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Eigenfunctions, eigenvalues, and time evolution of finite, bounded, undriven, quantum systems are not chaotic

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We prove here that the eigenvalues, eigenfunctions, and time evolutions for a broad class of spatially bounded, finite particle number, undriven, quantum systems can be computed by algorithms containing logarithmically less information than the quantities themselves. Algorithmic complexity theory asserts that such quantal systems are nonchaotic. These results are shown to be valid independent of the size of system parameters such as mass or Planck's constant, provided they are not set equal to zero or infinity. However, rather than confronting quantum mechanics with classical mechanics via the correspondence principle, we suggest a direct comparison of quantum mechanics with macroscopic laboratory reality. Specifically, we here propose the double pendulum—a simple, two-degree-of-freedom, macroscopic system exhibiting a transition to chaos as its amplitude increases—as a model suitable for testing whether a nonchaotic quantum mechanics to the performance of this comparison.

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I. INTRODUCTION

In this paper we rigorously prove that the eigenfunctions, eigenvalues, and time evolutions for a broad class of spatially bounded quantum systems containing a finite number of particles and governed by time-independent Hamiltonians are nonchaotic [1]. Here, spatially bounded refers to all quantum systems that can be confined within a box, and nonchaotic means that these systems exhibit no deterministic randomness [2]. Specifically, we establish that the information contained in these eigenfunctions, eigenvalues, and time evolutions is logarithmically compressed by the algorithms which compute them. Algorithmic complexity theory [3] then assures us that there is no chaos in such quantities. Since the proofs which appear in the following sections invoke unfamiliar theorems and involve tediously intricate arguments, it is perhaps worthwhile here at the outset to provide the reader with intuitively credible arguments that lend believability to our central conclusions even before they are proved. This intuitive presentation is especially relevant since many will view our conclusions as going against established opinion.

Recall that the procedure for calculating quantum eigenvalues and eigenfunctions is not only deterministic but computationally very straightforward; in fact, it is a computable [4] procedure, i.e., it involves only finite, recursive algorithms. Specifically, one begins with well-behaved operators $\hat{A}(\hat{q},\hat{p})$ obtained from smooth classical functions A(q,p). One then selects simple analytic functions as a basis set $\{\Phi_k\}$ for Hilbert space and determines the matrix elements of \hat{A} via the integral $A_{mn} = \int d\tau \Phi_n^* \hat{A} \Phi_m$. But integration is a smoothing

operation; hence, these matrix elements contain no element of chaos. Finally, one calculates the eigenfunctions and eigenvalues of the resulting matrix $[A_{mn}]$ using any of a number of computable diagonalization routines for finite matrices in concert with various computable limit procedures. One thus finds no hint of chaos in this entire process. On the other hand, if \hat{A} were a random matrix with elements generated by some random process, then its eigenvalues and eigenfunctions would most certainly be chaotic. Thus, out of the totality of all possible Hilbert space eigenfunction-eigenvalue equations, most of which have random solutions, quantum mechanics focuses on that subset which is computable and hence not random. In general then, one expects no chaos in the quantum eigenfunctions and eigenvalues.

In this regard, it is crucial not to confuse erratic with chaotic. The eigenvalues of the Hamiltonian describing the quadratic Zeeman effect [5], for example, have been computed by a relatively simple computer program which logarithmically compresses the information content of these eigenvalues. This eigenvalue set certainly looks erratic [5], but it is most assuredly not chaotic. A similar confusion exists in regard to the prime numbers. One frequently reads that the primes are random. However, the bit length of the algorithm to compute N primes, for large N, is almost totally exhausted by the log_2N bits needed to specify N. The primes are therefore not random because the information content contained in the first N primes is logarithmically compressible. Let us now examine the time evolution of the wave function Ψ .

Because the energy eigenvalues for the finite, bounded, quantum system of interest in this paper are discrete, the associated wave functions Ψ can always be written as

$$\Psi(\mathbf{x},t) = \sum_{k} \mathcal{A}_{k} U_{k}(\mathbf{x}) e^{-iE_{k}t/\hbar}, \qquad (1)$$

where x denotes all spatial variables, t denotes time, the E_k and $U_k(x)$ are energy eigenvalues and eigenfunctions, respectively, the \mathcal{A}_k are expansion coefficients, and \hbar is Planck's constant divided by 2π . Ψ is thus seen to be an almost periodic function [6], which means that Ψ , having achieved a value, makes near returns to this value throughout all time. Clearly, such time evolution precludes an approach to thermodynamic equilibrium or a decay of correlations. Moreover, this almost periodic behavior persists even in the density matrix description. However, in general, these near periods might be relevant only to long-time system behavior. If so, this would leave open the possibility for bounded systems to yield, or at least closely mimic, a chaotic time evolution over laboratory time scales. To address this possibility, we must examine Eq. (1) a bit more closely. Each time exponential in the sum of Eq. (1) is merely a rotating unit vector in the complex plane. At time zero, these vectors are phased such that the sum adds to $\Psi(x,0)$. As time increases, these unit vectors dephase at a constant rate. Consequently, the time evolution of Ψ involves nothing more than the phase mixing which characterizes laminar flow such as occurs in Couette flow or the spin-echo experiment [7]. Most assuredly, this type flow is not chaotic on either a short-time or a long-time scale. Additional details on this point are given in Ref. [3].

