Nonuniversal Behavior of the k-Body Embedded Gaussian Unitary Ensemble of Random Matrices

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Using a novel approach, we investigate the shape of the average spectrum and the spectral fluctuations of the k-body embedded unitary ensemble in the limit of a large matrix dimension. We identify the transition point between a semicircle and a Gaussian shape. The transition also affects the spectral fluctuations which deviate from the Wigner-Dyson form and become Poissonian in the limit $k \ll m \ll l$. Here m is the number of fermions and l the number of degenerate single-particle states.

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Introduction.—The stochastic behavior displayed by spectra and wave functions of quantum many-body systems (atoms, molecules, atomic nuclei, quantum dots) is usually and successfully modeled in terms of canonical random-matrix theory (RMT) [1,2]. However, this type of modeling is not completely realistic: All the above-mentioned many-body systems are effectively governed by one- and two-body forces, while canonical RMT is tantamount to assuming many-body forces between the constituents. Thus, a stochastic modeling of the one- and two-body interactions would yield a much smaller number of independent random variables than used in RMT. For instance, the number of independent two-body matrix elements in a shell-model calculation in atoms or nuclei is typically much smaller than the dimension N of the matrices involved, while the number of independent random variables in RMT is of order N^2. This difference poses the question whether a more realistic stochastic modeling of many-body systems might yield results which differ from RMT predictions. The question was addressed in the 1970s with the help of numerical simulations using matrices of fairly small dimensions. The main results were: In a certain limit, the average level density does not have the shape of a semicircle but is Gaussian; the ensembles are neither stationary nor ergodic; unfolding of the spectra yields Wigner-Dyson spectral fluctuation properties; see Ref. [3]. Interest in model Hamiltonians with random two-body interactions has resurged in recent years in several areas of many-body physics (see Ref. [4], and references therein), and the question of possible further differences between such models and RMT has resurfaced. It is the purpose of this Letter to shed new light on this question. In particular, we will show that for certain parameter values, the spectral fluctuation properties of realistic models differ from those of RMT. We discuss the implications of this novel and surprising result.

Focusing attention on the case of unitary symmetry, we use a paradigmatic model, the k-body embedded Gaussian random ensemble EGUE(k) introduced by Mon and French [5]. For this ensemble, a number of analytical results have been obtained [1,5,6]. However, as emphasized in Ref. [1], page 413, a comprehensive analytical approach to the spectral fluctuation properties of the ensemble is still lacking. This is due to the fact that, in contrast to RMT, embedded ensembles do not possess the (orthogonal or unitary) invariance in Hilbert space which is so essential for the successful analytical treatment of RMT.

We use three different methods: The supersymmetry approach, the "binary correlation approximation" of Mon and French [5], and the construction of two "limiting ensembles." We also make use of two fundamental and novel results on the second moment: The eigenvector expansion and duality. We compare our results with those of the Gaussian unitary ensemble (GUE) of random matrices.

Definitions.—Our Hilbert space is spanned by $N = \binom{l}{m}$ Slater determinants $|\mu\rangle$, $\mu = 1, \ldots, N$, obtained by distributing m spinless fermions over l degenerate single-particle states. The ratio $f = m/l$ is the filling factor. Using standard creation and annihilation operators $a_j^\dagger$ and a_j, $j = 1, \ldots, l$, we have $|\mu\rangle = \prod_{s=1}^{m} a_{j_s}^\dagger |0\rangle$. Here $|0\rangle$ is the vacuum state. The creation operators are written in ascending order of the indices j_s. The k-body interaction V_k has the form ($k = 1, \ldots, m$)

$$V_k = {\sum}' v_{j_1,\ldots,j_k;i_1,\ldots,i_k} a_{j_1}^\dagger \cdots a_{j_k}^\dagger a_{i_k} \cdots a_{i_1} . \qquad (1)$$

