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Introductory Chapter: Dynamical Symmetries and Quantum Chaos

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1. Introduction

Chaos and many ideas from the study of this area have permeated a very large number of areas of science especially those which rely on mathematics. It is hoped this will illustrate how deeply and powerfully these ideas have influenced such areas as chemistry and physics.

Nature seems to be far too complicated to be linear at all levels all of the time. The exact laws of nature cannot be linear, nor can they be derived from such, to quote Einstein. Quantum mechanics, which is formally linear, is believed to be the underlying system to understand nature [1–3]. These seemingly conflicting views urge one to ask whether quantum mechanics can encompass nonlinear phenomena as well. This question is related to the study of classical nonlinear phenomena [4, 5]. This leads one to wonder about the behavior of a quantum system if the classical version is chaotic. To understand chaos in quantum mechanics requires a more rigorous formulation of the fundamental structures of quantum theory [6, 7]. To do this, one needs to formulate the quantum-classical correspondence, and at present, such a formulation is lacking.

In classical mechanics a Hamiltonian system with N degrees of freedom is defined to be integrable if a set of N constants of motion $\{F_i\}$ exist which are in involution, so the Poisson bracket satisfies $\{F_i, F_j\} = 0$, with $i, j = 1, \dots, N$. When the system is integrable, motion is restricted to an invariant N torus in $2N$ -dimensional phase space and so is regular. If the system is perturbed by a small nonintegrable term, the Kolmogorov-Arnold-Moser (KAM) theorem states that its motion may still be restricted to the N -torus but be deformed. Chaos appears when such perturbations increase to such a degree that some tori are destroyed, and their behavior is characterized by positive Lyapunov exponents.

Attempts to investigate quantum chaos have focused on the quantization of classical nonintegrable systems. Since the former in principle is only a limiting case of the latter and most realistic quantum systems do not have a classical counterpart, the latter approach is more general and natural. The classical limit is most often approached by using Ehrenfest's theorem, and three popular ways to study the classical limit are given as follows. The Schrödinger approach is to develop a wave packet whose time evolution follows classical trajectories, so the time evolution of the coordinate and momentum expectation values solves not only Hamilton's equations but also Schrödinger's equation. Dirac's approach is to construct a quantum Poisson bracket such that the basic structure of classical and quantum mechanics is placed in one-to-one correspondence. The third approach is the Feynman path integral formalism, which expresses quantum mechanics in terms of classical concepts by integrating overall possible paths for a given initial and final state.

The problem may be reviewed based on the axiomatic structure of quantum mechanics, out of which the quantum dynamical degrees of freedom are defined

and permit the construction of quantum phase space. This allows us to propose an idea for what quantum integrability is as well as its relationship with dynamical symmetry.

Quantum chaos is related to the question of the quantum-classical correspondence at two levels, kinematical and dynamical. The kinematical quantum-classical correspondence is a kind of reconciliation of the quantum and classical degrees of freedom and their associated geometrical structures.

Consistency of quantum theory implies there must exist a fundamental structure which can be used to determine the system's Hilbert space structure before solving the quantum dynamical equations. The axiomatic structure of quantum mechanics implies such a fundamental structure is simply the given algebraic structure of the system. The quantum mechanical Hilbert space is realized as a unitary irreducible representation of an algebra denoted as \mathfrak{g} . For example, the harmonic oscillator is mentioned described by the Heisenberg algebra h_4 and specified by the operators $\{a, a^\dagger, a^\dagger a, I\}$. Here a, a^\dagger are creation and annihilation operators for the oscillator. There is the spin system given by $su(2)$ and spin operators $\{S_-, S_+, S_0\}$ and other systems such as the hydrogen and helium atoms. The associated covering group G of \mathfrak{g} carries a natural geometric manifold, and all representations of quantum mechanics can be represented on such a geometrical manifold. Consequently, the kinematical correspondence can be constructed out of the dynamical group structure of the system, and the general solution is as follows.