Many investigators accept these intuitive arguments regarding the nonchaotic time evolution of finite, bounded, quantum systems as essentially conclusive, but they quickly point out that Eq. (1) does not take measurement into account. Since repeated measurements might well mimic a random outside driving force which later can certainly introduce chaos even into harmonic-oscillator motion, this point needs to be addressed. Most investigators of quantum chaos, as in classical chaos, are interested in determining the intrinsic behavior of the system under study and not that due to outside influences. Nonetheless, if we are to maintain that Eq. (1) describes observable intrinsic behavior and not an idealized fantasy, we must be able to verify this fact by laboratory measurements that do not appreciably modify the behavior. Fortunately, Weigert [8] has applied the theory of quantum-nondemolition measurements to the question of intrinsic chaos (or its lack) in quantum systems and has concluded that, by proper choice of commuting observables, one can in fact make sequential measurements on a quantum system without disturbing its time evolution. Weigert's result thus opens the door to the legitimate study of the intrinsic behavior specified by Eq. (1). Another possibility for circumventing the destructive effects of measurement is to apply Eq. (1) to finite, bounded, undriven, macroscopic systems. Everyday experience teaches us that the time evolution of a macroscopic system is quite stable against the disturbance of macroscopic measuring devices [9]. This opportunity to circumvent the deleterious effects of both the classical and quantum measurement process becomes even more attractive if one chooses the macroscopic system to be one exhibiting

chaotic time evolution, for now one can directly test whether or not a nonchaotic quantum mechanics can correctly predict chaotic laboratory reality. We shall discuss this possibility in greater detail in a later section.

In this paper, we shall prove that the time flows for the quantum systems of interest to us exhibit no deterministic randomness over finite (as well as infinite) time intervals. However, since even experienced investigators express doubts regarding the ability of algorithmic complexity theory to distinguish randomness from nonrandomness in finite objects (digit strings), it behooves us to present at least an intuitive resolution of these doubts before burying the reader under the rigorous details of later sections. At this point, we shall seek to resolve only two of the most frequently voiced objections by confronting them with two very simple, illustrative examples. A more detailed discussion of these matters is to be found in Ref. [3].

We first consider the objection that emphasizes the lack of a sharp cutoff separating random from nonrandom finite binary digit strings. Let us resolve this issue by considering, for example, the set of all 100-bit binary sequences $(2^{100} \approx 10^{30} \text{ in all})$. The sum S of computer programs (algorithms) having (100-k-1) bits or less is given by the geometric series $S=2^1+2^2+2^3+\cdots$ +2^(100-k-1), since there are two programs with one bit, four programs with two bits, etc. Consequently, $S=2^{(100-k)}-2\simeq 2^{(100-k)}$. The fractional number of 100bit sequences which have the possibility of being computed by programs containing (100-k-1) bits or less is therefore 2^{-k} . This leaves a fraction $(1-2^{-k})$ of 100-bit sequences which cannot be computed by any algorithm having less than (100-k) bits. In terms of percentages, 50% of this 100-bit set cannot be computed by any algorithm having less than 99 bits, 75% cannot be computed be any algorithm with less than 98 bits, and 96% cannot be computed by any algorithm with less than 95 bits. A reasonable man thus concludes that an overwhelming majority of these 100-bit sequences cannot be computed by any algorithm having significantly less than 100 bits and that the matter of precise cutoff can hardly be regarded as a serious issue. At the other extreme reside the ordered 100-bit sequences of the type (1, 1, 1, 1, 1, ...) or $(1,0,1,0,1,0,\ldots)$ whose information contents are logarithmically compressible, i.e., which can be computed by programs with bit lengths proportional to $\log_2 100$. The distinction between these two extremes, called random and nonrandom, is not only clear but striking. Moreover, given the paucity of sequences lying in the border separating these two extremes, there is no difficulty in avoiding borderline cases in applications. However, it must be emphasized that, in this paper, we find ourselves facing only nonchaotic, nonrandom, logarithmically compressible objects [3].

Since logarithmic compressibility is such a pivotal concept in this paper, let us illustrate its occurrence in a familiar example. The digit string for the $\sqrt{2}$ reads in part

 $\sqrt{2} = 1.41421356237309504880168872\cdots$

Folklore asserts that this digit string is random, and indeed, as we scan these digits, certainly no order is ap-

parent. Nonetheless, this decimal representation can be by the simple, iterative algorithm computed $A_{n+1} = [(A_n^2 + 2)/2A_n]$, where A_n is the *n*th approximation. If we seek to compute a large number N of digits for the $\sqrt{2}$, encodement of the above short algorithm will occupy only a small part of the computer program. The majority of the program will be taken up by the encodement of $\log_2 N$. The information in the digits for the $\sqrt{2}$ is thus logarithmically compressible; this string is therefore not random. Even the algorithm alone exposes the meaning of informational compressibility. Setting $A_0 = 1.4$ in the above algorithm yields $A_1 = 1.414$, $A_2 = 1.41421356$, etc. Here, two digits yield four, four digits yield eight, ..., 1000 digits yield 2000, etc. Despite appearances, in the decimal representation for the $\sqrt{2}$, distant digits are rigidly determined by near digits. Let us now turn to the discussion of the second objection.

