Distribution of matrix elements of chaotic systems

Mario Feingold and Asher Peres
Department of Physics, Technion—Israel Institute of Technology, 32 000 Haifa, Israel
(Received 16 January 1986)

When a quantum system has a chaotic classical analog, its matrix elements in the energy representation are closely related to various microcanonical averages of the classical system. The *diagonal* matrix elements cluster around the classical expectation values, with *fluctuations* similar to the values of the *off-diagonal* matrix elements. The latter in turn are related to the classical autocorrelations. These results imply that quantum perturbation theory must fail, for chaotic systems, in the semiclassical limit $\hbar\to 0$: Two arbitrarily close Hamiltonians have, in general, completely different sets of eigenvectors.

I. INTRODUCTION AND THEORETICAL PREDICTIONS

If a quantum system has a chaotic classical analog, then, in the semiclassical limit $\hbar\to 0$, all the energy eigenfunctions $|E\rangle$ have roughly the same aspect: their Wigner distributions[1] fill the entire available phase space (namely, an "energy shell" with thickness ΔE of order $\hbar$) with an amplitude which fluctuates around the classical microcanonical phase-space density.[2] It follows that the expectation value $\langle E|\hat{A}|E\rangle$ of a "reasonable" operator $\hat{A}$ [that is, an operator having a well-behaved classical limit $A(p,q)$ as $\hbar\to 0$][3,4] tends to the microcanonical phase-space average[2,5,6]

$$\langle E|\hat{A}|E\rangle \simeq \{A(E)\} = \frac{\int A(p,q)\delta(E-H(p,q))dp\,dq}{\int \delta(E-H(p,q))dp\,dq} . \tag{1}$$

(In this paper, $\{\ \}$ denote the classical microcanonical average.) It is thus possible to obtain purely classical estimates of diagonal matrix elements. The purpose of this paper is to extend our previous work[6] to *off-diagonal* matrix elements and to evaluate the deviation of the quantum results from the classical ones.

Our theoretical predictions are listed below, in the present section. It is shown that although *individual* matrix elements, in the energy representation, can be considered as pseudorandom,[7] their *statistical* behavior follows well-defined rules governed by *classical* statistical mechanics. Section II reports the results of numerical simulations, which are in good agreement with our predictions. Section III discusses some implications of these results for the range of validity of perturbation theory.

The fundamental formula which is proved below is

$$\sum_k (E_j-E_k)^{2n}|A_{jk}|^2 \simeq \hbar^{2n}\{(d^nA/dt^n)^2\} , \tag{2}$$

where

$$A_{jk}=\langle E_j|\hat{A}|E_k\rangle , \tag{3}$$

and the right-hand side (rhs) of (2) is the microcanonical average at energy E_j. Equation (2) can be proved by induction, as follows. For $n=0$, we have

$$\sum_k A_{jk}A_{kj}=\langle E_j|A^2|E_j\rangle \simeq \{A^2\} , \tag{4}$$

as explained above. We now replace $\hat{A}$ by $[i\hat{H},\hat{A}]$ so that

$$A_{jk}\to\langle E_j|[i\hat{H},\hat{A}]|E_k\rangle = i(E_j-E_k)A_{jk} . \tag{5}$$

However, $[i\hat{H},\hat{A}]=d\hat{A}/dt$, whence it follows that

$$\sum_k (E_j-E_k)^2|A_{jk}|^2 \simeq \hbar^2\{(dA/dt)^2\} . \tag{6}$$

Here dA/dt may be expressed by the classical Poisson bracket $[A,H]_{\rm PB}$, if one wishes so. Replacing again and again $\hat{A}$ by $[i\hat{H},\hat{A}]$, we finally obtain (2).

