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# Ergodic properties of local spectral density for a conservative system of coupled quantum states

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**Abstract**

The shape and the inverse participation ratio (IPR) of local spectral density (LSD) are studied for a generic isolated system of coupled quantum states, the Hamiltonian of which is represented by a band random matrix with disordered leading diagonal. We find for the matrices with arbitrary small band that the lack of ergodicity for LSD can be associated with an exponential increase in IPR with the ratio $v/\Delta_c$ ($v$ is the root of the mean square for off-diagonal matrix elements and $\Delta_c$ is the energy spacing between directly coupled basis states). Criteria specifying transition to localization and ergodicity for LSD are considered.

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## 1. Introduction

The statistical properties of quantum systems attract considerable attention in a broad field of modern physics ranging from nuclear, atomic and molecular physics to condensed matter and quantum computing. Of special interest are the properties specifying the quantum chaos border for a system of many-body quantum states. Extensive investigations of many-body interacting systems such as nuclei, many-electron atoms, quantum dots, quantum spin glasses and quantum computer models [1–9] have shown that the border is associated with a crossover of level spacing statistics from the Poisson distribution to the Wigner–Dyson one and with a transition to an ergodic distribution for the eigenstate wavefunction over a large number of basis levels as in random matrix theory (RMT) [10, 11]. In a sense the interaction leads to dynamic thermalization without coupling to an external thermal bath. According to [2, 6, 12] this crossover takes place when the coupling matrix elements of the Hamiltonian become comparable to the energy spacing between directly coupled states.

We address this problem to a generic system of coupled quantum states, the Hamiltonian matrix $\boldsymbol{H}$ of which includes a leading diagonal with disordered random values and random off-diagonal elements inside a band of size $b$. This band random matrix with disordered diagonal (BRMDD) is a reasonable model describing the systems with strong imperfection in the basis

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state energies. Models based on the BRMDD have been applied to study the electron transport problem [13, 14] and the problem of interacting particles in a random potential [15–17]. The results obtained for these models are also of obvious interest in analysing such few-degrees-of-freedom physical objects as the vibrational quasicontinuum of polyatomic molecules [18] and a quantum computer [9].

The statistical properties of BRMDD-based systems have been studied in some detail [15, 16, 19–24]. The shape, the localization length and the inverse participation ratio (IPR) for the eigenfunction have been investigated with the help of numerical simulations [15, 16, 22] and the supersymmetry approach [22, 23]. These investigations have exhibited the Lorentzian shape for local spectral density (LSD) in circumstances when a non-perturbative localization regime is realized. The state–state interaction strength (at which the eigenstates are extended over the whole matrix size $N$ and the eigenenergy level spacing statistics has the Wigner–Dyson form) has been revealed for the BRMDD with sufficiently large band (when $2b + 1 \gg \sqrt{N}$) [16, 21–23]. Unfortunately the ergodic properties of LSD have not been investigated in detail. Another open question is the quantum chaos border for the BRMDD with arbitrary small band.

In the paper we study localization and ergodicity properties of LSD to be obtained from the BRMDD with arbitrary small band. The LSD was introduced in 1955 by Wigner [25] and successfully employed in RMT to describe statistically the localization effects for complex quantum systems [10, 11] (including the systems represented by band random matrices with reordered leading diagonal [26, 27]). This quantity is the Fourier transform for the correlation function $C(t) = \langle 0| \exp(-\mathrm{i}\boldsymbol{H}t/\hbar)|0\rangle$ and specifies spreading of the energy, initially concentrated in a specific unperturbed basis state $|0\rangle$, between the eigenstates due to state–state interaction. Generally the LSD may be characterized by the width $\Gamma$ measuring the energy scale in which the individual state $|0\rangle$ is localized. The number of eigenstates populating this scale is given in terms of the product

$$\xi_e = \rho_E \Gamma \tag{1}$$

designated here as *an ergodic localization length* of LSD ($\rho_E$ is the eigenstate density). Hence the quantity $\xi_e$ specifies the greatest possible number of eigenstates where the basis state $|0\rangle$ can be effectively admixed. The ergodic properties for the system can be identified with the structure of the LSD. The non-ergodic LSD is a strongly fluctuating spiked function and the IPR $\xi_{IPR}$, which gives the actual number of eigenstates involving the state $|0\rangle$, is low in comparison with $\xi_e$. In the ergodicity case the LSD is monotonic and the number $\xi_{IPR}$ approaches the value of $\xi_e$.