This second objection directs attention to the fact that

both random and nonrandom orbits in a fully chaotic dynamical system are dense, thereby permitting sufficiently close random and nonrandom orbits to be essentially indistinguishable over arbitrarily large finitetime intervals. This argument concludes that orbital randomness (or its lack) can be determined only in the infinite-time limit. In order to resolve this delicate issue, let us consider the one-dimensional Bernoulli shift $X_{n+1} = 2X_n \pmod{1}$, where, for reasons which will soon become apparent, each X_n is to be expressed in binary notation. Let us now focus on an orbit initiated at a rational point $X_0 = n/N$. Because X_0 is rational, it binary representation consists of an infinite repetition of some finite sequence of bits. Thus, we need to compute the binary representation of X_0 only out to the onset of the first repeat or at most to the second. In short, a calculation of finite accuracy serves to specify the full and precise binary representation for X_0 . The binary representation for a typical rational X_0 might read

 $X_0 = 0.1100010000 1100010000 1100010000 1100010000 \cdots$

The forward iterates of X_0 are now determined by moving the binary point sequentially to the right, each time dropping the integer part. This procedure makes it clear that this iteration sequence (orbit) is periodic with $X_{10n} = X_n$, for all n. As a consequence, this orbit is as obviously nonchaotic as an orbit of the simple pendulum. Indeed, a true picture of this orbit can be obtained simply by calculating its iterates to only three-bit accuracy: $X_0 = 0.110, \quad X_1 = 0.100, \dots, X_9 = 0.011, \quad X_{10} = X_0.$ Increased accuracy would move these iterates slightly but would leave their general location unchanged. In summary, we have determined the nonchaotic character of this orbit, in part and in whole, using finite accuracy to compute finite orbital segments. In deciding that this specific orbit is nonchaotic, we have encountered no need to consider long-time limits nor the character of nearby orbits. An alternative resolution of this objection points out that, if all we know about X_0 is the 40 bits explicitly given above, this finitely accurate X_0 is the same for all orbits initiated in the interval $(X_0, X_0 + 2^{-41})$. Nonetheless, the initial orbit segments for all these orbits are nonrandom, no matter that some orbits will later reveal their randomness; for even random digit strings can begin with nonrandom segments. Equally, had the 40 digits of X_0 been generated by a random coin, then all the initial orbital segments lying in the above interval would be regarded as random no matter that some orbits will later reveal periodicity; for even periodic digit strings can begin with random segments. In summary, it is quite meaningful to characterize finite orbital segments as random or nonrandom, no matter their subsequent behavior, for as established earlier, the notion of randomness (or its lack) in finite digit strings is a perfectly valid concept.

In Sec. II, we develop the basis set for Hilbert space which is relevant to later developments. Specifically, we

compute the eigenvalues and eigenfunctions for a free quantum particle moving inside a specified, though largely arbitrary, boundary. In the process, we establish that the algorithm which computes these eigenvalues and eigenfunctions logarithmically compresses the information they contain. Section III then calculates the eigenvalues and eigenfunctions for a broad class of finite, bounded, undriven, quantum systems, and we again prove that the algorithms used logarithmically compress the output data. Section IV then verifies that, as anticipated, the information in the time evolution of these systems is also logarithmically compressible. Section V proposes a laboratory experiment which can test the ability of a nonchaotic quantum mechanics to predict the chaos known to occur in many finite, bounded, undriven, macroscopic systems. Section VI summarizes our results and draws conclusions. Finally, it must be emphasized that, in proving logarithmic compressibility of output information, it is not required that the algorithm we invoke be optimal or even practical; it must simply be capable of actually computing the desired objects, in principle.

II. EIGENVALUES AND EIGENFUNCTIONS FOR A BOUNDED FREE PARTICLE

Reed and Simon [10] prove that a free quantum particle constrained to move in any open, bounded domain has a discrete set of eigenvalues and eigenfunctions. They also prove that this set of eigenfunctions is complete. When the domain has a simple shape, one can frequently obtain analytic expressions for the eigenvalues and eigenfunctions; however, when the shape is complicated, one must resort to numerical algorithms. For us, perhaps the most convenient algorithm for solving the time-independent Schrödinger equation $-(\hbar^2/2m)\nabla^2 U$ =EU is the method of finite differences. Convergence of the method has been established by Bramble and Hubbard [11] and by Kuttler [12] for both two and three dimensions and for boundaries whose local parametric representations are \mathbb{C}^2 . In the following paragraphs, we present our method of solution for two dimensions; its generalization to three dimensions is straightforward.