Here, and in Eqs. (2) and (9), the prime on the summation sign indicates that the sums over all indices run from 1 to l with the constraint that $j_1 < \cdots < j_k$ and $i_1 < \cdots < i_k$. The k-body interaction matrix $v_{j_1,\ldots,j_k;i_1,\ldots,i_k}$ is complex Hermitian. The independent matrix elements are uncorrelated Gaussian random variables with zero mean and a common second moment v^2. The value of $\sqrt{v^2}$ determines the overall energy scale and is set equal to unity without loss of generality. By taking matrix elements $\langle \nu | V_k | \mu \rangle$, we "embed" the random k-body interaction into an m-fermion system. This defines EGUE(k). The ensemble is invariant under unitary transformations of the single-particle states $1, \ldots, l$ and, for $k = m$, reduces to the standard GUE. As always in RMT, we are interested in the limit $N \to \infty$ ($l \to \infty$).

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Second moment.—The Gaussian distribution of the matrix elements in Eq. (1) implies that the $\langle\nu|V_k|\mu\rangle$'s are also Gaussian distributed random variables with zero mean value. All spectral properties of EGUE(k) are, therefore, determined by the second moment

$$A^{(k)}_{\mu\nu,\rho\sigma} = \overline{\langle\mu|V_k|\sigma\rangle\langle\rho|V_k|\nu\rangle} = {\sum}' \langle\mu|a^\dagger_{j_1}\cdots a^\dagger_{j_k}a_{i_k}\cdots a_{i_1}|\sigma\rangle \times \langle\rho|a^\dagger_{i_1}\cdots a^\dagger_{i_k}a_{j_k}\cdots a_{j_1}|\nu\rangle. \quad (2)$$

The bar denotes the ensemble average. We have $A^{(k)}_{\mu\nu,\rho\sigma} = A^{(k)}_{\rho\sigma,\mu\nu}$ and $(A^{(k)}_{\mu\nu,\rho\sigma})^* = A^{(k)}_{\sigma\rho,\nu\mu} = A^{(k)}_{\mu\nu,\rho\sigma}$. The matrix $A^{(k)}$ is Hermitian in the pairs of indices (μ,ν) and (ρ,σ). Moreover, it is easy to prove the "duality" relation $A^{(k)}_{\mu\nu,\rho\sigma} = A^{(m-k)}_{\mu\sigma,\rho\nu}$ which connects the second moments of the k-body and the $(m-k)$-body interactions.

Eigenvector expansion.—We construct the eigenvectors $C^{(sa)}$ and eigenvalues $\Lambda^{(s)}(k)$ of the Hermitian matrix $A^{(k)}$ satisfying $\sum_{\rho\sigma} A^{(k)}_{\mu\nu,\rho\sigma}C^{(sa)}_{\sigma\rho} = \Lambda^{(s)}(k)C^{(sa)}_{\mu\nu}$. Here $s = 0,\ldots,m$ and a labels the degenerate eigenvectors. We are guided by the example of the GUE where the second moment of the Hamiltonian H reads $\overline{H_{\mu\sigma}H_{\rho\nu}} = (\lambda^2/N)\delta_{\mu\nu}\delta_{\rho\sigma}$. The two Kronecker symbols display the unitary invariance of the GUE. The matrix $\delta_{\sigma\rho}$ is an eigenfunction of the second moment with eigenvalue λ^2. All traceless unitary matrices are likewise eigenfunctions but belong to eigenvalue zero. In the present case, we use the ansatz $C^{(sa)}_{\mu\nu} = \langle\mu|a^\dagger_{j_1}\cdots a^\dagger_{j_s}a_{i_s}\cdots a_{i_1}|\nu\rangle$. The label a enumerates all possible distinct choices of the indices $j_1 < \cdots < j_s; i_1 < \cdots < i_s$. It is easy to check that $C^{(sa)}$ is an eigenvector of the matrix $A^{(k)}$ if no two indices $(j_r, i_{r'})$ are equal. The corresponding eigenvalue is

