

## Odd-even binding effect from random two-body interactions

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Systematic odd-even binding energy differences in finite metallic particles are usually attributed to mean-field orbital energy effects or to a coherent pairing interaction. We show analytically and numerically that a purely random two-body Hamiltonian can also give rise to an odd-even staggering. We explore the characteristics of this chaotic mechanism and discuss distinguishing features with respect to the other causes of staggering. In particular, randomness-induced staggering is found to be a smooth function of particle number, and the mechanism is seen to be largely insensitive to the presence of a magnetic field.

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### I. INTRODUCTION

Interacting finite fermionic systems such as atomic nuclei, metallic clusters,<sup>1</sup> and small metallic grains<sup>2</sup> display an odd-even staggering in ground-state energies, i.e., the binding energy of an even-number system is larger than the arithmetic mean of its odd-number neighbors. There are two well-known mechanisms that can give rise to this staggering, namely, the Kramers degeneracy in the mean-field Hamiltonian and the BCS mechanism arising from an attractive effective interaction. In nuclei, the BCS pairing mechanism resulting from a residual nucleon-nucleon interaction is dominant,<sup>3</sup> but the mean-field or orbital energy effect may also be significant in the lighter nuclei.<sup>4</sup> Surprisingly, many basic phenomena normally associated with pairing can also arise from random interactions. The behavior of random-interaction ensembles has mostly been studied in a nuclear physics context<sup>5-11</sup> but there has also been some study of spectra in the context of small metallic grains.<sup>12</sup>

In the case of metallic clusters of fewer than a hundred atoms, the orbital energy effect is rather strong and staggering is seen for species that do not exhibit superconductivity. This effect can be easily understood using a jellium model or density functional theory.<sup>13</sup> On the other hand, the staggering effect seen in Ref. 2 may have some contribution from the BCS pairing mechanism. A number of theoretical studies have been made<sup>14</sup> using techniques applicable to large finite systems.<sup>15</sup> Taking a uniform mean-field spectrum and an attractive pairing interaction with constant coupling, one observes a smooth crossover from BCS superconductivity in the bulk to the few-electron regime. For small systems, the gap is of the size of the mean level spacing and thus ceases to be an indicator for pairing. Nevertheless, strong pairing correlations and odd-even staggering persist as the system size decreases.

In a grain with irregular boundaries, one expects that the electron orbitals will have a chaotic character and therefore the interaction will have a random as well as a regular part. In this paper we will introduce such an interaction and study its typical effects on the binding systematics. Our Hamiltonian thus includes attractive and repulsive pairing interactions as well as more general two-body interactions. The assumption of randomness is motivated as follows: For nu-

clei it is well known that the residual interaction leads to fluctuation properties in wave functions and energy levels that are similar to those of random matrices taken from the Gaussian orthogonal ensemble.<sup>16</sup> In the case of small metallic grains or quantum dots, one may assume that their irregular shape leads to chaoticity in the single-particle wave functions.<sup>17</sup> This in turn causes randomness in those two-body matrix elements that link four different orbitals with each other. Matrix elements between pairs of orbitals that are related by time-reversal symmetry need not necessarily be random, and these determine the “coherent” terms of the interaction.

A realistic Hamiltonian for quantum dots or small metallic grains would thus conserve total spin and include spin-independent one-body terms, random two-body interactions, and coherent interactions that are nonrandom but have attractive and repulsive components. The most general Hamiltonian to study generic properties when all these features are included may be written as

$$\begin{aligned}
 H = & \sum_{i,\sigma} \varepsilon_i c_{i\sigma}^\dagger c_{i\sigma} + \sum_i (u + u'_i) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} \\
 & + \sum_{ij} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} [(w_0 + w'_{0,ij}) \langle \sigma_1 | \sigma_2 \rangle \langle \sigma_3 | \sigma_4 \rangle \\
 & + (w_1 + w'_{1,ij}) \langle \sigma_1 | \vec{\sigma} | \sigma_2 \rangle \cdot \langle \sigma_3 | \vec{\sigma} | \sigma_4 \rangle] c_{i\sigma_1}^\dagger c_{j\sigma_2}^\dagger c_{j\sigma_3} c_{i\sigma_4} \\
 & + \sum_{ij} (g + g'_{ij}) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \\
 & + \sum_{ijkl} \sum_{\sigma_1 \sigma_2 \sigma_3 \sigma_4} [v_{0,ijkl} \langle \sigma_1 | \sigma_2 \rangle \langle \sigma_3 | \sigma_4 \rangle \\
 & + v_{1,ijkl} \langle \sigma_1 | \vec{\sigma} | \sigma_2 \rangle \cdot \langle \sigma_3 | \vec{\sigma} | \sigma_4 \rangle] c_{i\sigma_1}^\dagger c_{j\sigma_2}^\dagger c_{k\sigma_3} c_{l\sigma_4}. \quad (1)
 \end{aligned}$$

