

Fermi edge singularities in the mesoscopic regime: Anderson orthogonality catastrophe

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For generic mesoscopic systems, such as quantum dots or nanoparticles, we study the Anderson orthogonality catastrophe (AOC) and Fermi-edge singularities in photoabsorption spectra in a series of two papers. In the present paper we focus on AOC for a finite number of particles in discrete energy levels where, in contrast to the bulk situation, AOC is not complete. Moreover, fluctuations characteristic for mesoscopic systems lead to a broad distribution of AOC ground-state overlaps. The fluctuations originate dominantly in the levels around the Fermi energy, and we derive an analytic expression for the probability distribution of AOC overlaps in the limit of strong perturbations. We address the formation of a bound state and its importance for symmetries between the overlap distributions for attractive and repulsive potentials. Our results are based on a random matrix model for the chaotic conduction electrons that are subject to a rank-one perturbation corresponding, for example, to the localized core hole generated in the photoabsorption process.

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I. INTRODUCTION

Among the simplest many-body problems one can consider is a Fermi sea of electrons interacting with a static impurity. Such an impurity is, for example, suddenly formed when a core or valence electron is excited above the Fermi energy by an incident photon in a bulk-metal photoabsorption or photoluminescence experiment. Naively, one would expect a sharp onset of the absorption cross section at threshold with a signal proportional to the density of states in the conduction band above the Fermi energy. In experiments, deviations from this behavior were found in the form of peaked or rounded edges both in metals¹ and semiconductors.² These so-called Fermi-edge singularities (FES) are a clear indication of the importance of many-body processes that have been receiving enduring interest.

For (clean) macroscopic systems, an essentially complete understanding of the mechanisms causing the Fermi-edge singularities has been obtained by the late 1980s.³⁻⁷ In particular, these works have emphasized the role of two competing effects. The first one is the Anderson orthogonality catastrophe (AOC), which is a property of the overlap between many-body wave functions. However, in x-ray-absorption and photoabsorption processes, besides AOC there is another many-body response of the conduction electrons to the impurity potential,^{3,4,7,8} often referred to as Mahan's exciton, Mahan's enhancement, or the Mahan-Nozières-DeDominicis (MND) contribution. It counteracts the effect of AOC in situations where the dipole selection rules are fulfilled and causes the photoabsorption cross section to diverge at threshold.

In the present series of two papers we are interested in these many-body effects in mesoscopic systems,⁹⁻¹¹ such as quantum dots or nanoparticles, and, in particular, in the changes with respect to the macroscopic (or bulk) case due to the confined geometry. In this first paper, we focus on the orthogonality catastrophe mechanism for a finite system. We will more particularly consider the case of a contact (rank one), but not necessarily small perturbation, with the local-

ized perturbation presented by the core hole left behind in photoabsorption just being one example. In the second paper [12], we will discuss, in detail, Fermi-edge singularities and mesoscopic photoabsorption spectra that depend not only on AOC but crucially on the MND contribution.

In a bulk-metal x-ray-absorption experiment, the conduction electrons respond to the abrupt, nonadiabatic appearance of a core hole generated upon photoexcitation of an inner-shell electron into the conduction band by slightly adjusting their single-particle energies and wave functions. Since the core hole represents an effectively positive charge the scattering potential will be attractive, and the energy levels will be lowered. Although the overlap of the respective single-particle states before and after the perturbation is very close to one, the many-body ground-state overlap Δ tends to zero in the thermodynamic limit, $\Delta \propto M^{-\epsilon}$ with M the number of conduction electrons and the parameter $\epsilon > 0$. This effect, noted by Anderson in 1967,¹³ is the Anderson orthogonality catastrophe. As a result of AOC the cross section $A(\omega)$ for the absorption of photons with energy ω will be power-law suppressed near threshold, explaining the above-mentioned Fermi-edge singularity in the form of a rounded edge.

AOC plays an important role in all processes where a finite range scattering potential suddenly arises or changes. It is also prominent in the Mössbauer effect where AOC enables the recoilless emission or absorption of γ rays by the whole crystal, but not by a single nucleus.¹⁴ Another example is Kondo physics, except that in that case the impurity is dynamic, rather than static as considered here.

Turning from macroscopic to mesoscopic systems opens a different venue to the study of AOC. To start with, the confined geometry will naturally induce novel behavior associated with the mesoscopic regime, among which are the lack of translational or rotational invariance, the existence of interference effects, and the related mesoscopic fluctuations.⁹⁻¹¹ Furthermore, the advances in the fabrication of mesoscopic and nanoscopic devices provide a great flexibility in designing systems for which one can measure and con-

tol processes dominated by AOC. One example would correspond to the situation where an electron tunnels through a system of two quantum dots joined via a small constriction. In that case the boundary conditions of the electrons on the far dot are changed once the tunneling electron enters the first dot,^{15,16} and, as a consequence, a change of one electron appears as a sudden perturbation to the remaining electrons. Another example is a mesoscopic tunnel junction containing a localized impurity level such that tunneling from the junction to the lead leaves behind a hole bound to the impurity. The resulting power-law singularities in the current-voltage characteristics were studied in Ref. 17 and observed in experiments with two- and three-dimensional electrodes.¹⁸ Large optical singularities in one-dimensional electron gases formed in semiconductor quantum wires were observed in Ref. 19 and theoretically explained as Fermi-edge singularities.²⁰

Aspects of AOC in disordered or mesoscopic systems have been addressed in various publications.²¹⁻²⁴ AOC in disordered simple metals and its influence on x-ray-photoemission spectra (where the excited core electron leaves the metal and the edge behavior is determined by the AOC response alone) was studied by Chen and Kroha.²¹ In Ref. 23, Vallejos and co-workers studied AOC in chaotic mesoscopic systems for a weak perturbation modeled by a random matrix. They found large fluctuations of the AOC overlap that is nonzero, in general, due to the incomplete orthogonality. Small overlaps are correlated with avoided level crossings between the highest filled and the lowest empty level. This motivated the analytic study of a two-level model to which we refer below. Mesoscopic conductors with diffusive disorder were studied with respect to AOC by Gefen *et al.*²⁴ The dependence of the average AOC-overlap on the number M of electrons was found to be dimension dependent and to show a stronger dependence on M in two dimensions than in higher dimensions. In agreement with the results by Vallejos *et al.* [23] and the results we present here, a broad distribution of overlaps is seen, with the small-overlap tail of the distribution being related to few level statistics near the Fermi energy. Another key result was that the disorder-averaged AOC overlap depends non monotonically on the disorder. This becomes clear in the limit of strong disorder (where the electrons are strongly localized and cannot be sensitive to the addition of another impurity) and was confirmed in their numerical results.

As already mentioned, here we will more specifically consider the case of a short-range (rank one), not necessarily small, perturbation,^{3,4,7,22} which applies for the description of the perturbation created by the core hole. We will, furthermore, consider a generic chaotic mesoscopic system, such as a quantum dot or nanoparticle, for which a random matrix theory (RMT) model of the conduction electrons applies. This particular regime will show some similarities with both the diffusive systems studied in Ref. 24 and the non-rank-one perturbative regime investigated by Vallejos *et al.*,²³ but will also display interesting specific properties.