$$\Lambda^{(s)}(k) = \binom{m-s}{k}\binom{l-m+k-s}{k}. \quad (3)$$

When at least two indices $(j_r, i_{r'})$ are equal, $C^{(sa)}_{\mu\nu}$ is not an eigenfunction of $A^{(k)}$ but a linear combination of eigenfunctions with labels $s' \le s$. This is because an eigenfunction $C^{(s'a)}_{\mu\nu}$ with eigenvalue $\Lambda^{(s')}(k)$, $s' < s$, looks like a member of class s when the operator defining $C^{(s'a)}$ is multiplied by $(\sum_p a^\dagger_p a_p)^{s-s'} = m^{s-s'}$. To remove the components belonging to lower s' values, we orthogonalize (in the sense of the trace) all matrices $C^{(sa)}_{\mu\nu}$ in which at least two indices $(j_r, i_{r'})$ are equal, to all matrices generated from classes $s' < s$ in the manner just described. The resulting matrices are eigenvectors with eigenvalue $\Lambda^{(s)}(k)$. We choose Hermitian linear combinations of the degenerate eigenvectors which obey the orthonormality condition $\sum_{\mu\nu} C^{(sa)}_{\mu\nu}C^{(tb)}_{\nu\mu} = N\delta_{st}\delta_{ab}$. The number $D^{(s)}$ of linear independent eigenvectors in class s is given by $D^{(0)} = 1$ and

$$D^{(s)} = \binom{l}{s}^2 - \binom{l}{s-1}^2, \qquad s \ge 1. \quad (4)$$

We have $\sum_{s=0}^m D^{(s)} = N^2$ showing that the eigenvectors form a complete orthonormal set. Hence, the matrix $A^{(k)}$ possesses an eigenvalue decomposition of the form

$$A^{(k)}_{\mu\nu,\rho\sigma} = \frac{1}{N}\sum_{s=0}^{m}\Lambda^{(s)}(k)\sum_a C^{(sa)}_{\mu\nu}C^{(sa)}_{\rho\sigma}. \quad (5)$$

We note that the eigenvectors do not depend on the rank k of the interaction, only the eigenvalues do. Equation (3) shows that the sum over s actually terminates at $s = m-k$. For $k = m$ only $s = 0$ contributes, and the result reduces to the GUE expression with $\lambda^2 = \Lambda^{(0)}(m)$. Conversely, Eq. (5) extends the GUE result to EGUE(k) and constitutes a central result of this paper.

Moments of V_k.—Using the eigenvector decomposition of $A^{(k)}$, duality, and the orthonormality of the $C^{(sa)}$'s, we calculate the low moments of V_k and the kurtosis κ for which we write $\kappa = 2 + Q(k,m,l)$. We recall that $\kappa = 2(3)$ for the semicircle (Gaussian, respectively). We find $Q(k,m,l) = (1/N)\sum_{s=0}^{\min(m-k,k)} \times \{[\Lambda^{(s)}(k)\Lambda^{(s)}(m-k)]/[\Lambda^{(0)}(k)]^2\}D^{(s)}$. For $l \to \infty$ and keeping both k and m fixed, we have $Q(k,m,l) \to 0$ if $2k > m$ while $Q(k,m,l) \to \binom{m-k}{k}/\binom{m}{k}$ for $2k \le m$. This shows that the transition of the average spectrum from a semicircle to a Gaussian shape begins (with decreasing k) at $2k = m$. We ascribe the special role of the point $2k = m$ to duality. Likewise we can show that the relative fluctuations of the first and second moments of V_k and, thus, nonergodic features vanish for $l \to \infty$.

