# Semiclassical structure of Hamiltonians

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The structure of few-body Hamiltonian matrices is studied in the semiclassical regime. Given $(\hat{A}_1(\hat{\mathbf{q}},\hat{\mathbf{p}}), \hat{A}_2(\hat{\mathbf{q}},\hat{\mathbf{p}}))$, a pair of operators, it can be shown that, under quite general conditions, $\hat{A}_2$ takes the form of a banded matrix in the ordered eigenrepresentation of $\hat{A}_1$. Moreover, the bandwidth depends only on $\hbar$ and certain generalized microcanonical averages. In particular, if $H=H_0+\epsilon V$, this implies that the perturbed Hamiltonian is banded in the appropriately ordered unperturbed basis.

## I. INTRODUCTION AND THEORETICAL PREDICTIONS

Many of the predictions of semiclassical mechanics are limited to systems with an integrable classical analog. However, an expression for the density of states $\rho(E)$ has been derived which applies to both classically integrable and chaotic systems.[1-3] For the two-degrees-of-freedom case ($d=2$)

$$\rho(E)=\sum_n \delta(E-E_n)=\rho_0(E)+\rho_{\rm osc}(E)\ , \tag{1}$$

where to lowest order in $\hbar$

$$\rho_0(E)=\frac{1}{\hbar^2}\int d^2q \int d^2p\ \delta(E-H(\mathbf{q},\mathbf{p}))\ , \tag{2a}$$

$$\rho_{\rm osc}(E)=\frac{2}{h}\sum_j A_j \exp\left[i\frac{S_j}{\hbar}-i\nu_j\frac{\pi}{2}\right]\ . \tag{2b}$$

The summation in Eq. (2b) runs over all the periodic orbits. $S_j$ and $\nu_j$ are the action and number of conjugated points corresponding to the $j$th periodic orbit. The smooth part of $\rho(E)$,$\rho_0(E)$ can alternatively be obtained by convoluting the high-energy part of $\rho(E)$ with a smoothing function $f_{\gamma_0}(E)$ of width $\gamma_0$,

$$\rho_0(E)=\lim_{\hbar\to 0}\frac{\gamma_0}{\pi}\int_{-\infty}^{\infty} dE' f_{\gamma_0}(E-E')\rho(E')$$
$$\equiv F[\rho(E)]\ , \tag{3}$$

where $\gamma_0=h(\partial S_0/\partial E)^{-1}$ and $S_0$ is the action corresponding to the shortest periodic orbit.

The purpose of this paper is to derive a relation similar to that in Eqs. (2a) and (3) for diagonal matrix elements of operators[4-11] and to study some of its implications to the global structure of the corresponding matrices. In particular, we find that Hamiltonian matrices are quite often banded. In other words, the off-diagonal matrix elements decay in absolute value as a function of the distance from the diagonal. Our theoretical predictions are the subject of the present section. In order to illustrate our results, we proceed in Sec. II with a detailed study of some examples. Next, in Sec. III, we show that certain convergence properties of eigenvalues can be better understood by means of banded random matrices rather than the usual Gaussian orthogonal ensemble (GOE). We finally conclude our discussion in Sec. IV.

To start with, we discuss the expectation values $A(E)\equiv\langle E|\hat{A}|E\rangle$ of an operator $\hat{A}(\hat{q},\hat{p})$ with respect to the eigenstates of $\hat{H}=(\hat{q},\hat{p})$, $\hat{H}|E\rangle=E|E\rangle$. Our aim is to relate the smoothed diagonal elements function to some phase-space integral involving the classical analogs of $\hat{A}$ and $\hat{H}$. Since

$$A(E)=\begin{cases}\langle E_n|\hat{A}|E_n\rangle\ , & E=E_n\\ 0\ , & E\neq E_n\end{cases} \tag{4}$$

a similar smoothing procedure as the one in Eq. (3) leads to a function which is identically zero. As a consequence, from the smoothing viewpoint one needs to distinguish between the class of functions with a finite integral, as $\rho(E)$ for example, and those with a vanishing integral. In the first case, it is natural to use the $F$ transformation which is described in Eq. (3). For functions of the second type, however, a discrete averaging over an energy inter-

val of length $\gamma_0$ is appropriate. We shall refer to this as a $\tilde{F}$ transformation

$$\tilde{F}[A(E)]=\lim_{\hbar\to 0}\frac{1}{\rho(E)\gamma_0}\sum_{E_n>E-(\gamma_0/2)}^{E_n<E+(\gamma_0/2)}\langle E_n|\hat{A}|E_n\rangle$$
$$=\frac{1}{\rho_0(E)}\lim_{\hbar\to 0}\int_{-\infty}^{\infty}f_{\gamma_0}(E-E')\langle E'|\hat{A}|E'\rangle \times\rho(E')dE' , \quad (5)$$

where we have chosen

$$f_\gamma(E)=\begin{cases}\frac{1}{\gamma}, & |E|\le\gamma/2\\ 0, & |E|>\gamma/2 .\end{cases} \quad (6)$$

Next, we need to specify the nature of the classical analogs of the $\hat{A}$ and $\hat{H}$ operators. This task is straightforward if the explicit dependence of $\hat{A}(\hat{\mathbf{q}},\hat{\mathbf{p}})$ on $\hbar$ can be expressed in the form of a Laurent series but has no essential singularity at $\hbar=0$. We shall confine our studies to this case. Then $A(\mathbf{q},\mathbf{p})$ has the same functional dependence on $(\mathbf{q},\mathbf{p})$ as the dependence on $(\hat{\mathbf{q}},\hat{\mathbf{p}})$ of the lowest order in this expansion. A similar statement defines $H(\mathbf{q},\mathbf{p})$. Littlejohn[12] refers to $A(\mathbf{q},\mathbf{p})$ as the *principal symbol* of $\hat{A}(\hat{\mathbf{q}},\hat{\mathbf{p}})$. In this notation

$$\tilde{F}[A(E)]=\{A\}_E \equiv\frac{\int d\mathbf{q}\int d\mathbf{p}\,A(\mathbf{q},\mathbf{p})\delta(E-H(\mathbf{q},\mathbf{p}))}{\int d\mathbf{q}\int d\mathbf{p}\,\delta(E-H(\mathbf{q},\mathbf{p}))} . \quad (7)$$

