Geometry of Quantum Riemannian Hamiltonian Evolution

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This work concerns a study of the quantum mechanical extension of the work of Horwitz et al. [1] on the stability of classical Hamiltonian systems by geometrical methods. Simulations are carried out for several important examples; these show that the quantum mechanical extension of the classical method, for which trajectories are plotted as expectation values of the corresponding quantum operators, appears to work well, providing results consistent with the corresponding classical problems. The results appear to provide a new contribution to the subject of quantum chaos.

I. INTRODUCTION

A classical Hamiltonian of the standard form

$$H = \delta_{ij} \frac{p^i p^j}{2m} + V(y)$$  (1)

can be cast into the Riemannian form [1]

$$H_G = \frac{1}{2m} g^{ij}(x) p^i p^j$$  (2)

by choosing

$$g_{ij}(x) = \Phi(x) \delta_{ij}$$  (3)

with, for $H$ and $H_G$ on the same energy shell $E$, the constraint

$$\Phi(x)(E - V(y)) = E$$  (4)

It follows from the classical Hamilton equations that [2][3] the motion generated by the Riemannian Hamiltonian (2) satisfies the geodesic relation

$$\ddot{x}_l = -\Gamma_{lmn} \dot{x}_m \dot{x}_n$$  (5)

where the connection form is given by (here $g^{ij}$ is the inverse of $g_{ij}$)

$$\Gamma_{lmn}^{mn} = \frac{1}{2} g^{ik} \left\{ \frac{\partial g^{kn}}{\partial x^m} + \frac{\partial g^{km}}{\partial x^m} - \frac{\partial g^{mn}}{\partial x^k} \right\}$$  (6)

Let us now define the variable $y^j$ for which

$$y^j \equiv g^{ij}(x) \dot{x}_i = \frac{p^j}{m}$$  (7)

The last equality follows from the Hamilton equations based on the Riemannian Hamiltonian (2), and the geodesic equation (5) implies that the variables $\{y\}$ then satisfy the equation

$$\ddot{y}_l = -M_{lmn} y_m y^n$$  (8)

where

$$M_{lmn} = \frac{1}{2} g^{jk} \frac{\partial g_{nm}}{\partial y^k}$$  (9)

corresponds to an affine connection governing the motion in the $\{y\}$ description. Application of the constraint (4) to the definition (9) results in precisely the Hamilton equations derived from (1). Therefore, the evolution (8) corresponds to a geometric embedding of the usual Hamiltonian motion described by (1). With (7) a functional correspondence can be established between the variables $x_i$ and $y^j$ [4].

An equivalence principle becomes accessible for the Hamiltonian (1) through the mapping defined by (3) and (4), since the connection form (5) is compatible with the metric (3). Moreover, it is shown in [1] that the "geodesic deviation" computed from (8) results in a Jacobi equation for which the eigenvalues associated with the resulting curvature tensor, constructed from the $M$ connection (9), have remarkable
We then construct the quantum counterpart of the variables corresponding with a general operator valued Hermitian Riemannian Hamiltonian

\[ \hat{H}_G = \frac{1}{2m} p^i g_{ij}(\mathbf{x}) p^j \]  

We shall show here that the variables corresponding to \{x\} in the Heisenberg picture, satisfy dynamical equations closely related to those to the classical system, and therefore that when the Ehrenfest correspondence is valid, the expectation values of these variables would describe a corresponding flow.

We then construct the quantum counterpart of the relations (7), (8), (9) and show that these results are related to the quantum dynamics associated with a Hamiltonian operator of the form (1).

First we study the basic operator properties of coordinate and momentum observables associated with a Hamiltonian operator of type (10) (with \( g_{ij} \) invertible). Thus the canonical momentum is defined, both classically and quantum mechanically, as the generator of translation on a Euclidean space, and thus has a Schrodinger (coordinate) representation as a simple derivative.

II. HEISENBERG ALGEBRA ON THE GEOMETRIC HAMILTONIAN

The coordinates \{x_i\} form a commuting set, as do the \{p^j\}. The Heisenberg equations for the coordinates (\( \hbar = 1 \)):

\[ \dot{x}_k = i[H_G, x_k] \]  

with the canonical commutation relations

\[ [x_i, p^j] = i \delta^j_i \]  

result in

\[ \dot{x}_k = \frac{1}{2m} \{ p^j, g^{kl} \} \]  

The corresponding classical result leads directly, by inverting \( g_{ik} \), to an expression for \( p^i \) in terms of \( \dot{x}_k \). We can nevertheless invert equation (13). The anticommutator of \( \dot{x}_k \) with \( g^{kl} \) becomes

\[ \dot{x}_k g^{kl} + g^{kl} \dot{x}_k = \frac{1}{2m} \left[ \left( p^i g_{ik} + g_{ik} p^i \right) g^{kl} + g^{kl} \left( p^i g_{ik} + g_{ik} p^i \right) \right] 
\]

\[ = \frac{1}{2m} \left[ p^l \delta_{il} + g_{ik} p^l g^{kl} + g^{kl} p^l g_{ik} + \delta_{il} p^l \right] 
\]

\[ = \frac{1}{2m} \left[ 2 p^l + p^l g_{ik} g^{kl} + [g_{ik}, p^l] g^{kl} + g^{kl} g_{ik} p^l + g^{kl} [p^l, g_{ik}] \right] 
\]

\[ = \frac{1}{2m} 4 p^l = \frac{2}{m} p^l \]  

so that

\[ p^l = \frac{m}{2} \{ \dot{x}_k, g^{kl} \} \]  