The main attention of our study is paid to the perturbative and localized regimes for LSD. Therefore we restrict the study to a moderate strength of state–state interaction. This restriction implies that the width $\Gamma$ is essentially small as compared with the energy scale bounding the location of the eigenstate levels ($\xi_{IPR}, \xi_e \ll N$). The finite-size effects are ignored. Hence the quantities $\xi_e$ and $\xi_{IPR}$ can be considered as functions of the interaction strength and the relative width of band.

We investigate the LSD shape and determine the ergodic localization length. Then we analyse the behaviour of IPR for ergodic and non-ergodic LSD. From this analysis we obtain criteria specifying the transition to localized and ergodic regimes for the LSD.

## 2. Model description

We consider a BRMDD that represents the Hamiltonian matrix $\boldsymbol{H}$ in the basis of unperturbed states $|k\rangle$ ($k = -K, \ldots, K$) for an isolated system of $N = 2K + 1$ quantum states. The BRMDD is a real symmetric matrix with statistically independent random elements

$$H_{mk} = E_k^{(0)}\delta_{mk} + V_{mk} \tag{2}$$

where off-diagonal elements $V_{mk} = V_{km}$ specify the state–state interaction. The values of $V_{mk}$ are distributed uniformly in the interval $[-V, V]$ with $\langle V_{mk}\rangle = 0$ and $v^2 = \langle V_{mk}^2\rangle = V^2/3$ if $|m-k| \leqslant b$ or are zero otherwise. The diagonal elements $E_k^{(0)}$ corresponding to energy levels for the states $|k\rangle$ are uniformly distributed according to the Poisson statistics with the mean spacing $\Delta$ between adjacent energy levels: $-K\Delta \leqslant E_k^{(0)} \leqslant K\Delta$. The energy level $E_0^{(0)}$ for a probing state $|0\rangle$ is located in the midpoint of interval $[-K\Delta, K\Delta]$: $\langle E_k^{(0)}\rangle \approx E_0^{(0)} = 0$.

The perturbation of an individual basis state depends on the relative level position for unperturbed states which are coupled directly with the state by interaction. Therefore the strength of state–state interaction for BRMDD can be specified in terms of the ratio $v/\Delta_c$, where

$$\Delta_c = \frac{\Delta}{\beta} \tag{3}$$

is the energy spacing between directly coupled unperturbed states. Here the relative band width

$$\beta = \frac{b}{K} \tag{4}$$

gives the relative number of states coupled directly with the individual state.

Depending on the relation between $v/\Delta_c$ and $b$, three important regimes can be distinguished [15,16,22,23]. When the coupling matrix elements are weak and $v/\Delta_c \ll 1$ the perturbative regime is realized. In this regime the Hamiltonian (2) can be treated within the framework of perturbation theory. The condition $1 \ll v/\Delta_c \ll \sqrt{b}$ characterizes a regime at which the eigenstates are localized. The strong interaction at $v/\Delta_c \gg \sqrt{b}$ is responsible for a delocalized regime for the eigenfunctions. In the regime the eigenstates are extended over the whole matrix size $N$.

The eigenfunctions $|\alpha_n\rangle$ and the eigenenergies $E_n$ are obtained from diagonalization of (2). The quantity $W_{n0} = |\langle\alpha_n|0\rangle|^2$ gives the probability of finding the probing state $|0\rangle$ in the eigenstate $|\alpha_n\rangle$. The numerical simulation is performed for a wide range of matrix parameters: $2 < N < 3200$, $1 < b < 1600$ and $10^{-3} < v/\Delta < 10^2$. The number of disorder realizations lies in the range from 100 to 1000.