The validity of this expression is further restricted to Hamiltonians with discrete spectra and operators for which the integrals on the right hand side are finite. It is important to realize that these restrictions are not pertinent only to pathological situations. For example, the evolution operator $\hat{U}=\exp[-(i/\hbar)t\hat{H}]$ is excluded due to its essential singularity at $\hbar=0$. Likewise, projection operators are inadequate because they cannot be expressed as functions of canonical variables. When valid, Eq. (7) [like Eq. (3)] relates a quantum-mechanical object, namely, the smoothed expectation values, to a purely classical quantity, the microcanonical average.

In order to establish Eq. (7) we shall use the properties of the corresponding Weyl symbols $A_W(\mathbf{q},\mathbf{p})$. These have been introduced as a representation independent, symplectic invariant association between operators on Hilbert space and functions on phase space.[13] On one hand, this association is not unique; other phase-space functions can be defined, e.g., the coherent-state symbol. On the other hand, whenever the various symbols have at most pole singularities at $\hbar=0$, the corresponding lowest order is identical to the principal symbol, $\lim_{\hbar\to 0}A_W(\mathbf{q},\mathbf{p})=A(\mathbf{q},\mathbf{p})$. One can show that it is sufficient that $\hat{A}$ have a no-essential-singularity Laurent expansion in $\hbar$ in order for the corresponding symbols to also have one. Accordingly, this requirement does not represent an additional constraint on the class of operators for which Eq. (7) holds. Although the Wigner-Weyl formalism has been reviewed several times in the past,[14,12,15] we have included a summary of the relevant formulas in the Appendix. Applying the $F$ transformation to the left-hand side of Eq. (A13) and replacing $\hat{A}$ with $\hat{A}\delta(E-\hat{H})$ we obtain

$$F[\mathrm{Tr}[\hat{A}\delta(E-\hat{H})]]=F\left[\sum_n\langle E_n|\hat{A}|E_n\rangle\delta(E-E_n)\right]$$
$$=\lim_{\hbar\to 0}\int_{-\infty}^{\infty}f_{\gamma_0}(E-E')\sum_n\langle E_n|\hat{A}|E_n\rangle\delta(E'-E_n)dE'$$
$$=\lim_{\hbar\to 0}\int_{-\infty}^{\infty}f_{\gamma_0}(E-E')A(E)\rho(E)dE'=\tilde{F}[A(E)]\rho_0(E) . \quad (8)$$

Next we notice that in the $\hbar\to 0$ limit $f_{\gamma_0}$ tends to a $\delta$ function and the Weyl symbol becomes the principal symbol. Thus, under the $F$ transformation the corresponding right-hand side of Eq. (A13) reduces to the phase-space integral of the principal symbol. Equating the two sides and using Eq. (2a) for $\rho_0$, one immediately obtains Eq. (7).

In order to illustrate the behavior of the individual matrix elements and how it leads to Eq. (7), it is useful to consider Eq. (A15). It has been conjectured long ago,[14,16] that the semiclassical Wigner function corresponding to an eigenstate is concentrated on the region explored by a typical trajectory over infinite times. At present, the exact interpretation of this conjecture is subject to controversy mainly due to the scaring in the stadium eigenfunctions found by Heller.[17] While it is certainly not clear whether deviations from the conjectured Wigner functions vanish in the semiclassical limit, for the sake of the argument, we shall assume this to be the case. The region explored by a classical trajectory over infinite times is the entire energy shell for a strongly chaotic (ergodic) system and a torus for an integrable system. As a consequence, the semiclassical Wigner function for the former is a homogeneous distribution over the energy shell and Eq. (A15) leads to a version of Eq. (7) which holds for *individual* matrix elements. At finite values of $\hbar$, the fluctuations of the individual matrix elements around the microcanonical average are obviously related to the devia-

tions of the Wigner functions from the homogeneous form. On the other hand, in the case of integrable systems the energy surface is represented by a curve in action space. A finite number of tori in the neighborhood of this curve $N$ satisfy the quantization conditions. At fixed energy, $N$ is $O(\hbar^{-1})$ and therefore, these tori divide the energy shell into $N$ segments of length $O(\hbar)$ each. Moreover, the tori are homogeneously covering the angle directions and thus the associated Wigner functions are characterized by an $O(\hbar)$ spread in the actions. Under these circumstances, the only way to simulate a Wigner function which is homogeneous over the energy shell is to average over all the $N$ tori. Inserting this averaged Wigner function into Eq. (A15) one immediately retrieves Eq. (7). It should be stressed, however, that at fixed energy, the deviations of the individual matrix elements from the microcanonical average do not decay as $\hbar\to 0$.