Beyond AOC, Fermi-edge singularities in the mesoscopic regime were considered in Refs. 8, 16, and 17. We will consider the full mesoscopic x-ray edge problem and the resulting FES in photoabsorption spectra of quantum dots or nano-

particles in [12], and concentrate on AOC in the present paper.

This paper is organized as follows. In Sec. II we will introduce our model of a rank-one perturbation on discrete (bulklike or chaotic) energy levels and apply it to the study of AOC. We investigate the properties of the ground-state overlap probability distribution $P(|\Delta|^2)$ and show that the phase shift at the Fermi energy determines the overlap fluctuations. The presence of a bound state is addressed in Sec. III, and its role for the symmetry of overlap distributions for positive and negative perturbations is discussed. Knowing that the origin of the fluctuations lies in the levels nearest to the Fermi energy allows us to derive an analytic formula for the overlap distribution in the limit of strong perturbations in Sec. IV. We end with a summary on AOC in generic mesoscopic systems.

II. ANDERSON ORTHOGONALITY CATASTROPHE FOR MESOSCOPIC CHAOTIC SYSTEMS

Anderson orthogonality catastrophe refers to the vanishing of the overlap Δ between the system's many-body ground states, before and after a finite range scattering potential is suddenly applied, and is complete only in the thermodynamic limit.¹³ In this section we will discuss the effect of a finite number of particles in a mesoscopic system as well as the role of mesoscopic fluctuations. As the spin variable does not play a particular role here, we shall not take it into account (except for the discussion of the Friedel sum rule). We, therefore, describe the unperturbed system by the Hamiltonian

$$\hat{H}_0 = \sum_{k=0}^{N-1} \epsilon_k c_k^\dagger c_k, \quad (1)$$

where the operator c_k^\dagger creates a particle in the unperturbed eigenstate $\varphi_k(\mathbf{r})$ corresponding to the eigenenergy ϵ_k . We want to consider a situation where the perturbing potential is created by the hole left by a core electron excited into the conduction band, which, because of screening by the other electrons, is a short-range potential. We shall, therefore, use for the perturbation a rank-one contact potential

$$\hat{V}_c = v_c \Omega f^\dagger(\mathbf{r}_c) f(\mathbf{r}_c), \quad (2)$$

[$f(\mathbf{r}_c) = \sum_k \varphi_k(\mathbf{r}_c) c_k$], that only acts at the location \mathbf{r}_c of the core hole (Ω is the volume in which the electrons are confined and the parameter v_c defines the strength of the potential). Introducing \tilde{c}_κ^\dagger as creator of a particle in the perturbed orbital $\psi_\kappa(\mathbf{r})$ (we will use Greek indices to indicate the perturbed system), we obtain the diagonal form of the perturbed Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V}_c = \sum_{\kappa} \lambda_{\kappa} \tilde{c}_{\kappa}^{\dagger} \tilde{c}_{\kappa}. \quad (3)$$

We will refer to the many-body, Slater-determinant ground states of the unperturbed and the perturbed systems as $|\Phi_0\rangle$ and $|\Psi_0\rangle$, respectively. Their overlap is $\Delta = \langle \Psi_0 | \Phi_0 \rangle$. In the ground state the M conduction electrons fill the lowest of the

N levels, i.e., the levels $i=0, \dots, M-1$ [see also Fig. 7(a)]. Whenever practical, we will use the index i (μ for perturbed levels) for levels below E_F and j (γ) for levels above E_F , and k (κ) when reference to all levels is made.

A. Bulklike systems

In the bulk the orbital momentum l is a good quantum number, and, because the core hole potential (2) is rotationally invariant, only the $l=0$ sector couples to the perturbation. Within this sector, the unperturbed energy levels $\{\epsilon_k\}$ near the Fermi energy can be taken equidistantly spaced and, with a proper choice of the origin of the phase of the wave functions, we can take $\phi_k(\mathbf{r}_c) = \text{const} = 1/\sqrt{\Omega}$.

In the following, we will call ‘‘bulklike’’ a model that, as the $l=0$ sector of a bulk system, has no fluctuations for the eigenlevel spacing or for the amplitude of the wave function at the impurity. We shall, however, assume finite the number of levels within the bandwidth. In this subsection we shall review briefly some properties of this bulklike system.

In the absence of mesoscopic fluctuations, the perturbation is

$$\hat{V}_c = v_c \sum_{kk'} c_k^\dagger c_{k'}.$$

Introducing the transformation matrix $\mathbf{a} = (a_{k\kappa})$,

$$\psi_\kappa = \sum_{k=0}^{N-1} a_{k\kappa} \varphi_k, \quad (4)$$

one can check easily that the perturbed eigenstates $\{\lambda_\kappa\}$ and the coefficients $a_{k\kappa}$ fulfill the familiar equations⁷

$$0 = 1 - v_c \sum_{k=0}^{N-1} \frac{1}{\lambda_\kappa - \epsilon_k}, \quad (5)$$

$$a_{k\kappa} = - \frac{v_\kappa}{\lambda_\kappa - \epsilon_k}, \quad (6)$$

$$\frac{1}{|v_\kappa|^2} = \sum_{k=0}^{N-1} \frac{1}{(\lambda_\kappa - \epsilon_k)^2}. \quad (7)$$

Equation (5) allows one to find the perturbed eigenvalues λ_κ as a function of the unperturbed energies ϵ_k and the perturbation strength v_c . This is illustrated in Fig. 1 where the perturbed eigenvalues λ_κ are found as intersection points of the function

$$f(\lambda) = \sum_k^{\text{def}} \frac{1}{\lambda - \epsilon_k}$$

with the horizontal line $1/v_c$. We have assumed a negative perturbation $v_c < 0$ to account for the attractive perturbation caused by the core hole potential.

The effect of the perturbation and the shift between perturbed and unperturbed levels is generally characterized by the partial-wave phase shifts δ_l at the Fermi energy for the orbital channel l . The phase shifts obey the Friedel sum rule

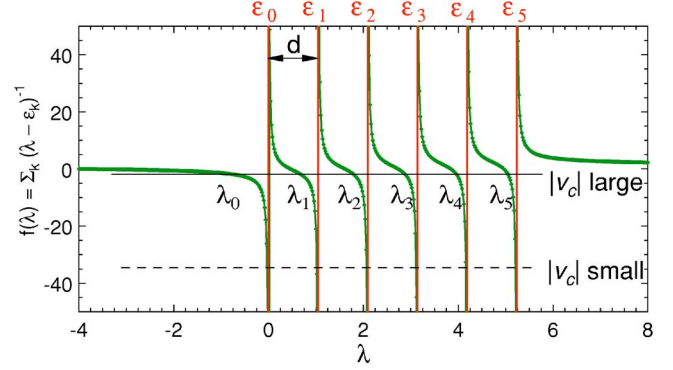


FIG. 1. (Color online) Perturbation of a bulklike material with six initially equidistant energy levels ϵ_k ($0 \leq \epsilon_k \leq 2\pi$, mean level spacing d) by a rank-one perturbation of strength $v_c < 0$. The perturbed eigenvalues λ_κ arise from a graphical solution of Eq. (5) and are shifted to lower energies (attractive interaction). This shift increases as the perturbation becomes stronger; see the horizontal lines corresponding to two different potential strengths. The strongest perturbation shifts the perturbed levels right to the middle of two neighboring unperturbed levels $\epsilon_k, \epsilon_{k+1}$ (strictly, this applies in the center of the band; see the discussion of boundary effects).

$$Z = \sum_l 2(2l+1) \delta_l / \pi, \quad (8)$$

where the factor of two accounts for spin and $Z = -1$ in the case of photoabsorption. For a localized rank-one perturbation, which, as mentioned above, is spherically symmetric, all δ_l with $l \neq 0$ are zero. In this case the Friedel sum rule, Eq. (8) implies $\delta_0 = -\pi/2$.