We have thereby obtained a semiclassical approximation for all the moments of the off-diagonal matrix elements, from which one can derive, in principle, the distribution of the $|A_{jk}|^2$ themselves. This can, however, be done more directly as follows. Consider

$$\sum_k \exp[i(E_j-E_k)t/\hbar]|A_{jk}|^2 = \sum_k \langle E_j|\exp(iE_jt/\hbar)\hat{A}|E_k\rangle\exp(-iE_kt/\hbar)\langle E_k|\hat{A}|E_j\rangle$$
$$= \langle E_j|e^{iHt/\hbar}\hat{A}e^{-iHt/\hbar}\hat{A}|E_j\rangle = \langle E_j|\hat{A}(t)\hat{A}(0)|E_j\rangle , \tag{7}$$

where $\hat{A}(t)$ and $\hat{A}(0)$ are now given in the Heisenberg picture. In the semiclassical limit, this ought to tend to

$$C(t)=\{A(t)A(0)\}=\lim_{T\to\infty}\frac{1}{T}\int_0^T A(t+\tau)A(\tau)d\tau , \tag{8}$$

because, for an ergodic system, the microcanonical average is the same as the time average. Here, $C(t)=C(-t)$ is the *autocorrelation* of the classical dynamical variable A. Its Fourier transform

$$S(\omega)=\int_{-\infty}^{\infty} C(t)e^{-i\omega t}dt , \tag{9}$$

is called the power spectrum[8] of A.

There is, however, a difficulty. Equation (7) contains a constant term $A_{jj}^2 \simeq \{A\}^2$. If this does not vanish, $C(t)$ tends to $\{A\}^2$ as $t \to \infty$, so that $S(\omega)$ is singular for $\omega = 0$. We must therefore replace $\hat{A}$ by $\hat{A} - \mathrm{diag}(\hat{A})$ or, more simply, if we deal with a narrow energy range, by $\hat{A} - \{A\}$. This is equivalent to subtracting A_{jj}^2 from Eq. (7), or $\{A\}^2$ from Eq. (8). We obtain

$$\sum_k{}' \exp[i(E_{j-E_k})t/\hbar] \, |A_{jk}|^2 \simeq C(t) - \{A\}^2 . \tag{10}$$

where $\sum'$ excludes the term with $k = j$. The rhs of (10) falls off for $t \to \infty$ and its Fourier transform gives a well-defined power spectrum $S(\omega)$. We shall henceforth assume that we have subtracted $\{A\}$ from $\hat{A}$, so that the new $\hat{A}$ satisfies $\{A\} = 0$. We may now return to Eq. (9), from which we obtain

$$|A_{jk}|^2 \simeq S((E_j - E_k)/\hbar)/2\pi\rho(E) , \tag{11}$$

where

$$\rho(E) = h^{-N} \int \delta(E - H(p,q)) d^N p d^N q , \tag{12}$$

is the coarse-grained density of states.[9] The latter must appear here because when we perform the Fourier transform from t to ω, we must replace the discrete sum in (7) by an integral:

$$\sum_k \cdots \to \int \cdots \rho(E_k) dE_k . \tag{13}$$

It does not matter whether one uses E_j or E_k in Eq. (12) since both must coincide in the semiclassical limit $\hbar \to 0$, as otherwise $S((E_j - E_k)/\hbar)$ tends to zero.

Unfortunately, it is extremely tedious to compute the rhs of (8) and (9). However, a reasonable approximation to (9) may be obtained from the *periodogram*[8]

$$S(\omega, T) = \frac{1}{T} \left| \int_0^T A(t) e^{i\omega t} dt \right|^2 . \tag{14}$$

Although $S(\omega, T)$ itself does not converge to a well-defined limit for $T \to \infty$,[10] and may even be a Cantor set,[11] a suitable ensemble average $\langle S(\omega, T) \rangle$, taken over a family of classical orbits, does converge:[12]

$$\lim_{T \to \infty} \langle S(\omega, T) \rangle = S(\omega) . \tag{15}$$

(Here, the angular brackets $\langle \ \rangle$ do not denote a quantum average, but a *classical* ensemble average, such as one obtained by randomizing initial conditions.)

The limit $\omega \to 0$ ought to be considered carefully:

$$S(0) = \int_{-\infty}^{\infty} [C(t) - \{A\}^2] dt , \tag{16}$$

$$= \lim_{T \to \infty} \left\langle \left| \int_0^T [A(t) - \{A\}] dt \right|^2 \Big/ T \right\rangle , \tag{17}$$

where we have returned to the original definition of A. This expression thus gives $|A_{jk}|^2$ for $|E_j - E_k| \to 0$, but *not* of course the diagonal element itself, $A_{jj} \simeq \{A\}$, which has been subtracted from it. We shall now argue that (16) is related to the *deviation* of A_{jj} from $\{A\}$.