Various global properties of the operator matrix $A_{nk}=\langle E_n|\hat{A}|E_k\rangle$ can be studied employing the formalism we have just developed. For example, we can define a bandwidth for operator $A$, $\Delta E_A$, at energy $E_n$

$$(\Delta E_{n,A})^2\equiv\frac{\sum_k (E_n-E_k)^2|A_{nk}|^2}{\sum_{k\neq n}|A_{nk}|^2}=\frac{\langle E_n|([i\hat{H},\hat{A}])^2|E_n\rangle}{\langle E_n|\hat{A}^2|E_n\rangle-\langle E_n|\hat{A}|E_n\rangle^2}\ . \tag{9}$$

Replacing the quantum commutator with the corresponding Poisson bracket $[\ ]_{\rm PB}$ and using Eq. (7) we obtain

$$(\tilde{\Delta}E_{n,A})^2\equiv\tilde{F}[(\Delta E_{n,A})^2]=\hbar^2\frac{\{[H,A]^2_{\rm PB}\}_{E_n}}{\{A^2\}_{E_n}-\{A\}^2_{E_n}}\ . \tag{10}$$

For a given value of $\hbar$, the bandwidth $\tilde{\Delta}E_{n,A}$ is finite and therefore the $A_{nk}$ matrix elements must be a decaying function of $|E_k-E_n|$. This is the origin of a quasidiagonal (banded) structure. The width of this band can be easily translated to the number of states it includes, $\tilde{\Delta}M_{n,A}=\rho_0(E_n)\tilde{\Delta}E_{n,A}$. Remarkably, $\tilde{\Delta}M_{n,A}=O(\hbar^{-1})$ and therefore diverges as $\hbar\to 0$. It is, however, important to mention that if only a fixed range of energy is considered, the size of the $\hat{A}$ matrix is $M=O(\hbar^{-2})$. As a consequence, for an operator matrix which has been truncated according to a classical criterion the bandwidth diverges in the $\hbar\to 0$ limit slower than the matrix size. We shall return to this point in Sec. II.

We now turn to the last part of this section in which it is shown that our conclusions concerning the structure of operators apply to Hamiltonians as well. This is true simply because any operator can play the role of a Hamiltonian. Let us first stress that the statements in Eqs. (7) and (10) generalize in a straightforward manner to a pair of operators $(\hat{A}_1,\hat{A}_2)$ subject to the same restrictions as in the case of $(\hat{H},\hat{A})$ pairs. The first member of the pair $A_1$ fixes the basis (its eigenvectors, $v_{1n}$) and its appropriate arrangement (in increasing order of the eigenvalues $a_{1n}$). Consequently, the second member $\hat{A}_2$ will have a smoothed band-width

$$(\tilde{\Delta}a_{1n,(A_1,A_2)})^2\equiv\tilde{F}[(\Delta a_{1n,(A_1,A_2)})^2]=\tilde{F}\left[\frac{\sum_k (a_{1n}-a_{1k})^2|\langle v_{1n}|\hat{A}_2|v_{1k}\rangle|^2}{\sum_{k(\neq n)}|\langle v_{1n}|\hat{A}_2|v_{1k}\rangle|^2}\right]=\hbar^2\frac{\{[A_1,A_2]^2_{\rm PB}\}_{a_{1n}}}{\{A_2^2\}_{a_{1n}}-\{A_2\}^2_{a_{1n}}} \tag{11}$$

and similarly $\tilde{\Delta}M_{n,(A_1,A_2)}=\rho_0(a_{1n})\tilde{\Delta}a_{1n,(A_1,A_2)}$. Here

$$\{A_2\}_{a_{1n}}=\frac{\int d\mathbf{q}\int d\mathbf{p}\ A_2(\mathbf{q},\mathbf{p})\delta(a_{1n}-A_1(\mathbf{q},\mathbf{p}))}{\int d\mathbf{q}\int d\mathbf{p}\,\delta(a_{1n}-A_1(\mathbf{q},\mathbf{p}))} \tag{12}$$

and

$$\rho_0(a_{1n})=h^{-2}\int d\mathbf{q}\int d\mathbf{p}\,\delta(a_{1n}-A_1(\mathbf{q},\mathbf{p}))\ . \tag{13}$$

Evidently, in our original discussion pairs of the type $(\hat{H},\hat{A}_2)$ were treated. However, for understanding the semiclassical structure of Hamiltonians we need to study $(\hat{A}_1,\hat{H})$ pairs. Fortunately, all these cases are equally well described by Eqs. (11)–(13). One can alternatively interpret the $(\hat{A}_1,\hat{H})$ pairs as specifying the representation in which $\hat{H}$ is banded. In Sec. II we present several examples in order to support our heuristic arguments.

## II. EXAMPLES

We open the series of examples with the study of coupled harmonic oscillators

$$H=\sum_{i=1}^{2}H_{0i}+\epsilon V=\tfrac{1}{2}\sum_{i=1}^{2}(p_i^2+x_i^2)+\epsilon V(x_1,x_2)\ . \tag{14}$$

The actions for $\epsilon=0$ are just $J_i=H_{0i}$ and semiclassically these assume only a countable number of values $J_i=\hbar(m_i+\frac{1}{2})$. Therefore, in the quantum number space the eigenstates of $H_0$ form a square lattice. In the language of Sec. I, we shall study the band properties of $H$ as the second member of the $(H_0,H)$ pair. There is some freedom in arranging the $|m_1,m_2\rangle$ basis due to the degeneracy in the eigenvalues of $H_0$,

$$E_{0,M}\equiv E_{0,m_1,m_2}=\hbar\sum_{i=1}^{2}(m_i+\tfrac{1}{2})\ .$$

This degeneracy is irrelevant to our argument and therefore we suppose that it is removed by an infinitesimal perturbation such that $E_{0,m_1+1,m_2}>E_{0,m_1,m_2+1}$. The ordering appropriate to this setting is indicated in Fig. 1(a).

