Localized states in the chaotic Ce atom

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We show that the energy-averaged entropy localization length for the eigenstates of the Ce atom is well approximated by the prediction of the Wigner ensemble.

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In Ref. [1], predictions of the Wigner ensemble [2] of banded random matrices are compared with the results obtained in a model of the Ce atom. In particular, it is shown that, in the basis of single-electron orbitals arranged in increasing order of the corresponding energies, the eigenstates of Ce are localized (see Fig. 12 of Ref. [1]). This finding, although in agreement with recent predictions [3–8] contradicts the widely accepted expectation that the eigenstates of time-independent strongly chaotic systems are generically extended [9], and therefore it is important.

On the quantitative side, the comparison between the average shape of the Wigner-ensemble squared eigenvectors, $\langle |e_{ij}|^2 \rangle = w(i-j)$, where i is the index of the eigenvectors and j is the index of the basis states, and the eigenstates of Ce leads to some agreement, the extent of which is, however, unclear (see Figs. 13 and 20 of Ref. [1]). This comparison is hampered by the fact that w is only implicitly known as the solution of a complicated nonlinear integral equation [2]. It can be explicitly obtained only for $|i-j| < b$ and $|i-j| \gg b$, where b is the bandwidth of the random matrices [10]. Accordingly, in Ref. [1], $\rho_w(u) \equiv w((i-j)/b)$ was separately compared in the two regimes with the corresponding Ce eigenfunctions. In the small-u range, ρ_w is found to be close to the Lorentzian predicted by the Wigner ensemble but having lower tails. Furthermore, in the large-u regime, where better agreement is claimed, ρ_w is compared with partially averaged (over 20 neighbors) eigenvectors of Ce rather than with a fully averaged one. Since in the Ce atom the parameters corresponding to those of the random matrix ensemble, b and α, are varying with energy, it is unjustified to expect such detailed agreement between the two. In what follows, we propose that instead a more global feature of the eigenvectors, e.g., the *average* entropy localization length [11] L should be used as a measure of the agreement between the properties of the Ce atom and the predictions of the Wigner ensemble. Moreover, we show that the values of L for the two models are extremely close to each other.

We use the data of Ref. [1] to calculate the energy-averaged values of b, α, and L, b_{Ce}, α_{Ce}, and L_{Ce}, respectively (see Figs. 3, 14, 21, and 22 of Ref. [1]). In addition, the root mean square of the off-diagonal matrix elements is 0.1 eV (see Table II and text of Ref. [1]). One obtains $b_{\mathrm{Ce}}=78.7$, $\alpha_{\mathrm{Ce}}=0.027$, and $L_{\mathrm{Ce}}=131$ for the $J^{\pi}=4^{-}$ states (odd). Moreover, N_{Ce}, the size of the single-electron-orbital basis used in the calculations of the Ce-atom model, is 260. On the other hand, the numerical computation of L for 100 random matrices with the same parameters gives $L_W=137.4\pm0.8$ for $b=78$ and $L_W=138\pm1$ for $b=79$. We incline to regard this result as being in very good agreement with that for the Ce atom. However, one should estimate the size of the error of L_{Ce} in order to strengthen this statement. This error is due to both our approximate handling of the data of Ref. [1] and the energy variation of the parameters in the Ce atom, which is not accounted for by the Wigner ensemble. It is expected to be of the order of a few percent.

It is worthwhile to point out the relation of these results to the recent studies on the behavior of L_W. It was shown [3–8] that in the scaling regime, namely, for $z \equiv \alpha^{-1} b^{-1/2} \gtrsim 0.3$, $L_W = b^2 f(x,y)$ where $x = b^2/N$ and $y = \alpha b^{3/2}$. In the Ce atom, $z=0.42$, not too far from the edge of the scaling regime. Moreover, $x_{\mathrm{Ce}}=23.8$ and $y_{\mathrm{Ce}}=185.9$, which according to Ref. [6] corresponds to a regime with Anderson-like behavior and $L_W=118.7$. Since the values of x and y for the Ce atom are much larger than the largest ones considered in Ref. [6], the inaccuracy in the predicted value of L_W is not surprising. As far as the spacing distribution $P(s)$ is concerned, the prediction of the Wigner ensemble is that it should follow the Wigner distribution (see Fig. 4 of Ref. [6]). This is indeed observed in the experimental spectrum of the Ce atom (see Fig. 2 of Ref. [1]), in that of the model studied in Ref. [1] for Ce (see Fig. 5 in Ref. [1]), and in all the strongly chaotic models studied up to now. It is presently not clear, however, whether or not strongly chaotic systems can have values of x and y for which the $P(s)$ of the corresponding Wigner ensemble deviates from the Wigner distribution [7].

Finally, we suggest that a simpler model than the Ce atom should be studied in order to verify the predictions of the Wigner ensemble. In particular, the classical dynamics for such a model should be studied to make sure that it is fully chaotic.

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