The cancellation in (14) that leads to this result follows from the fact that \( [g_{ik}, p^l] \) depends only on \( \mathbf{x} \) and commutes with \( g^{kl} \). This result implies that the Hamiltonian does not correspond to a simple bilinear form in \( \dot{x}_i \), but a bilinear in anticommutators of the type (15). As we shall see, this correspondence carries over to the analog of the geodesic type formula for \( \dot{x}_i \). The classical form of eq. (15) (as in the classical theory) does not correspond to the usual relation between momentum and velocity; moreover, by Eq. (14) the separate components of \( \dot{x}_k \) do not commute with each other, or, with \{x_i\}. For example, it is straightforward to show that

\[ [\dot{x}_k, x_l] = -\frac{i}{m} g_{lk} \]  

and

\[ [\dot{x}_k, \dot{x}_l] = \frac{i}{2m^2} \left( p^i (g_{im} \frac{\partial g_{kl}}{\partial x_m} - g_{km} \frac{\partial g_{il}}{\partial x_m}) \right) \]  

Thus, the velocities do not commute. Let us define, in analogy to the classical case, a new set of operators (analogous to what were called \{y\} in our discussion above of the classical case; here we use the same notation)

\[ \dot{y}^j = \frac{1}{2} \{ \dot{x}_k, g^{kl} \} \]  

so that, by (15),

\[ p^j = m \dot{y}^j \]  

The \{\dot{y}^j\} form a commutative set. Furthermore, it follows from (16) that

\[ [\dot{y}^j, x_m] = \frac{1}{2} \{ \dot{x}_k, g^{kl} \}, x_m \} = g^{kl} [ \dot{x}_k, x_m ] = -\frac{i}{m} \delta^j_m \]
We now turn to the second order equations for the dynamical variables. Since from (19)

\[ \dot{y}^i = -\frac{i}{m} [p^i, \hat{H}_G] = \frac{1}{2m^2} p^i [p^j, G_{ij}(x)] p^j = -\frac{1}{2m^2} p^i \frac{\partial G_{ij}}{\partial x_l} p^j \]

(22)

Using (19) again, we arrive at the simple result

\[ \ddot{y}^i = -\frac{1}{2} \ddot{y}^j \frac{\partial G_{ij}}{\partial x_l} y^j \]

(23)

closely related to the form obtained in the classical case \[1\] for the "geodesic" equation with reduced connection. In the classical case, this formula was used to compute geodesic deviation for the geometrical embedding of Hamiltonian motion (for Hamiltonian of the form \( \frac{p^2}{2m} + V(y) \)) \[1\], as discussed above, for which the corresponding metric was of the conformal form given in Eq. (3). It follows from the Heisenberg equations applied directly to (18) that

\[ \dot{y}^i = i[\hat{H}_G, \dot{y}^i] = \frac{i}{2} [\hat{H}_G, \dot{x}_k g^{ki} + \dot{g}^{ki} \dot{x}_k] = \frac{1}{2} \dot{x}_k g^{ki} + \frac{i}{2} \dot{x}_k [\hat{H}_G, \dot{y}^i] + \frac{i}{2} [\hat{H}_G, \dot{g}^{ki}] \dot{x}_k + \frac{1}{2} \dot{g}^{ki} \dot{x}_k \]

(24)

Computing the commutator \([\hat{H}_G, \dot{g}^{ki}]\) in relation (24),

\[ [\hat{H}_G, \dot{g}^{ki}] = \frac{1}{2m} \{ p^m g_{mn} p^n, \dot{g}^{ki} \} \]

\[ = \frac{1}{2m} \{ p^m \dot{g}_{mn} p^n + p^m g_{mn} \dot{p}^n, \dot{g}^{ki} \} \]

\[ = \frac{1}{2m} \{ -i \frac{\partial \dot{g}^{ki}}{\partial x_l} g_{mn} p^n + p^m g_{mn} (\frac{i}{2m} \frac{\partial \dot{g}^{ki}}{\partial x_l}) \} \]

\[ = \frac{i}{2m} \frac{\partial \dot{g}^{ki}}{\partial x_l} g_{mn} p^n \]

(25)

and therefore

\[ \ddot{y}^i = \frac{1}{2} \{ \ddot{x}_k, g^{ki} \} + \frac{i}{2} \{ \dot{x}_k, [\hat{H}_G, \dot{g}^{ki}] \} \]

\[ = \frac{1}{2} \{ \ddot{x}_k, g^{ki} \} + \frac{1}{4m} \{ \dot{x}_k, \frac{\partial \dot{g}^{ki}}{\partial x_l} g_{mn} p^n \} \]

(26)

Furthermore, with relation (15), \( p^m = \frac{m}{2} \{ \dot{x}_k, g^{kn} \} \), relation (26) results in

\[ \ddot{y}^i = \frac{1}{2} \{ \ddot{x}_k, g^{ki} \} + \frac{1}{8} \{ \dot{x}_k, \frac{\partial \dot{g}^{ki}}{\partial x_l} g_{mn} \{ \dot{x}_m, g^{kn} \} \} \]

(27)

The relation between \( \ddot{y}^i \) and \( \ddot{x}_k \) therefore contains nonlinear velocity dependent inhomogeneous terms. It appears, however, that there should be a strong relation between instability, sensitive to acceleration, in \( x \) and \( y \) variables.