It was suggested long ago by Pechukas[2] that the *fluctuations* of the diagonal matrix elements should be of the same order of magnitude as the elements *near* the diago-

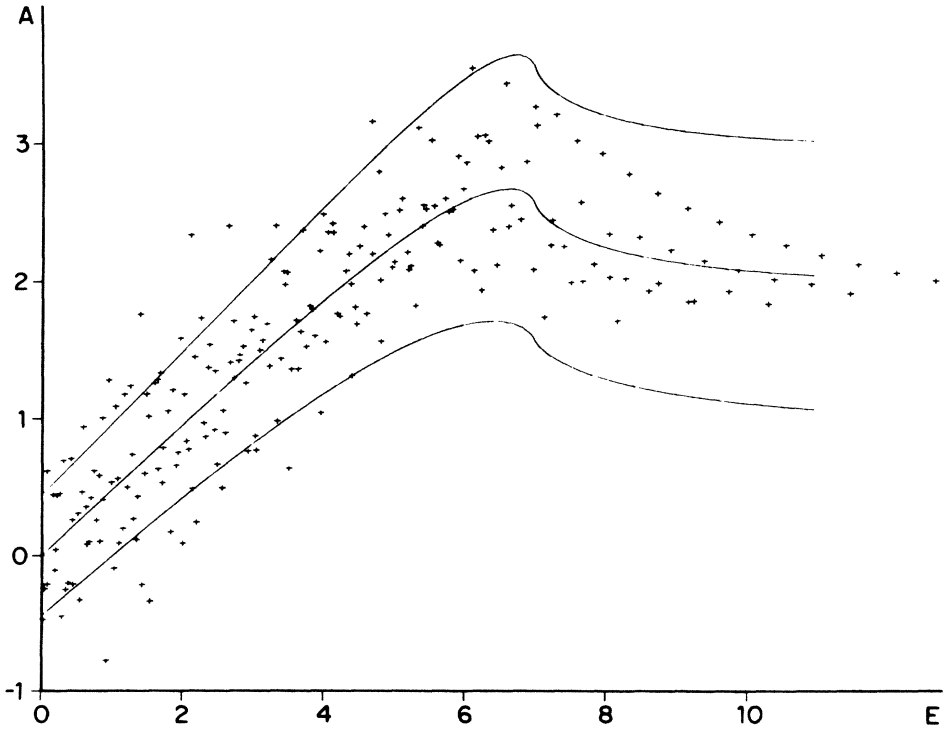

FIG. 1. Diagonal matrix elements A_{jj} (crosses) and their semiclassical value $\{A\}$ (solid lines). The three solid lines represent $\{A\}$ and $\{A\}$ plus and minus the expected quantum fluctuations, as functions of the energy E. There is good agreement for low E, in the classically chaotic domain, but not for large E, in the classically regular domain, where the quantum fluctuations turn out smaller than expected. Negative values of E correspond to opposite values of A_{jj} and $\{A\}$.

nal. This prediction is supported by the following argument. Consider two energy levels E_j and E_k which are close to each other (but not necessarily consecutive) and define two new orthonormal states

$$|\pm\rangle = 2^{-1/2}(|E_j\rangle \pm |E_k\rangle) , \tag{18}$$

so that

$$H|\pm\rangle = \tfrac{1}{2}(E_j+E_k)|\pm\rangle + \tfrac{1}{2}(E_j-E_k)|\mp\rangle . \tag{19}$$

Since $|E_j-E_k|$ is very small (of order $\hbar^N$) we see that $|\pm\rangle$ are "almost eigenstates" of H, with energy $(E_j+E_k)/2$. We therefore expect that these two functions are qualitatively similar to $|E_j\rangle$ and $|E_k\rangle$: namely, they fill the entire energy shell with a probability distribution fluctuating around the classical microcanonical phase-space density.

