Quantum Kolmogorov-Arnol'd-Moser-like Theorem: Fundamentals of Localization in Quantum Theory

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A quantum Kolmogorov-Arnol'd-Moser-like theorem is formulated with use of an existence condition of a unique transformation between eigenstates of integrable and nonintegrable Hamiltonians. This condition determines the ability to assign local quantum numbers to eigenstates of nonintegrable Hamiltonians and explains localization phenomena.

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For systems with nonintegrable Hamiltonians the theorem named after Kolmogorov, Arnol'd, and Moser (KAM) established the existence in classical mechanics of localized stable motion, namely quasiperiodic orbits in coordinate space or invariant tori in phase space (for the generalized existence conditions and the proof, cf. Arnol'd[1]). For purposes of analogy with what shall be done below the important points of KAM theorem are reviewed. Assume that a nonintegrable Hamiltonian in N degrees of freedom may be written as $H=H_s(J)+\lambda V(J,\theta)$, where H_s is an integrable Hamiltonian cyclic in N action variables θ. Since H_s is integrable it generates phase-space trajectories that are conditionally periodic; that is they lie on N-dimensional surfaces in phase space called tori. The points (p_i, q_i) on a torus satisfy N relations $p_i=\partial S(J)/\partial q_i$, where S is the generating function that solves the Hamilton-Jacobi equation for H_s. Each torus is completely determined by N values of the action variables J. The KAM theorem states that for sufficiently small perturbations ($\lambda \ll 1$), most of the unperturbed tori of H_s do not vanish but are only "slightly deformed," so that most of the trajectories generated by the perturbed H are still conditionally periodic. The proof of the KAM theorem rests on a convergence argument of perturbation theory, where starting from an unperturbed (and nonresonant) torus of H_s, and if $\lambda \ll 1$, a perturbed torus can be found by convergent perturbation solution of the Hamilton-Jacobi equation for the nonintegrable H. The perturbation method is a sequence of successive canonical transformations, each of which is close to the identity transformation, that if convergent can be truncated to eliminate the angle-dependent terms and to yield an integrable Hamiltonian close to the fully perturbed H. The same sequence of canonical transformations generates the perturbed torus from the unperturbed one, and is therefore the generating function that solves (in a convergent perturbation manner) the Hamilton-Jacobi equation. The existence of a torus that is the limit of a convergent sequence allows the calculation of the actions from the N action integrals $\oint \vec{p}\cdot d\vec{q}$ defined for N independent closed paths about the torus. These actions are local since they are defined on a torus which itself is local and they impose the N relations (action integrals) on original dynamical variables $\vec{p}$ and $\vec{q}$ which causes localization in both position and phase space.

The motivation for seeking a similar theorem in quantum mechanics follows. In quantum theory localization and the ability to assign uniquely (or equally important, the inability to assign) N quantum numbers to an eigenfunction of a nonintegrable H has never been demonstrated as the existence conditions which must be satisfied have never been given. Of course, no end of solutions have been found in various problems that physically show localization phenomena: for example, narrow resonances behind potential barriers which could be modeled as arising from bound states in the continuum,[2] and the successful assignment of atomic states according to LS or jj coupling schemes. Many other localizations are only explained approximately. For example, the chemical bond (a truly localized quantity) in ground and excited states is explained by obtaining wave functions and energies that show that the bond exists only after the Born-Oppenheimer adiabatic approximation has been made. Even if an exact (or nearly exact) solution to the wave function could be obtained without the adiabatic approximation and which did show localization in bond regions, the chemical

bond would still be hard to explain in the sense that the total molecular bare potential generally shows no walls or barriers that would confine the electron cloud to the bonds. Fano[3] has recently called attention to other problems in atomic and molecular physics where an exactly similar situation occurs, namely the quadratic Zeeman effect, certain doubly excited autoionizing states in helium, and collinear chemical reactions such as $I+HI \rightarrow IH+I$.[4] In all of these cases the solution of the wave equation exhibits localizations which could only be explained in the limit of weak perturbations or in an adiabatic picture.

In a recent paper[5] we have established a criterion to test for quantum states that correlate with the classical quasiperiodic trajectories that yield the quantum energy levels by semiclassical quantization. Our criterion is essentially an existence criterion for the convergence of perturbation-iteration expansion for the energy starting from an unperturbed eigenstate of an integrable Hamiltonian. We had not realized it at the time, but this existence criterion (slightly modified below) is in essence the quantum analog of the classical KAM theorem. As such it is precisely the existence condition for assigning N quantum numbers to eigenfunctions of nonintegrable Hamiltonians, and in the same way is the explanation for unexpected localizations.[3,4] We rederive our criterion in the spirit of the classical KAM theorem.