Supersymmetry.—We calculate spectrum shape and spectral fluctuation properties of EGUE(k) using the supersymmetry approach [7,8]. After averaging over the ensemble, the integrand of the generating functional contains an exponential whose argument depends linearly on the matrix $A^{(k)}$. With the eigenvalue decomposition (5), the argument of the exponential becomes a sum of squares of bilinear forms in the integration variables. This allows us to perform the Hubbard-Stratonovich transformation. For each pair (s,a) we introduce a supermatrix $\sigma^{(sa)}$ of composite variables. The resulting integral over the composite variables contains the factor $\exp(-\mathcal{L}_{\rm eff})$. The effective Lagrangian $\mathcal{L}_{\rm eff}$ is given by

$$\frac{N}{2}\sum_{sa}\mathrm{trg}[\sigma^{(sa)}]^2 + \mathrm{tr}_\mu\,\mathrm{trg}\ln\left[\left(E - \frac{1}{2}\epsilon L\right)\delta_{\mu\nu} - \sum_{sa}\lambda^{(s)}(k)\sigma^{(sa)}C^{(sa)}_{\mu\nu} - J_{\mu\nu}\right]. \quad (6)$$

Here, $\lambda^{(s)}(k) = +[\Lambda^{(s)}(k)]^{1/2}$. The energy arguments E_1 and E_2 of the advanced and the retarded Green function define $E = (1/2)(E_1 + E_2)$ and $\epsilon = E_2 - E_1$, while J stands for the source terms. The diagonal supermatrix L distinguishes the retarded and advanced cases and is defined in Ref. [8]. The saddle-point equation has the solution $\sigma^{(sa)}_{\rm s.p.} = \delta_{s0}\tau^{(0)}$

where $\tau^{(0)}$ is the standard GUE saddle-point solution. Thus, the saddle-point condition yields a semicircular spectrum and universal GUE spectral fluctuations. To determine the range of validity of this solution, we have calculated the first nonvanishing term in the loop expansion. The expansion is obtained by writing $\sigma^{(sa)} = \sigma^{(sa)}_{\text{s.p.}} + \delta\sigma^{(sa)}$ and expanding in powers of $\delta\sigma^{(sa)}$. We recall that for the GUE, each term of the loop expansion vanishes in the limit $N \to \infty$ with an inverse power of N. For the one-point function, we find that the loop correction is proportional to $Q(k, m, l)$. This is consistent with the result of the previous paragraph and reaffirms our conclusion that the transition from a semicircular to a Gaussian shape sets in at $2k = m$. It would be desirable to show that all higher terms of the loop expansion vanish likewise asymptotically for $2k > m$ but this proof is beyond our means. For the two-point function, the loop correction yields nonuniversal spectral fluctuations of the type first considered by Kravtsov and Mirlin [9]. The amplitude of this correction (given in units of the inverse mean level spacing) vanishes, however, for $l \to \infty$. It does so as N^{-2} for $k = m$ but only as $(\ln N)^{-2k}$ for both k and f fixed. We see that for $l \to \infty$, the supersymmetry approach does not yield a limit on the range of validity of the universal GUE spectral fluctuations of EGUE(k).

The case $k \ll m \ll l$.—For this case where the supersymmetry method does not yield relevant information on spectral fluctuations, we use a modification of the binary correlation approximation [1,5]. In the average two-point function $\overline{g(z_1)g(z_2)}$, we expand [6] both traced Green functions g in powers of V_k. We collect the terms containing equal powers of V_k. The ensemble average is taken by Wick-contracting pairs of V_k's in all possible ways. We evaluate all pairs located on the same Green function as in Ref. [5]. For the rest, we use simple counting arguments. We show that for $k \ll m \ll l$, terms where s pairs of V_k's are not on the same Green function, are smaller by at least a factor l^{-sk} than the terms with $s = 0$. Thus, the connected part of $\overline{g(z_1)g(z_2)}$ vanishes asymptotically compared to the disconnected part, and the two-point correlation function

$$R_2(z_1, z_2) = \frac{\overline{g(z_1)g(z_2)}}{\overline{g(z_1)} \cdot \overline{g(z_2)}} - 1 \tag{7}$$

approaches zero in the limit $k \ll m \ll l$. For similar reasons, all higher correlation functions also vanish in the same limit, and the spectral fluctuations become Poissonian.