Here the coherent parts of the interaction are represented by the terms with coefficients  $u$ ,  $w_s$ , and  $g$ . The fluctuating parts of the interaction are represented by the terms containing  $u'$ ,  $w'_s$ ,  $g'$ , and  $v_s$ . These fluctuating parts are typically taken from ensembles with a Gaussian distribution; they are thus characterized by the width of the Gaussian. The single-particle term  $\varepsilon_i$  sets the energy scale and may often be taken

to give a uniform spacing of levels without loss of generality. This full Hamiltonian is difficult to study due to its many parameters. There have been many studies in the limit in which fluctuation effects are only included in the single-particle Hamiltonian  $\varepsilon_i$ .<sup>18–21</sup> We consider a very different limit, neglecting the coherent terms in the interaction and assuming the  $v_s$  term to dominate the fluctuating parts. Properties of such random two-body interaction ensembles have been studied extensively in nuclear physics.<sup>22–25</sup>

When the Hamiltonian of the nuclear shell model was modeled in this way, it was found that the spectral properties were quite regular for the ground states. As examples we mention  $J^P=0^+$  ground-state dominance in shell model calculations with random interactions,<sup>5–9</sup> band structure in interacting boson models with random couplings,<sup>10</sup> structure in ground-state wave functions of two-body random ensembles,<sup>26</sup> and an odd-even binding effect in filling a large shell.<sup>11</sup> In the context of quantum dots, the random two-body interactions were found strongly to favor singlet ground-state spins.<sup>12,27</sup> Recently, this structure has been investigated using the group symmetry of the random Hamiltonians.<sup>28</sup> These findings suggest that the structure of interacting many-body systems is to some extent already determined by the rank of the interaction alone, and one does not need all the details of the interaction. We will show that odd-even staggering also fits into this picture and is not solely a consequence of an attractive pairing force.

This paper is organized as follows. In Sec. II we introduce the Hamiltonian and discuss the odd-even effects arising from the one-body part alone. Section III contains analytical results for the odd-even staggering due to a random two-body interaction (some technical details of this analytical analysis are included in the Appendix). The crossover between the mean-field regime and the regime of strong interactions is numerically investigated in Sec. IV. The effects of breaking time-reversal symmetry are studied in Sec. V. Finally, we give a summary.

## II. HAMILTONIAN AND STAGGERING INDICATOR

As discussed in the Introduction, we will consider ensembles of Hamiltonians including only a single-particle energy and a random two-body interaction. We write this in the form

$$H = \sum_{i=1}^M \varepsilon_i (c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow}) + C_0 \sum_{\alpha, \alpha' \text{ spin-0 pairs}} v_{0\alpha\alpha'} A_{0\alpha}^\dagger A_{0\alpha'} + C_1 \sum_{\beta, \beta' \text{ spin-1 pairs}} v_{1\beta\beta'} A_{1\beta}^\dagger A_{1\beta'}. \quad (2)$$

The first term represents the mean-field contribution, where  $\varepsilon_i$  is the single-particle energy associated with orbital  $i$ , and  $c_{i\uparrow}$ ,  $c_{i\downarrow}$  are the one-particle annihilation operators for that orbital. As usual, we assume an ordering  $\varepsilon_j \leq \varepsilon_{j+1}$ . The second and third terms represent the interaction for pairs having spin  $S$  equal to 0 and 1, respectively. The operators  $A_{0\alpha}$  in the second term are spin-singlet two-particle annihilation operators  $A_{0\alpha} = (c_{i\downarrow} c_{j\uparrow} - c_{i\uparrow} c_{j\downarrow}) / \sqrt{2(1 + \delta_{ij})}$  with  $\alpha$  standing

for the set of orbital pairs  $ij$ . The  $A_{1\beta}$  in the third line are similarly defined for spin-triplet pairs.

The randomness assumption tells us that there is no preferred basis within either the  $S=0$  or  $S=1$  sector of two-body states. The couplings  $v_{s\alpha\alpha'}$  then should be taken from the Gaussian orthogonal random-matrix ensemble (GOE). We fix the variance of the  $v_s$  to be unity for off-diagonal elements. The GOE then satisfies

$$\langle v_{0\alpha\alpha'}^2 \rangle = 1 + \delta_{\alpha\alpha'}, \quad (3)$$

where  $\langle \dots \rangle$  indicates an ensemble average and similarly for  $v_{1\beta\beta'}$ . We are concentrating for now on the case of time-reversal symmetry, so the matrices  $v_0$  and  $v_1$  are real and symmetric. The case of broken time-reversal symmetry in the presence of a magnetic field will be considered in Sec. V.

The prefactors  $C_0$  and  $C_1$  allow us to consider arbitrary strengths of the spin-0 and spin-1 couplings relative to each other and relative to the single-particle level spacing. As we will see below, several qualitatively different regimes for ground-state staggering are possible within this simple random model, depending on the values  $C_0$  and  $C_1$  as well as on particle density.