When E_F is in the middle of the conduction band, δ_0 is related to the potential v_c and the mean-level spacing d by²²

$$\delta_0 = \arctan \frac{\pi v_c}{d}. \quad (9)$$

$\delta_0 = -\pi/2$, therefore, corresponds to a strong perturbation $|v_c/d| \gg 1$. We will therefore be mainly interested in AOC in this limit, although we shall also consider other cases.

For the finite number of particles that we consider in the following, boundary effects are important. First, the phase shift varies (monotonically) with the level number, and Eq. (9) holds only for levels at the band center. For levels off center, the number of energy levels on the left and right is unbalanced and leads to additional pushing from the side with the surfeit. This can already be guessed from inspecting Fig. 1.

This effect can easily be taken into account by noting that, for any perturbed level λ_κ [assuming for instance $0 \leq \kappa \leq (N-1)/2$], Eq. (5) can be rewritten as

$$\sum_{k=0}^{2\kappa-1} \frac{1}{\lambda_\kappa - \epsilon_k} = \frac{1}{v_\kappa}, \quad (10)$$

where we have defined

$$\frac{1}{v_\kappa} \stackrel{\text{def}}{=} \frac{1}{v_c} - \sum_{k=2\kappa}^{N-1} \frac{1}{\epsilon_k - \lambda_\kappa}. \quad (11)$$

Since κ is now in the middle of the range $[0, 2\kappa-1]$, we see that Eq. (9) can be generalized to give a level-dependent phase shift $\delta_\kappa = \arctan(\pi v_\kappa/d)$, where evaluating the sum as an integral yields

$$\frac{1}{v_\kappa} = \frac{1}{v_c} + \frac{1}{d} \ln \frac{N - \frac{1}{2} - \kappa}{\kappa + \frac{1}{2}} \text{ if } \kappa \in \left(0, \frac{N-1}{2}\right),$$

$$\frac{1}{v_\kappa} = \frac{1}{v_c} - \frac{1}{d} \ln \frac{N - \frac{1}{2} - \kappa'}{\kappa' + \frac{1}{2}} \text{ if } \kappa \in \left(\frac{N-1}{2}, N-1\right). \quad (12)$$

Note that away from the band center, δ_κ is no longer confined to the interval $[-\pi/2, \pi/2]$ but can take values in the range $[-\pi, \pi]$.

A second boundary effect becomes important for strong perturbations $v_c/d \lesssim -1$ that induce a large shift of the lowest perturbed energy level toward $-\infty$ (see Fig. 1). We will discuss the effect of such a bound state in detail in Sec. III.

A remarkable property of rank-one perturbations, such as a contact potential, is that the overlap between the many-body ground states $|\Phi_0\rangle$ and $|\Psi_0\rangle$ of \hat{H}_0 and \hat{H} can be expressed as⁷

$$|\Delta|^2 = |\langle \Psi_0 | \Phi_0 \rangle|^2 = \prod_{i=0}^{M-1} \prod_{j=M}^{N-1} \frac{(\lambda_j - \epsilon_i)(\epsilon_j - \lambda_i)}{(\lambda_j - \lambda_i)(\epsilon_j - \epsilon_i)}. \quad (13)$$

In other words, all the required information is contained in the eigenvalues $\{\epsilon\}$, $\{\lambda\}$. In the bulklike situation we have considered thus far, the $\{\lambda\}$ are uniquely determined from the $\{\epsilon\}$, yielding the bulklike overlap $|\Delta_b|^2$. Analytic formulas for $|\Delta_b|^2$ were discussed in Ref. 7. For half filling, $M=N/2$, and assuming a level-independent phase shift, the relation

$$|\Delta_b|^2 = \left(\frac{N}{2}\right)^{-\langle \delta_0^2 / \pi^2 \rangle} e^{-\langle \delta_0^2 / \pi^2 \rangle \mathcal{F}} \quad (14)$$

is easily derived. The factor $\mathcal{F} \approx \frac{1}{2} \sum_{k=1}^{\infty} (1/k^2) \approx 0.822$ is a correction to the exponent due to the discreteness of the levels.

B. Mesoscopic systems

We now consider a generic chaotic mesoscopic system. In that case, because of the confinement, both energies and wave functions will display mesoscopic fluctuations from level to level or as an external parameter is varied.⁹⁻¹¹ This implies that the effective strength of the contact potential felt by electron k cannot be assumed constant. More precisely, introducing $u_k \equiv \sqrt{\Omega} \varphi_k(\mathbf{r}_c)$, such that $\langle |u_k|^2 \rangle = 1$, we now have

$$\hat{V}_c = v_c \sum_{kk'} u_k^* u_{k'} c_k^\dagger c_{k'}.$$

Accordingly, the generalized versions of Eqs. (5)–(7) for the perturbed energy levels λ_κ read

$$0 = 1 - v_c \sum_{k=0}^{N-1} \frac{|u_k|^2}{\lambda_\kappa - \epsilon_k}, \quad (15)$$

$$a_{k\kappa} = -\frac{v_\kappa u_k}{\lambda_\kappa - \epsilon_k}, \quad (16)$$

$$\frac{1}{|v_\kappa|^2} = \sum_{k=0}^{N-1} \frac{|u_k|^2}{(\lambda_\kappa - \epsilon_k)^2}, \quad (17)$$

$$u_k^2 = \frac{1}{v_c} \frac{\prod_{\kappa=0}^N \lambda_\kappa - \epsilon_k}{\prod_{\kappa \neq k} \epsilon_\kappa - \epsilon_k}, \quad (18)$$

$$\tilde{u}_\kappa = \sum_{k=0}^{N-1} a_{k\kappa} u_k \equiv -\frac{v_\kappa}{v_c}, \quad (19)$$

and the bulklike situation is recovered by setting $u_k^2 = \langle |u_k|^2 \rangle = 1$. Note that we can choose the phase in the wave functions φ_k and ψ_κ such that their value at \mathbf{r}_c is real. It is then evident that u_k , $a_{k\kappa}$, and \tilde{u}_κ are also real.

For a chaotic system, a good model for the eigenvalues and eigenvector fluctuations is given by the classic ensembles of random matrix theory (RMT).^{25,26} Most commonly, the Gaussian orthogonal (unitary) ensembles, GOE (GUE), are used to describe the energy eigenvalues of chaotic systems in the presence (absence) of time-reversal symmetry. Here, however, because we would like to model systems with constant mean density of states, we will rather consider the corresponding circular ensembles COE and CUE,²⁶ which display the same fluctuations but have, by construction, a mean density of eigenphases $\exp(i\epsilon_k)$ that is uniformly distributed on the unit circle. Since time-reversal symmetry can easily be broken by applying a magnetic field, we will address both ensembles.