## 3. Shape of LSD

The shape of the LSD is studied for an eigenenergy scale no larger than $5\Gamma$. For this scale the interaction-induced variations in level density are negligible and the eigenenergies are homogeneously distributed with the density $\rho_E \approx 1/\Delta$. Then the LSD can be defined as

$$\rho_W(E) = \rho_E \frac{\langle\sum_n W_{n0}\delta(E-E_n)\rangle}{\langle\sum_n \delta(E-E_n)\rangle}, \tag{5}$$

where $\langle\ldots\rangle$ means the averaging over disorder (that is, over many random matrices). Numerical investigation confirms that the LSD is described by the well known Breit–Wigner distribution of the Lorentzian shape

$$\rho_{BW}(E) = \frac{\Gamma}{2\pi}\frac{1}{E^2 + \Gamma^2/4} \tag{6}$$

(see the inset in figure 1) with the width $\Gamma$. This shape is observed for any $v$, $\Delta_c$, $b$ and $N$ satisfying $\xi_e \ll N$ (including the parameter region where $\Gamma \ll \Delta$). We find the ergodic localization length $\xi_e$ from (1) where the width $\Gamma$ is estimated by fitting of the Lorentzian (6)

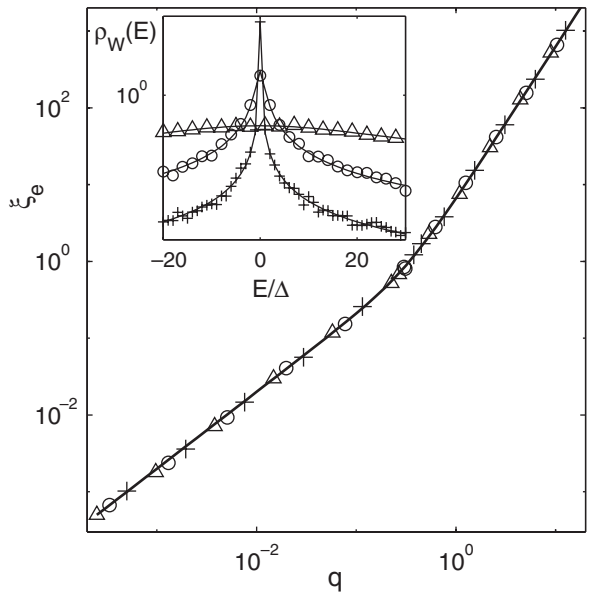


**Figure 1.** Dependence of the ergodic localization length $\xi_e$ on $q$ for $\beta = 1$ (+), 0.5 (○) and 0.04 (△). The solid curve gives the approximation (9). The inset shows a semilog plot for the LSD $\rho_W(E)$ for $\beta = 1$ at $v/\Delta_c = 0.089$ (+, 1000 disorder realizations), $v/\Delta_c = 0.45$ (○,100 disorder realizations) and $v/\Delta_c = 2.82$ (△, 100 disorder realizations). The solid curves give the Breit–Wigner distribution (6) with $\xi_e = 0.05$, 1.3 and 50.

to an averaged LSD. Our analysis of numerical data obtained for different values of $v$, $\Delta_c$ and $\beta$ shows that the quantity $\xi_e$ can be considered as a function of the single parameter

$$q = \frac{v}{\Delta_c\sqrt{\beta}}, \tag{7}$$

which essentially defines the localization of LSD in the eigenenergy scale. When the coupling of the basis states by perturbation is sufficiently strong and $q \gg 1$ the quantity $\xi_e$ satisfies the Fermi golden rule: $\xi_e\Delta = \Gamma \approx 2\pi q^2\Delta = 2\pi v^2/\Delta_c \gg \Delta$. At low values of $q$ ($q \ll 1$) the length $\xi_e$ can be described by a linear function of $q$: $\xi_e \approx 2q$. The width $\Gamma$ is then much smaller than the spacing $\Delta$. Figure 1 demonstrates the behaviour of $\xi_e$ in a wide range of $q$ at three fixed magnitudes of $\beta$.

The linear dependence of $\xi_e$ and $\Gamma$ on the strength of state–state coupling for small $q$ can be explained in terms of a simple perturbation approach to the eigenenergy levels $E_n$ located in the vicinity of $E_0^{(0)}$: $|E_n - E_0^{(0)}| \lesssim v \ll \Delta$. In this approach the eigenstate $|\alpha_n\rangle$ is considered as a superposition of the nearest basis states $|0\rangle$ and $|n\rangle$. The probability $W_{n0}$ of finding the basis state $|0\rangle$ in the eigenstate $|\alpha_n\rangle$ can be then estimated from a two-state (the states $|0\rangle$ and $|n\rangle$) approximation. According to this approximation the dependence of $W_{n0}$ on $E_n$ for an individual disorder realization is Lorentzian-like

