ТЕОРЕТИЧЕСКАЯ ХИМИЯ

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QUANTUM CURVATURE ANALYSIS FOR SIMPLE VIBRATIONAL SYSTEMS

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We introduce quantum mechanical counterparts of line curvatures and surface curvatures for estimating the degree of nonlinearity and complexity in quantum states of the corresponding dynamic systems. The measures are used to discuss the peculiarities of the systems in the context of quantum chaos. The use of the fluctuations of the curvatures for distinguishing chaotic from regular behaviour is considered. The method is applied to analyze the Henon-Heiles and Yang-Mills model systems.

Introduction

Curvature analysis for dynamical systems has a long history, the earliest work in this field was evidently the time-honored paper by Hadamard [1] providing a fundamental example of a chaotic motion of a point particle on the surface of constant negative curvature. A special attention to the curvatures associated with complex dynamical systems was given in the remarkable study by Krylov on the foundations of statistical mechanics [2]. Finally, the seminal investigation by Anosov [3] generated a great body of papers considering ergodic properties of dynamic systems on closed Riemannian manifolds with negative curvature [4-7].

Within chemical physics problems, in particular the transition-state theory, the Krivoshey's paper [9] provided the first semi-quantitative applications of Anosov's results on the exponential divergence of many nearby geodesics on Riemannian manifolds of negative curvatures (specifically, in the vicinity of a saddle point on the potential energy surfaces). This work is closely related with the general aspects of the geometrisation of classical dynamics considered in detail in many comprehensive reviews and original works [10-17]. In application to molecular problems the relevant simplified study is also given in Ref. [18] and termed by us the *chemical geometro-dynamics*. The recent detailed and extended study [17] reflects a very wide scope of possibilities for exploring the dynamical chaos in rather complex systems by geometrical methods. In this context it is also worth referring to the curvature analysis of dynamical trajectories in Ref. [19]. In all these works the dynamical problems are treated in the framework of the conventional classical mechanics.

A special branch of the differential-geometrical approach is an appropriate quantum description. Rather than discussing in detail the conceptual difficulties of the quantum chaos, that is the fingerprints of deterministic chaos in quantum mechanics, we confine ourselves to quoting the most important general reviews [20 - 27].

The quantum molecular kinematics developed in [28] should also be mentioned. In this and subsequent works [29-31] special quantum complexity measures are derived from the differential geometrical properties of the spatial curves associated with the electron paths in molecules. In particular, we studied a model of the folding process in oligopeptides [31] concurrently using the quantum-chemical chirality measures (defined previously in Ref. [28]) and molecular dynamic simulation extended by the analysis of the dynamical complexity [32].

A logical step to a broader use of quantum kinematics is to study quantum complexity for generic dynamical systems in which the classical deterministic chaos is clearly detected. Thus, the main goal of the present work is to define appropriate quantum curvature measures beyond the quantum-chemical approach given in [28-31] and to demonstrate their advantages for typical dynamical systems investigated previously by other methods [19-27].

1. Quantum counterparts of curvature measures

Here we sketch of our main approach [29] and give only few necessary definitions modified to fit a broader context. From the classical kinematics as differential geometry of particle paths we take the key notions such as the trajectory length (one might term it as a zero-order curvature) and the usual (the first-order) curvature which we call the 1-curvature. The higher-order curvatures, such as the tor-

sion for 3-dimentional spatial trajectories, are not considered here (the torsion, however, can be directly applied to chiral quantum systems [28]).

Introducing a position vector $\mathbf{r} = \mathbf{r}(t)$ as a function of time t we define conventionally a mechanical momentum as a time derivation $\mathrm{p} = \dot{\mathbf{r}}(\mathrm{t})$ (masses can be included in coordinates by passing to the so-called mass-weighted coordinates). The explicit expressions for the above mentioned length and 1-curvature are

$$L^{cl} = \int |\mathbf{p}|\, dt \ , \tag{1}$$

$$K^{cl} = \left| \mathbf{p} \wedge \dot{\mathbf{p}} \right| / |\mathbf{p}|^3 , \tag{2}$$

where $\wedge$ stands for the vector product operation. Proceeding to the quantum-mechanical treatment we have to replace the momentum and its time derivatives (in particular, the force vector) by their quantum analogues that are the corresponding operators. In doing so, time-averaged quantities become the conventional quantum-mechanical averages over a given state vector $|\Psi\rangle$:

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

where $\hat{A}$ is the associated operator for the classical dynamical quantity a. In accordance with the theory of linear operators, a modulus of a dynamic quantity is translated into a positive semidefinite operator, that is the operator modulus. Therefore, the quantum length L, being associated with classical quantity (1), is defined:

$$L = \langle |\hat{\mathbf{P}}| \rangle \tag{3}$$

In the same fashion, the quantum 1-curvature K is the average value

$$K = \langle \hat{K} \rangle \tag{4}$$

where, strictly speaking, one must deal with the associated quantum curvature operator, $\hat{K}$ of the form

$$\left| \hat{\mathbf{P}} \wedge \dot{\hat{\mathbf{P}}} \right| \ |\hat{\mathbf{P}}|^{-3} \tag{5}$$

or its more symmetric form that guarantees the Hermiticity. However, $|\hat{\mathbf{P}}|^{-1}$ is not a well defined operator due to the appearance of the zero eigenvalues in $\hat{\mathbf{P}}$. This causes a problem not only for practical computations, and in this work we follow the same prescriptions as in [29] where the singular denominator is removed and the Hermitian curvature operator is taken to be

$$\hat{K} = \frac{1}{2} \left| \hat{\mathbf{P}} \wedge \dot{\hat{\mathbf{P}}} - \dot{\hat{\mathbf{P}}} \wedge \hat{\mathbf{P}} \right| \ . \tag{6}$$

In [29,30] we directly computed the quantities (3), (4) using rough simplifications for the operators $|\hat{\mathbf{P}}|$ and (6), which were treated at a certain semiempirical level of quantum chemistry. With this, the indices (3) and (4) were considered, following quantum kinematics, the molecular complexity measures. This viewpoint can be straightforwardly extended to quantum dynamics.

Now we add to these measures an additional quantum measure derived from the geometrised classical dynamics mentioned in the Introduction. The typical geometrisation is based on the Maupertuis-Jacobi metric generating a specific Riemann space. The average curvature R (an analogue of the Gauss curvature for 2-D surfaces) takes the form

$$R = (N-1) \left\{ \frac{\nabla^2 U}{(E-U)^2} - (N-6) \frac{\nabla U \cdot \nabla U}{4(E-U)^3} \right\}, \tag{7}$$

where N stands for the number of degrees of freedom, E is the total energy (a motion integral for the real trajectory) and $U = U(\mathbf{r})$ is the potential function, such that $-\nabla U$ is a force vector. The above expression (7) is derived (ignoring misprints) many times [13,14,18] and recently this quantity has been reconsidered in the review [17] as well. As it is stressed in this work and in [33], the Maupertuis-

Jacobi metric is not suitable for the practical use. In quantum mechanics the singularities caused by the denominators in Eq. (7) are also objectionable. If we neglect these denominators and the gradient terms we just arrive at the expression proposed in [16,17] for the geometrisation scheme given by the Eisenhart metrics. It means that in our study the quantum operator for a dynamical curvature is defined in a simple form

$$\hat{K}_E = \nabla^2 U \tag{8}$$

The subscript E reflects the fact that Eq. (8) essentially expresses a curvature due to Eisenhart [11]. Therefore, the term $E-$curvature is rather appropriate in this case, and we define such $E-$curvature as follows

$$K_E = \left\langle \hat{K}_E \right\rangle. \tag{9}$$

As a result, our approach leads to three quantum complexity measures (3), (4), and (9) and the associated operators $\left|\hat{\mathbf{P}}\right|$ and (6), (8).

Along with K_E the curvature of the potential energy function is also a useful quantity, and in 2-dimentional case it can be defined via the Hessian of U, specifically,

$$K_U^{cl} = \frac{U_{xx}U_{yy} - (U_{xy})^2}{[1 + (U_x)^2 + (U_y)^2]^2}, \tag{10}$$

where $U_x = \partial U / \partial x$ and so on. As in the previous case of 1-curvature (2), we neglect the denominator and introduce the corresponding U-curvature operator

$$\hat{K}_U = U_{xx}U_{yy} - (U_{xy})^2, \tag{11}$$

such that the quantity

$$K_U = \left\langle \hat{K}_U \right\rangle \tag{12}$$

is used as an additional curvature index. Note that in the theory of dynamical systems the corresponding classical quantity is widely used for a simplified analysis of the trajectory instability within the Brumer-Duff-Toda (BDT) approach [34-36].

2. Some properties of quantum curvatures

The usefulness of the above defined curvature measures can be elucidated by specific calculations on generic systems some of which are discussed below and in the next section. Here we give only some simplest properties helping us to realise a possible range of applications of the quantum curvatures.

We start with the quantum length (3) which cannot disappear for bound states due to the interrelation between $\left|\hat{\mathbf{P}}\right|$ and the kinetic energy operator $\hat{T}$, namely

$$\left|\hat{\mathbf{P}}\right| = (2\hat{T})^{1/2} \tag{13}$$

(recall also the quantum virial theorem). Therefore, the index (3) is a nonzero quantity even for one-dimensional systems. For estimations the inequality

$$L \le \sqrt{2}\left\langle \hat{T} \right\rangle^{1/2}$$

can be used (it trivially follows from the Cauchy- Swarz inequality). An additional information can be obtained from the fluctuations of the index (3). Owing to Eqs. (3) and (13) the relative fluctuations

$$\delta L = (\left\langle 2\hat{T} \right\rangle - L^2)^{1/2} / L \tag{14}$$

are zeroed for a free motion such as that of a particle in a potential box. Then the relative fluctuation of the quantum length can be viewed as a general measure of nonlinearity.