The fluctuations in the $\{\epsilon\}$ and $\{\lambda\}$ are not independent. Under the hypothesis that the unperturbed eigenenergies are distributed according to the circular ensembles and, accordingly, that the eigenvectors follow a Porter-Thomas distribution, the joint probability distribution $P(\{\epsilon\}, \{\lambda\})$ was shown by Aleiner and Matveev²² to be

$$P(\{\epsilon\}, \{\lambda\}) \propto \frac{\prod_{i>j} (\epsilon_i - \epsilon_j)(\lambda_i - \lambda_j)}{\prod_{i,j} |\epsilon_i - \lambda_j|^{1-\beta/2}} e^{-(\beta/2) \sum_i (\lambda_i - \epsilon_i)/v_i} \quad (20)$$

with the constraint $\epsilon_{i-1} \leq \lambda_i \leq \epsilon_i$ and $\beta=1$ in the COE case, whereas $\beta=2$ for CUE. In the middle of the band $v_i = v_c$, away from the band center, boundary effects have to be taken into account according to Eq. (12). It is interesting that a joint probability distribution can also be found in the more general, non-rank-one case,²⁷ which we do not consider here.

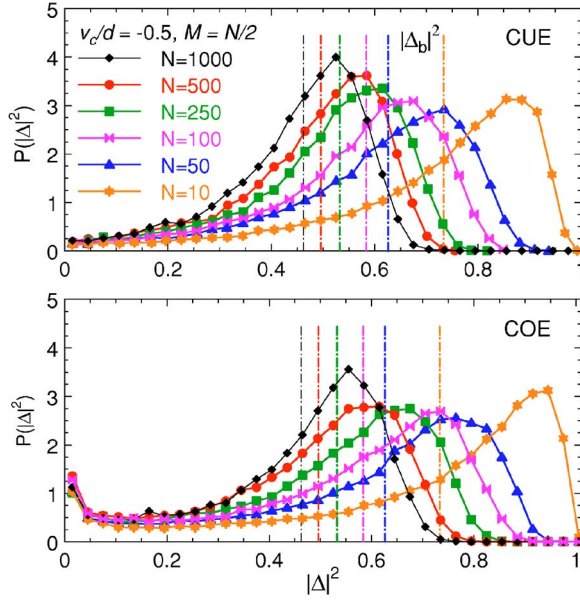


FIG. 2. (Color online) Distribution of ground-state overlaps in a mesoscopic system as the number of particles is increased at half filling, $M=N/2$, for the (a) CUE and (b) COE cases. The perturbation strength is chosen intermediate, $v_c/d=-0.5$. The dashed-dotted lines indicate the bulklike overlaps $|\Delta_b|^2$. The curves illustrate the power-law characteristic of AOC, which makes it a truly thermodynamic-limit effect; even with $M=1000$ electrons in the system, the most probable overlap $|\Delta|^2$ is as big as 0.46, indicating that a bulk-based discussion of AOC in mesoscopic systems can be inaccurate. Note that for this intermediate perturbation strength the overlap distribution exhibits a clear maximum and a difference in CUE vs COE for small overlaps. (In order to make the statistical error essentially negligible, 20 000 realizations of the random matrix were used in producing each curve.)

The ground-state overlap Δ is expressed entirely in terms of the unperturbed and perturbed eigenvalues $\{\epsilon\}$ and $\{\lambda\}$ [see Eq. (13)]. Therefore, the joint distribution (20) contains all the information required to build the overlap distribution $P(|\Delta|^2)$.

In Sec. IV, we shall see that a slightly different route is actually more effective to obtain analytic expressions for $P(|\Delta|^2)$. However, the present approach is perfectly adapted to numerically constructing this distribution for any value of the parameters M , N , v_c , and β . Indeed, we can use Eq. (20) as the basis of a simple Metropolis algorithm to generate ensembles of $(\{\epsilon\}, \{\lambda\})$ with the proper joint probability distribution. Applying Eq. (13), we then build the distribution of ground-state overlaps. Examples for overlap distributions obtained in this way are shown in Fig. 2 for systems with and without time-reversal symmetry and an intermediate perturbation strength. The evolution of AOC as the number of particles is increased is clearly visible as a shift of the probability density to smaller values of $|\Delta|^2$. However, since AOC is a power-law effect even $N=1000$ is far away from the thermodynamic limit [cf. Eq. (14), which can also be used as a rough estimate for the mean overlap in the mesoscopic case]. We point out the different behavior for very small overlaps in the CUE versus COE case. It originates in the

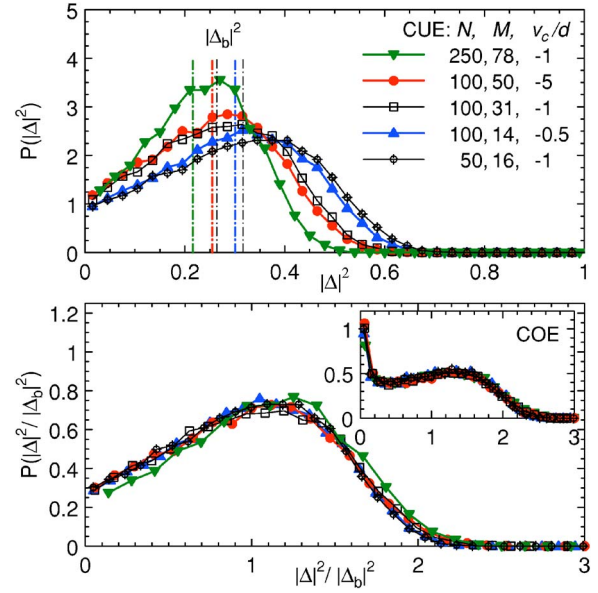


FIG. 3. (Color online) Ground-state overlap in the absence of time-reversal symmetry (CUE case) for different parameter realizations corresponding to a phase shift of approximately $-\pi/2$ at the Fermi energy. (a) Before and (b) after scaling with the bulklike result $|\Delta_b|^2$ (dashed-dotted lines, $|\Delta_b|^2$ increases with the legend entries). The scaled result for COE is given in the inset of (b), see Ref. 8 for the unscaled result in that case.

difference of the Porter-Thomas distributions and will be discussed in Sec. IV.

In the metallic x-ray edge problem all relevant properties are known to depend only on the phase shift at the Fermi energy, and a natural question is whether this remains true in the mesoscopic case for the ground-state overlap. In Fig. 3(a) we therefore compare overlap distributions for different parameter sets $\{N, M, v_c/d\}$ all of which yield a phase shift $\delta_F \approx \arctan(\pi v_{i=M}/d) \sim -\pi/2$ at the Fermi energy E_F . The curves differ, as do the corresponding bulklike overlaps $|\Delta_b|^2$ indicated by the vertical lines. However, after scaling by the bulklike overlaps all curves coincide, Fig. 3(b). Therefore, although the individual $P(|\Delta|^2)$ depends independently on N , M , and v_c/d , the fluctuations of the overlap depend on the value of δ_F alone.

This fact allows one to provide the overlap distribution as a universal curve for a given phase shift δ_F . In Figs. 4(a) and 5(a) results are shown for $N=100$ levels subject to a strong perturbation. The phase shift δ_F is varied by increasing the filling of the band from 2 to 98 electrons. The distributions are *not* scaled by the bulk overlap in order to allow easier comparison of the curves when they all range from 0 to 1.