A quantum system possesses a well-defined dynamical group G over a Hilbert space \mathcal{H} . This can be regarded as an irrep space. The number of quantum dynamical degrees of freedom of the system is just the same number as the M independent non-fully degenerate quantum numbers necessary to specify the space \mathcal{H} . The quantum phase space \mathcal{P} is realized uniquely on a $2M$ - dimensional coset space G/H where $H \subset G$ is the maximal stability subgroup of a fixed state $|\psi_0\rangle \in \mathcal{H}$ of the system. The coset space G/H and its global properties give a precise realization to the kinematical quantum-classical correspondence sought after. The fixed state $|\psi_0\rangle \in \mathcal{H}$ is the lowest (highest) weight state of \mathcal{H} when G is compact. When G is a non-compact group, it is the lowest bound state of \mathcal{H} .

To see what can be extracted from this statement, consider now some nontrivial examples. In particular, let us clarify the idea of quantum dynamical degrees of freedom. The non-fully degenerate quantum numbers are defined by the nonconstant eigenvalues of a complete set of commuting operators in the associated basis.

The harmonic oscillator whose dynamical group is the Heisenberg-Weyl group H_4 and Hilbert space is the Fock space with $|n\rangle$ as its basis is specified by the non-fully degenerate quantum number n .

Next consider the spin system whose dynamical group is $SU(2)$. In its Hilbert space, a given irrep space of $SU(2)$ labeled $|j, m\rangle$, the total spin quantum number is a constant. The only non-fully degenerate quantum number to specify the basis is m , and the quantum dynamical degree of freedom is one, as its Hilbert space, which is an irrep space of $SU(2)$ often denoted as $\{|j, m\rangle\}$, has total quantum number one.

In the central potential problem, the dynamical group is $SU(1, 1)$, and its quantum degree of freedom is one. The Hilbert space of $SU(1, 1)$ is specified by two quantum numbers k and n . The first is related to angular momentum, and the second is the principal quantum number. Since the angular momentum is conserved, the quantum number k is fully degenerate.

The hydrogen atom and the relativistic free Dirac particle are perhaps the simplest and most realistic both having the dynamical group $SO(4, 2)$. For hydrogen the three quantum dynamical degrees of freedom correspond to three non-fully

degenerate quantum numbers, the principle quantum number n , angular momentum quantum number j , and z -component m . These label the Hilbert space completely, $\{|n, j, m\rangle\}$.

For the harmonic oscillator, to construct the phase space, the fixed state used is the vacuum state. The phase space is then $H_4/U(1) \otimes U(1)$, where $U(1) \otimes U(1)$ is invariant with respect to the vacuum. The phase space structure is determined by coherent state $|z\rangle$ of $H_4/U(1) \otimes U(1)$:

$$D(\alpha)|z\rangle = |z + \alpha\rangle, \quad D(\alpha) \in H_4/U(1) \otimes U(1).$$

The phase space is not complicated, just a one-dimensional complex space or two-dimensional real space.

For a spin system, the dynamical group is $SU(2)$, and in an irrep space $\{|j, m\rangle\}$, the fixed state is $|j, -j\rangle$. The phase space is $SU(2)/U(1)$, and is isomorphic to a two-sphere, and there is the coherent state:

$$|\Omega\rangle = D(z)|j, -j\rangle = \exp(zS_+ - z^*S_-)|j, -j\rangle, \quad (1)$$

where s_{\pm} are spin raising and lowering operators. In a geometrical representation, $D(z)$ is

$$\exp \left(\begin{pmatrix} 0 & z \\ -z^* & 0 \end{pmatrix} \right) = \begin{pmatrix} \cos |z| & \frac{z}{|z|} \sin |z| \\ -\frac{z^*}{|z|} \sin |z| & \cos |z| \end{pmatrix} = \begin{pmatrix} x_o & x \\ -x^* & x_o \end{pmatrix}, \quad (2)$$

where x_o is real and $x = x_1 + ix_2$. Unitarity of $D(z) \in SU(2)/U(1)$ requires $x_o^2 + x_1^2 + x_2^2 = 1$, which describes a two-sphere. The phase space is nontrivial, and canonical coordinates can be obtained from the coherent state basis as

$$q = \sqrt{4j\hbar} \sin \frac{\theta}{2} \cos \phi, \quad p = -\sqrt{4j\hbar} \sin \frac{\theta}{2} \sin \phi.$$