Let us denote the ground-state energy of the  $N$ -body system as  $E(N)$ . A useful staggering indicator is the empirical pairing gap

$$\Delta(N) \equiv \frac{1}{2} [E(N+1) - 2E(N) + E(N-1)]. \quad (4)$$

This three-point observable is essentially the ‘‘curvature’’ or second derivative of the binding energy with respect to particle number  $N$ . Positive (negative)  $\Delta(N)$  indicates that the binding energy of the  $N$ -body system is larger (smaller) than the arithmetic mean of the binding energies of its neighbors. We have an odd-even staggering whenever  $\Delta(N)$  staggers with  $N$ .

It is instructive to consider the trivial case where residual interactions are negligible, i.e.,  $C_0 = C_1 = 0$ . Then the  $N$ -particle ground-state energy is given by  $E(N) = 2\sum_{i=1}^{N/2} \varepsilon_i$  for  $N$  even and  $E(N) = E(N-1) + \varepsilon_{(N+1)/2}$  for  $N$  odd. Here  $N$  may range between 0 and  $2M$ , where  $M$  is the number of available orbitals. One obtains for the empirical pairing gap

$$\Delta(N) = \begin{cases} (\varepsilon_{(N/2)+1} - \varepsilon_{N/2})/2 \geq 0 & \text{for } N \text{ even,} \\ 0 & \text{for } N \text{ odd.} \end{cases} \quad (5)$$

Thus, there is a trivial odd-even staggering due to the mean-field alone. In what follows we will mainly be interested in the effects of interactions, and in the effects of adding a magnetic field. For odd-number systems, a nonzero value of the empirical pairing gap must be due to interactions, and this allows one easily to discriminate mean-field effects from interactions. Such a discrimination is more difficult for even-number systems and has recently been studied in mean-field plus pairing Hamiltonians.<sup>4,29,30</sup> We will see in Sec. IV how mean-field effects can be distinguished from staggering caused by complex (or random) interactions. Note that an

electric charging energy  $E_{\text{charge}} = cN(N-1)$  leads only to a  $N$ -independent constant shift  $\Delta(N) \rightarrow \Delta(N) + c$  and can therefore be neglected.

### III. EFFECTS FROM RANDOM TWO-BODY INTERACTIONS

We now imagine the opposite situation from that of the previous section, i.e., we consider the regime  $\varepsilon_i = 0$  where mean-field effects are negligibly weak compared with the random two-body interaction. In this limit one might assume that all odd-even effects should disappear. Surprisingly, this turns out not to be the case. Instead, we find persistent odd-even staggering arising only from the random two-body interactions; stronger binding energies for even- $N$  systems are typically obtained in numerical simulations.

To understand this result analytically, we first note that the spectral density of a system with two-body interactions approaches a Gaussian shape in the many-body limit  $N \rightarrow \infty$ .<sup>31,32</sup> The ground-state energies for different particle number or spin sectors are then largely determined by the widths  $\sqrt{\text{Tr}H^2}$  (Refs. 12,27) of the corresponding Gaussians, scaling as

$$E \approx b \sqrt{\text{Tr}H^2}, \quad (6)$$

where it is assumed without loss of generality that  $\text{Tr}H = 0$ . The prefactor  $b$  depends of course on the details of the deviations of the spectral shape from an exact Gaussian form, since these deviations cut off the tails of the Gaussian. Following an analysis along the lines of Ref. 31, where the spectral shape is expanded in terms of Hermite polynomials, and then estimating the coefficients of these polynomials, one may conjecture that the prefactor  $b$  should scale as  $\ln N$  with the number of particles in the system. In any case, for our purposes it is sufficient that this prefactor varies smoothly with  $N$  without significant staggering, which is confirmed by numerical simulations. Equation (6) is known to provide a good qualitative explanation for some observed behavior of low-lying spectra, even for moderate numbers of particles where the Gaussian approximation is far from valid. For example, a comparison of  $\text{Tr}H^2$  for different spin sectors helps to explain  $J=0$  total spin dominance among the ground states of random interacting many-body systems.<sup>12,27</sup>

#### A. Dilute limit

Applying this approach to the present problem, we need then to understand how  $\text{Tr}H^2$  depends on the number of particles and other parameters of the system. For simplicity, we consider first the dilute limit  $N \ll M$  with a pure  $S=0$  two-body coupling ( $C_1 = 0$ ).