To find the second order equation for the operators \( x_1 \), we proceed directly from (10), using (19), to write the Hamiltonian as

\[ \hat{H}_G = \frac{m}{2} \ddot{y}^i G_{ij}(x) \dot{y}^j \]

(28)

We may now compute

\[ \ddot{x}_l = i[\hat{H}_G, \dot{x}_l] \]

(29)

and use (17) and (18) to obtain the quantum mechanical form of the "geodesic" equation generated by the Hamiltonian \( \hat{H}_G \):

\[ \ddot{x}_l = \frac{1}{16} \{ \{ s^{\mu n}, \dot{x}_m \}, \frac{\partial s^{\mu n}}{\partial x_l} \}, G_{ij} \{ s^{ip}, \dot{x}_p \} \]

\[ - 2 \{ s^{ip}, \dot{x}_p \} g_{ln} \frac{\partial \ddot{g}_{ij}}{\partial x_n} (g^{hi}, \dot{x}_q) \]

(30)

In the classical limit, where all anticommutators become just (twice) simple products, a short computation yields

\[ \ddot{x}_l = -\Gamma_{pq}^l \dot{x}_p \dot{x}_q \]

(31)

with

\[ \Gamma_{pq}^l = \frac{1}{2} g_{ln} \left( \frac{\partial s_{np}^{\mu}}{\partial x_p} + \frac{\partial s_{np}^{\mu}}{\partial x_q} - \frac{\partial s_{np}^{\mu}}{\partial x_n} \right) \]

(32)

i.e., the classical geodesic formula generated by a classical Hamiltonian of the form (2) \([1]\). Therefore, (30) is a proper quantum generalization of the classical geodesic formula.

We finally express the quantum "geodesic" formula (30) explicitly in terms of the canonical momenta using (18) and (19). We use the canonical commutation relations to write the result in terms of a bilinear in momentum ordered to bring momenta to the left and right. In this form we may describe the quantum
state in terms of the variables \( \{ x_i \} \) canonically conjugate to the \( \{ p^j \} \) in the sense of (20-22), for which

\[
p^j \rightarrow -i \frac{\partial}{\partial x_j}
\]

on \( \psi(x) \).

We then find that expression (30) for the quantum mechanical form of the "geodesic" equation \( \ddot{x}_i \) could be written as

\[
\ddot{x}_i = \frac{1}{2m^2} p^j (\frac{\partial g_{ij}}{\partial x_n} g_{nj} + \frac{\partial g_{ij}}{\partial x_n} g_{nl} - \frac{\partial g_{ij}}{\partial x_n} g_{ln}) p^j + \frac{1}{4m^2} \frac{\partial}{\partial x_j} (\frac{\partial^2 g_{ln}}{\partial x_i \partial x_n} g_{ij})
\]

(34)

The first term is closely related to the classical connection form; the second term, an essentially quantum effect.

III. LOCAL RELATION BETWEEN THE TWO COORDINATE BASES

We shall need some algebraic relations. Using definition (19) and relations (13) and (18), it follows that

\[
[g_{ij}, \dot{y}_l] = \frac{1}{2m} [g_{ij}, \{ p^m, g_{ln} \}]
\]

\[
= \frac{1}{2m} p^n [g_{ij}, g_{nl}] + \frac{i}{2m} [g_{ij}, g_{nl}] p^n
\]

\[
= -i \frac{m}{2m^2} p^n \frac{\partial g_{ij}}{\partial x_i} - i \frac{m}{2m^2} \frac{\partial g_{ij}}{\partial x_i} p^n
\]

\[
= -i \frac{m}{2m} \{ g_{ij}, \frac{\partial g_{nl}}{\partial x_i} \}
\]

(35)

so that

\[
[y_i, \dot{x}_l] = -i \frac{m}{2m} \{ g_{ij}, \frac{\partial g_{nl}}{\partial x_i} \}
\]

(36)

Furthermore

\[
[g_{ij}, \dot{x}_l] = \frac{1}{2m} [g_{ij}, \{ p^m, g_{ln} \}]
\]

\[
= \frac{1}{2m} [g_{ij}, p^m] g_{nl} + \frac{1}{2m} g_{nl} [g_{ij}, p^m]
\]

\[
= \frac{i}{m} \frac{\partial g_{ij}}{\partial x_n}
\]

(37)

so that

\[
[g_{ij}, \dot{x}_l] = \frac{i}{m} \frac{\partial g_{ij}}{\partial x_n}
\]

(38)

We also have that

\[
[g_{ij}, \dot{y}^l] = \frac{i}{m} \{ g_{ij}, \dot{x}_k, \hat{G}^{kl} \}
\]

\[
[g_{ij}, \dot{y}^l] = \frac{i}{2m} [g_{ij}, \dot{x}_k, \hat{G}^{kl}]
\]

(39)

so that

\[
[g_{ij}, \dot{y}^l] = \hat{G}^{kl}[g_{ij}, \dot{x}_k]
\]

(40)