Consider H and H_s to be respectively nonintegrable and integrable Hamiltonians in N degrees of freedom. Let J represent a set of N commuting observables (dynamical variables) that commute with H_s but not with H. Since $[H_s, J]=0$, the eigenfunctions of H_s could be chosen simultaneously as eigenfunctions of the set J. When H_s has a degenerate spectrum it has several sets of commuting observables; the corresponding eigenbases are related through unitary transformations within the degenerate subspaces of H_s For a given basis, each eigenfunction is uniquely labeled by N quantum numbers that represent the eigenvalues of the observables J that define the basis. To see the analogy with the classical KAM theorem it suffices to consider one set J. In the classical limit[6] the eigenfunctions of H_s that are labeled by the set J are usually identified with the unperturbed tori of the classically integrable H_s that commutes (in the Poisson-bracket sense) with the action variables J.

Let Ψ and Φ be eigenfunctions of H and H_s, respectively. If there exists a one-to-one transformation relation between the particular states Φ and Ψ, then since Φ is uniquely labeled by N quantum numbers, so will Ψ be. The existence condition of a one-to-one transformation between Φ and Ψ is[5]

$$|\langle\Phi|\Psi\rangle|^2 > 0.5, \tag{1}$$

where Ψ and Φ are both normalized to unity. It can be immediately seen that condition (1) establishes one-to-one correspondence between the states Φ and Ψ. Since $\langle\Phi|\Phi\rangle=1$, it is guaranteed that if one eigenfunction of the nonintegrable H satisfies condition (1) for a particular Φ, then it is the only one that does so. The converse follows trivially. Note that if Φ does not satisfy condition (1) for any eigenstate of H, then it is possible that two eigenstates of H would have equal weights on that Φ. What must be realized is that condition (1) provides a quantitative measure as to how close in Hilbert space the eigenstates Φ of H_s and Ψ of H should be, so that a unique transformation shall exist from the unperturbed Φ to the perturbed Ψ. Classically, this condition is vaguely stated[1] as "sufficiently small pertrubation." It is shown below that in a manner similar to the KAM theorem, condition (1) will also guarantee the existence of an energy-independent effective Hamiltonian defined on part of the Hilbert space, the unperturbed Φ, and which is close to H in the sense that when operating on Φ it gives the same energy (to any desired accuracy) as does H while operating on the perturbed Ψ. This is analogous to shifting the unperturbed torus onto the perturbed energy shell in the classical phase space.

Unlike the KAM theorem, the present theorem does not prove *a priori* existence in terms of analytic properties of H_s, albeit by placing almost unacceptable restrictions on the perturbation. The new theorem, in fact, places no unusual limitations on H and in this sense is more general. Here condition (1) is a test for existence given the exact solution Ψ which has been constructed as below or by other methods. Existence in general is then demonstrated by simply recalling that the eigenstates of a Hamiltonian which is known to be nonintegrable[6] have already been shown[5] to satisfy condition (1). Numerous other examples are available from, say, the success of the normal-mode model to describe the low-lying vibrational states of molecules.

By use of the projector operator onto Φ, $P=|\Phi\rangle\langle\Phi|$, and its complement $Q=1-P$, it is possible to transform the Schrödinger equation

for the nonintegrable Hamiltonian, $H\Psi = E\Psi$, into a nonlinear equation for an energy-dependent effective Hamiltonian defined on Φ,[7]

$$H_{\text{eff}}(E)P\Psi = [PHP + PHQ(E - QHQ)^{-1}QHP]P\Psi = EP\Psi. \quad (2)$$

The perturbed wave function is obtained from $P\Psi$ by the wave-operator transformation[8] that yields Ψ expanded in the basis of H_s,

$$\Psi = A(E)P\Psi = [P + (E - QHQ)^{-1}QHP]P\Psi. \quad (3)$$

Multiplying (2) by Φ^* and integrating, we obtain, after eliminating $\langle\Phi|\Psi\rangle$ from both sides of the equation,