From previous work, it is known that for even  $N$  the ground state comes always from the sector of total spin  $J = 0$ . In the dilute limit, a typical basis state in this sector has the form

$$|\Psi_{J=0}\rangle = 2^{-N/2} \prod_{z=1}^{N/2} (a_{i_z \downarrow}^\dagger a_{j_z \uparrow}^\dagger - a_{i_z \uparrow}^\dagger a_{j_z \downarrow}^\dagger) |0\rangle, \quad (7)$$

where the  $N$  orbitals  $i_z, j_z$  are all distinct. One easily checks that the number of  $S=0$  pairs in this state is  $(N^2 + 2N)/8$ , since the particles on orbitals  $i_z$  and  $j_z$  for a given  $z$  are in an  $S=0$  combination by construction, while the remaining  $(N^2 - 2N)/2$  pairs have a probability 1/4 of being in a singlet combination. Any of these  $S=0$  pairs, labeled by  $\alpha'$  in Eq. (2), may be annihilated by the  $C_0$  term in the Hamiltonian. Another  $S=0$  pair  $\alpha$  must then be created; there are  $M^2/2$  choices for  $\alpha$  in the dilute limit. Thus, simply by counting the number of terms in the  $C_0$  part of the Hamiltonian in Eq. (2) that may act on a total spin  $J=0$  basis state we find

$$\text{Tr}_{(\text{even } N \ll M)} H^2 = C_0^2 \frac{M^2(N^2 + 2N)}{8} \quad (8)$$

for  $N$  even and  $N \ll M$ .

Similarly, for odd  $N$  the preferred many-body ground state has total spin  $J = 1/2$ . The typical basis state has the form

$$|\Psi_{J=1/2}\rangle = 2^{-N/2} a_{k \uparrow}^\dagger \prod_{z=1}^{N/2} (a_{i_z \downarrow}^\dagger a_{j_z \uparrow}^\dagger - a_{i_z \uparrow}^\dagger a_{j_z \downarrow}^\dagger) |0\rangle, \quad (9)$$

where we take  $J_z = +1/2$  without loss of generality, and the indices  $i_z, j_z$ , and  $k$  are all distinct. This state contains only  $(N^2 + 2N - 3)$  singlet pairs, resulting in

$$\text{Tr}_{(\text{odd } N \ll M)} H^2 = C_0^2 \frac{M^2(N^2 + 2N - 3)}{8}. \quad (10)$$

The  $O(1/N^2)$  difference in the widths explains the odd-even staggering in ground-state energies. Intuitively, the result is easy to understand: the ground state of the odd- $N$  system is forced to have a slightly higher total spin, resulting in a slightly smaller fraction of spin-0 pairs and consequently a smaller effect of the  $C_0$  term in the Hamiltonian. This in the end is what leads to weaker binding for the odd- $N$  system.

The above analysis also gives a quantitative prediction for the size of the staggering effect. Assuming in accordance with Eq. (6) that the ratio of ground-state energies is proportional to the ratio of the widths, we find

$$|E_{\text{even}N}| = |E_{\text{odd}N}| \left( 1 + \frac{3}{2N^2} \right) \quad (11)$$

for large  $N$  in the dilute limit and therefore

$$\Delta(N)_{C_0} = (-1)^N \frac{3}{2N^2} |E(N)| \quad (12)$$

to leading order. We may compare this with the size of the pairing gap for the mean-field dominated system. In the previous section, we saw that  $\Delta(N) = \Delta/2$  on average for  $N$  even, where  $\Delta$  is the mean level spacing of the single-particle spectrum. This can be normalized, however, in units of the binding energy. This binding energy, i.e., half the many-body spectral width, is  $|E| \approx MN\Delta/2$  in the mean-field case. So the average pairing gap has the size

$$\Delta(N)_{\text{mean-field}} = \frac{1}{MN} |E(N)| \quad (13)$$

for even  $N$ , which surprisingly is *smaller* than the pure interaction-induced pairing gap in the dilute limit  $N \ll M$ .

At finite particle density  $\rho = 2N/M$ , mean-field-induced and interaction-induced stagger are of comparable size, a characteristic difference being the vanishing of the pairing gap  $\Delta(N)$  for odd  $N$  in the mean-field case, Eq. (5), which is absent for the pure interacting theory. In addition, in the presence of fluctuations in the single-particle spectrum, mean-field induced  $\Delta(N)$  will itself fluctuate between successive even values of  $N$ , while interaction-induced stagger is predicted to be smooth. These analytic predictions will be verified numerically in Sec. IV below.

### B. General results for finite density

The above derivation, though strictly valid only in the dilute limit, in fact provides a correct intuitive explanation of the stagger at any density for a pure  $S=0$  two-body interaction. Handling the  $S=1$  interaction requires more care, since the qualitative behavior will depend strongly on the density  $\rho$ . We therefore need the exact expressions for  $\text{Tr}H^2$  in various particle number and spin sectors. These expressions may be straightforwardly, though perhaps rather tediously, obtained by applying the original Hamiltonian, Eq. (2), to various basis states and evaluating the norm.

The full results are presented in the Appendix. There we find that for a pure singlet random interaction, the prediction of Eq. (12) for the size of the staggering, obtained above only in the dilute limit, is in fact confirmed as a lower bound for arbitrary densities in the many-body limit  $N \rightarrow \infty$ :

$$(-1)^N \Delta(N)_{C_0} \geq \frac{3}{2N^2} |E(N)|. \quad (14)$$

The situation is more complex for a pure triplet coupling ( $C_0=0$ ), since here the ground state may be a state of either minimal or maximal spin. In this case we see using formulas given explicitly in the Appendix that a critical density  $\rho_{\text{crit}}$  exists below which there is no staggering, while above which interaction-induced staggering of order  $|E(N)|/N^2$  appears, just as in the singlet case. As the singlet coupling is turned on,  $\rho_{\text{crit}}$  decreases, reaching 0 at  $C_0=C_1$ . Thus, odd-even staggering with stronger binding for even- $N$  systems is predicted to be a very general consequence of random two-body interactions, present for pure-singlet and pure-triplet interactions as well as in the intermediate case.