$$W_{n0} \approx \frac{V_{n0}^2}{V_{n0}^2 + (E_n - E_0^{(0)})^2} \tag{8}$$

with the width of $2|V_{n0}|$. If the states $|0\rangle$ and $|n\rangle$ are not coupled by interaction the dependence (8) is considered as a function the width of which is negligible in comparison with $v$. The probability that the states $|0\rangle$ and $|n\rangle$ are coupled by interaction is equal to $\beta$. As a result the shape of the disorder-averaged LSD is described by the Lorentzian-like contour with the

width $\Gamma \approx 2\beta v$. It seems that this perturbation approach can also be applied for the eigenstates with $|E_n - E_0^{(0)}| \gg \Delta$, when the probability $W_{n0}$ is essentially small as compared with the contributions of other basis states. In this limit equation (8) gives $W_{n0} \approx V_{n0}^2/(E_n^{(0)} - E_0^{(0)})^2$, as predicted in the framework of a standard perturbation approach for non-degenerate states (see, for instance, in [28]).

In order to estimate the localization properties of LSD at intermediate values of $q$ we approximate the behaviour of ergodic length for a wide range of $q$ ($10^{-3} < q < 15$). The analysis of numerical data shows that the length $\xi_e$ can be well approximated by

$$\xi_e \approx L_1 q \sqrt{1 + (L_2 q)^2} \tag{9}$$

with the fitted coefficients $L_1 = 2.01 \approx 2$ and $L_2 = 3.16 \approx \pi$. According to (9) an accurate boundary between the linear and quadratic dependences of $\xi_e$ on $q$ is obtained at $q \approx 1/L_2$ where $\xi_e \approx 0.9$. Notice that this boundary separates the ranges where the value of $\xi_e$ is low or high as compared with 1.

## 4. Participation ratio for LSD

The IPR $\xi_{IPR} = (\langle \sum_n \mid W_{n0}^{(s)} \mid^2 \rangle_s)^{-1}$ is associated with the parameters $q$ and $\beta$, which specify respectively the ergodic localization length $\xi_e$ for LSD and the band width for BRMDD. This association depends on whether or not the LSD is ergodic. In the ergodic case the probing state is monotonically spread over eigenstates in the energy scale $\Gamma$. Then the IPR is a function of the only parameter $q$ and approaches the ergodic length $\xi_e$. The ergodic LSD can be realized from BRMDD with large band. Our analysis of calculated data for the matrices with $\beta \sim 1$ shows that the best approximation for ergodic IPR is

$$\xi_{IPR} \approx 1 + D_1 q \sqrt{1 + (D_2 q)^2} \approx 1 + \xi_e. \tag{10}$$

The fitted coefficients $D_1 = 3.16$ and $D_2 = 1.94$ are obtained for full Hamiltonian matrices (2) with $\beta = 1$ where all $2K$ basis states are directly linked with the state $|0\rangle$. Notice that the approximation (10) gives the maximum allowable magnitude of IPR for BRMDD at fixed $q$.

An essentially non-ergodic LSD can be obtained from BRMDD with $\beta \ll 1$. Then the IPR is significantly low in comparison with $\xi_e$ and should be considered as a function depending both on the parameter $q$ and on $\beta$. The analysis of numerical data for matrices with low magnitudes of $q$ and $\beta$ shows that the lack of ergodicity for LSD can be clearly identified with an exponential increase in IPR with the quantity $q\sqrt{\beta} = v/\Delta_c$

$$\xi_{IPR} \approx \exp(Cq\sqrt{\beta}). \tag{11}$$

At fixed $\beta$ the IPR is shown in figure 2 to increase exponentially with the rate $C\sqrt{\beta}$ ($C \approx 3.0$–3.2) as the parameter $q$ rises if $\xi_{IPR} \ll \xi_e$. The increase is observed up to the point where $\xi_{IPR} \sim \xi_e$. Then the IPR approaches asymptotically the length $\xi_e$ from below with increasing $q$. At high magnitudes of $q$ and $\beta$, when the exponential (11) gives higher values of $\xi_{IPR}$ in comparison with $\xi_e$, the LSD is ergodic and the IPR can be determined from (10).