We first rewrite the time-independent Schrödinger equation as the familiar Helmholtz equation $\nabla^2 U(x,y) + \lambda U(x,y) = 0$. We now replace $\nabla^2 U(x,y)$ by the finite difference operator $\Delta_{\epsilon} U(x,y)$ defined on a grid of squares having width ϵ . Specifically, we require

$$\Delta_{\epsilon} U(x,y) \equiv \epsilon^{-2} [U(x+\epsilon,y)+U(x-\epsilon,y)+U(x,y+\epsilon) + U(x,y-\epsilon)-4U(x,y)], \qquad (2)$$

where the continuum variables x and y now take on only the discrete values $x = m\epsilon$ and $y = n\epsilon$. Equation (2) is valid for all grid points whose nearest neighbors lie within the boundary. For a grid point whose nearest x neighbor lies, say, to the right of the boundary, Eq. (2) must be modified. If the boundary point lying on the line connecting these two neighbors lies a distance $\alpha\epsilon$ from the grid point in question, then Eq. (2) becomes

$$\Delta_{\epsilon} U(x,y) = \frac{1}{\epsilon^2} \left[\frac{1}{\alpha} U(x+\epsilon,y) + U(x-\epsilon,y) + U(x,y+\epsilon) + U(x,y-\epsilon) - \left[3 + \frac{1}{\alpha} \right] U(x,y) \right]. \quad (3)$$

Generalization of Eq. (3) to other near-boundary points is straightforward. The net result is that we now have one unique Helmholtz difference equation $\Delta_{\epsilon} U(x,y)$ $+\lambda U(x,y)=0$ for each grid point.

In fact, Eq. (2) and its companion Eq. (3) make it clear that these linear, coupled Helmholtz difference equations can be brought to matrix form. In preparation for the later use of a standard diagonalization algorithm, we elect to write the Helmholtz difference equations in terms of a square, two-subscript matrix \mathcal{R}_{ij} . To this end, we sequentially number all the grid points lying within the boundary with a single integer. Consider grid point *j* and let U_j be the value of U(x,y) at the *j*th grid point. Then we may write $\Delta_{\epsilon}U + \lambda U = 0$ at point *j* as $\sum_{u,j} \mathcal{R}_{ij}U_j + \lambda'U_j = 0$ or, more succinctly, as

$$\mathcal{R}\mathbf{U} + \lambda'\mathbf{U} = 0 , \qquad (4)$$

where U is a column vector with components U_j and where $\lambda' = \epsilon^2 \lambda$. To determine the matrix elements of \mathcal{R} , let the nearest neighbors of the point *j* be points *k*, *l*, *m*, and *n*. Then, according to Eq. (2), the *j*th row of Eq. (4) can be written $(U_k + U_l + U_m + U_n - 4U_j) + \lambda' U_j = 0$. The matrix elements of \mathcal{R} for the *j*th row are thus $\mathcal{R}_{jj} = -4$, $\mathcal{R}_{ij} = 1$ for i = k, l, m, or *n* and zero otherwise. When one of the nearest neighbors of the point *j* lies outside the boundary, say point *n* at which $U_n = 0$, then according to Eq. (3) we have $\mathcal{R}_{ii} = -(3 + \alpha^{-1})$, $\mathcal{R}_{ij} = 1$ for i = k, l, m, and zero otherwise. The generalization to two or three nearest neighbors lying outside the boundary is straightforward. For us, the essential point is that the matrix \mathcal{R} is not only real but also symmetric. This latter property follows from the fact that $\mathcal{R}_{ij} = 1$ if points *i* and *j* are nearest neighbors and zero otherwise.

Because \mathcal{R} is real and symmetric, it can be diagonalized using the sequential rotations of the Jacobi method [13]. Here, one performs sequential similarity transformation in the form of rotations reducing the off-diagonal elements of \mathcal{R} to zero. A convergence proof for the Jacobi method has been given by Golub and van Loan [13], while Schonhage [14] has shown that the Jacobi iteration scheme yields quadratic convergence of the off-diagonal elements to zero. Once the diagonalization of \mathcal{R} is completed to the desired accuracy, its eigenvalues can be read off its diagonal representation. The corresponding eigenfunctions are the columns of the composite rotation matrix which makes \mathcal{R} diagonal. Each one-variable eigenfunctions U(j) must then be mapped into the twovariable eigenfunction $U(m\epsilon, n\epsilon)$, but this involves only a trivial matter of relabeling points. Much more significant is the issue of obtaining accuracy estimates for the final eigenvalues and eigenfunctions. A bound on the error in the eigenvalues produced by the Jacobi method can be obtained using the Wielandt-Hoffmann theorem [15,1]. Upper and lower bounds on the deviation of the eigenvalues produced by the finite difference method from the true eigenvalues have been established by Weinberger [16] and by Ilg [1]. Pointwise error bounds on the eigenfunctions can be derived from the relationships given by Bramble and Hubbard [11] as has been shown by Ilg [1]. We elect not to write out these error estimates here, since for our purposes, it is sufficient to note that the computation of these error bounds involves nothing more than perhaps repeated use of the finite difference method plus the Jacobi method as outlined above [1]. Again, generalizing the above arguments to three dimensions is straightforward. Indeed, in the following paragraphs we assume that this generalization has been made.