## IV. CROSSOVER BETWEEN MEAN-FIELD REGIME AND STRONG TWO-BODY INTERACTIONS

The analytical results of the previous sections were obtained for pure one-body or pure two-body interactions. In this section we will study the odd-even staggering for the full Hamiltonian (2) numerically. To this purpose we draw the random matrices  $v_0$  and  $v_1$  in Eq. (2) from the GOE and compute the ground-state energies of Hamiltonian of Eq. (2) for several particle numbers  $N$ . This procedure is repeated many times for each  $N$  to obtain ensemble-averaged values for the ground state energies  $E(N)$  and the empirical pairing gap defined in Eq. (4). In what follows we set the number of

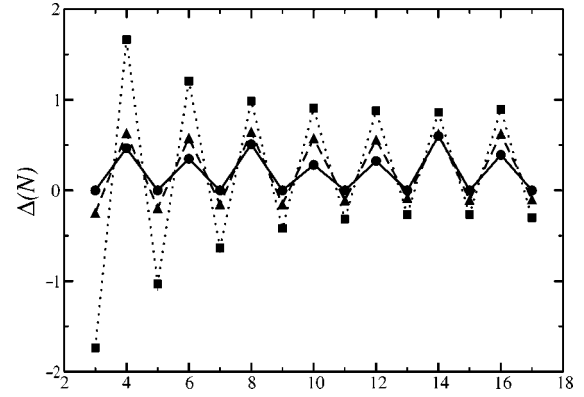


FIG. 1. Empirical pairing gap as a function of particle number for parameter  $\varphi=0$  (full line),  $\varphi=\pi/12$  (dashed line), and  $\varphi=\pi/2$  (dotted line; graph scaled by a factor 1/2 for display purposes) shows the transition from the mean-field regime to strong interactions in the spin-0 channel. Note that the pairing gap  $\Delta(N)$  is dimensionless here and in all following figures; the energy scale in our calculation is set by the overall energy scale of the Hamiltonian (see text).

single-particle orbitals to  $M=10$ , and obtain ensemble averages from 200 runs. The largest matrices of the ensemble have dimension 63 504; their ground states are computed using the sparse matrix solver ARPACK.<sup>33</sup>

We have to assign values to the single-particle energies  $\varepsilon_i$  of the mean field and to the coupling constants  $C_0$  and  $C_1$  of the two-body interactions. We assume a mean-field spectrum with level spacings  $\varepsilon_{i+1}-\varepsilon_i$  that are Wigner distributed. This is consistent with the assumption that our quantum dot or metallic grain has irregular shape. To study the transition, we multiply the single-particle energies with a factor  $\cos\varphi$  and set the spin-0 coupling  $C_0(\varphi)=\sin\varphi$ . Here  $\varphi$  is in the range  $\varphi \in [0, \pi/2]$  and thus parametrizes the transition from the mean field to the regime of strong interactions. The spin-1 coupling  $C_1$  is set to zero. Figure 1 shows the empirical pairing gap (4) as a function of particle number  $N$  for parameter values  $\phi=0, \pi/12, \pi/2$ .

We see from Fig. 1 that the odd-even staggering persists throughout this transition. In the absence of the mean field ( $\phi=\pi/2$ ), the staggering decreases slowly with increasing  $N$  and then increases again very close to the maximal filling, when the number of holes becomes small and  $\rho$  approaches unity in Eq. (A4). Its envelope depends smoothly on  $N$  if only even or only odd values of  $N$  are considered. These qualitative results are fully consistent with the analytical predictions obtained in Sec. III and in the Appendix. The absence of such a smooth envelope thus indicates that the staggering is instead dominated by mean-field effects, as in the  $\varphi=0$  line in Fig. 1. Similar observations have been made for pairing-plus-quadrupole in Ref. 29. Note that the random interactions drive the empirical pairing gap  $\Delta(N)$  to negative values for odd  $N$ ; in this sense the staggering is more pronounced in the presence of interactions than in the mean-field regime. Note also that the magnitude of the staggering itself contains only little information since the transition from the noninteracting to the interacting Hamiltonian does not correspond to a transition in a physical system.