Furthermore, the left term of relation (40) results in

\[
[g_{ij}, \dot{y}^l] = \frac{i}{2m} [g_{ij}, \{ p^m, g_{mn} p^n, y^l \}]
\]

\[
[g_{ij}, \dot{y}^l] = \frac{i}{2m} [p^m, y^l] g_{mn} [g_{ij}, p^n] + \frac{i}{2m} [g_{ij}, p^m] g_{mn} [p^n, y^l]
\]

(41)

We assume that the operator \( p^j \), on the Hilbert space representation \( \chi(y) \in \mathcal{H}_x \), constructed in accordance with the (Hermitian) operator form of (1), is represented by

\[
p^j \rightarrow -i \frac{\partial}{\partial y^j}
\]

(42)

This assumption is analogous to the "dynamical equivalence" assumption of ref [3], for which the classical momenta in the two descriptions are taken to be identical for all time. The quantum mechanical momenta then generate translations in \( \psi(x) \in \mathcal{H}_x \) and \( \chi(y) \).

Therefore, applying relation (42) along with (33) to (41) results in (as a formal definition)

\[
[g_{ij}, \dot{y}^l] = i m \frac{\partial g_{ij}}{\partial x_n} \equiv \frac{i m}{2m} \frac{\partial g_{ij}}{\partial y^l}
\]

(43)

We may apply relation (42) to the right side of relation (40)

\[
\hat{G}^{kl}[g_{ij}, \dot{y}^l] = \frac{1}{2m} g^{kl} [g_{ij}, p^m] g_{nk} + \frac{1}{2m} \frac{\partial}{\partial y^l} \hat{G}^{kl} g_{nk} [g_{ij}, p^m]
\]

\[
= \frac{i}{m} \frac{\partial g_{ij}}{\partial y^l}
\]

(44)

which is consistent with relation (43). As a result of relation (43) we may think formally of a transformation between the two coordinate bases, \( \{ x_i \} \) and \( \{ y^l \} \), defined locally by

\[
\frac{\partial g_{ij}}{\partial y^l} \equiv \frac{\partial g_{ij}}{\partial x_n}
\]

(45)
It should be emphasized that, in the classical case, Horwitz et al. [1] identified an effective embedding of the Hamiltonian dynamics into a non-Euclidean manifold, equipped with a connection form and a metric. Derivatives of functions on \{y^i\} could then be related to derivatives of functions of \{x_i\} [4], but the global relation between these manifolds is not determined. As a result of the differential relations found by [4], the relation
\[
\frac{\partial g_{ij}}{\partial x_m} = g^{mn} \frac{\partial g_{ij}}{\partial y^n} \tag{46}
\]
is, however, valid.

**IV. RELATION TO POTENTIAL MODEL HAMILTONIANS**

As we have pointed out above, the acceleration satisfies the "geodesic" type equation (23). The truncated connection form in this equation is similar in form to that derived for the classical case and used in a large number of applications [9] to generate, by geodesic deviation, a criterion [1] for stability of a Hamiltonian of the potential model form (1)
\[
H = \delta_{ij} \frac{p^i p^j}{2m} + V(y) \tag{47}
\]
where we have assigned the variable \(y\) to correspond to the configuration space of the potential model.

For a Hamiltonian of form (1), we wish to make a correspondence, as in the classical case, with a geometric Hamiltonian of the form (10). Let us suppose that \(g_{ij}(x)\) has the form (3) for this case as well. Then,
\[
\hat{H}_G = \frac{1}{2m} p^i \Phi(x) p^i \delta_{ij} \tag{48}
\]
In the semiclassical limit, we choose states in \(\mathcal{H}_x\) and \(\mathcal{H}_y\) that are localized in \(p^i\), and, for consistency in the application of the Ehrenfest approximation [1], fairly well localized in \(x\) and \(y\) as well (within the uncertainty bonds). Then, for such a wave function
\[
\langle \hat{H}_G \rangle_{\chi_p} \approx \frac{1}{2m} p^2 \Phi(x) \tag{49}
\]
and
\[
\langle \hat{H} \rangle_{\psi_p} \approx \frac{1}{2m} p^2 + V(y) \tag{50}
\]
Assigning a common value \(E\) to \(\langle \hat{H}_G \rangle_{\chi_p}\) and \(\langle \hat{H} \rangle_{\psi_p}\), we see that the choice (as in (4))
\[
\Phi(x) = \frac{E}{E - V(y)} \tag{51}
\]
is effective in this approximation as well. The relation between the functions on the left and right hand sides established by (45) and ref. [4] is valid in this contest as well. We now return to (23), which can be written, with the help of (45), as
\[
\dot{y}^i = -\frac{1}{2} \frac{\partial g^{ij}}{\partial y} \delta_{ij} \tag{52}
\]
Using the relation (51), this becomes
\[
\dot{y}^i = -\frac{1}{2} \frac{\partial V(y)}{\partial y} y^i \frac{\partial V(y)}{\partial y} y^i \tag{53}
\]
so that (we do not distinguish upper and lower indices of \(y^i\) here)
\[
\dot{y}^i = -\frac{1}{2m^2} p^i \frac{\partial V(y)}{\partial y} y^i \frac{\partial V(y)}{\partial y} p^i \tag{54}
\]
The expectation values of \(\dot{y}^i\) in the state \(\chi_p\) is the
\[
\langle \dot{y}^i \rangle_{\chi_p} \approx \langle \dot{\Phi} \rangle_{\chi_p} \tag{55}
\]
recovering, in this semiclassical limit, the quantum evolution of the particle in the Ehrenfest approximation. Thus, as pointed out above, a calculation of "geodesic deviation" based on the quantum formula (23) could provide a new criterion for quantum chaos, consistent with the Bohigas conjecture [6] due to the similar structure of the classical and quantum criteria (see below).