We have now presented algorithmic procedures which can be used to compute the eigenvalues and eigenfunctions to any desired accuracy. Therefore, we are at last in a position to estimate the amount (in bits) of input information required to generate a specified amount of output information. To this end, let us begin by requesting as output the first M eigenvalues, each to an accuracy of $2^{-(N+1)}$. Moreover, let us require the corresponding set of M eigenfunctions evaluated at all lattice points [K] $(\sim \epsilon^{-3})$ in number], each value having an accuracy of $2^{-(N+1)}$. The output information in the eigenvalues contains no less than MN binary digits while that in the eigenfunctions contains no less than KMN binary digits. Let us now determine the amount of input information needed to compute the above (K+1)MN binary digits of output information. To this end, we now outline, at the block-diagram level, a computer program which could in principle actually print out the desired result.

Our first task is to compute the boundary of the domain D in which our free particle moves. Here we shall assume that the boundary can be divided into sections, in each of which the boundary is specified by a parametric representation X = X(u,v), Y = Y(u,v), and

Z = Z(u, v), where X, Y, and Z denote computable [4] functions. Without going into the technical details, for us "computable" means that the functions X, Y, and Z in each section of the boundary can be computed by repeated iteration of a finite set of computer instructions. The essential pieces of information we must supply the program which computes the boundary are the number L of its points to be determined and their accuracy $2^{-(N+1)}$. With only the additional input of the initial grid cube width ϵ , the program can compute all grid points in a large cube C which completely encloses the domain Dand can also compute the boundary points at which grid lines intersect the boundary, thereby determining all the α in the three-dimensional generalization of Eq. (3). Summarizing to this point, our computer program must be given the input data L, N, and initial ϵ which will take up $\log_2 L$, $\log_2 N$, and $\log_2 \epsilon$ bits of the program. In addition, the program must also be given the fixed length algorithms defining the parametric representation of the boundary. Those knowledgeable in complexity theory will immediately recognize that here the printable output information—L boundary plus K grid points having no less than N digits each—exponentially exceeds the input when K and L are large, but let us not dwell on this intermediate situation.

With the boundary and grid mesh now in place, the program can start at one corner of the cube C and work its way sequentially through the entire grid. If a given point is not inside D, skip to the next point. If the grid point lie within D, then generate one row of \mathcal{R} . Upon completion of this process, \mathcal{R} is fully determined. The program now utilizes the quadratically convergent Jacobi rotation method to decrease the size of the off-diagonal elements of \mathcal{R} sequentially. At each stage, the program uses the Wielandt-Hoffmann theorem [15] to check the accuracy of the eigenvalues of \mathcal{R} . If the error is not less than $2^{-(N+1)}$, another Jacobi rotation is initiated; otherwise the program continues to the next stage. To establish the closeness of these \mathcal{R} eigenvalues to the true eigenvalues of the problem, the program now repeats the above procedure twice, first for a set of cubes whose boundary lies totally within or on D and second for a set of cubes whose boundary lies totally outside or on D. These two additional run throughs provide upper and lower bounds on the true eigenvalues [1,16]. If the eigenvalues of $\mathcal R$ are not within the preassigned error value of $2^{-(N+1)}$ of the true eigenvalues, the program then decreases ϵ , recomputes the grid (and boundary, if necessary), and repeats the above procedure. When the error criterion is met, the eigenvalues are printed out. The eigenfunctions are now the columns of the composite Jacobi rotation matrix. The program now checks for pointwise accuracy [1,11] of these eigenfunctions. If the accuracy criterion $2^{-(N+1)}$ is met, the eigenfunctions are printed out; otherwise ϵ is decreased and the entire above procedure is repeated. Finally, to guarantee that the computer is using a sufficient number of digits to meet the accuracy criteria, a tally of the round-off error is maintained and an increase in precision from single to double to triple, etc., is made as needed.

Aside from the fixed bit length of the program itself,

the program requires $\log_2 M$ bits to specify the number of eigenvalues and eigenfunctions, $\log_2 N$ bits to specify the accuracy of all calculated quantities, $\log_2 \epsilon$ bits to specify the initial value of cube width, and $\log_2 L$ bits to specify the initial number of boundary points. When M and Nbecome large, the total bit length of this program equals $(\log_2 M + \log_2 N)$ to a good approximation. For this amount of input information, we obtain M eigenvalues each having no less than N bits, and M eigenfunctions evaluated at $K \ (\approx \epsilon^{-3})$ points having no less than N bits each. The output thus contains no less than (K+1)MNbits. It is now clear that our algorithm logarithmically compresses the information in the eigenvalues and eigenfunctions of the free-particle problem for all M and N, no matter how large. The full infinite set of eigenvalues and eigenfunctions is therefore not chaotic (random) because the information in all its finite subsets is logarithmically compressible [17,18].

This set of free-particle eigenfunctions forms a complete, orthonormal basis for Hilbert space. Although the eigenfunctions have been evaluated only on a countably dense set, continuity of the eigenfunctions permits analytic continuation, if required. Finally, the above program has computed only the one-particle eigenvalues and eigenfunctions. However, the many-particle eigenvalues are simply sums of the one-particle eigenvalues while many-particle eigenfunctions are simply products of oneparticle eigenfunctions.