C. Fluctuations of levels beyond the Thouless energy

Strictly speaking a random matrix model applies only to chaotic energy levels on a scale of the Thouless energy E_{Th} .^{10,11,28,29} In the semiclassical limit E_{Th} is much larger than the mean-level spacing, but significantly smaller than the Fermi energy E_F . Therefore one may question the model

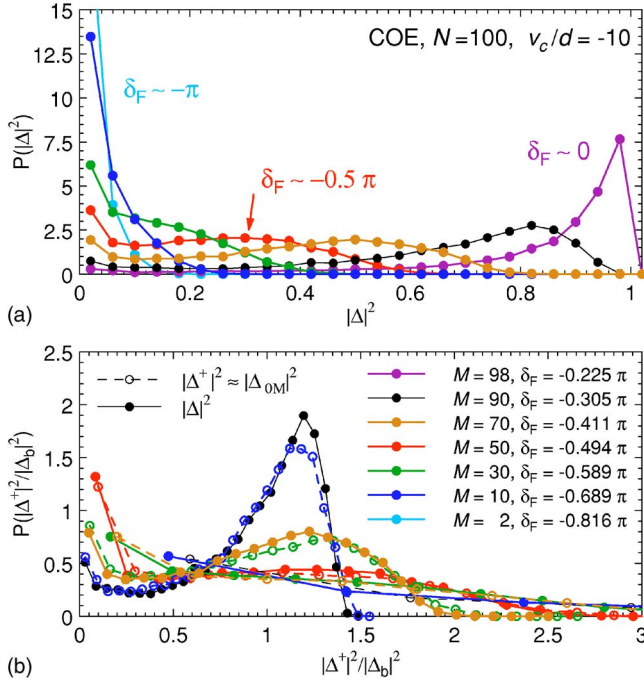


FIG. 4. (Color online) (a) Probability distribution $P(|\Delta|^2)$ for the ground-state overlap (COE, $N=100, v_c/d=-10$). The number M of electrons is varied, corresponding to a varying phase shift δ_F at the Fermi energy. The curves (here not scaled by the bulklike overlaps) illustrate the characteristics of $P(|\Delta|^2)$ for a given phase shift. For comparison, recall that at constant filling, a decreasing phase shift corresponds to increasing perturbation strength. (b) Comparison of the bulk-scaled probability distributions of the ground-state overlaps for a negative (solid line, $|\Delta|^2$) and positive (dashed line) perturbation. The overlap $|\Delta^+|^2$ is, up to the negligible influence of the runaway states, equivalent to the overlap $|\Delta_{0M}|^2$ shown here as a dashed line. It will be of importance in the discussions of the x-ray-absorption part. The pairing of curves whose phase-shift moduli add up to π is nicely illustrated in this graph.

we use where the full bandwidth is described by RMT. It turns out, however, that the overlap distributions depend only on the fluctuation of the levels near the Fermi energy. In order to demonstrate this, we introduce a *range- n approximation* in which only n of the levels on either side of the Fermi energy are left free to fluctuate, while all the others are kept fixed at their mean position. To gauge the accuracy of this approximation, we perform a Kolmogorov-Smirnov test.³⁰ In Fig. 6 the result of this test, namely, the maximum deviation of the range- n cumulative distribution from the exact cumulative distribution of the overlap, is shown. Clearly, the deviation decreases to almost zero as soon as the fluctuations of a few levels near E_F are included. Furthermore, the convergence with n appears faster for the larger perturbation strengths in which we are interested for the x-ray edge problem. This retrospectively justifies the use of a full random matrix to model the statistical properties of our chaotic systems, as the levels beyond the Thouless energy for which such a description does not hold, do not affect the overlap distribution.

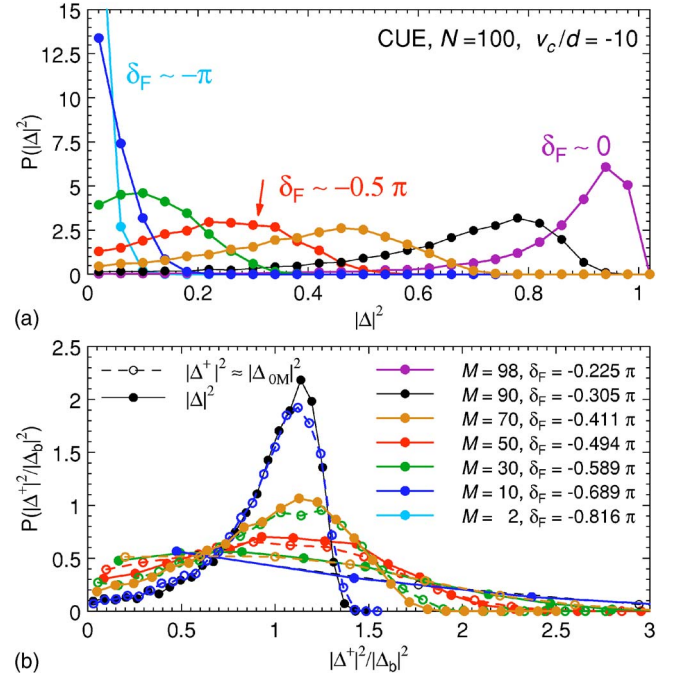


FIG. 5. (Color online) Same as in Fig. 4, but for CUE. Note the difference in the distributions for small overlaps $|\Delta|^2$.

III. BOUND STATES AND SYMMETRY BETWEEN POSITIVE VERSUS NEGATIVE PERTURBATION

As soon as the perturbation strength becomes significant, i.e., for attractive perturbations $v_c/d \lesssim -1$, the shift of the lowest perturbed level, $\lambda_0 - \epsilon_0$, starts to become large. Analogously, for positive perturbation strengths larger than $v_c/d \gtrsim 1$, the same boundary effect now shifts the highest perturbed level λ_{N-1} to very high energies (see Figs. 1 and 7). These so-called runaway levels correspond to the formation of a bound state,^{7,31–33} which entirely screens the impurity. They can be found, respectively, at

$$\lambda_0 - \epsilon_0 = -\frac{Nd}{e^{d|v_c|} - 1} \quad (v_c < 0),$$

$$\lambda_{N-1} - \epsilon_{N-1} = +\frac{Nd}{1 - e^{-dv_c}} \quad (v_c > 0).$$

The fluctuations of these levels will be neglected,³⁴ since in the limit of very strong perturbations, $|v_c|/d \gg 1$, the runaway level does not affect the value for the overlap [Eq. (13)] because the terms involving λ_0 (or λ_{N-1} , respectively) yield ratios of one. Therefore, one has only to consider the N unperturbed levels $\{\epsilon\}$ and the $N-1$ perturbed levels λ_κ “in between.” In this case of very strong perturbations, the perturbed levels are maximally shifted: in the center of the band, the λ_κ lie, on average, exactly in the middle between the two neighboring unperturbed levels $\epsilon_{\kappa-1}$ and ϵ_κ (or ϵ_κ and $\epsilon_{\kappa+1}$). Therefore, a strong negative perturbation v_c (i.e., $v_c/d \ll -1$, $\delta_F = -\pi/2$) and a strong positive perturbation v_c^+ (i.e., $v_c^+/d \gg 1$, $\delta_F^+ = \pi/2$) are indistinguishable, see Fig. 7. This means, in particular, that the corresponding overlap distributions $P(|\Delta|^2)$ and $P(|\Delta^+|^2)$ are identical.

