepsilon=0$  will depend on the density of  $\Delta\varepsilon=\text{const}$  lines close to the ellipse (A13).

The interaction  $\tilde{V}$  which determines  $J_1$  and  $J_3$  is just  $V^A$  when the two levels  $\varepsilon_1$  and  $\varepsilon_2$  are not degenerate. In this case we find from (A6)  $J_{ab}=[(V_{1212}-V_{1221})/2]\delta_{ab}$ . Thus for a positive (negative) definite,<sup>23</sup> i.e., repulsive (attractive) interaction  $J_1=J_3>0$  ( $J_1=J_3<0$ ). When the levels are degenerate one must extend the two levels treatment to include all degenerate wave functions. However, if the degeneracy is due to spin and the wave functions are separable spin-space products, one can define an equivalent two level problem for the orbital parts with the interaction  $\tilde{V}=V^A+V$ . For this case  $J_1=(V_{1212}-2V_{1221}-V_{1122})/2$  and  $J_3=[2V_{1212}-V_{1221}-(V_{1111}+V_{2222})/2]/2$ . For such  $\tilde{V}$  the signs of  $J_1$  and  $J_3$  are not uniquely related to the nature of the interaction. In particular they may both be positive even for a repulsive interaction. However, if this happens, we expect to find, due to a general argument,<sup>23</sup> another HF solution (e.g., lacking spin degeneracy) with lower total energy for which the levels do not cross.

The case  $J_1=J_3=J$  is particularly simple since the ellipse degenerates into a circle and one obtains

$$\Delta\varepsilon(B,J)=2|B+J|, \quad (\text{A14})$$

where  $B=\sqrt{B_1^2+B_3^2}$ . For positive  $J$  this result leads, after choosing for simplicity  $P(B)$  of a Gaussian form, to the shifted Wigner distribution, Eq. (22). For negative  $J$  (attractive interaction) we find

$$P(s;J)=\left\{\begin{array}{l} \frac{\pi}{2\Delta^2}[(2|J|-s)e^{-\pi/4[(2|J|-s)/\Delta]^2}+(2|J|+s)e^{-\pi/4[(2|J|+s)/\Delta]^2}]s<2|J| \\ \frac{\pi}{2\Delta^2}(2|J|+s)e^{-\pi/4[(2|J|+s)/\Delta]^2} \quad s\geq 2|J| \end{array}\right\}. \quad (\text{A15})$$

This distribution is a sum of two, mirror reflected and shifted Wigner distributions resulting from the two roots of  $s=\Delta\varepsilon(B,J)$ . The most important feature to note in (A15) is the nonzero probability  $P(s=0)$ . This is a consequence of the linear dependence of  $\Delta\varepsilon(B,J)$  at  $B=|J|$ .

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