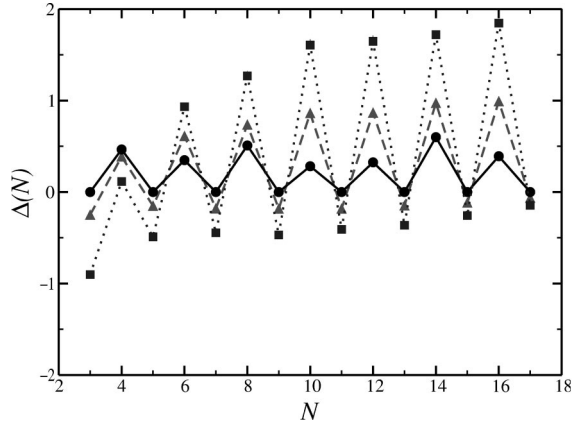


FIG. 2. Empirical pairing gap as a function of particle number for parameter  $\varphi=0$  (full line),  $\varphi=\pi/12$  (dashed line), and  $\varphi=\pi/2$  (dotted line; graph scaled by a factor 1/2 for display purposes) shows the transition from the mean-field regime to strong interactions in the spin-1 channel.

We repeat these calculations in Fig. 2 for the case of vanishing spin-0 coupling,  $C_0=0$ , and set the spin-1 coupling to  $C_1(\varphi)=\sin\varphi$ . Again, odd-even staggering persists throughout the transition. In the regime of strong interactions the magnitude of the empirical pairing gap increases with increasing  $N$  for even  $N$ . The situation is reversed for odd values of  $N$ . Leaving out very small systems ( $N=3$ ), the envelopes for even and odd  $N$  are still smooth enough to discriminate mean-field effects from interaction-induced pairing.

Finally, we consider the case of equally strong spin-0 and spin-1 couplings and set  $C_0(\varphi)=C_1(\varphi)=\sin\varphi$ . Figure 3 shows that this case is qualitatively similar to the case of pure spin-1 coupling, since triplet pairs outnumber singlet pairs by a 3:1 ratio in the large- $N$  limit. Again, the interaction-induced staggering exhibits a smooth envelope and can therefore clearly be distinguished from mean-field effects.

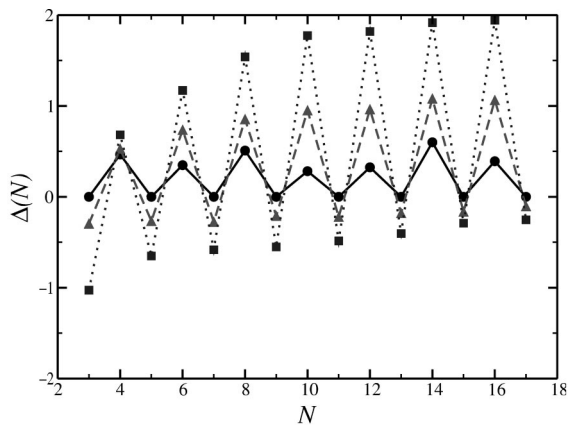


FIG. 3. Empirical pairing gap as a function of particle number for parameter  $\varphi=0$  (full line),  $\varphi=\pi/12$  (dashed line), and  $\varphi=\pi/2$  (dotted line; graph scaled by a factor 1/2 for display purposes) shows the transition from the mean-field regime to strong interactions.

## V. MAGNETIC FIELD EFFECTS

BCS-like pairing results from strong correlations between fermions in time-reversed orbitals. Thus, these correlations can be destroyed by a sufficiently strong breaking of time-reversal symmetry. Examples of this well-known phenomenon are the breakdown of electronic superconductivity in the presence of sufficiently strong magnetic fields and the reduction of pairing correlations in rapidly rotating and deformed nuclei. In this section we want to study how breaking time-reversal symmetry affects the odd-even staggering in systems with a random two-body interaction. Having metallic grains in mind we thus consider the effect of a magnetic field. To be definite, we take a uniform  $B$  field in the  $z$  direction. This leads to Zeeman splitting and adds the following one-body term to the Hamiltonian:

$$H_B = \mu B \sum_{i=1}^M (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}), \quad (15)$$

which also breaks rotational symmetry, i.e., only the projection of the total spin  $J_z$  remains conserved. Here,  $\mu$  is an appropriate constant. A second effect consists of the modification of the random two-body interaction. Provided the time-reversal symmetry breaking induces splittings that are larger than the mean level spacing, the random matrices  $v_{0\alpha\alpha'}$  and  $v_{1\beta\beta'}$  in the Hamiltonian (2) have to be drawn from the Gaussian unitary ensemble (GUE). Accordingly, Eq. (3) for the  $S=0$  matrix  $v_{0\alpha\alpha'}$  and the corresponding formula for the  $S=1$  matrix  $v_{1\beta\beta'}$  have to be replaced by

$$\langle |v_{0\alpha\alpha'}|^2 \rangle = \langle |v_{1\beta\beta'}|^2 \rangle = 1. \quad (16)$$

This reduces the variance of the diagonal matrix elements by a factor of two when compared to the GOE. Considering the random two-body interaction alone, this effect introduces only small corrections of order  $1/N^2$  to the results presented in the previous sections and in the Appendix.