**V. STABILITY RELATIONS AS A CRITERION FOR UNSTABLE BEHAVIOR**

Following the classical notion of inducing an infinitesimal translation of a trajectory around a given initial point along the trajectory we refer to a corresponding quantum mechanical notion of "geodesic deviation" based on the quantum formula (23).

For "geodesic deviation" we then induce a translation as follows (where we define \(\xi\) as a common number):
\[
\psi_t(x) \rightarrow \psi_t(x + \xi) \tag{56}
\]
that is
\[ \psi_t(x + \xi) = e^{i y^i x_i} \psi_t(x) \]  
(57)

Computing \( \delta(\psi_t, y^i \psi_t)(t) \), assuming now the physical system is supposed almost classical, results in
\[ \frac{1}{2} < \psi_t | y^i (\frac{\partial}{\partial x_a} (\frac{\delta g_{ij}}{\delta x_i}) \frac{\partial}{\partial y_j}) \psi_t > \xi^a \overset{\text{def}}{=} \hat{\xi}^a(t) \]  
(58)

where the left side of expression (58) is defined as the second derivative with respect to the common number \( \xi^i \), the distance between the two trajectories as a function of time, which is expected to coincide in the Ehrenfest approximation with Horwitz et al. study [11]. Substituting relation (45) for a local transformation between the two coordinate basis \( \{ x_i \} \) and \( \{ y^i \} \) results in
\[ \frac{1}{2} < \psi_t | y^i (g^{am} \frac{\partial}{\partial y^m}(g^{jn} \frac{\partial g_{ij}}{\partial y^n})) y^j | \psi_t > \xi^a \overset{\text{def}}{=} \hat{\xi}^a(t) \]  
(59)

Thus one may write expression (59) as the sum of two terms
\[ \frac{1}{2} < \psi_t | y^i (g^{am} \frac{\partial}{\partial y^m}(g^{jn} \frac{\partial g_{ij}}{\partial y^n})) y^j | \psi_t > \xi^a \]
\[ \frac{1}{2} < \psi_t | y^i (g^{am} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n}) y^j | \psi_t > \xi^a \overset{\text{def}}{=} \hat{\xi}^a(t) \]  
(60)

We then define
\[ \hat{\xi}^a \overset{\text{def}}{=} - \frac{1}{2} y^i g^{am} (\frac{\partial g_{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{jn} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n}) y^j \]  
(61)

which we call the operator geodesic deviation.

The expectation values associated with this operator correspond in the Ehrenfest approximation to a measure of deviation between the expectation values of two neighboring evolutions of \( y^i \) which in the classical analogy are characteristic of the geodesic deviation between two near by trajectories in space. In the Ehrenfest approximation they are expected to determine the dynamic flow of the position variable’s expectation values. Based on the sensitivity to the local instability criterion it is expected that in Ehrenfest approximation one can characterize the “local” stability properties of the dynamic flow of the coordinate expectation variables. We use these matrix coefficients’s eigenvalues to determine “local” instability. If one of them is negative, it is sufficient to imply “local” instability. One can map out the regions of instability over the physically admissible region using these formulas. We shall also follow the orbits to see their behavior, as exhibited by the expectation values. We have found, so far, a remarkable correlation between the simulated orbits and the predictions of “local” instability in this way. Note that these curves of the expectation values of \( y^i \) do not necessarily correspond to classical particle trajectories in the sense of Ehrenfest. As pointed out above, the Ehrenfest theorem fails after some time [8]. We see, however, that the expectation values contain important diagnostic behavior [10], and could well be incorporated into a new definition of “quantum chaos”, corresponding to deviation under small perturbation (change of initial conditions). Although the Ehrenfest correspondence fails rapidly in case of chaotic behavior, from the behavior of the solutions it appears that this criterion may nevertheless provide a good definition for quantum chaotic behavior. The correspondence between the classical and quantum definitions provides, furthermore, support for the Bohigas conjecture [6], i.e., that a classical Hamiltonian generating chaotic dynamics goes over to a quantum theory exhibiting characteristics of chaotic quantum behavior. Our simulations indicate that this will be true, for the examples we consider below.

We will show below through simulation by numerical analysis that this formula works well beyond the Ehrenfest approximation.

VI. QUANTUM DYNAMICS STABILITY PROPERTIES VS. CLASSICAL DYNAMICS STABILITY PROPERTIES

In this section we wish to define a manifold which we suggest as corresponding to the classical Gutzwiller manifold presented by [1]. We then work through an analytical analysis to investigate the stability properties of the trajectories covering this manifold and we derive local stability criteria which we assume to be related to the stability behaviors of the corresponding quantum mechanical dynamics. We will show some computational examples in which applying these stability criteria predicts correctly the stability properties of the quan-
tum dynamics. This might suggest that the trajectories have the same stability properties as in the underlying quantum case and through the local criterion it seems that one may predict chaotic quantum mechanical behavior as well.