2. Quenched quantum mechanics

The dynamical correspondence of quantum-classical mechanics is a fundamental idea which should be addressed. In order to study the resultant singularity structures which result in a transition to chaos, it must be stated more precisely what this limit entails. Quenched quantum mechanics suggests a possible origin for a parameter which maps out this limit. Instead of considering $\hbar \rightarrow 0$, it involves allowing a parameter referred to as the quenching index τ , which is dimensionless, to tend to infinity. In cases where τ turns out to be a fixed parameter, the system does not possess a classical limit. To understand properties of τ , let us consider the case in which the associated Lie algebra splits up in the form $g = h \oplus k$ with $[h, h] \in h$, $[h, k] \in k$, $[k, k] \in h$, where h is the Lie algebra of H and the explicit form of $K(z, \bar{z})$ is

$$K(z, \bar{z}) = \det(I \pm Z^\dagger Z)^{\pm\tau} \quad (3)$$

In Eq. (3), $+$ ($-$) refers to the case where G is compact (non-compact) and Z a matrix with elements z and τ is related to the matrix element $\langle 0|h_i|0\rangle$ with $h_i \in h$.

This gives rise to a geometrical interpretation for τ . This can be seen by looking at the propagator on G/H .

To study quenched quantum mechanics, the propagator is expressed as

$$U = \int D\mathbf{x} \exp\left(\frac{i}{\hbar}S\right). \quad (4)$$

In Eq. (4), $D\mathbf{x}$ is the integration measure and S is the effective action given as

$$S = \theta - \mathcal{H}dt.$$

where v is the one-form of G/H and \mathcal{H} the expectation value of the Hamiltonian operator $H = H(T_i)$, $T_i \in G$, that is,

$$V = i\frac{\hbar}{2} \left(\frac{\partial \ln K}{\partial z^i} dz^i - \frac{\partial \ln K}{\partial \bar{z}^i} d\bar{z}^i \right), \quad \mathcal{H} = \langle \Omega | H(T_i) | \Omega \rangle. \quad (5)$$

The quantum equations depend on τ . Upon expanding with respect to this parameter and not \hbar , the semi-quantal equations describing a classical-like system result. This arises from purely quantum structures and provides a way to achieve a classical limit:

$$\lim_{Q \rightarrow \infty} \mathcal{H} = \mathcal{H}_C = H(\langle \Omega | H | \Omega \rangle). \quad (6)$$

This limit may be divergent, since the phase space derived from the quantum geometry has not been scaled. Scaled canonical coordinates must be introduced to obtain a convergent limit as

$$\frac{1}{\sqrt{2\tau\hbar}}(q + ip) = \frac{Z}{\sqrt{I + Z^\dagger Z}}. \quad (7)$$

Expectation values of observables in coherent states can have correct dimensions in terms of p and q in such a coordinate system, and the semi-quantal dynamics in terms of (p, q) in (7) is determined by the Hamilton equations:

$$\frac{dq_i}{dt} = \frac{\partial(p, q)}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i} \quad (8)$$

The difference between semi-quantal dynamics and classical mechanics is called the quantum fluctuation or correlation $\mathcal{H} - \mathcal{H}_c = f(z, z^*, \eta)$, which is clearly an explicit function of η . Once the quantum fluctuation is fixed in a quantum system, its dynamical evolution is determined by \mathcal{H} not \mathcal{H}_c .

3. Dynamical symmetry

Let us discuss now some basic concepts related to chaos. One way to proceed is to study the behavior of quantum systems at the semi-quantal level by explicitly exploring the dynamical effects of quantum fluctuations on classical chaos. It would be good to find some general set of conditions which determine without great effort whether systems become chaotic and when.

The central idea of quantum integrability is dynamical symmetry. Integrability is a fundamental concept in the study of dynamical systems. Usually, the function

of symmetry restricts the possible forms of Lagrangian, but not the associated dynamics.