Let us consider the trivial case where residual interactions can be neglected. The  $B$ -dependent pairing gap then becomes

$$\Delta(N, B) = \begin{cases} \frac{1}{2} (\varepsilon_{N/2+1} - \varepsilon_{N/2}) - \mu B & \text{for } N \text{ even,} \\ \mu B & \text{for } N \text{ odd.} \end{cases} \quad (17)$$

The odd-even staggering thus decreases with increasing magnetic field and disappears when the Zeeman splitting  $2\mu B$  equals half the mean level spacing  $\langle \varepsilon_{i+1} - \varepsilon_i \rangle$ . Note that Eq. (17) ceases to be applicable for stronger magnetic fields. In the limit of very large  $B$  fields, the ground state becomes spin polarized (i.e., has maximal spin  $J=N/2$ ) and any odd-even staggering disappears. Note also that a breaking of time-reversal symmetry leads to a positive pairing gap at odd  $N$  and can thereby easily be distinguished from the effects of interactions.

We now include again the random two-body interactions and compute the empirical pairing gap as the magnetic field is switched on. The number of single-particle orbitals is  $M=6$ . At vanishing magnetic field we assume an equidistant mean-field spectrum with unit spacing. The two-body ran-

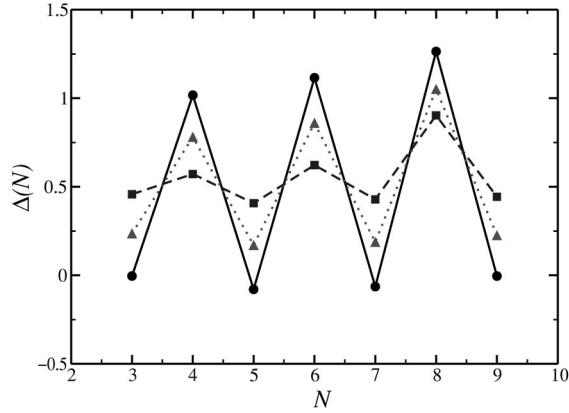


FIG. 4. Empirical pairing gap as a function of particle number for various strengths of the magnetic field:  $2\mu B/\langle\varepsilon_{i+1}-\varepsilon_i\rangle = 0, 1/4, 1/2$  (full line, dotted line, dashed line).

dom interactions have fixed couplings  $C_0=C_1=1/10$ . We add the Zeeman Hamiltonian (15) to the system and increase the Zeeman splitting  $2\mu B$  from zero to its maximal value  $\langle\varepsilon_{i+1}-\varepsilon_i\rangle/2$ . Simultaneously, the variance of the imaginary part of the random matrix elements is increased from zero to one, being held proportional to the Zeeman splitting. Figure 4 shows that the odd-even staggering decreases with increasing Zeeman splitting. The remaining staggering is due to the interactions, which are relatively weak in this example; the transition from the GOE to the GUE in the random two-body matrix is very mild. For strong two-body interactions the odd-even staggering remains strong when time-reversal symmetry is broken. Thus, the breaking of time-reversal invari-

ance has only mild effects on the ground-state structure in strongly interacting systems. This finding is consistent with a recent study of time-reversal symmetry breaking in the nuclear shell model with random two-body interactions.<sup>34</sup>

## VI. SUMMARY

We have shown analytically and numerically that random two-body interactions cause an odd-even staggering in interacting few-fermion systems such as small metallic grains or quantum dots. Interactions tend to smooth out the odd- $N$  and even- $N$  dependence of the pairing gaps and can thereby be discriminated from the nonsmooth mean-field staggering. As expected, the breaking of time reversal symmetry leads to a decrease of the odd-even staggering; this trend can, however, be countered by sufficiently strong two-body interactions.

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## APPENDIX

The derivation of interaction-induced staggering in Sec. III was obtained in the dilute limit  $N \ll M$ . For general values of  $N$  and  $M$  and couplings  $C_0$  and  $C_1$ , a straightforward counting procedure results in the exact expressions

$$\begin{aligned} \text{Tr}_{J=0} H^2 &= \frac{C_0^2 + 3C_1^2}{64} N^2 (2M - N)^2 + \frac{N}{16} [C_0^2 (2M^2 + MN - N^2) - 3C_1^2 (2M^2 - 7MN + 3N^2)] \\ &\quad + \frac{N}{16} \{C_0^2 [6M + N - 2Nd(1-d)] - 3C_1^2 [10M - 13N - 2Nd(1+d)]\} + \frac{N}{16} [8C_0^2 - 24C_1^2(2+d)] \quad (\text{A1}) \end{aligned}$$

$$\begin{aligned} \text{Tr}_{J=1/2} H^2 &= \frac{C_0^2 + 3C_1^2}{64} N^2 (2M - N)^2 + \frac{N}{16} [C_0^2 (2M^2 + MN - N^2) - 3C_1^2 (2M^2 - 7MN + 3N^2)] \\ &\quad + \frac{1}{16} \{C_0^2 (-3M^2 + 9MN - N^2/2) + 3C_1^2 [M^2 - 15MN + 31N^2/2 + 2N^2d(1+d)]\} \\ &\quad + \frac{1}{16} [C_0^2 (-9M + 11N - 2Nd) + 3C_1^2 (9M - 31N - 8Nd)] + \frac{3}{64} [-13C_0^2 + 73C_1^2] \quad (\text{A2}) \end{aligned}$$

$$\text{Tr}_{J=N/2} H^2 = \frac{C_1^2}{4} [N^2 (M - N)^2 - N(M^2 - 5MN + 4N^2) + N(7N - 3M) - 4N]. \quad (\text{A3})$$