It follows that $\langle +|\hat{A}|+\rangle \simeq \langle -|\hat{A}|-\rangle \simeq \{A\}$ and, moreover, that $\langle -|\hat{A}|+\rangle$ is roughly of the same order of magnitude as A_{jk}. Thus

$$A_{jk} \simeq \langle -|\hat{A}|+\rangle = \tfrac{1}{2}(A_{jj}-A_{kk}+A_{jk}-A_{kj}) . \tag{20}$$

The last two terms in the rhs mutually cancel, if A_{jk} is a real matrix (at most, their difference has the same order of magnitude as the lhs of the equation). Now define the "fluctuation" of A as

$$F_j = A_{jj} - \{A\} . \tag{21}$$

We have from (20)

$$\tfrac{1}{2}(F_j - F_k) \simeq A_{jk} . \tag{22}$$

Assuming that the various F_j are statistically independent, we obtain, as a rms average,

$$\langle F_j^2\rangle = \langle F_k^2\rangle = 2\langle |A_{jk}|^2\rangle , \tag{23}$$

where $\langle\ \rangle$ now denote a statistical average over a set of *neighboring* levels.

II. NUMERICAL SIMULATION

To test the validity of these various predictions, we have used the double-rotator model which was extensively discussed in previous publications.[1,13–15] The Hamiltonian is

$$\hat{H} = \hat{L}_z + \hat{M}_z + \hat{L}_x\hat{M}_x , \tag{24}$$

where **L** and **M** are independent angular momenta. Since $L^2=\hbar^2 l(l+1)$ and $M^2=\hbar^2 m(m+1)$ are constants of the motion, the Hamiltonian is, for given l and m, a *finite*-dimensional matrix. Therefore all our calculations are *exact* (there is no need of truncation) except for numerical noise, such as round-off errors. We take

$$\hat{A} = \hat{L}_z + \hat{M}_z , \tag{25}$$

and use the same numerical data as in our preceding work, namely $l=m=20$ and $\hbar=0.1707825$, so that $L=M=3.5$. An investigation of the corresponding *classical* problem[13] shows that low energies (say $|E|<5$) correspond to mostly chaotic orbits, while high energies ($|E|>8$) involve mostly regular orbits.

A plot comparing A_{jj} and $\{A\}$ is given in Fig. 1, where the three solid lines represent $\{A\}$ and $\{A\}\pm\langle F_j^2\rangle^{1/2}$. The quantum fluctuations $\langle F_j^2\rangle$ can be predicted with various levels of reliability and (difficulty) as explained below. Before we do this, it is good to have a look at Fig. 2, which shows the "thickness" ΔE of the energy shell where the Wigner distribution[1] is appreciably different from zero:

$$(\Delta E)^2 = \frac{\sum_k |A_{jk}|^2 (E_j-E_k)^2}{\sum_k' |A_{jk}|^2} \simeq \frac{\hbar^2\{[H,A]^2_{\rm PB}\}}{\{A^2\}-\{A\}^2} . \tag{26}$$

Note that this ΔE depends on E_j and also on the choice of the dynamical variable A. Figure 2 compares both expressions for ΔE, with $\hat{A}$ given by (25) and $E_j=0$. (Note that $E_j=0$ is an eigenvalue of $\hat{H}$, lying in the chaotic region of phase space.)[13–15] The agreement is quite satisfactory, up to quantum fluctuations similar to those of Fig. 1.

We now turn our attention to these quantum fluctuations. Their most reliable estimate is given by Eqs. (11) and (23):