To understand the geometric contest of our formality let us define a manifold as follows [9]:

- Let $\mathcal{H}$ be a Hilbert space corresponding to a given quantum mechanical system and let $H_G$ be the self-adjoint Geometric Hamiltonian generating the evolution of the system.
- Let $\varphi(t) = U(t)\varphi = e^{-iH_Gt}\varphi$ be the state of the system at time $t$ corresponding to an initial localized state $\varphi(0) = \varphi \in \mathcal{H}$ such that (as long as) $\varphi(t)$ is localized too, i.e. the width of a well-localized state is extremely narrow compared to the characteristic variation in the matrix function $g_{ij}(x)$ which is the relevant system dimension.
- Define the trajectory $\Phi_\varphi$ corresponding to an initial localized state $\varphi \in \mathcal{H}$ to be $\Phi_\varphi := \{U(t)\varphi\}_{t \in \mathbb{R}^+} = \{\varphi(t)\}_{t \in \mathbb{R}^+}$ i.e., $\Phi_\varphi$ is the set of localized states reached in the course of the evolution of the system from an initial localized state $\varphi$.
- Next, let us denote by $M(\Phi_\varphi) = \{(\varphi, M\varphi) | \varphi \in \Phi_\varphi\}$ the collection of all expectation values of $M$ for localized states in $\Phi_\varphi$ (up to a multiplicative normalization constant).
- Next, let us denote by $\{M(\Phi_\varphi) | \Phi_\varphi \in \mathcal{H}\} = \{M(\Phi_\varphi) | \Phi_\varphi \in \mathcal{H}\}$ the collection of all expectation values of $M$ for all possible trajectories $\Phi_\varphi$ in $\mathcal{H}$, i.e. $\{M(\Phi_\varphi) | \Phi_\varphi \in \mathcal{H}\} \subseteq \mathbb{R}^n$ where $\mathbb{R}^n$ is the $n$-dimensional Euclidean space. We call $\{M(\Phi_\varphi) | \Phi_\varphi \in \mathcal{H}\}$ the expectation values manifold.

The classical limit of the corresponding collection of all possible trajectories evolved in this way in the course of a long period of time appear to be valid beyond localization [10].

Consider the coordinate bases $\{x_i\}$ and $\{y^j\}$. Given relation (45), we may think of the transformation matrix $A = \{a^j_i\}$ between the two sets of bases vectors [11]

$$\delta_i \equiv \{\frac{\partial}{\partial x_i}\} \rightarrow \hat{\delta}^i \equiv \{a^j_i \frac{\partial}{\partial x_i}\} \equiv \{g_{ij} \frac{\partial}{\partial x_i}\} \quad (62)$$

thus the set $\{\hat{\delta}^i\}$ forms another set of basis vectors associated with the coordinate basis defined previously $\{y^j\}$. Then we have a new set of basis vectors locally for each tangent space on the manifold. We would like our new frame to be orthonormal at all points. That is,

$$g(\hat{\delta}^i, \hat{\delta}^j) = g(a^n_i a^n_j g_{nk} = \delta_{ij}) \quad (63)$$

This equation can be rearranged

$$a^n_i g_{nk} (a^n_k)^T = \delta_{ij} = AGA^T = I \quad (64)$$

We get the matrix (we choose $A$ to be symmetric) solution $A = G^{-\frac{1}{2}}$. If the matrix component, $g_{ij}(\varphi)$, is considered as a slowly varying function on the coordinates basis in the position representation then we can expand this solution in a power series around $G = I$

$$A = G^{-\frac{1}{2}} = I + \sum_{n=1}^{\infty} (-1)^{n+1} \cdot 3 \cdot (2n - 1) \cdot n! \cdot 2^n \cdot \tilde{c}^n$$

where $G \overset{def}{=} G - I \quad (65)$

In terms of components the first few terms are;

$$a^n_i = \delta_{ij} - \frac{1}{2} \tilde{g}_{ij} + \frac{3}{8} \sum_{k=1}^{N} \tilde{g}_{ik} \tilde{g}_{kj} - \ldots \quad (66)$$

Substituting the zero order of the matrix expansion applied to $g^{mn}$ in relation (60) where the localization construction is required to be valid results in

$$\tilde{g}^{ij} \approx \frac{1}{2} \tilde{y}^{i \rho} \tilde{y}^{j \rho} \left(\frac{\partial^2 \tilde{S}^{mn}}{\partial y^m \partial y^n} \right) \tilde{y}^{\rho} \tilde{\zeta}^a$$

$$= \frac{1}{2} \tilde{y}^{i \rho} \left(\frac{\partial^2 \tilde{S}^{mn}}{\partial y^m \partial y^n} \right) \tilde{y}^{\rho} \tilde{\zeta}^a \quad (67)$$

This zero order expansion is precisely the form obtained in the classical case for the second order geodesic deviation equations (considering the second term only of a zero order) (see eq. (22) in [11]). It is implied that in the quantum case the orbit deviation equations become oscillatory.

Thus one may conclude that in the classical limit the
first order of the matrix expansion (66) applied to $g^{am}$ in relation (60) may be considered as a quantum mechanical effect

$$ -\frac{1}{2} \gamma' g^{am} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) \gamma' \xi^a $$  (68)

which could be viewed as the low order expansion of expression (60) around the classical relation of a "geodesic" deviation equation \[1\].