A quantum system with dynamical group G has a dynamical symmetry if and only if the Hamiltonian of the system can be written in terms of the Casimir operators of any particular subgroup chain G^α of G : $H = f(C_{ki}^\alpha)$, where $k = s^\alpha, \dots, 1$; $i = 1, \dots, l_k^\alpha$. Here α is fixed and labels the particular subgroup chain, C_{ki}^α is the i -th Casimir operator of subgroup G_k^α and l_k^α the rank of subgroup G_k^α .

Dynamical symmetry is less restrictive on the system than pure, since the Hamiltonian and ground state are not necessarily invariant under a transformation of G . Quantum integrability can be formulated from the classical definition once dynamical degrees of freedom are specified and the quantum-classical correspondence of dynamics is elaborated. The Heisenberg equation, the quantum dynamical equation, has a similar structure to the classical dynamical system.

A quantum system with M independent dynamical degrees of freedom and $2M$ -dimensional quantum phase space is integrable if and only if there are M quantum constants of the motion or good quantum numbers. The corresponding constants of the motion have operators which commute with the Hamiltonian. From the definition of dynamical symmetry and quantum integrability, it can be shown that a quantum system with a dynamical group G is integrable if such a system possesses a dynamical symmetry of G .

Consider the example of an N -independent level system to illustrate the consistency of quantum and classical integrability. Introduce annihilation and creation operators for the state $|i\rangle$ such that $|i\rangle = b_i^\dagger|0\rangle$, $|0\rangle = b_i|i\rangle$ and $[b_i, b_j^\dagger] = \delta_{ij}$, $[b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0$. Then the general form of the Hamiltonian is

$$H = \sum_{i,j=1}^n H_{ij} b_i^\dagger b_j. \quad (9)$$

The generators of the dynamical group $SU(N)$ are given as $E_{ij} = b_i^\dagger b_j$, and H is a linear operator composed of the E_{ij} . From group theory, it is always possible to assume there is a $U(N)$ transformation such that $H = \tilde{H} = gHg^{-1}$ where $g \in U(N)$ and

$$\tilde{H} = \sum_{i=1}^N \tilde{H}_{ii} E_{ii}. \quad (10)$$

It follows that \tilde{H} and H have the following dynamical symmetry

$$U(N) \supset \dots \supset C = U(1) \otimes U(1) \otimes \dots \otimes U(1), \quad (11)$$

where C represents the Cartan subalgebra which is defined to be a product of N factors of $U(1)$ with the generators E_{ii} . This implies the system is integrable. Consider now the phase space representation of this operator from quenched quantum mechanics, with phase space representation of E_{ij} :

$$\begin{aligned} \mathcal{E}_{11} &= N - \frac{1}{2}(p^2 + q^2), \\ \mathcal{E}_{ij} &= \frac{1}{2}(q_j + ip_j) \sqrt{2N - p^2 - q^2} \quad j \neq 1, \quad \mathcal{E}_{ij} = \frac{1}{2}(q_j + ip_j)(p_i + iq_i), \\ \mathcal{E}_{ji} &= (\mathcal{E}_{ij})^\dagger, \quad i, j \neq 1. \end{aligned} \quad (12)$$

where

$$p^2 + q^2 = \sum_{i=2}^N (p_i^2 + iq_i^2). \quad (13)$$

The \mathcal{E}_{ij} has the same algebraic structure as the E_{ij} , and the Hamiltonian function is only a decoupled function of $p_i^2 + q_i^2$ in quadrature. All of this implies that the system is integrable, as might be expected on account of dynamical symmetry.

There is an important consequence of the results mentioned above. Nonintegrability of a quantum system implies breaking of dynamical symmetry. This means that if chaos is present, dynamical symmetry of the system must be broken.

To develop this idea, if a system with l -rank, n -dimensional dynamical Lie group G is nonautonomous, dynamical symmetry breaking implies the system becomes nonintegrable. For an autonomous system, the energy is conserved, and it becomes nonintegrable, and this means it is broken such that more than one of the $M \leq (n - l)/2$ constants of motion are destroyed. It may be asked how much dynamical symmetry needs to be broken so that perturbative expansions about the dynamical symmetry basis will not converge.