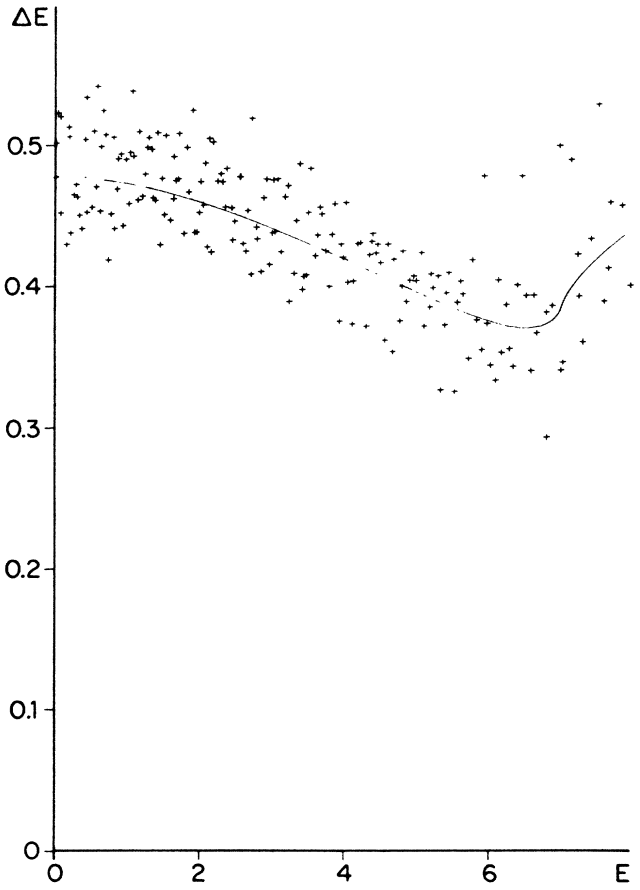

FIG. 2. Thickness of the "energy shell" ΔE for each energy level E_j. The crosses are given by the quantum expression, and the solid line by the classical expression in Eq. (26). The Wigner distribution in the classical phase space is appreciably different from zero for $|H(p,q)-E_j| < \Delta E$. Note that Fig. 1 involves only the diagonal matrix elements, while Fig. 2 involves only the off-diagonal ones.

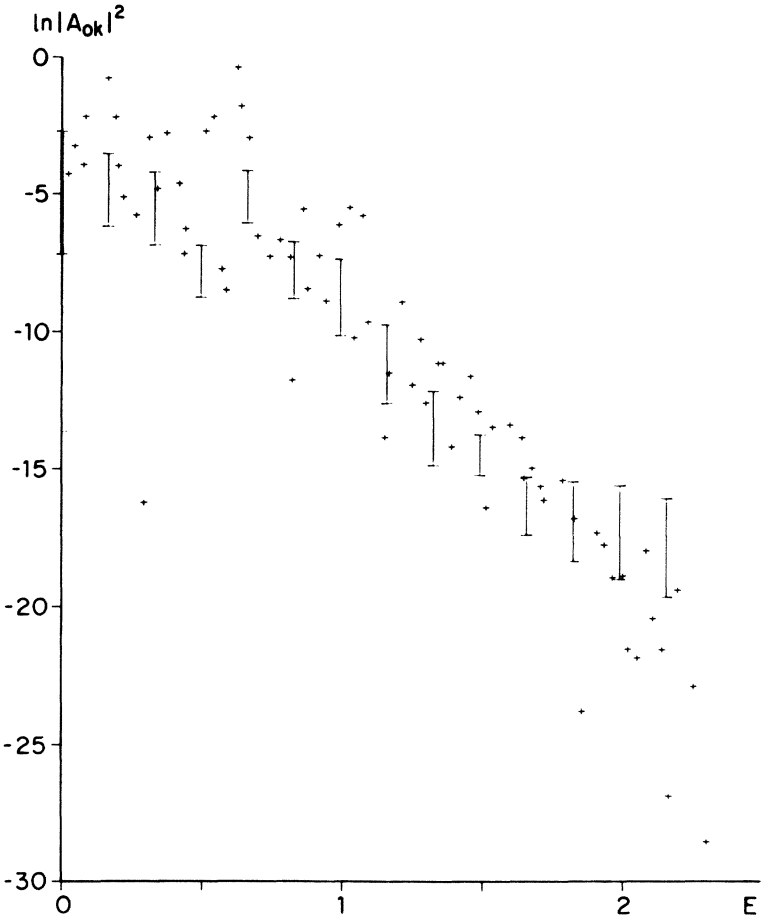

FIG. 3. Numerical test of Eq. (11). Each cross represents the value of an off-diagonal matrix element; each error bar is, on the same scale, the value of the rhs of (11), as approximated by the periodogram (14). The agreement deteriorates for larger values of E_k because of round-off errors in the computer.

$$|\langle F_j^2\rangle| = S(0)/\pi\rho(E_j)\ . \tag{27}$$

However, in practice, it is extremely tedious to compute $S(\omega)$ from its definition in Eqs. (8) and (9) and one replaces it by the approximation (15), which is based on an ensemble average.[8,12] We have performed this ensemble average for a single energy, $E_j=0$, by choosing in a random way 30 classical orbits of duration $T=6694.07$ (about 1000 oscillations of the double rotator). All these orbits had $L=M=3.5$ and $E=0$. The result is shown in Fig. 3 where we plot, on a logarithmic scale, the lhs and rhs of Eq. (11) for $E_j=0$ and for various k. The average results for the 30 classical orbits are represented by error bars in the standard way. The agreement of the quantum results and the semiclassical approximation is excellent.