Then the low orders expansion of the quantum mechanical "geodesic deviation" in the classical limit results in

$$ \ddot{\xi}^i (t) \approx -\frac{1}{2} \gamma' \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) \gamma' \xi^a $$

$$ -\frac{1}{2} \gamma' g^{am} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) \gamma' \xi^a $$  (69)

In the classical limit one may refer to expression (69) as a measure of deviation between the two dynamics of $\gamma'$'s expectation values which becomes the corresponding quantum second order "geodesic deviation" equations. On this view, the quantum dynamics may be identified as chaotic provided the flow of the quantum expectation values approximately follow a chaotic classical trajectory.

Moreover, one may claim that in the classical limit expression (69) is expected to admit the emerging of a corresponding quantum "local" criterion for stability properties of the dynamical flow of the position variable’s expectation values in correspondence with the sensitivity to the local stability criterion for unstable behavior derived by \[1\] in the classical case.

Then one may write in the classical limit a corresponding quantum mechanical "local" criterion which reflects the stability of the trajectories associated with the position expectation values (average particle's position). This view may be expressed as

$$ \ddot{\xi} (t) = -(\mathcal{V}) P \xi $$  (70)

where

$$ \mathcal{V}_{ija} \overset{\text{def}}{=} \frac{1}{2} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) $$

$$ + \frac{1}{2} s^{am} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) $$  (71)

and $p^{ij} = \delta^{ij} - \langle \gamma' \rangle < \langle \gamma' \rangle \langle \gamma' \rangle$, defining a projection into a direction orthogonal to the average velocity, $< \gamma' >$, i.e. the component orthogonal to the flow of the position expectation values.

"Local" instability should occur if at least one of the eigenvalues of the matrix $\mathcal{V}_{ija}$ is negative.

We define for brevity

$$ C_{ija} \overset{\text{def}}{=} \frac{1}{2} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) $$

$$ Q_{ija} \overset{\text{def}}{=} \frac{1}{2} s^{am} \left( \frac{\partial g^{ln}}{\partial y^m} \frac{\partial g_{ij}}{\partial y^n} + g^{ln} \frac{\partial^2 g_{ij}}{\partial y^m \partial y^n} \right) $$  (72)

Since the matrix $\mathcal{V}$ embeds in its structure a sum of two terms, i.e. expression (71), where the first one as mentioned previously carries the precise structure as the matrix involved in the classical case \[1\], while the second term is a quantum effect, then it is implied by equation (70) that the position expectation trajectories may demonstrate "local" instabilities while the classical corresponding trajectory defined by Hamilton’s equations of motion is stable and conversely.

Those cases may be expressed by the following inequalities for "local" instabilities. Given $\{\lambda_1, \lambda_2, \lambda_3, ..., \lambda_n\}$ are the matrix eigenvalues of $C_{ija}$ and $\{\alpha_1, \alpha_2, \alpha_3, ..., \alpha_n\}$ are the matrix eigenvalues of $Q_{ija}$, then

$$ \text{if } \exists (\lambda_i, \alpha_i) \text{ such that } 0 < \alpha_i < -\lambda_i $$

quantum instability is in correspondence with classical instability

(73)

But

$$ \text{if } \exists (\lambda_i, \alpha_i) \text{ such that } 0 < \lambda_i < -\alpha_i $$

classical stability vs. quantum instability may emerge

(74)

while

$$ \text{if } \exists (\lambda_i, \alpha_i) \text{ such that } 0 < -\lambda_i \leq \alpha_i $$

quantum stability vs. classical instability may emerge

(75)

As Zaslavsky \[8\] has pointed out, however, the Ehrenfest correspondence fails rapidly in case of chaotic behavior. Nevertheless, Ballentine, Yang, and Zibin \[10\] compared quantum expectation values and classical ensemble averages for the low-order moments for initially localized states. This
correspondence suggests that the statistical properties of Liouville mechanics continue to last even after Ehrenfest’s approximation fails. The correspondence with Liouville mechanics, given fixed system size, was shown to be accurate for a longer time period under conditions of classical chaos.

In the Ehrenfest approximation and beyond, i.e. even after Ehrenfest correspondence fails in case of chaotic behavior, the collection \( y(\Phi_{\rho}) \) will satisfy dynamical equations closely related to those for which the classical ensemble averages describe the possible configurations for a classical system in phase space.

VII. SIMULATIONS

In this section we study the stability characters of the quantum dynamics through numerical simulations. We present here three approaches. One which uses a direct time evolution of the wave packet simulated by the Schroedinger time dependent equation. In each time step, the position expectation values are computed, directly, by the wave function (using a narrow coherent state wave packet). Moreover, each simulation is repeated by a small change in the initial condition (small change in the initial average momentum of the wave packet) and the two trajectories are computed. The following diagrams (fig.1 and fig.2) show the orbits of the particles in the presence of the regions of instability described above. One sees that the instability of the orbits, demonstrated by crossing trajectories and complexity, reflects the divergence of nearby trajectories which can lead to chaotic behavior.