In each of the three above expressions for minimal and maximal spin states, terms are ordered by their relative importance in the many-body limit at finite density, i.e., in the limit  $N \rightarrow \infty$  with  $\rho \equiv N/2M = \text{const}$ . The leading term is  $O(N^4)$  in

the many-body limit, and this leading term is seen to be manifestly symmetric under particle-hole exchange  $N \rightarrow 2M - N$  for the minimal-spin states (of course the maximal spin states  $J = N/2$  exist only for  $N \leq M$ ). At subleading order, the

symmetry is broken due to anticommutation relations between the creation and annihilation operators in Eq. (2). At both leading and first subleading order,  $\text{Tr}H^2$  is clearly identical for the  $J=0$  and  $J=1/2$  states, indicating that the staggering can occur only at  $O(1/N^2)$ , entirely consistent with our dilute analysis in Sec. III. It is also at this second subleading order that we first encounter the dimensionless quantity  $d$ , which we did not need to consider in the dilute approximation.  $d$ , taking values  $0 \leq d \leq 1$ , represents the fraction of particles in the basis state that live on doubly occupied orbitals.

As discussed above, for a pure  $S=0$  coupling ( $C_1$  vanishing), ground states come always from the sector of minimal spin, and thus we are led to consider the quantity

$$\frac{\text{Tr}_{S=0}H^2 - \text{Tr}_{S=1/2}H^2}{\text{Tr}_{S=1/2}H^2} = \frac{3 - 6\rho(1-\rho) - 8\rho^2d(1-d)}{N^2(1-\rho)^2} \geq \frac{3}{2N^2}, \quad (\text{A4})$$

where terms of higher order in the  $1/N$  expansion have been dropped, and the last inequality is easily checked for all possible values of filling fraction  $\rho$  and double occupancy fraction  $d$ . Thus, our original estimate, Eq. (12), obtained using the dilute approximation, is confirmed as a lower bound to the amount of predicted pairing gap

$$(-1)^N \Delta(N)_{C_0} \geq \frac{3}{2N^2} |E(N)|. \quad (\text{A5})$$

The situation is more complex for a pure  $S=1$  coupling ( $C_0=0$ ), since here the ground state may be a state of either minimal or maximal spin, depending on the density  $\rho$ . Comparing Eqs. (A1), (A2) with Eq. (A3) at leading order in the many-body limit, we see easily that  $J=N/2$  is preferred at

very low density,  $\rho < \rho_{\text{crit}} = (5 - 2\sqrt{3})/13 \approx 0.118$ , but as density increases a transition should occur to ground states of minimal spin. The preference for maximal spin at low density is obvious, since high-spin states clearly maximize the fraction of particle pairs with aligned spins ( $S=1$  instead of  $S=0$ ). On the other hand, the physical reason for the transition to minimal-spin ground states even with a pure  $S=1$  coupling for  $\rho > \rho_{\text{crit}}$  is that at high enough density there are relatively few other high-spin states that a given high-spin state can couple to.

The relevant result for our purpose here is that at low densities there is no predicted stagger in the many-body limit, in accordance with Eq. (A3), but for  $\rho > \rho_{\text{crit}}$  minimal-spin states again become dominant. A calculation completely analogous to the one in Eq. (A4) tells us that once again the pairing gap  $\Delta$  is positive (negative) for even (odd)  $N$  and proportional to  $1/N^2$  times the magnitude of the binding energy. Thus,

$$\begin{aligned} \Delta(N)_{C_1} &= 0 \quad (\rho < \rho_{\text{crit}}), \\ (-1)^N \Delta(N)_{C_1} &\geq \frac{0.027}{N^2} |E(N)| \quad (\rho > \rho_{\text{crit}}). \end{aligned} \quad (\text{A6})$$

The above analysis generalizes easily to the generic case where the two coefficients  $C_0$  and  $C_1$  are both nonzero. For  $C_0 > C_1$ , ground states are always expected to come from the minimal-spin sector, leading to positive pairing gap  $\Delta$  proportional to  $1/N^2$  times the binding energy. For  $C_1 > C_0$ , on the other hand, there will be a transition between no pairing gap at low density to positive pairing gap at higher density, the critical density  $\rho_{\text{crit}}$  approaching 0.118 for  $C_1 \gg C_0$  and approaching 0 at  $C_0 = C_1$ .

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