Suppose now $\epsilon$ is made finite and $V$ is a $p$-order polynomial. Writing the potential in terms of raising and lowering operators it is easy to see that given a site on the square lattice, $|m_1,m_2\rangle$

$$\langle m_1,m_2|H|m_1+j,m_2\rangle=\begin{cases}\text{finite or } 0\ , & |j|\le p\\ 0\ , & |j|>p\ .\end{cases} \tag{15}$$

Therefore, at most $2p+1$ rows in each direction $m_i$ are connected by nonvanishing matrix elements and as a

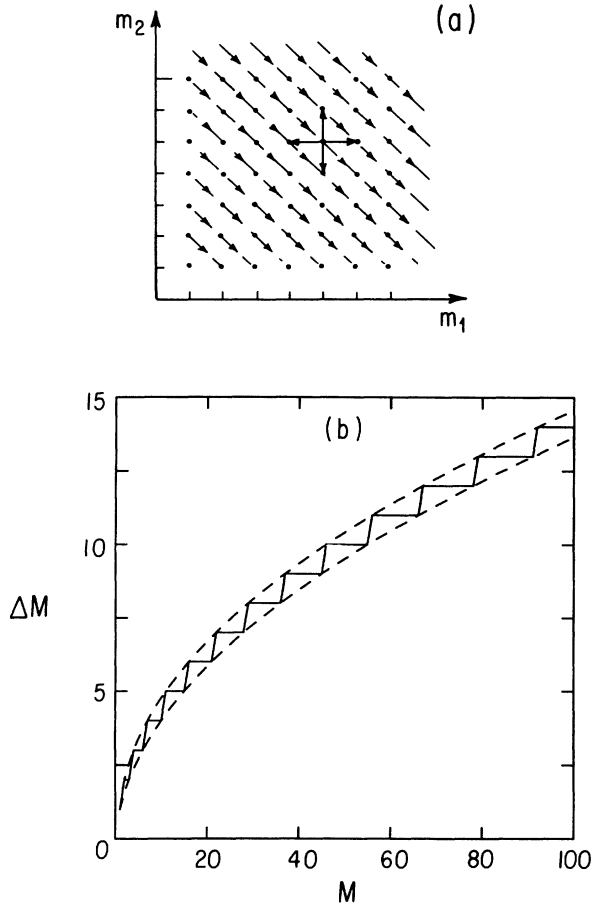


FIG. 1. Properties of the system in Eq. (14) with $\epsilon V(x_1,x_2)=ax_1+bx_2$. (a) Quantum number lattice for $H_0$. The solid arrows depict the nonvanishing matrix elements at a lattice point. The dashed arrows describe the way in which the basis is ordered. Notice that at the end of a diagonal we return to the beginning of the next one when arranging the basis. (b) Bandwidth $\Delta M$ vs $M$ (solid). The dashed curves correspond to the bounds on $\Delta M$ given in Eq. (16).

consequence, $H$ is banded. Let us restrict our attention to the case $p=1$ which is obviously the easiest to study. It corresponds to a potential $\epsilon V(x_1,x_2)=ax_1+bx_2$ for which $H$ is exactly integrable. Since $\{H\}_{E_0}=E_0$, Eq. (7) is immediately satisfied. Moreover, due to the quadratic form of the Hamiltonian the fluctuations vanish and the $\tilde{F}$ transformation is unnecessary. Using the quantum-mechanical definition in the left-hand side of Eq. (11) one obtains $\Delta E_0 \equiv \Delta E_{0M,(H_0,H)}=\hbar$. Exactly the same result is obtained from the classical calculation corresponding to the right-hand side of Eq. (11). Since $\rho_0(E_0)=\hbar^{-2}E_0$, we obtain $\Delta M \equiv \Delta M_{M,(H_0,H)}=\hbar^{-1}E_0$. As is shown in Fig. 1(b), $\Delta M$ is a steplike function of the row number $M$. However, at fixed $\Delta M$

$$\frac{\Delta M^2-\Delta M+2}{2}<M<\frac{\Delta M^2+\Delta M}{2} \tag{16}$$

and therefore $\lim_{M\to\infty}\Delta M=\sqrt{2M}$. As a consequence, $M=O(\hbar^{-2})$ which is in agreement with our predictions.

In order of increasing complexity, after studying a pair where both members are integrable, we proceed to an example where the first pair member $H$,

$$H=L_{1z}+L_{2z}+L_{1x}L_{2x} \tag{17}$$

is nonintegrable. Specifically, the corresponding classical motion changes gradually from regular to strongly chaotic as the energy of the system is lowered.[4] The second member of this pair

$$A_2 \equiv H_0=L_{1z}+L_{2z} \tag{18}$$

is once again exactly integrable. The angular momenta in Eqs. (17) and (18) satisfy $L_i=(L_{ix}^2+L_{iy}^2+L_{iz}^2)^{1/2}$ and therefore the energy is bounded. When $L_1=L_2=L$,