We also see in Fig. 3 that $\ln|A_{0k}|^2$ is roughly parabolic in E_k. In other words, $|A_{0k}|^2$ can be approximated by a Gaussian distribution. There is no theoretical justification for this result and it should not be expected to hold for other models. However, if we have reasons to believe that, for some model, it is a good approximation to take

$$|A_{jk}|^2 \simeq a\exp[-b(E_j-E_k)^2]\ , \tag{28}$$

then the constants a and b can be readily evaluated, without going through the tedious calculation of (8) and (9), or (14). We simply substitute

$$\sum_k (E_j-E_k)^{2n}|A_{jk}|^2 \to \rho a\int E^{2n}e^{-bE^2}dE\ , \tag{29}$$

whence we obtain, after an elementary calculation using Eq. (2),

$$(\rho a)^2 = (\{A^2\}-\{A\}^2)^3/2\pi\hbar^2\{[A,H]^2_{\rm PB}\}\ . \tag{30}$$

This gives, for $A=L_z+M_z$ and $E=0$, a result $a=0.10$, in good agreement with the data on Fig. 3. It is therefore Eq. (30) which we used to draw the upper and lower lines in Fig. 1.

On the other hand, the value of b obtained in the same way is too low by about a factor of 2. The lack of agreement should not be a matter of concern, because the matrix elements for $E_k>1$, which are those giving the "parabolic" aspect to the plot of Fig. 3, have a negligible weight in the sum (29).

In fact, Eq. (30) could also be derived, except for the factor 2π, by simple dimensional analysis: from the defi-

nition (28), the lhs of (30) must have the dimensions of $(A^2/\text{energy})^2$, it must be multiplied by c^2 if $A \to cA$, for any constant c, and it must be *invariant* under $A \to A+c$. Then, if only $\hbar$, $\{A\}$, $\{A^2\}$, and powers of $[A,H]_{PB}$ are admitted in the rhs of (30), this determines this rhs completely, except for the numerical factor 2π.

III. IMPLICATIONS FOR PERTURBATION THEORY

Consider a Hamiltonian $\hat{H}=\hat{H}_0+\hat{V}$. Let $E_j, E_k, \ldots$ be eigenvalues of $\hat{H}_0$. As is well known, elementary perturbation theory fails if these eigenvalues are degenerate or, more precisely, if $|E_j-E_k| < |V_{jk}|$. Indeed, a necessary (but not a sufficient) condition for the eigenvectors of $\hat{H}$ to be close to those of $\hat{H}_0$ is that

$$|V_{jk}| \ll |E_j-E_k| \ . \tag{31}$$

For *regular* systems, having selection rules, *most* V_{jk} vanish so that (31) is trivially satisfied. On the other hand, in a chaotic system, the V_{jk} are *pseudorandom*.[7] For neighboring levels, $|E_j-E_k| \simeq \rho^{-1}$ and Eq. (31) reduces to $\rho^2 a \ll 1$, with a defined by (28). Thus, by virtue of (12) and (30) we obtain the condition[16]

$$\hbar^{2N+2} \gg \frac{\left[\int \delta(E-H)d^N p d^N q\right]^2 (\{V^2\}-\{V\}^2)^3}{[V,H_0]^2_{PB}} \ . \tag{32}$$

The rhs of this equation involves only *classical* quantities. Therefore perturbation theory can *never* be valid in the semiclassical limit $\hbar \to 0$: for an arbitrarily small but *finite* perturbation, the nth eigenvectors of $\hat{H}_0$ and $\hat{H}$ are nearly always nearly orthogonal to each other. This result is similar to the orthogonality of bare and dressed states in quantum field theory.[17] [Naturally, for *finite* $\hbar$, it is always possible to make V small enough so that (32) is valid. This does not guarantee, of course, that the perturbation series will then converge.]