$$E = \langle\Phi|PHP + PHQ(E - QHQ)^{-1}QHP|\Phi\rangle. \quad (4)$$

Assuming, without loss of generality, that the eigenvalues of QHQ are known, we can proceed to solve Eq. (4) for the perturbed energy by an iteration procedure starting from an initial guess; for example $E^{(0)} = E_s$, the unperturbed energy. The advantage of this iteration procedure over other methods (e.g., the Newton-Raphson method) of solving Eq. (4) is that only here does the iteration sequence $E^{(i)}$ uniquely give, via Eqs. (2) and (3), sequences of $H_{\text{eff}}(E^{(i)})$ and $\Psi(E^{(i)})$ which show the evolution of H_{eff} and Ψ to their limits. Note that while the function series $\Psi(E^{(i)})$, if convergent, yields the exact eigenfunction of H, the limit of $H_{\text{eff}}(E^{(i)})$ is not the exact Hamiltonian. This is fortunate as it is seen below that H_{eff} is integrable but H by definition is not. In the case where $P = |\Phi\rangle\langle\Phi|$, the iteration procedure leads to a simple formal continued-fraction expression for H_{eff},

$$H_{\text{eff}} = PHP + PHQ\left(\cfrac{1}{-QHQ + \langle\Phi|HP + PHQ\cfrac{1}{-QHQ + \langle\Phi|HP + PHQ\cfrac{1}{\ddots\cfrac{}{-QHQ + E_s}}QH|\Phi\rangle}QH|\Phi\rangle}\right)QHP. \quad (5)$$

The infinite continued-fraction expression (5) is strictly equivalent to $H_{\text{eff}}(E)$ defined in Eq. (2). If the iteration procedure diverges, it means that H_{eff} is defined only at the perturbed energy (or by infinite continued fraction) and is therefore energy dependent. However, if the iterations converge, then to any desired accuracy there exists a finite continued-fraction approximation to H_{eff}. This truncated H_{eff} is analogous to the classical Hamiltonian which is "close" to the exact nonintegrable H. Furthermore, comparing Eqs. (2) and (3) it is seen that $H_{\text{eff}}(E) = PHA(E)$; it is clear therefore that any finite continued-fraction H_{eff} yields a finite continued-fraction expression for the wave operator A that performs the transformation from the unperturbed Φ to the perturbed Ψ. The crucial point is that the iteration procedure generates a sequence of functions in Hilbert space, as each iteration step is equivalent to a finite continued-fraction transformation from the unperturbed Φ. Convergent iterations produce therefore a sequence of functions which begins with the unperturbed Φ and has a definite limit, the perturbed Ψ. This is exactly the situation in the classical KAM theorem whereby a sequence of canonical transformations from the unperturbed torus has as its limit the "slightly deformed" torus.

Now H_{eff} is defined only in P space; it vanishes in Q space. Since the P space is just Φ which is an eigenfunction of N commuting observables J, the latter must also commute with H_{eff}. However, this commutativity means that the observables J are constants of the motion for H_{eff} only when the latter is energy independent; i.e., it is a convergent continued-fraction Hamiltonian. We have previously shown[5] that condition (1) is the convergence condition for the iteration solution of Eq. (4). Hence, Eq. (1), and its one-to-one correspondence property, is an existence condition for a unique energy-independent H_{eff} that would generate a unique wave-operator transformation from the unperturbed Φ to the perturbed Ψ. The exact constants of the motion for H_{eff} defined on Φ are therefore the local (as Φ is only a part of Ψ) actions for Ψ. No other eigenstate of H can have the same local actions as Ψ which is therefore uniquely assigned by the corresponding quantum numbers that label Φ.

In summary, the convergence condition of perturbation theory, $\lambda \ll 1$ in the classical case and

$|\langle\Phi|\Psi\rangle|^2 > 0.5$ in the quantum case, is a criterion of localization, as it guarantees the existence of an integrable Hamiltonian which is "close" to the exact nonintegrable H so as to generate a unique transformation between the unperturbed and the perturbed classical tori, or quantum wave functions. Physically Ψ, an eigenfunction of a nonintegrable Hamiltonian, is localized because it is dominated in the probability-density sense by an eigenfunction, Φ, of an integrable H_s. In this respect condition (1) is the quantum localization condition analogous to N local actions in classical mechanics, $\oint \vec{p} \cdot d\vec{q}$. Both "hold" the solutions in place. Hence, it is a necessary and sufficient condition for a solution with N local quantum numbers to exist.

Finally, we mention that the KAM theorem, as well as the present derivation of its quantum analog, is applicable to bound systems. Yet it is well known that quasiperiodic trajectories were found in regions where no potential walls exist to enforce classically bound motion,[9] and were shown to be related to resonances in the continuum.[10] Complex dilatation analysis,[11] prior to the perturbation analysis, provides a continuum KAM analog and a way for a unique assignment of resonances.

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