$$|E| \le \begin{cases} 2L\ , & L<1 \\ 1+L^2\ , & L>1\ . \end{cases} \tag{19}$$

The equations of motion for this system

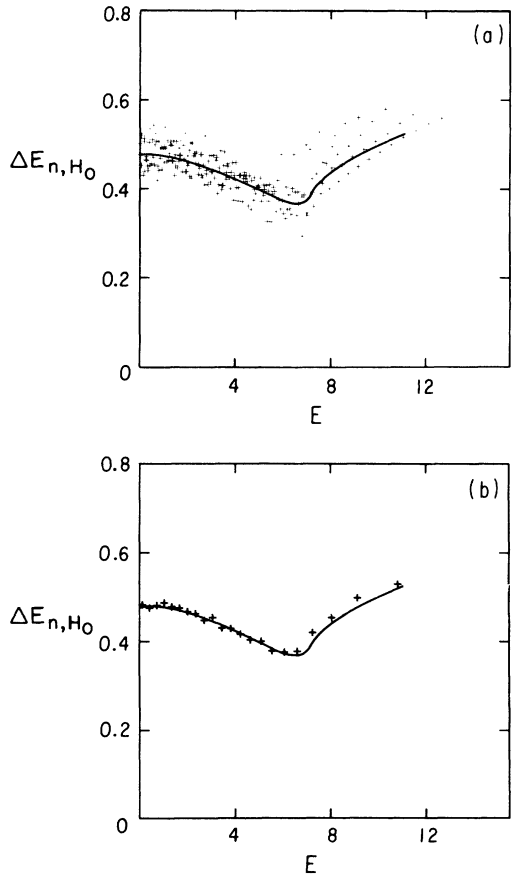


FIG. 2. Semiclassical value for $\tilde{\Delta}E_{n,H_0}$ as given by the right-hand side of Eq. (10) vs energy (solid) for the $(H,H_0)$ pair [see also Eqs. (17) and (18)] is compared with (a) the exact quantum-mechanical values of $\Delta E_{n,A}$ as defined in Eq. (9) (crosses). (b) $\tilde{\Delta}E_{n,A}$ values obtained from smoothing $\Delta E_{n,A}$ with the $f_\gamma$ of Eq. (6) (crosses).

$$\dot{L}_i=[\mathbf{L}_i,H]_{\mathrm{PB}} \tag{20}$$

can be obtained using the standard angular-momentum algebra. Apparently, the operators in Eqs. (17) and (18) are not functions of canonical variables and therefore do not satisfy one of the basic requirements of our formalism. However, one can find a transformation from angular-momentum variables to canonical ones[18] and consequently avoid this inconsistency. When $L_1=L_2=3.5$ most trajectories are chaotic if $|E|\leq 6.6$ and regular for $|E|\geq 9.1$. For energies in the range $6.6\leq|E|\leq 9.1$ regular and chaotic trajectories coexist. Quantum mechanically, $H$ is represented in the $H_0$ eigenbasis by a matrix of finite size $M$. Since $L_i^2=\hbar^2 l_i(l_i+1)$, $M=(2l_1+1)(2l_2+1)$, and therefore $M=O(\hbar^{-2})$ as $\hbar\to 0$. This again coincides with our conclusions from Sec. II.

In previous work, Eq. (7) was numerically checked for the $(H,H_0)$ pair (see Fig. 4 in Ref. 5 and Figs. 5 and 6 in Ref. 9) and good agreement with theory was found in all regimes: chaotic, regular and mixed. Presently, in Fig. 2(a) we compare the quantum-mechanical bandwidth for individual rows as defined in Eq. (9) with the semiclassical bandwidth [see the right-hand side of Eq. (10)] for this pair. As before, we set $l_1=l_2=20$ and therefore $\hbar=0.170\,782\,5$. Notice that the fluctuations around the semiclassical curve are apparently random in the chaotic regime while for the regular case these form a slightly distorted square lattice.[18] Next, in Fig. 2(b) we show that the two sides of Eq. (10) nicely agree with each other even though $N\equiv\gamma\rho_0$ was rather arbitrarily set to 10.

## III. RANDOM MATRICES

Instead of pursuing more examples, in the following we bring indirect but generic support to the proposed semiclassical structure of Hamiltonian matrices. For this purpose Gaussian orthogonal ensemble (GOE) random matrices are used.[19] We claim that if the Hamiltonian matrices of strongly chaotic systems were typical members of the GOE, then, one could never obtain converged eigenvalues using truncated approximations to the full Hamiltonian. However, this method is frequently used in numerical calculations of eigenvalues and the lower bounds on the corresponding errors are only due to limited computational power.[20] We shall show that the two facts can be at least partially reconciled if a band is superimposed on the GOE matrices.

The quantity considered $\Delta_0$ is the error induced in the eigenvalue closest to zero $e_0$ by fluctuations of matrix elements which are outside an $M\times M$ block. Accordingly, we shall study the behavior of $\Delta_0$ as a function of $M$. Since the eigenvalue distribution for the GOE is given by the Wigner semicircle law[21]

$$P(e)=\begin{cases}\dfrac{(4S\sigma^2-e^2)^{1/2}}{2\pi S\sigma^2}, & e^2\leq 4S\sigma^2\\ 0, & e^2>4S\sigma^2\end{cases} \tag{21}$$

where $S$ is the matrix size and is assumed to be large, there are on average $(S-1)/2$ eigenvalues greater than the one we focus on. In this sense, $e_0$ is the eigenvalue which is farthest from the fluctuating elements. The latter correspond to the matrix elements which are arbitrarily set to zero in the truncation approximation to Hamiltonian matrices.

Four different settings are studied. In the first (scheme *I*) to a fixed $M\times M$ random matrix $B$, a *frame* of fluctuating elements $F$ is added. The frame consists of two columns of Gaussian distributed elements one on each side of the original matrix and similarly two rows such that the resulting matrix $B_F$ is symmetric. The distribution of $e_0, P(e_0)$ is obtained by numerically diagonalizing $B_F$ for $q_F$ different realizations of the frame. $\Delta_0$ is defined as the standard deviation of $P(e_0)$ and is averaged over $q_B$ different realizations of $B$. In all our numerical experiments, $q_F=25$ and $q_B=10$. Here, the size of $B_F, S$ is $M+2$. In Fig. 3(a), $\Delta_0(M)$ is compared with the corresponding power-law best fit $\Delta_0=cM^{-\alpha_{\mathrm{I}}}$, where $\alpha_{\mathrm{I}}=0.550\pm 0.034$. One might be tempted to conclude that the eigenvalues do converge as the size of $B$ is increased. However, this convergence is the consequence of a rather artificial effect. Namely, for $|e_0|\ll 2\sigma\sqrt{S}$ there is an $O(M^{1/2})$ increase in the density of states following from the change in the size of $B_F$. The number of eigenvalues $n$ in a given interval $(e_1,e_2)$ is

$$n=M\int_{e_1}^{e_2}P(e)de\ . \tag{22}$$

Using Eq. (21) and setting $e_1=-\Delta e/2$, $e_2=\Delta e/2$, and $n=1$ in Eq. (22) we obtain that $\Delta e\propto M^{-1/2}$ for large enough $M$. In other words, the fluctuations of $e_0$ are restricted to lie within $\Delta e$. As a consequence, we expect that $\Delta_0(M)$ behaves similarly to $\Delta e$. This prediction is in good agreement with the numerical result for $\alpha_{\mathrm{I}}$.