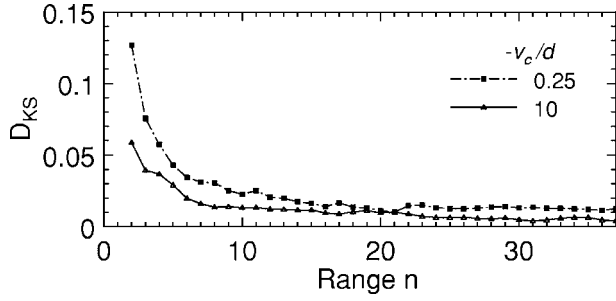


FIG. 6. Accuracy of the range- n approximation using the Kolmogorov-Smirnov test (COE, $N=100, M=50$). The maximum deviation of the range- n cumulative distribution from the exact cumulative distribution of the overlap is shown as a function of n . The rapid approach to 0, especially in the strong perturbation case, shows that fluctuation of only those levels near E_F is important.

In the case of intermediate perturbation strengths $v_c/d \sim \pm 1$, a level shift δ_F associated with the negative perturbation corresponds to a phase shift $\delta_F^+ = \pi - |\delta_F|$ when the level scheme is interpreted as originating from some positive perturbation v_c^+ ($\neq |v_c|$, in general), see Fig. 7(c). We therefore expect again the two corresponding bulk-scaled overlap distributions to be identical, and the (symmetry) relation

$$P\left(\frac{|\Delta|^2}{|\Delta_b|^2}\right)_{v_c, \delta_F} = P\left(\frac{|\Delta^+|^2}{|\Delta_b^+|^2}\right)_{v_c^+, \delta_F^+ = \pi - |\delta_F|} \quad (21)$$

to hold.

In Figs. 4 and 5 overlap distributions for phase shifts $0 > \delta_F > -\pi$ are shown. Starting with an almost full band ($M=98$ particles on $N=100$ levels) and a small negative phase shift, δ_F is lowered (the effective potential strength raised) as the filling is decreased, passing $\delta_F \approx -\pi/2$ at half filling. The corresponding overlap distributions are shown in Fig. 4(a) for the COE situation and in Fig. 5(a) for a CUE case. In Figs. 4(b) and 5(b), overlap distributions belonging to a negative phase shift δ_F (and $v_c < 0$) and the associated positive phase shift $\delta_F^+ = \pi - |\delta_F|$ (and $v_c^+ > 0$) are compared and seen to (almost) coincide pairwise after scaling by the

respective bulk overlaps (the small deviations are due to the finite number of discrete levels available). Note that the bulk overlaps $|\Delta_b|^2$ are very similar in each pair, but rather different for different pairs, thereby causing the stretching of the x -axis.

In the context of the x-ray edge problem (strong negative perturbation), a situation that is equivalent to a *positive* perturbation becomes of importance when the core electron is excited to the level λ_M just above the Fermi energy E_F . The consequences and more details will be discussed in [12].

IV. ANALYTIC RESULTS FOR THE OVERLAP DISTRIBUTION

We finish with the derivation of analytic results for the overlap distribution. We argued in Sec. II C that the fluctuations in the ground-state overlap are dominated by fluctuations of the energy levels around the Fermi energy (see Fig. 6). We now want to deepen this discussion and investigate to what extent an analytic understanding of overlap probability distributions $P(|\Delta|^2)$ is possible. In particular we want to understand two characteristic qualitative features of the overlap distribution (see, for example, Fig. 3): first, $P(|\Delta|^2=0)$ is finite and characteristically different for the COE versus CUE situation, and second, $P(|\Delta|^2=1)$ is zero [i.e. $P(|\Delta|^2)$ drops to zero before the natural bound $|\Delta|^2=1$ is reached].

To begin, remember that in Eq. (13) for the overlap $|\Delta|^2$ all energy differences are taken between empty ($j \geq M$) and occupied ($i \leq M-1$) levels. The smallest differences (of the order of the mean-level spacing d) contain the energy levels ϵ_M , ϵ_{M-1} , and λ_M . We expect, therefore, that the small Δ part of the overlap distribution will be mainly given by the fluctuation of these terms.

To gain an analytic understanding of the overlap distribution, we therefore consider only the level closest to the Fermi energy as fluctuating, whereas all other levels are assumed at their bulklike values (range-1 approximation). We therefore want to evaluate fluctuations of $(\lambda_M - \epsilon_{M-1}) / (\epsilon_M - \epsilon_{M-1})$. For simplicity, we consider the half-filled case. Note that a similar two-level problem was studied by Vallejos *et al.*,²² moti-

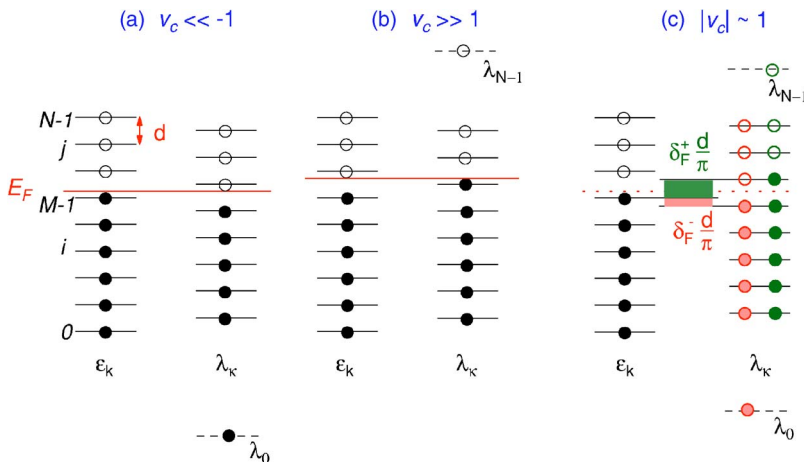


FIG. 7. (Color online) Runaway level for strong perturbation that is (a) positive or (b) negative. For simplicity, the bulklike situation is shown. In the case of intermediate perturbations (c), the perturbed levels λ_k are not shifted to the center of the unperturbed level interval ϵ_k . The phase shifts δ_F^- (negative perturbation) and δ_F^+ (positive perturbation) are related by $|\delta_F^-| + \delta_F^+ = \pi$. In the case of strong negative perturbations, as in the x-ray problem, λ_0 forms a bound state that screens the perturbation.

vated by their observation that very small AOC overlaps were related to avoided level crossings at the Fermi energy. In our present model, Eq. (15) for the rank-one perturbation determines the position of the perturbed levels as solutions of

$$f(\lambda) = d \sum_k^{\text{def}} \frac{A_k}{\lambda - \epsilon_k} \equiv \frac{d}{v_c}, \quad (22)$$

where $A_k = |u_k|^2$ are the Porter-Thomas distributed wave-function intensities,

$$P(A) = \begin{cases} e^{-A} & \text{for CUE} \\ \frac{1}{\sqrt{2\pi A}} e^{-A/2} & \text{for COE} \end{cases}. \quad (23)$$