The case $k = 1$ with $k \ll m \ll l$ illustrates this result. Taking first $m = k = 1$, we construct the eigenvalues ϵ_α and eigenfunctions Ψ_α of a given realization of EGUE(1) by diagonalization. The ϵ_α's obey GUE spectral statistics; the average spectrum has a semicircle shape, and the coefficients $U_{\alpha j}$ in the expansion $\Psi_\alpha = \sum_{j=1}^{l} U_{\alpha j} a_j^\dagger |0\rangle$ in terms of the single-particle basis are Gaussian distributed random variables. For $m > 1$ and every realization of the ensemble, the eigenfunctions are Slater determinants χ of the Ψ_α's, the eigenvalues are sums of the ϵ_α's, and the average spectrum is an m-fold convolution of the semicircle. This shows immediately that for $m \gg 1$, the spectrum has a Gaussian shape, and that the spectral fluctuations are Poissonian. We have also shown that the states χ are localized.

Regular graphs.—Further insight into the spectral properties of EGUE(k) is gained by using yet another approach involving regular graphs and limiting ensembles. A graphical representation of EGUE(k) is obtained by assigning to each Hilbert-space vector $|\mu\rangle$ a vertex μ, and to each nondiagonal element $\langle\nu|V_k|\mu\rangle$ which does not vanish identically, a link connecting the vertices ν and μ. The diagonal matrix elements $\langle\mu|V_k|\mu\rangle$ are represented by loops attached to the vertices μ. The number of vertices is N. The number M of links emanating from a given vertex is the same for all vertices and given by

$$M = \sum_{s=1}^{k} \binom{m}{s} \binom{l-m}{s}. \tag{8}$$

For $k < m$, we have $M < N - 1$ while $M = N - 1$ for $k = m$. The resulting graphical structure is called a "regular graph" in the mathematical literature. The total number P of links is given by $P = (1/2)MN$. The number K of uncorrelated matrix elements of EGUE(k) is given by $K = \binom{l}{k}^2$. It is interesting to study the ratio K/P. For fixed m and $f \le 1/2$, K/P grows monotonically with k, starting out with very small values and reaching the limit $2N/(N-1)$ for $k = m$. This suggests that deviations of EGUE(k) from universal GUE behavior are caused by the fact that the number of independent random variables is too small in comparison with the number of links, making it impossible for the system to become thoroughly mixed.

Limiting ensembles.—To test this hypothesis, we have constructed and analyzed two limiting ensembles. The first, $\text{EGUE}_{\min}(k)$, is given by the matrix elements $\langle\nu|V_k^{\min}|\mu\rangle$ of the interaction $V_k^{\min} = v \sum{}' a_{j_1}^\dagger \cdots a_{j_k}^\dagger a_{i_k} \cdots a_{i_1}$. The factor v is a Gaussian complex random variable. The ensemble $\text{EGUE}_{\min}(k)$ has the same graphical representation as EGUE(k) but possesses only a single random variable. We succeeded in proving that for $k = 1$ and $k = m$, $\text{EGUE}_{\min}(k)$ is fully integrable, has a Gaussian average spectrum, and spectral fluctuations which are not of a GUE type. We are convinced that these properties hold for all k. The second limiting ensemble, $\text{EGUE}_{\max}(k)$, carries the maximum number of uncorrelated random variables consistent with the graph structure of EGUE(k) and has Hilbert-space matrix elements given by

$$v_{\nu\mu} \sum{}' \langle\nu|a_{j_1}^\dagger \cdots a_{j_k}^\dagger a_{i_k} \cdots a_{i_1}|\mu\rangle. \tag{9}$$