It is possible that the decay of $\Delta_0(M)$ is further enhanced due to the decrease in the ratio between the number of fluctuating elements in $B_F$ and the number of fixed ones. This might be the reason for the fact that $\alpha_{\mathrm{I}}$ is slightly bigger than $\frac{1}{2}$. In order to distinguish between the two effects a second scheme, II, is studied. Here, the size of $B_F, S$, is kept fixed while $M$ grows. Therefore, the frame consists of $S-M$ columns and an equal number of rows. All its elements are allowed to fluctuate according to a Gaussian distribution. All other characteristics of this scheme are the same as in the previous one. We obtain $\alpha_{\mathrm{II}}=0.193\pm 0.112$ [see Fig. 3(b)] suggesting that the change in the density of states is not the only reason for the decaying of $\Delta_0(M)$. In this case it is particularly obvious that the power-law ansatz is not an appropriate description to the behavior of $\Delta_0(M)$ for an arbitrary convergence scheme. Therefore, the $\alpha$ exponents should be, in general, regarded merely as indicators for the decay rate.

When truncating a matrix of *infinite* size to an $M\times M$ block the fraction of erroneous elements is constant as $M$ is increased. Moreover, while in a random matrix the density of states increases $O(M^{1/2})$, in a true Hamiltonian system it is fixed by $\hbar$ and the classical volume of the energy surface. Accordingly, we study a third scheme, III, in which both effects leading to the decay of $\Delta_0(M)$ in

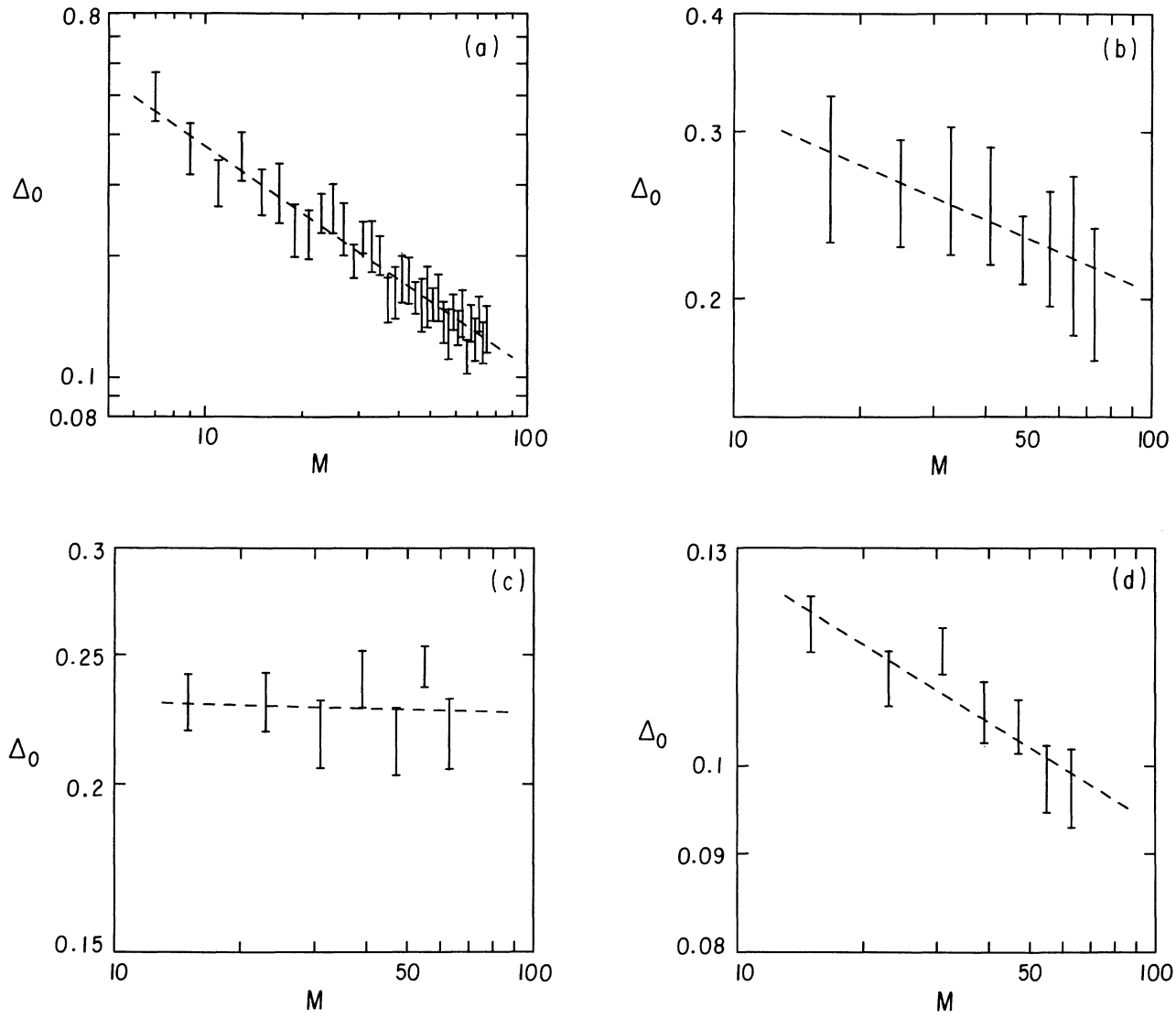


FIG. 3. $\Delta_0$ vs $M$ (error bars) are compared with the best fit $\Delta_0 = cM^{-\alpha}$ (dashed). (a) Scheme I, (b) scheme II, (c) scheme III, and (d) scheme IV (see text).