III. EIGENVALUES AND EIGENFUNCTIONS FOR THE FULL PROBLEM

We now turn our attention to systems governed by Hamiltonians having the form

$$\mathbf{H} = \sum_{k=1}^{3N} \left(P_k^2 / 2m_k \right) + \mathbf{V}(Q_1, Q_2, Q_3, \dots, Q_{3N}) , \quad (5)$$

where m_K is the mass of the kth particle and N is the number of particles. As before, motion is confined to lie within a bounded, open domain whose boundary is specified by a computable, parametric representation. The potential V is required to be a sum of pair potentials in which each pair potential is a member of the Rollnik class [19], a general category of potentials which includes, among many others $V(r) = -r^{-\alpha}$ for $0 < \alpha < 2$, any V(r) which is a sum of an L^2 and an L^{∞} function, any V(r) continuous in $\mathbb{R}^3/\{0\}$ which goes to zero at infinity and for which $|V(r)| < C|r|^{-2}(1-\ln|r|)^{-\alpha}$ when |r| < 1 for some C and some $\alpha < 1/2$. For this broad class of finite, bounded, undriven quantum systems, Reed and Simon [10] prove that their eigenvalue spectrum is discrete and that their eigenfunction set is complete. Of course, there are additional systems, such as the harmonic oscillator, for which proofs of discreteness and completeness appear in the literature. However, contrary to popular opinion, not all spatially bounded, finite, undriven quantum systems have discrete spectra. Chirikov, Israilev, and Shepelyansky [20] discuss one of these exceptions. In any event, the broad class defined above is adequate for our purposes.

We obtain the eigenvalues and eigenfunctions of Hamiltonian (5) using the Raleigh-Ritz procedure whose convergence is guaranteed when the basis set of trial functions is complete [21]. Specifically, finding the minima of the functionals involved in the Raleigh-Ritz technique is equivalent [22] to the eigenvalue-eigenfunction problem for Hamiltonian (5). We thus must now obtain the matrix elements of $\mathbf{H}=\mathbf{H}_{\text{free}}+\mathbf{V}$, where $\mathbf{H}_{\text{free}}=\sum_{k}(P_{k}^{2}/2m_{k})$. Since we here already know the matrix elements of \mathbf{H}_{free} , we have only to obtain an algorithm for the matrix elements of \mathbf{V} , where, without significant loss of generality, we assume that \mathbf{V} is a computable function whose information content is logarithmically compressible. The matrix elements of \mathbf{V} can then be determined by

$$\mathbf{V}_{kl} = \int_{D} d^{3N} Q \ U_l(Q_s) \mathbf{V} U_k(Q_s) \ , \tag{6}$$

where N is particle number, D is the bounded open domain, and the $U_k(Q_s)$ are the real eigenfunctions of the free-particle problem. We may evaluate the integral in Eq. (6) by approximating it as the Riemann sum

$$\mathbf{V}_{kl} = \epsilon^{3N} \sum \cdots \sum U_l \mathbf{V} U_k , \qquad (7)$$

where the summation is to be carried out over all grid points inside the hyperdomain D^{3N} . Since the information in both the eigenfunctions U_k and the potential Vare logarithmically compressible and since the summations in Eq. (7) require only a fixed-length repetitive algorithm, the matrix elements \mathbf{V}_{kl} are computable, i.e., "information in" is the logarithm of "information out." Hence, the eigenvalues and eigenfunctions of \mathbf{H} can now be obtained using the Jacobi rotation technique [13] discussed earlier. It is straightforward to find theorems in the literature which prove that the above procedures do converge, but in order to establish the number of accurate output bits of information relative to the input at each stage, we must obtain accurate error estimates. It is to this matter we now turn.

Since we are using the free-particle eigenfunctions as our basis for Hilbert space, we can, as shown in Sec. II, determine the matrix elements of \mathbf{H}_{free} as accurately as we desire. The computation of the matrix elements \mathbf{V}_{kl} for the potential V, on the other hand, are subject to three sources of error which we now discuss. The first error is due to discretization of the integral in Eq. (6). Davis and Rabinowitz [23] provide a reliable estimate of this error which depends on the size of the domain D, the number of particles N, and the number of grid points nwithin D. The second source of error arises from the fact that the summation in Eq. (7) is taken over all grid points. Once each grid point in D^N is multiplied by the hypervolume ϵ^{3N} , the total hypervolume in Eq. (7) exceeds the hypervolume of D^N . A reliable estimate of this second error is again given by Davis and Rabinowitz [23]. The third source of error arises from the fact that, in practical computations, the Riemann sum of Eq. (7) will be evaluated using only approximate values for the free-particle eigenfunctions U_k . An estimate for this error is provided by Ilg [1]. Turning now to the full Hamiltonian H, an exact solution of the eigenvalueeigenfunction requires the diagonalization of the infinite

Hamiltonian matrix, whereas numerical algorithms cannot handle more than a finite, increasingly large number of matrix elements. We thus elect to diagonalize increasingly large square blocks of H in order to obtain increasingly good approximations to the eigenvalues and eigenfunctions of H. Specifically, the eigenvalues of the finite matrices are upper bounds for the true eigenvalues of H [1]. Lower bounds are given by Weinberger [21]. An additional error is induced in the computation of eigenvalues because of finite accuracy in the basis set; bounds for this error have been obtained by Ilg [1]. Turning now to eigenfunctions, as before we need a pointwise bound on the values for each eigenfunction. This bound can be obtained in terms of a bound on the norm for the difference between precise eigenfunction and Raleigh-Ritz eigenfunction [24]. From this bound, Weinberger [24] obtains a pointwise bound between true and approximate eigenfunctions. Weinberger's derivation assumes that the potential \mathbf{V} is positive and continuous within D and on its We have not sought to improve on boundary. Weinberger's conditions because they are not severe and, more important, because they still permit us to expose a broad class of finite, bounded, quantum systems which are not chaotic.