Let us say that *chaos will appear* in a nonintegrable system when the breaking of the dynamical symmetry is accompanied by a structural phase transition. So if a structural phase transition takes place in a quantum system such that certain control parameters are altered, then it passes from one dynamical symmetry limit to another. Different dynamical symmetries connote different toroidal structures in G/H , so the torus structure must also alter from one to another. Consequently, dynamical symmetry breaking means that some or even all constants of motion are destroyed along with the corresponding tori giving rise to chaotic phenomenon.

Let us present a simple model which consists of two-spin coupled system governed by the Hamiltonian:

$$H = (1 - \alpha)\hbar(S_{1z} + S_{2z}) + \alpha\hbar^2 S_{1x} S_{2x}. \quad (14)$$

In (14), α is a coupling constant. This system has the possible dynamical symmetries:

$$SU^1(2) \otimes SU^2(2) \supset \begin{cases} SO^1(2) \otimes SO^2(2), & (i) \\ SU^{1+2}(2) \supset SO^{1+2}(2). & (ii) \end{cases} \quad (15)$$

The Hilbert space basis which carries the irreducible representations $(j_1 j_2)$ of $SU^1(2) \otimes SU^2(2)$ are $\{|j_1, j_2; m_1, m_2\rangle: m_1 = -j_1, \dots, j_1, m_2 = -j_2, \dots, j_2\}$ and $\{|j_1, j_2; j, m\rangle, j = j_1 + j_2, \dots, |j_1 - j_2|, m = -j \dots j\}$ for the dynamical symmetry chains (i) and (ii).

The dynamical symmetries of H are classified as: for $\alpha = 0$, H has symmetries (i) and (ii). For $\alpha = 1$, the system is just in (i). However, when $0 < \alpha < 1$, dynamical symmetries are broken. The semi-quantal description can be used to see whether there has been a structural phase transition in the symmetry breaking phase.

Coherent states are used to state the phase space is $S^2 \otimes S^2$ and given as

$$|p, q\rangle = \exp \sum_{i=1}^2 (z_i J_{i+} - z_i^* J_{i-}) |j_1, j_2; -j_1, -j_2\rangle. \quad (16)$$

where the canonical coordinates (p, q) are given as

$$\frac{1}{\sqrt{4j_i\hbar}}(q_i + ip_i) = \frac{z_i}{|z_i|} \sin |z_i| = \sin \frac{\theta_i}{2} e^{-i\varphi_i} \quad (17)$$

and $p_i^2 + q_i^2 \leq 4j_i\hbar$. The Hamiltonian determined by semi-quantal dynamics is

$$\mathcal{H} = \langle p, q | H | p, q \rangle = (1 - \alpha) \left[\frac{1}{2} (p_1^2 + q_1^2) + \frac{1}{2} (p_2^2 + q_2^2) - (j_1\hbar + j_2\hbar) \right] + \frac{\alpha}{4} q_1 q_2 \sqrt{4j_1\hbar - p_1^2 - q_1^2} \sqrt{4j_2\hbar - p_2^2 - q_2^2}. \quad (18)$$

Finally, it may be stated that to understand quantum chaos, one has to understand the dynamical behavior of a nonintegrable system when it deviates from the classical dynamics by taking into account nonvanishing quantum fluctuations. It may be asked whether the global phase space structure of classical dynamics can survive when quantum fluctuations are included. There is also the question of what governs the evolution of quantum fluctuations. It is required to have on hand a procedure which allows one to obtain the classical limit from a quantum system when one can only compute the deviations of the dynamics both close to and far from the classical limit. These deviations provide knowledge as to whether quantum fluctuations may alter classical dynamics and in what way. This is also deepening the understanding of the quantum-classical correspondence. Based on this, it may be asked whether the global phase space structure of classical mechanics can survive when quantum fluctuations are included and what actually governs the evolution of quantum fluctuations.

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