scheme I are eliminated. To the extent to which GOE matrices are equivalent to the Hamiltonians of ergodic systems, this is the correct configuration for simulating a truncation approximation to the eigenvalue problem. The same setting as in scheme II is used only that here a fixed number, independent of $M$, of frame elements are allowed to fluctuate. The fluctuating subset of the frame is now random in both its positions in $F$ and in the values it assumes. As shown in Fig. 3(c), $\alpha_{\rm III} = 0.008 \pm 0.064$ and therefore agrees very well with the nonconverging situation $\alpha = 0$. Since the $B_F$ matrix is completely homogeneous and there is no natural distance between its different regions, this behavior is to be expected. In other words, none of the average properties of $B_F$ change if two of its rows (and accordingly two columns such as to preserve $B_F^T = B_F$) are interchanged. As a consequence, the positions of the fluctuating elements have no influence on the behavior of $\Delta_0(M)$. Since this result contradicts previous experience concerning the influence of truncation on eigenvalue convergence, we conclude that GOE is not a faithful representation of ergodic systems.

Finally, in the fourth scheme, IV, a band of width $\sigma_b$ is imposed on the matrices generated by scheme III,

$$(\tilde{B}_F)_{ij} = (B_F)_{ij} \exp[(i-j)^2/2\sigma_b^2] \ .$$

Moreover, the diagonal elements which in the context of Sec. II correspond to the spectrum of $A_1$, are arranged in increasing order. As we can see in Fig. 3(d), the decay of $\Delta_0(M)$ reappears with an exponent $\alpha_{\rm IV} = 0.135 \pm 0.045$ at $\sigma_b = 10$. This convergence suggests that banded random matrices are more appropriate for modeling properties of ergodic Hamiltonians than the usual GOE.

## IV. CONCLUDING REMARKS

Using standard methods from phase-space semiclassical theory, examples, and random matrices we have shown that under certain conditions, given a pair of operators $(A_1, A_2)$, $A_2$ has a banded structure in the representation determined by $A_1$. The appropriate representation is determined by the eigenvectors of $A_1$ arranged in increasing order of the corresponding eigenvalues. Accordingly, the bandwidth of $A_2$ is $O(\hbar)$ in units of $A_1$ eigenvalues and $O(\hbar^{-1})$ in the number of states. All our results can be easily extended to systems with an arbitrary number of degrees of freedom $d$ by appropriately adjusting Eq. (2a).

We shall end by pointing out some similarities between the eigenvalue equation of a banded Hamiltonian and the Anderson localization problem.[22] Suppose that $H \equiv A_2$. Since in the ordered eigenrepresentation of $A_1, H_{nk}$ are very small whenever $|a_{1n}-a_{1k}| \geq b\tilde{\Delta}a_{1n,(A_1,H)}$ and $b \gg 1$, it is an arbitrarily good approximation to set all these matrix elements to zero. The larger $b$ the better is the approximation. In turn, the eigenvalue equation corresponding to this approximation can be converted into transfer matrix form. The asymptotic properties of the eigenvectors are determined by the smallest positive eigenvalue of infinite products of these transfer matrices. On one hand, it is known that for random sequences of transfer matrices almost all the eigenvectors are exponentially localized. In the context of electronic states on random lattices this is known as Anderson localization. On the other hand, for the periodic case extended solutions are obtained. In between the two extremes there is a wide range of possibilities (pseudorandom,[23] quasiperiodic,[24] etc.), which has recently received much attention. The eigenvalue problem of banded matrices also lies in this largely unknown territory.

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## APPENDIX

In the following we shall briefly remind the reader of the Wigner-Weyl formalism. First of all, we define the Heisenberg operator

$$\hat{T}(\mathbf{q}_0,\mathbf{p}_0)=e^{(i/\hbar)(\mathbf{p}_0\cdot\hat{\mathbf{q}}-\mathbf{q}_0\cdot\hat{\mathbf{p}})} \tag{A1}$$

which represents the quantum analog of a displacement in phase space

$$\hat{T}^{\dagger}(\mathbf{q}_0,\mathbf{p}_0)(\hat{\mathbf{q}},\hat{\mathbf{p}})\hat{T}(\mathbf{q}_0,\mathbf{p}_0)=(\hat{\mathbf{q}}+\mathbf{q}_0,\hat{\mathbf{p}}+\mathbf{p}_0)\ . \tag{A2}$$

Its action on the wave function is

$$[\hat{T}(\mathbf{q}_0,\mathbf{p}_0)\Psi](\mathbf{x})=e^{(i/\hbar)(\mathbf{p}_0\cdot\mathbf{x}-\mathbf{p}_0\cdot\mathbf{q}_0)}\Psi(\mathbf{x}-\mathbf{q}_0) \tag{A3}$$

and accordingly for the product of two Heisenberg operators we obtain

$$\hat{T}(\mathbf{q}_0,\mathbf{p}_0)\hat{T}(\mathbf{q}_1,\mathbf{p}_1)=e^{i(\mathbf{p}_0\cdot\mathbf{q}_1-\mathbf{q}_0\cdot\mathbf{p}_1)/2\hbar}\hat{T}(\mathbf{q}_0+\mathbf{q}_1,\mathbf{p}_0+\mathbf{p}_1)\ . \tag{A4}$$