We are now in a position to describe in block-diagram form an algorithm which can compute the eigenvalues and eigenfunctions for the H of Eq. (5). We may then compare the amount of input information to output information. This program starts by running the algorithms which compute the eigenvalues and eigenfunctions for the free-particle problem. The output data for the free-particle problem is then used to compute the matrix elements of the full H along with the error estimates for these matrix elements. If they are not satisfactory, decrease the size of ϵ and repeat all earlier steps until the error is acceptable. Diagonalize H via Jacobi rotations and determine the error bounds; if not satisfactory, decrease ϵ , increase the number M of free-particle eigenvalues and eigenfunctions, and return to the start of the program. If the error is acceptable, print the eigenvalues and eigenfunctions. As input, this program requires all the input used by the free-particle problem -N, initial M, L, and ϵ —plus the number \mathcal{M} of desired full **H** eigenvalues and eigenfunctions (each evaluated at $\mathcal{H} \approx \epsilon^{-3N}$ grid points) and the accuracy $2^{-(N+1)}$ of each. Thus when \mathcal{M} and \mathcal{N} become large, an input of about $\log_2 \mathcal{M}$ and $\log_2 \mathcal{N}$ bits yields an output of about $(\mathcal{H}+1)\mathcal{M}\mathcal{N}$ bits, paralleling a similar result for the free-particle case. Finally then, we note that the infinite set of eigenvalues and eigenfunctions for the full H is not chaotic because the information in all its finite subsets is logarithmically compressible [17,18].

Since the arguments in both this and the previous section are a bit tedious, let us try to expose the forest hidden behind all these trees. Even including such input information as m_k or \hbar , the dominant input parameters we must give the program are simply the number of eigenvalues or eigenfunctions we wish as output along with their accuracy. Since we know all the relevant error bounds, we may simply write the program to iteratively reduce the error until it produces the desired result. Program run times may therefore be incredibly long, but run time is of no concern to us since convergence assures us that run time is finite, however, long. Moreover, computer storage space for either the program or the intermediate results is not a problem, because algorithmic complexity theory assumes that storage space, though finite, can be as large as we please.

IV. TIME EVOLUTION OF Ψ FOR THE FULL PROBLEM

Since the finite, bounded, undriven, quantum systems we consider have discrete spectra, their wave functions can always be written as

$$\Psi(\mathbf{x},t) = \sum_{k} A_{k} U_{k}(\mathbf{x}) e^{-iE_{k}t/\hbar}, \qquad (8)$$

where x denotes all spatial variables, t denotes time, the E_k and $U_k(x)$ are energy eigenvalues and eigenfunctions of **H**, respectively, the $A_k = \int dx \ U_k(x) \Psi(x,0)$ are expansion coefficients, and \hbar is Planck's constant divided by 2π . As we turn to proving that the information in $\Psi(x,t)$ is logarithmically compressible, we may not only avail ourselves of the results of Sec. III, but we may also considerably shorten the required proof. When the information in a quantity is logarithmically compressible, let us simply say that the quantity is compressible. Turning now to Eq. (8), all quantities in the exponent of each exponential are compressible. This is clearly true for the E_k ; it is also true for the time provided we restrict t to the rationals or to compressible irrationals like the $\sqrt{2}$; finally, it is true for \hbar provided we follow its known binary digits with any compressible digit string, such as all zeros. As a consequence, the product $(iE_k t/\hbar)$ is compressible. But each exponential in the sum may be iteratively computed from its power-series representation, thus each $e^{-iE_k t/\hbar}$ is compressible and the product $U_k(x)e^{-iE_k t/\hbar}$ is thus also compressible. Representing A_k by its Riemann sum, we observe that A_k is compressible provided we make the very mild assumption that $\Psi(x,0)$ is compressible. The sum of compressible factors in Eq. (8) may itself be computed by a recursive algorithm. Finally then, $\Psi(x,t)$ is compressible because the sum in Eq. (8) is compressible.

At this point, we may note that increasing or decreasing the size of compressible parameters such as m_k or \hbar by multiplying them say by $2^{\pm\beta}$, where β is a positive integer, does not affect their compressibility. If in this way we let $\hbar \rightarrow 0$, a serious question then arises regarding whether the compressible quantal description of finite, bounded, undriven, systems will always properly limit to the correct noncompressible chaotic behavior of classical dynamics. Indeed, it would appear that the quantal description of classically chaotic systems must, of necessity, exhibit the same unexpected behavior as the Arnol'd cat [3]. However, we elect not to pursue this question further here. Rather, we now propose an experimental test to determine whether quantum mechanics can predict the laboratory observable chaotic behavior of finite, bounded, undriven, macroscopic systems.