[$\langle A \rangle = 1$ and $\langle A \rangle^2 = 2(3)$ for CUE (COE)]. We will explicitly only take the fluctuations of the amplitudes A_{M-1} and A_M for the wave functions ϕ_{M-1} and ϕ_M into account. Accordingly, we separate the first two terms of the sum and comprise the remaining terms in a function δf , which is assumed to be a Gaussian random variable and contains the joint effect of all other levels and intensities,

$$f(\lambda) = \frac{dA_{M-1}}{\lambda - \epsilon_{M-1}} + \frac{dA_M}{\lambda - \epsilon_M} + \delta f \equiv \frac{d}{v_c}. \quad (24)$$

Equation (24) makes it possible, already, to understand at a qualitative level the finite probability for having $|\Delta|^2 = 0$, which corresponds to having $\lambda_M - \epsilon_{M-1} = 0$. However, setting $\lambda = \lambda_M$ in Eq. (24) we see that the ratio $A_{M-1}/(\lambda_M - \epsilon_{M-1})$ has to be finite. We conclude that having $\lambda_M - \epsilon_{M-1} = 0$ is related to having $A_{M-1} = 0$. From Eq. (23) we find $P(A=0) = 1$ [or ∞] in the CUE [COE] case, thereby explaining both $P(|\Delta|^2 = 0) > 0$ and the peak at $|\Delta|^2 = 0$ in the COE case.

To obtain a more quantitative description, we investigate δf more closely. According to the assumptions of the range-1 approximation, we replace the energy levels in δf by their bulklike values. Furthermore, we neglect boundary effects that would make the phase shift dependent on the level number, which is a good approximation for $N \rightarrow \infty$ at half-filling. Fixing the energy origin in the middle of the mean position of ϵ_{M-1} and ϵ_M , we express δf in the symmetric form

$$\delta f = \sum_{k=1}^{\infty} \left(\frac{A_{k+M}}{\frac{\lambda}{d} - \left(k + \frac{1}{2}\right)} + \frac{A_{-(k+1)+M}}{\frac{\lambda}{d} + \left(k + \frac{1}{2}\right)} \right). \quad (25)$$

Fluctuations in δf are due to the fluctuations in the intensities $A_{\pm k}$ that follow the Porter-Thomas distributions given in Eq. (23). Expanding the mean value $\langle \delta f \rangle$ about the center of the band, $\lambda = 0$, yields in lowest order $\langle \delta f \rangle = -2\lambda S_1$ with

$$S_1 = \sum_{k=1}^{\infty} \frac{1}{\left(k + \frac{1}{2}\right)^2} \approx 0.9348. \quad (26)$$

Comprising *all* the randomness of the amplitudes $A_{k \neq M-1, M}$ in one random Gaussian variable ξ with $P(\xi) = e^{-\xi^2/2}/\sqrt{2\pi}$,

and explicitly writing the scale var δ of the fluctuations around the mean value, we arrive at the approximation

$$\delta f = \langle \delta f \rangle + \sqrt{\text{var } \delta f} \xi = -2\lambda S_1 + \sqrt{\text{var } \delta f} \xi \quad (27)$$

with

$$\text{var } \delta f = \begin{cases} 2S_1 & \text{for CUE} \\ 4S_1 & \text{for COE.} \end{cases} \quad (28)$$

Setting $\epsilon_M - \epsilon_{M-1} = s$, the probability distribution $P(\lambda|s)$ is obtained by integrating over the distributions of A_{M-1} , A_M , and ξ . These integrals can only partially be solved analytically and, leaving out the further details of the calculation, the result for the CUE case [$\mu = \alpha_M - \alpha_{M-1}$, $\alpha_0 = A_{M-1}/(\lambda + s/2)$, $\alpha_1 = -A_M/(\lambda - s/2)$] is

$$P(\lambda|s) = \frac{1}{2s\sqrt{\pi S_1}} \int_{-\infty}^{\infty} d\mu \exp \left[\mu\lambda - |\mu| \frac{s}{2} \right] \times \exp \left[-\frac{1}{4S_1} \left(2S_1\lambda + \frac{1}{v_c} + \mu \right)^2 \right] \times \left[2S_1 \left(\frac{s^2}{4} - \lambda^2 \right) + \mu\lambda + |\mu| \frac{s}{2} + 1 \right], \quad (29)$$

and for the COE case

$$P(\lambda|s) = \frac{1}{\sqrt{(2\pi)^3 4S_1} \left(\frac{s^2}{4} - \lambda^2 \right)} \int_{-\infty}^{\infty} d\mu \exp \left[-\frac{1}{8S_1} \left(2S_1\lambda + \frac{1}{v_c} + \mu \right)^2 + \mu\lambda \right] \left\{ \left[2S_1 \left(\frac{s^2}{4} - \lambda^2 \right) + \mu\lambda \right] \times K_0 \left(\left| \frac{s\mu}{4} \right| \right) + 2 \left| \frac{s\mu}{4} \right| K_1 \left(\left| \frac{s\mu}{4} \right| \right) \right\}, \quad (30)$$

with K_0 , K_1 the modified Bessel functions.

The remaining integral over μ can be performed in the CUE case using the (inverse) error function. Splitting the μ integration into integration from 0 to ∞ and from $-\infty$ to 0, yielding results $P_+(\lambda|s)$ and $P_-(\lambda|s)$, and using the substitutions $A = 2S_1\lambda + 1/v_c$, $B = 2S_1(s^2/4 - \lambda^2)$, $a = 1/(4S_1)$, and $b_{\pm} = [s \pm 1/(S_1 v_c)]/2$, we find

$$P_{\pm}(\lambda|s) = \frac{\exp(-A^2 a)}{2aC} \left\{ \pm \left(\lambda \pm \frac{s}{2} \right) + \sqrt{\frac{\pi}{a}} \exp \left(\frac{b_{\pm}^2}{4a} \right) \text{erfc} \left(\frac{b_{\pm}}{2\sqrt{a}} \right) \left[Ba \mp \frac{b_{\pm}}{2} \left(\lambda \pm \frac{s}{2} \right) \right] \right\}, \quad (31)$$

and their sum yields $P(\lambda|s) = P_+(\lambda|s) + P_-(\lambda|s)$.

This expression simplifies considerably in the limit of very strong perturbations, $|v_c| \gg 1$. Then, the result becomes independent of v_c (in particular, independent of the sign—very strong attractive and repulsive interactions are equivalent), and takes the form

$$P_\infty(\lambda|s) = \frac{\exp(-\lambda^2 S_1)}{s\sqrt{\pi}} \left[s\sqrt{S_1} + \sqrt{\pi}(1-2\lambda^2 S_1) \exp\left(\frac{s^2 S_1}{4}\right) \operatorname{erfc}\left(\frac{s\sqrt{S_1}}{2}\right) \right]. \quad (32)$$

Clearly, this probability distribution is symmetric with respect to $\lambda=0$ as it should be.