The matrix $v_{\nu\mu}$ is complex Hermitian. Elements not connected by symmetry are uncorrelated complex Gaussian random variables with mean value zero and variance

$\overline{v_{\nu\mu}v_{\nu'\mu'}} = \delta_{\mu\nu'}\delta_{\nu\mu'}$. Using supersymmetry, we have shown that $\mathrm{EGUE}_{\max}(k)$ has an average spectrum of semicircle shape, that the spectral fluctuations are of universal GUE type, and that for $l \to \infty$ the leading term of the loop expansion vanishes both for the one-point and for the two-point functions. We conclude that the spectral properties of $\mathrm{EGUE}_{\max}(k)$ coincide with those of GUE.

Conclusions.—We have studied the shape of the average spectrum and the eigenvalue fluctuations of the embedded ensemble EGUE(k) in the limit of infinite matrix dimension, attained by letting the number l of degenerate single-particle states go to infinity. We have shown that for sufficiently high rank k of the random interaction ($2k > m$ where m is the number of fermions), EGUE(k) behaves generically: The spectrum has a semicircle shape, and the eigenvalue fluctuations obey Wigner-Dyson statistics. This does not come as a surprise. A transition to a different regime takes place at or near $2k = m$. It has long been known that the average spectrum changes into a Gaussian shape, although the point of departure from the semicircle shape was not known previously. We have presented conclusive evidence that in addition—and contrary to general expectations—the level fluctuations also change and are not of a Wigner-Dyson type for $2k \lesssim m$. In the extreme case $k \ll m \ll l$, the spectral fluctuations are Poissonian, and the eigenfunctions are likely to display localization in Fock space. We cannot pin down precisely the k value where such change occurs nor can we penetrate deeply into the intermediate regime. This is not surprising as we do not know of any other case where such an aim would have been achieved. We cannot even say definitively whether the transition from Wigner-Dyson to Poissonian statistics is smooth or sudden. But we have circumstantial evidence for a smooth transition: (i) The nonuniversal fluctuations calculated from the loop correction set in smoothly. (ii) In the case $k = 1$, the transition from GUE (for $m = 1$) to Poisson behavior (for $k \ll m$) is smooth. (iii) The ratio K/P of the number of uncorrelated random variables over the number of links changes smoothly with k for fixed m.

Formally and using diagrammatic language, we ascribe the deviations from universal GUE behavior to the fact that with decreasing k, intersecting Wick contraction lines gain increased weight. Universal GUE results are obtained whenever such contributions are negligible. This apparently is the case for $2k > m$. We ascribe the special role of the transition point $2k = m$ to duality.

Physically, our results can be understood in terms of the ratio K/P of the number of uncorrelated random variables over the number of links. We have shown that if all links were to carry uncorrelated random variables, the ensemble would have GUE spectral fluctuations. Conversely, if all links were to carry the same random variable, the ensemble would be completely integrable and display Poissonian statistics. These statements hold for all values of k. The actual situation is located between these two limits. EGUE(1) is closest to the integrable case, and EGUE(m) corresponds to the GUE. This shows that deviations from GUE behavior are not caused by the number of zeros in the matrix representation of the interaction but are strictly due to correlations between the matrix elements carried by the links.

As mentioned in the introduction, numerical simulations have shown good agreement between the spectral fluctuations of EGUE(k) and those of GUE. We ascribe this result to the fact that the dimensions of the matrices used were quite small. It is easy to see that the ratio K/P is relatively close to unity for typical values such as $k = 2$, $m = 8$, and $l = 20$. It is only in the limit $l \gg 1$ that K/P becomes very small, resulting in significant deviations of EGUE(k) spectral fluctuation behavior from Wigner-Dyson statistics.

Details, further results, and the extension to EGOE(k), the orthogonal case, are given in Ref. [10].

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