In the second approach we are searching for “local” instabilities as they are defined through the operator geodesic deviation, \( \xi_{al} \) (eq. (61)), i.e. the expectation values associated with this operator are characterizing in the Ehrenfest approximation a measure of deviation between two dynamic flows of \( \hat{y}^a \)’s expectation values which in the classical analogy are a characteristic of a geodesic deviation between two nearby trajectories in space and “local” instability will be defined by computing the matrix’s eigenvalues where if one of them is negative, it is sufficient to determine “local” instability. In the following, we display a set of graphs (fig.3) showing the unstable regions. It is expected that the trajectories, i.e. \( < y >, \) of the particles will be deflected strongly when they pass through these unstable regions, causing instability of the motion [9]. We use as initial wave function the coherent state wave packet:

\[
\psi(x,y,0) = \frac{1}{\pi} e^{-\frac{1}{2}(x-x_0)^2+ip_0^x x - \frac{1}{2}(y-y_0)^2+ip_0^y y}
\]

(76)

where

\[
< x >= x_0 \quad < p_x >= p_0^x \\
< y >= y_0 \quad < p_y >= p_0^y
\]

(77)

We examine simulations of a set of five quantum 2D wells while increasing the energy hypersurface, approaching the separatrix of the centered well. As can be easily observed, the centered well becomes an unstable dynamical region as the threshold energy is approached. This phenomena takes place due to the quantum effect terms which seem to “sense” the unstable regions outside the accessible classical region. The same behavior is observed also for the rest of the wells. Moreover, one may think of the quantum mechanical terms as acting as a “driving force” (the system, as will be shown shortly, could be thought of as a driven quantum 2D five well anharmonic oscillator) which is quite significant due to the energy interval range of influence as it is manifested in the following simulations (fig.3). It is suggested that the “fluctuating” term of the “local curvature” of the energy hypersurface might be quite significant near the separatrix of the wells. This would turn the undriven system to be effectively a driven dynamics with the same stability properties and dynamic behavior. As Lin and Ballentine pointed [12], the tunneling rate of an electron through a semiconductor double quantum well structure can be enhanced by means of a dc bias or ac field (i.e. a driven anharmonic oscillator). Our work implies that it is reasonable to assume that also by approaching to the separatrix of a well tunneling might be enhanced. This phenomena we are presenting here has never been previously observed. Further research is required to confirm this idea. In the third approach we continue to examine the instability inequalities relations (eq.73-75). We follow the work of Feit and Fleck [13] which simulated wave packet dynamics and chaos in the Henon-Heiles system. The evolution of wave packets under the influence...
of a Henon-Heiles potential was investigated in [13] by direct numerical solution of the time-dependent Schrödinger equation, i.e. coherent state Gaussians with a variety of mean positions and momenta were selected as initial wave functions. Four cases were simulated by [13]; two of the wave packets can be reasonably judged to exhibit regular or nonchaotic behavior and the remaining two chaotic behavior. All of the four cases exhibit corresponding classical motions which are regular.

Following the instability inequalities relations we are able to derive analytically (eqs.(73)-(75)) those simulated results where the conformal structure (eq.3-4) has been applied. Those analytic results are summarized in table 1 below. We wish to emphasize that case (d) reflects our definition of "local" instability as an appropriate definition for a quantum mechanical analogy of the classical notion of "local" instability since it corresponds to the Feit and Fleck [13] findings for case (d) where the behavior at early times appears regular.

| Case   | Instability Inequality Relations | Behavior |
|--------|----------------------------------|----------|
| case (a)| $0 \leq (-\alpha_l) \leq \lambda_l$ | regular  |
| case (b)| $0 \leq (-\alpha_l) \leq \lambda_l$ | regular  |
| case (c)| $0 \leq \lambda_l < (-\alpha_l)$ | chaotic  |
| case (d)| $0 \leq (-\alpha_l) \leq \lambda_l$ | regular  |

VIII. CONCLUSIONS

We have introduced a new generalized analytic approach and on this basis we have derived a new diagnostic tool for identifying a quantum chaotic behavior. This might serves as a new definition for quantum Hamiltonian chaos. We have shown results of simulation of the quantum motion in two dimensions, showing in certain cases that the transition from predominantly regular to predominantly irregular trajectories (of expectation values) takes place over a narrow energy range about some energy $E_c$. We have shown an independent stability behavior of the quantum dynamics from the classical correspondence. We were able to predict local stability properties depending on energy, but even more surprising, on the initial conditions of the wave packets and identifying zones of local stability and instability (on the level of the space expectation values). Moreover, this last demonstrates a possible KAM-like transition, which by itself could serve as a new criterion and definition for quantum chaos very much like in the classical case.

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Figure 1: (a) Henon-Heilles quantum dynamical simulation corresponding to a low classical energy, in a range known to be a non chaotic for classical dynamic. The two trajectories (blue and green) are closely together, reflecting no divergence of nearby trajectories, which indicates, on the basis of our theory, a stable dynamics. (b) Zoomed picture of fig.1 above, presenting parallel trajectories, no complexity and nearby trajectories, indicating stability of the wave packet dynamics.

Figure 2: Henon-Heilles quantum dynamical simulation corresponding to a higher classical energy, in a range known to be a chaotic classical dynamics. The two trajectories starting from the same initial position’s expectation value, separate along the time evolution of the dynamics, presenting broken trajectories (the trajectories are crossing themselves) and complexity indicating a chaotic dynamical behavior.
Figure 3: (a) Five 2D well dynamical stability analysis for $E=-36.6709$. Stable dynamical regions are presented through 5 wells, separated by highly chaotic areas. Green lines indicating the classical hypersurface of classical energy as was discussed previously. (b) Five 2D well dynamical stability analysis for the separatrix of the centered well.

Figure 4: Five 2D well dynamical stability analysis for the separatrix of the off-centered wells.