The contribution to the overlap [Eq. (13)] that contains the energy levels closest to the Fermi energy is represented by $(\lambda_M - \epsilon_{M-1})/(\epsilon_M - \epsilon_{M-1}) \equiv (\lambda + s/2)/s$ in our present notation. To obtain the probability distribution $P^{F1}(\lambda)$ of this quantity, we have to take into account the distribution of nearest-neighbor spacings $s = \epsilon_M - \epsilon_{M-1}$ according to the Wigner surmise,

$$P(s) = \begin{cases} \frac{32}{\pi^2} s^2 \exp\left(-\frac{4}{\pi}s^2\right) & \text{for CUE} \\ \frac{\pi}{2} s \exp\left(-\frac{\pi}{4}s^2\right) & \text{for COE.} \end{cases} \quad (33)$$

The final result then reads

$$P^{F1}(\lambda) = \int_0^\infty ds s P(\lambda|s) P(s). \quad (34)$$

This integrated result is, however, essentially indistinguishable from $P(\lambda|s=1)$.

The probability distribution of the range-1 approximation, $P^{r1}(|\Delta^r|^2)$, is straightforwardly obtained from $P^{F1}(\lambda)$ by scaling with the bulklike quantity $|\Delta_b|^2/(1 - \delta_F/\pi)$ [cf. Eq. (35)] and shifting the argument by $1/2$. The resulting curves are presented in Fig. 8 for weak, intermediate, and strong perturbations. This analytic range-1 result is compared to the full overlap distribution $P(|\Delta|^2)$ as well as the exact range-1 and range-2 approximations³⁵ [CUE case (see Ref. 8 for the corresponding COE figure)]. The agreement between the analytic approximation and the exact range-1 results is excellent. The analytic range-1 result provides, in particular, a very good estimate for the full overlap distribution at small overlaps, independent of the perturbation strength. Moreover, in the limit of strong perturbations, in which we are especially interested for the x-ray edge problem, it provides a reasonable estimate of the full probability distribution $P(|\Delta|^2)$. The increase in the degree of symmetry of the range-1 result (with respect to the maximum of the curve) as the perturbation strength is increased is clearly visible and confirmed by Eq. (32).

We would like to mention that Vallejos and co-workers in Ref. 23, and, based on their work, Gefen and co-workers in Ref. 24, found similar results, in particular, that the distribution of small overlaps is well represented by a two-level analytic model. However, there are a few differences. For example, the difference between the (Gaussian) orthogonal and unitary case was less pronounced in their models, especially the increase of the probability $P(|\Delta|^2)$ toward $|\Delta|^2 \rightarrow 0$, characteristic of our model, was not seen. Furthermore, simple analytic expressions similar to the expressions

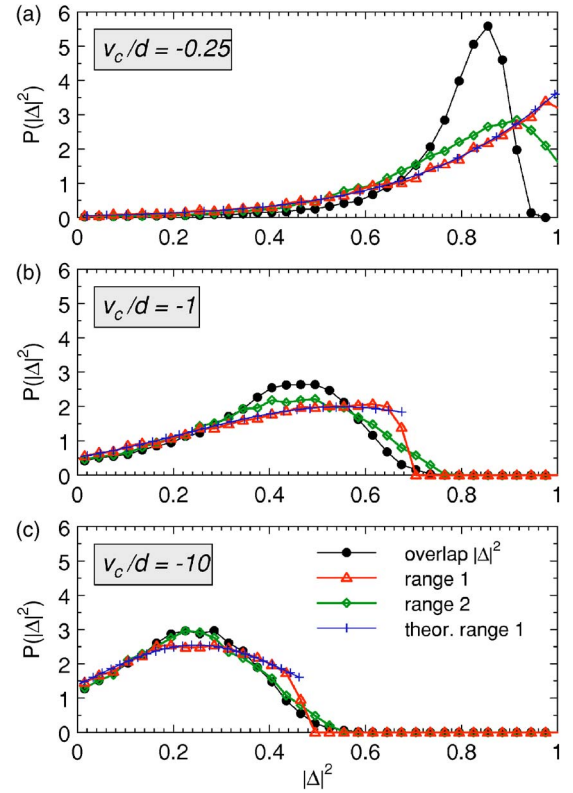


FIG. 8. (Color online) Probability distributions $P(|\Delta|^2)$ for the ground-state overlap ($N=100$, $M=50$, CUE) for increasing potential strength: (a) weak ($v_c/d=-0.25$), (b) intermediate ($v_c/d=-1$), and (c) strong ($v_c/d=-10$) perturbation. Shown are the exact distribution (dots) as well as the range-1 (triangles) and range-2 (diamonds) approximations. Clearly, the fluctuations come from the levels closest to the Fermi energy, and the range-1 approximation provides a good estimate already for intermediate perturbation strengths as in (b). The crosses denote the analytic result for the range-1 approximation, showing excellent agreement with the numerical results.

(29) and (30) could only be found for the orthogonal situation in Ref. 23.

Eventually, we briefly remark on having $P(|\Delta|^2=1)=0$ for finite perturbation strength. Within a range-1-like approximation scheme, Eq. (13) can be written as

$$|\Delta^{r1}|^2 = \frac{(\lambda_M - \epsilon_{M-1})}{(\lambda_M - \lambda_{M-1})} \frac{d}{d \left(1 - \frac{\delta_F}{\pi}\right)} |\Delta_b|^2, \quad (35)$$

where we have normalized all differences by their bulklike values. Only the first term is fluctuating, between 0 and 1, whereas the last two terms are numbers that are strictly smaller than 1 and, furthermore, get smaller as the perturbation gets stronger. Accordingly, the upper boundary 1 of the first term is shifted to a value $|\Delta_{\max}^{r1}|^2 < 1$ that decreases with increasing perturbation strength, as is clearly visible in Fig. 8. The value $|\Delta_{\max}^{r1}|^2$ provides a good estimate for the upper boundary of the overlap $|\Delta|^2$, although there are, of course, corrections from higher-order approximations that smear the

(total) overlap distribution $P(|\Delta|^2)$ about $|\Delta_{\max}^{r1}|^2$ [see, for example, Fig. 8(b)].

V. SUMMARY AND CONCLUSIONS

In this paper we have studied the Anderson orthogonality catastrophe in generic mesoscopic systems with a finite number of electrons in discrete energy levels. Motivated by the study of mesoscopic photoabsorption spectra that will be the subject of a second paper in this series,¹² we have used the model of a rank-one perturbation describing the perturbation left behind after the photoexcitation of a core electron into the conduction band. However, the basic underlying physics is much more general, and the model can be applied to any situation where a sudden, localized (rank-one) perturbation acts on a finite number of chaotic electrons.

As a result of such a sudden perturbation, the overlap between the unperturbed and perturbed many-body ground states vanishes in the thermodynamic limit (AOC). In mesoscopic systems, even with few thousand electrons, this effect will be incomplete. Fluctuations cause a broad

distribution of overlaps that is, however, bounded from above by a value smaller than 1 (for not too small perturbations), whereas there is a nonzero probability for having zero overlap. The distribution of small overlaps is distinctly different for systems with or without time-reversal symmetry (COE versus CUE) and traces back to the difference in the Porter-Thomas distribution of their single-particle wave-function intensities. The fluctuations originate from the levels around the Fermi energy (within a range smaller than the Thouless energy for systems in which we are interested), and we derived an analytic expression for the lowest-order (range-1) result that reproduces the distribution of small overlaps and is a good approximation for the whole distribution in the case of strong perturbations.

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introduced by hand, neglecting possible fluctuations.

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