For a broad range of $q$ and $\beta$ satisfying $\xi_{IPR} < \xi_e/2.7$, mean square fitting gives the coefficient $C = 3.15 \pm 0.01$. Figure 3 demonstrates a good accordance between the calculated and fitted values of IPR for non-ergodic LSD. Unfortunately we can give no heuristic explanation of the exponential rise in IPR with $q\sqrt{\beta}$. Notice only that this rise is observed under conditions when the eigenstates are essentially localized and $l_{sb}/N \approx q^2\beta^2 \ll 1$ ($l_{sb}$ is the eigenstate localization length).

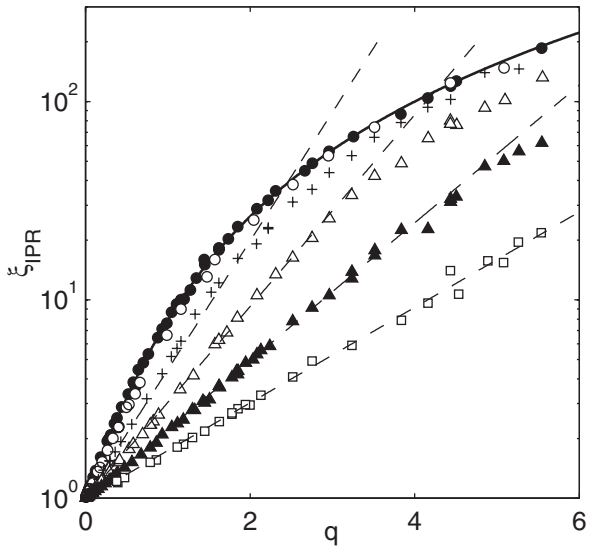


**Figure 2.** Dependence of the IPR $\xi_{IPR}$ on $q$ for $\beta$ =1 (●), 1/2 (○), 1/4 (+), 1/8 (△), 1/16 (▲) and 1/32 (□). The dashed lines give the exponential (11) for $\beta = 1/4$ ($C = 2.99$), 1/8 ($C = 3.15$), 1/16 ($C = 3.19$) and 1/32 ($C = 3.13$). The solid curve shows the ergodic approximation (6) of the IPR.

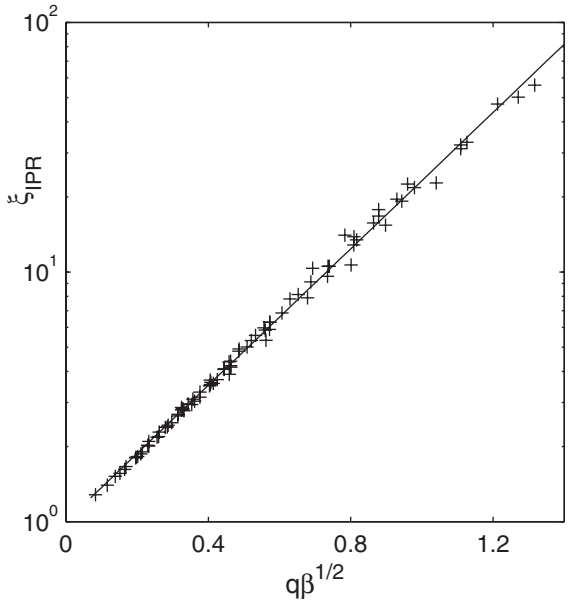


**Figure 3.** Dependence of the IPR $\xi_{IPR}$ on the product $q\sqrt{\beta}$ for a broad range of $q$ ($0.01 < q < 10$) and $\beta$ ($\beta > 0.001$) satisfying the requirement $\xi_{IPR} < \xi_e/2.7$ (+). The solid line shows the approximating exponential (11) with $C = 3.15$.

## 5. Criteria of localization and ergodicity of LSD

We associate the localized regime for LSD with a high magnitude of IPR. For BRMDD with arbitrary small band the requirement $\xi_{IPR} \gg 1$ is seen from (10) and (11) to result in

$$v/\Delta_c = q\sqrt{\beta} > q_d\sqrt{\beta_d} = 1/C_0 \sim 1/\pi, \tag{12}$$

no matter what the ergodic properties of LSD and the magnitude of $\beta$. The parameters $q_d$ and $\beta_d$ then define a localization border on the plane $(q, \beta)$, that is a boundary between regions where the perturbative ($\xi_{IPR} \sim 1$) or localized ($\xi_{IPR} \gg 1$) regimes are realized. Notice that, as for LSD, the criterion (12) specifies a transition to the localized regime for the eigenstate [15, 16, 22, 23].