V. PROPOSED LABORATORY TEST OF QUANTUM MECHANICS

The quantal analysis of the preceding sections is subject to comparison with macroscopic laboratory reality. In making this comparison, no correspondence limits are to be taken nor is Newtonian dynamics to be invoked. Planck's constant is to be given its standard value and the generally large macroscopic system parameters are to be used in Schrödinger's equation. Quantum mechanics is designed to predict observables, so let it predict direct laboratory observations of a macroscopic finite, bounded, undriven system. It is crucial here to remember that macroscopic objects as well as their time evolution are quite stable under measurement by macroscopic instruments. Quantum effects, such as collapse of the wave function, spreading of wave packets, errors induced by the uncertainty principle, are here quite negligible, in general [9].

Nonetheless, macroscopic objects are many-body systems which, for the most part, are as intractable in the quantum domain as in the classical; even the gravitational three-body problem has, for example, successfully resisted all attempts at analytic solution. On the other hand, consider the simple pendulum. Any physical realization of this system is certainly a many-body problem, yet both classical and quantum mechanics treat it as a one-degree-of-freedom system. Here, the oscillatory motion is sufficiently isolated from pendulum internal degrees of freedom and the environment that these oscillations can be treated as quite independent. Of course, the effect of the internal degrees of freedom and the environment is to introduce damping into the pendulum's oscillations, but with sufficient experimental care, the pendulum can swing, as if undamped, over many periods. Here, one could construct a macroscopically sharp, but far from minimum, wave packet for the pendulum, having the form $\Psi(\theta,t) = \sum_{n} A_n U_n(\theta) e^{-iE_n t/\hbar}$, and expect it to predict laboratory observation to within experimental error. Our confidence in this regard is bolstered by the fact that the pendulum is "integrable" in both classical and quantum mechanics. But the classical pendulum is never chaotic, not even for large amplitude motion. Thus, let us take one step up and consider the double pendulum in which each pendulum bob is free to swing through 360°.

For small-amplitude motion of this two-degree-offreedom, double-pendulum system, we would expect a wave-packet description to agree with laboratory observation just as well as it does for the single-pendulum case. But for large-amplitude motion, the double pendulum exhibits a transition to chaos which is just as visible in the laboratory as is the transition to turbulence in a rising column of cigarette smoke [25]. But how can we observe the distinction, if any, between the nonchaotic quantal description of the motion and the chaotic motion perceived in the laboratory? One, though not the only, way is to perform a "crude," macroscopic time reversal of both the quantal and the laboratory motion. A number [3] of numerical experiments have shown that, in the domain of chaotic motion, the quantal description reverses back to its initial state to high accuracy whereas the classical

description does not. Here, "time reversal" means only that the signs of system velocities or momenta are reversed while time continues forward. The possibility of such a laboratory time reversal arises precisely because we are dealing with a macroscopic, two-degree-offreedom system. At this point, as a check, one might wish to verify that the chaotic motion of the double pendulum agrees with the classical prediction [26], if not the quantal. The essence of this proposed comparison is to reveal that quantum mechanics is "simple" whereas the macroscopic world is "complex." Clearly, this test of quantum mechanics will not be easy to conduct; few significant experiments are. Nonetheless, it is difficult to avoid guessing the outcome even before the experiment is performed.

The double pendulum is only one of several laboratory systems which might be used to test quantum mechanics. Experiments involving the Paul trap, superconducting quantum interference devices, Josephson junctions, or microwave excitation of Rydberg hydrogen immediately leap to mind. But to our minds, the virtues of the double pendulum lie in its simplicity, its ready availability, and its opportunity to demonstrate yet again the significance of chaos in simple, two-degree-of-freedom systems which have existed since the time of Newton.

VI. SUMMARY

Most investigators accept the lack of chaos in finite, bounded, undriven, quantum systems with the same ease they accept the statement that a simple closed curve divides the plane into an inside and an outside. Yet the

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- This paper is based in part on the Master's thesis of Matthias Ilg, Georgia Institute of Technology, 1991 (unpublished). A copy may be obtained upon request (from J.F.).
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proof of both these results contains many subtleties. Indeed, some finite, bounded quantum systems are chaotic [20]. Nonetheless, as we have shown, a broad class of such systems are nonchaotic, a result which may have quite deep consequences. To illustrate the possible consequences, we have elected not to investigate the correspondence limit, but to appeal directly to laboratory observation via a proposed experimental test. We have suggested the double pendulum as a viable macroscopic candidate, but other systems are available. But whatever the macroscopic system, the central issue is whether or not the motion of a chaotic, finite, bounded, undriven, macroscopic classical system can be predicted by a nonchaotic quantum-mechanical description. Strictly speaking, the issue is not whether quantum mechanics will fail in this regard, for fail it must. Indeed, it would be a logical contradiction for a compressible quantum description to correctly predict a noncompressible laboratory result. Rather, the issue is whether or not laboratory accuracy can detect the failure. Nonetheless, even (v^2/c^2) effects have been observed in the past and perhaps can also be observed in the present situation. In fact, it is possible that a time reversal using only "crude" macroscopic accuracy may elevate the quantum-laboratory discrepancies above the (v^2/c^2) level.

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