ACKNOWLEDGMENTS

This work is part of a thesis by M.F. Various results were obtained by A.P. during visits to the University of Bristol, the University of California at Santa Barbara, and the Centre International de Sciences Mécaniques at Udine. The hospitality of these institutions is gratefully acknowledged. Work done at Technion was supported by the Gerard Swope Fund, the New York Metropolitan Fund, and the Fund for Encouragement of Research.

APPENDIX

The results obtained here allow us to sharpen those of a previous article.[7] It was shown in Ref. 7 that the time average of the quantum fluctuations of a time-dependent operator $\hat{A}(t)$ is given by

$$F^2=\langle[\langle\hat{A}(t)\rangle_Q]^2\rangle_T-[\langle\langle\hat{A}(t)\rangle_Q\rangle_T]^2 \tag{33}$$

$$=\sum_j\sum_k |\rho_{jk}|^2|A_{jk}|^2-\sum_j|\rho_{jj}A_{jj}|^2 \ . \tag{34}$$

This can be written as

$$F^2=\sum_j{\sum_k}' |\rho_{jk}|^2|A_{jk}|^2 \ , \tag{35}$$

which involves *only off-diagonal matrix elements*. Assuming statistical independence, this is

$$F^2=\langle|A_{jk}|^2\rangle\sum\sum'|\rho_{jk}|^2 \ , \tag{36}$$

where $\langle\ \rangle$ denotes an ensemble average. Since $\sum_k'|A_{jk}|^2=\{A^2\}-\{A\}^2$, this ensemble average is about $(\{A^2\}-\{A\}^2)/N$, where N is the number of energy levels involved.

On the other hand, $\sum_j\sum_k'|\rho_{jk}|^2$ may take values from 1 (for a pure state) to N^{-1} (for an ideal mixture). The practical situation is usually closer to a mixture and one obtains

$$F^2\simeq(\{A^2\}-\{A\}^2)/N^2 \ , \tag{37}$$

which is smaller by a factor N than the estimate of Ref. 7. This *strengthens* the validity of the results claimed in that paper.

[1] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[2] P. Pechukas, Phys. Rev. Lett. **51**, 943 (1983).
[3] L. G. Yaffe, Rev. Mod. Phys. **54**, 407 (1982).
[4] K. B. Kay, J. Chem. Phys. **79**, 3026 (1983).
[5] R. A. Marcus, Extended Abstracts, 27th Annual Conference on Mass Spectroscopy, Seattle, 1979 (Am. Soc. Spectroscopy), p. 568 (unpublished); also in *Horizons of Quantum Chemistry*, edited by K. Fukui and B. Pullman (Reidel, Dordrecht, 1980), p. 107.
[6] M. Feingold, N. Moiseyev, and A. Peres, Chem. Phys. Lett. **117**, 344 (1985).
[7] A. Peres, Phys. Rev. A **30**, 504 (1984).
[8] W. B. Davenport, Jr. and W. L. Root, *An Introduction to the Theory of Random Signals and Noise* (McGraw-Hill, New York, 1958), pp. 102–108.
[9] M. V. Berry, in *Chaotic Behavior of Deterministic Systems*, Vol. 36 of *Les Houches Summer School Proceedings*, edited by G. Iooss, R. H. G. Helleman, and R. Stora (North-Holland, Amsterdam, 1983).
[10] G. E. Powell and I. C. Percival, J. Phys. A **12**, 2053 (1979).
[11] J. E. Avron and B. Simon, J. Func. Anal. **43**, 1 (1979), Appendix 1.
[12] M. Born and E. Wolf, *Principles of Optics* (Pergamon, Oxford, 1980), pp. 498 and 503.
[13] M. Feingold and A. Peres, Physica (Utrecht) D **9**, 433 (1983); Phys. Rev. A **31**, 2472 (1985).
[14] M. Feingold, N. Moiseyev, and A. Peres, Phys. Rev. A **30**, 509 (1984).
[15] A. Peres, Phys. Rev. A **30**, 1610 (1984); Phys. Rev. Lett. **53**, 1711 (1984).
[16] A. Peres, Bull. Am. Phys. Soc. **31**, 47 (1986).
[17] G. Barton, *Introduction to Advanced Field Theory* (Interscience, New York, 1963).