The attainment of ergodic LSD for BRMDD is defined by the relative width of the band. For the matrices with $\beta \sim 1$ the localized LSD is nearly ergodic and the ergodicity criterion can be represented by the condition (12). This condition is in good agreement with a quantum chaos border for many-body systems and gives the crossover of level spacing statistics from the Poisson to Wigner–Dyson distribution for a nucleus model ($C_0 = 3.0$ [12]) and for a generic model of a quantum computer ($C_0 = 2.5$ [6]). In (12) the factor $C_0$ is assumed to be equal to $C \approx D_1 \approx \pi$.

For BRMDD with $\beta \ll 1$ we should take into account the exponential growth (11) of IPR with $v/\Delta_c$. The criterion of LSD ergodicity can then be determined from the requirement $\exp(Cq\sqrt{\beta}) > \xi_e$, that results in

$$v/\Delta_c = q\sqrt{\beta} > q_e\sqrt{\beta_e} = \frac{\ln(2\pi q_e^2)}{C} \approx \frac{\ln(2\pi q_e^2)}{\pi}, \tag{13}$$

where the values of $q_e$ and $\beta_e$ specify an ergodicity border on the plane $(q, \beta)$. Notice that the condition (13) is a more severe restriction imposed on the parameters $q$ and $\beta$ than the criterion (12).

Our study reveals some distinctive features in behaviour of LSD for BRMDD with arbitrary small band. These features are outlined on the plane $(q, \beta)$ in figure 4 to depend on the relation between $v/\Delta_c$ and $\beta$. As for the eigenstates, the perturbative regime for LSD can be associated with the requirement $v/\Delta_c \ll 1/3$. In contrast to the eigenstates, the localization properties of the LSD are essentially defined by the magnitude of $q$. In the limit $q \ll 1/3$ (that is, $v/\Delta_c \ll \sqrt{\beta}/3$) the ergodic localization length is a linear function of $q$ and $\xi_e \approx 2v/\Delta_c\sqrt{\beta}$. Due to weak state–state interaction the LSD is a delta-like function confined in an eigenstate: $\xi_e \ll \xi_{IPR} \sim 1$. At higher values of $q$ ($1 \ll 3q \ll 1/\sqrt{\beta}$ or $\sqrt{\beta} \ll 3v/\Delta_c \ll 1$) the quantity $\xi_e$ satisfies the Fermi golden rule: $\xi_e \approx 2\pi v^2/\Delta_c^2\beta$. Despite the wide spreading of basis states over the eigenenergy scale, the actual number of eigenstates associated with an individual basis state for this parameter region remains small: $\xi_e \gg \xi_{IPR} \sim 1$.

The criterion (12) specifies a transition from the perturbative to the localized regime both for the eigenstates and for the LSD. Depending on the ergodicity properties of the localized LSD, one can distinguish two important parameter ranges. An area located between the borders (12) and (13) on the plane $(q, \beta)$ corresponds to the parameter region $1 \ll 3v/\Delta_c \ll \ln(\xi_e)$ where $\xi_e \approx 2\pi v^2/\Delta_c^2\beta \ll \xi_{IPR} \approx \exp(Cv/\Delta_c) \gg 1$. For this region the neighbouring eigenstates are weakly coupled by interaction since the density $\xi_{IPR}/\Gamma$ of eigenstates involving the probing state is negligible in comparison with the total state density $\rho_E = \xi_e/\Gamma$. This means that the level spacing statistics $P(S)$ should exhibit a Poisson-like distribution as shown in figure 5. We identify this region with a non-ergodic localized regime for LSD. The regime of ergodic localization for LSD at $v/\Delta_c \gg \ln(\xi_e)/3$ is represented by a domain above the ergodicity border (13) where $\xi_e \approx 2\pi v^2/\Delta_c^2\beta \sim \xi_{IPR} \gg 1$. For this domain the level spacing statistics is close to the Wigner–Dyson distribution (see figure 5), usually associated with quantum chaos. In a sense the condition (13) can be considered as a quantum chaos criterion.