As a consequence, the Heisenberg operators do not form a group. A slight extension of their definition as to include the phase factor

$$\hat{T}(\mathbf{q}_0,\mathbf{p}_0,\eta)=e^{i\eta/\hbar}\hat{T}(\mathbf{q}_0,\mathbf{p}_0) \tag{A5}$$

leads to the Heisenberg group with the following product rule:

$$\hat{T}(\mathbf{q}_0,\mathbf{p}_0,\eta_0)\hat{T}(\mathbf{q}_1,\mathbf{p}_1,\eta_1)=\hat{T}(\mathbf{q}_0+\mathbf{q}_1,\mathbf{p}_0+\mathbf{p}_1,\eta_0+\eta_1+\tfrac{1}{2}(\mathbf{p}_0\cdot\mathbf{q}_1-\mathbf{q}_0,\mathbf{p}_1))\ . \tag{A6}$$

It is now easy to define the *alternative Weyl symbol* of some operator $\hat{A}$ as its expansion coefficient in a linear combination of Heisenberg operators

$$\hat{A}=h^{-d}\int d\mathbf{q}\int d\mathbf{p}\ \tilde{A}_W(\mathbf{q},\mathbf{p})\hat{T}(\mathbf{q},\mathbf{p})\ . \tag{A7}$$

Finally, the Weyl symbol itself is obtained

$$A_W(\mathbf{q},\mathbf{p})=h^{-d}\int d\mathbf{q}\int d\mathbf{p}\ \tilde{A}_W(\mathbf{q},\mathbf{p})e^{-i(\mathbf{p}_0\cdot\hat{\mathbf{q}}-\mathbf{q}_0\cdot\hat{\mathbf{p}})/\hbar}\ . \tag{A8}$$

It can be also expressed as the Fourier transform of the configuration-space off-diagonal matrix element of $\hat{A}$

$$A_W(\mathbf{q},\mathbf{p})=\int d\mathbf{s}\,e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}\langle\mathbf{q}+\tfrac{1}{2}\mathbf{s}|\,\hat{A}\,|\mathbf{q}-\tfrac{1}{2}\mathbf{s}\rangle\ . \tag{A9}$$

The Weyl symbol of a product of operators $\hat{C}=\hat{A}\hat{B}$ is related to the individual symbols

$$C_W(\mathbf{q},\mathbf{p})=h^{-2d}\int d\mathbf{q}_0\int d\mathbf{p}_0\int d\mathbf{q}_1\int d\mathbf{p}_1 e^{i(p_0\cdot q_1-\mathbf{q}_0\cdot\mathbf{p}_1)/2\hbar}A_W(\mathbf{q}+\tfrac{1}{2}\mathbf{q}_0,\mathbf{p}+\tfrac{1}{2}\mathbf{p}_0)B_W(\mathbf{q}-\tfrac{1}{2}\mathbf{q}_1,\mathbf{p}-\tfrac{1}{2}\mathbf{p}_1)\ . \tag{A10}$$

Alternatively, Eq. (A10) can be formally written as a power series in $\hbar$

$$C_W(\mathbf{q},\mathbf{p}) = A_W(\mathbf{q},\mathbf{p}) \exp\left[\frac{i\hbar}{2}\overleftrightarrow{\mathrm{L}}\right] B_W(\mathbf{q},\mathbf{p}) , \tag{A11}$$

where $\overleftrightarrow{\mathrm{L}}$ is the *Janus operator*. Let $\mathbf{z} \equiv (\mathbf{q},\mathbf{p})$ and $J$ be the basic symplectic matrix, then

$$\overleftrightarrow{\mathrm{L}} = \frac{\overleftarrow{\partial}}{\partial z_\alpha} J_{\alpha\beta} \frac{\overrightarrow{\partial}}{\partial z_\beta} . \tag{A12}$$

In the present formalism the trace of an operator takes a simple form

$$\mathrm{Tr}\,\hat{A} = h^{-d} \int d\mathbf{q} \int d\mathbf{p}\; A_W(\mathbf{q},\mathbf{p}) \tag{A13}$$

and so does the trace of a product

$$\mathrm{Tr}(\hat{A}^{\dagger}\hat{B}) = h^{-d} \int d\mathbf{q} \int d\mathbf{p}\; A_W^*(\mathbf{q},\mathbf{p}) B_W(\mathbf{q},\mathbf{p}) . \tag{A14}$$

Probably the best known Weyl symbol is the one corresponding to the projection operator $\hat{P}_\Psi = |\Psi\rangle\langle\Psi|$. It is referred to as the Wigner function $W(\mathbf{q},\mathbf{p})$ and it represents the quantum-mechanical analog of a Liouville distribution. Unlike the latter, however, the Wigner function is normalized on phase space to $h^d$ instead of unity and can take on negative values. If one of the operators in Eq. (A14) is a projection, one obtains an expression for the expectation value

$$\langle\psi|\hat{A}|\psi\rangle = h^{-d} \int d\mathbf{q} \int d\mathbf{p}\; W(\mathbf{q},\mathbf{p}) A_W(\mathbf{q},\mathbf{p}) . \tag{A15}$$

One can easily retrieve the standard description of quantum-mechanical behavior in terms of wave functions from the Wigner function description

$$|\psi(\mathbf{q})|^2 = h^{-d} \int d\mathbf{p}\; W(\mathbf{q},\mathbf{p}) . \tag{A16}$$

Likewise

$$|\phi(\mathbf{p})|^2 = h^{-d} \int d\mathbf{q}\; W(\mathbf{q},\mathbf{p}) . \tag{A17}$$

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