## 6. Conclusion

We have analysed the properties of LSD for a generic conservative system of coupled states, the Hamiltonian of which is represented in terms of a BRMDD. As for the eigenstates, the

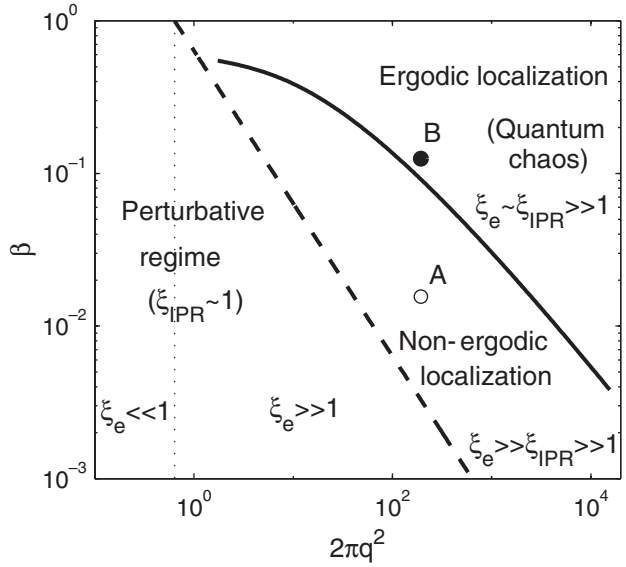


**Figure 4.** Localization regimes depending on the parameters $q$ and $\beta$. The thick dashed line shows the localization border (12). The thick solid curve gives the LSD ergodicity border (13). The dotted line indicates a boundary between the regions with $\xi_e < 1$ and $\xi_e > 1$. The points A ($q = 5.55$, $\beta = 0.016$) and B ($q = 5.55$, $\beta = 0.125$) give the parameter sets used to obtain the level spacing statistics represented in figure 5.

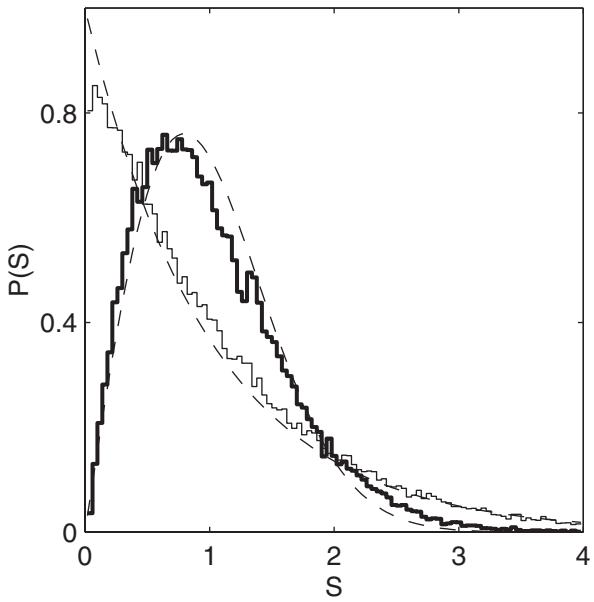


**Figure 5.** Level spacing statistics $P(S)$ at $\xi_e = 193.5$ for non-ergodic ($\beta = 0.016$, $\xi_{IPR} = 10.3$, solid steps) and ergodic ($\beta = 0.125$, $\xi_{IPR} = 150.5$, thick steps) LSD localization regimes, represented respectively by the points A and B in figure 4. The dashed curves show the Poisson and Wigner–Dyson distributions.

transition from the perturbative to the localized regime for LSD can be associated with the same requirement to be imposed on the strength of state–state interaction. Nevertheless, our study has revealed some distinctive features in the properties of LSD. We have determined localization and ergodicity borders for LSD obtained from BRMDD with arbitrary small band. For the matrices with large band ($\beta \sim 1$) the borders coincide with each other and are in good agreement with the quantum chaos border for some generic many-body systems. For the matrices with small band ($\beta \ll 1$) the criterion of LSD ergodicity is a more severe requirement imposed on the band size and the interaction strength than the localization criterion. In the parameter range between the borders the IPR is found to increase exponentially with the ratio $v/\Delta_c$, which specifies the strength of state–state interaction. We suppose that such an effect can be observed for any isolated system of coupled states with strong imperfection in non-perturbed energies.

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