A different situation is with the 1-curvature measure (4). By definition, it should vanish for the systems with one degree of freedom. Moreover, the index itself vanishes identically for any system consisting of harmonic coupled oscillators. This fact is simply proved by transforming to an equivalent uncoupled system in terms of the normal coordinates. Then each new independent subsystem possesses one degree of freedom giving no contribution to the spatial curvature. Therefore, the quantum 1-qurvature gives a more appropriate measure of nonlinearity automatically eliminating from consid-

eration the trivial systems with the potential energy having a quadratic form. We stress that the index K tracing only nonlinearity cannot distinguish between systems with regular motion (in classical understanding) and those with chaotic behaviour. The description of quantum chaos is too complicated problem to be resolved by a limited set of indices. Nevertheless, we hope that, again, the relative fluctuations

$$\delta K = (\langle \hat{K}^2 \rangle - K^2)^{1/2} / K \tag{15}$$

would allow us to recognize certain differences between the chaotic and regular states at the level of such simplified quantum description.

Now we consider the quantum $E-$curvature (9). Apart from the occasional cases of null values, this index vanishes for U satisfying the Laplace equation, that is for harmonic functions. It means that some special cases of nonlinearity cannot be directly treated by K_E. In the case of coupled harmonic oscillators the index will be constant, so in order to exclude this trivial case the usual fluctuation analysis is a suitable tool. In other words, the quantity δK_E calculated as in Eq. (12) is a more appropriate index of the quantum complexity and nonlinearity. Note that the similar fluctuation of the classical quantity $\nabla^2 U$ is first introduced in [15], and actually, this fluctuation is a base of the whole geometrical approach exposed in the review [17].

Nevertheless, aforementioned vanishing of K_E for the harmonic functions somewhat narrows the range of its applicability. This peculiarity is seen in the case of the so-called Henon-Heiles system, very popular for exploring chaos and nonlinearity, The corresponding potential is

$$U = (\omega_x{}^2 x^2 + \omega_y{}^2 y^2)/2 + \alpha\,(x^2 y + \beta\, y^3), \tag{16}$$

where ω_x, ω_y are the usual harmonic frequencies, and α and β are the nonlinearity constants. For the special Henon and Heiles choice $\beta = -1/3$ we have $\nabla^2 U = \omega_x{}^2 + \omega_y{}^2$, that is a non-informative behaviour, whereas for this and other choices of β the system is rather complicated and develops a chaotic regime as well (see [37] or numerous textbooks and reviews such as [21,22,34,36]). Admittedly, the potentials of such kind are rare, and normally K_E and δK_E should help too.

As for the U-curvature (12) it is worth noting that generally it is not a positive definite quantity. Moreover, in classical dynamics the appearance of the negative values of K_U^{cl} gives a rough estimation of the critical energy associated with the developed chaotic motion. In the quantum description K_U (12) can serve similar purposes. Nevertheless, there are many situations where BDT estimations are not reliable for detecting classical chaos, and the same is evidently possible for our index K_U. However, for our analysis a distribution of the curvature values over the whole range of the quantity is more essential. Therefore, K_U will be useful as well.

3. Numerical examples

We study two well-known nonlinear systems, the Henon-Heiles (H-H) coupled oscillators with the potential energy (16), and the classical Yang-Mills (Y-M) system with

$$U = (x^2 + y^2)/2 + \alpha\,(x^4 + y^4)/4 + \beta\, x^2 y^2/2, \tag{17}$$

where α and β are nonlinearity constants. Both systems are thoroughly explored with classical dynamics methods as well as quantum-mechanical ones (see [21,22,26,34-40] and references therein). The cited quantum mechanical investigations were aimed to find what are the quantum manifestations of classical stochasticity in the discrete level structure. It would be overoptimistic to say that the studies provided a clear solution of this problem, although bright ideas and techniques appeared when seeking the quantum chaos phenomena. Thus, new approaches are desirable, and the quantum curvature method allows us to obtain an additional information.

The remarkable property of the H-H and Y-M systems is their classical integrability for some exceptional sets of parameters ω_x, ω_y, α and β (for more general problems see [41]). This peculiarity makes the considered problems very suitable for testing new schemes of analysis.

For the H-H system the parameters for the integrable regime are given, for example, in [20], Chapter 8. For example,

$$\omega_x, \omega_y \text{ are arbitrary,}$$
$$\alpha = 1,\ \beta = 2.$$

In our study we specified these integrable case parameters as follows

$$\begin{aligned} &\omega_x = 4,\ \ \omega_y = 7.1, \\ &\alpha = 1,\ \ \beta = 2. \end{aligned} \tag{18}$$

For other cases the system allows coexistence of chaotic and regular classical trajectories. As such non-integrable case parameters we take the set from [42]:

$$\begin{aligned} &\omega_x = \omega_y = 1, \\ &\alpha = 0.1118,\ \beta = -1/3 \end{aligned}. \tag{19}$$

For the Y-M system the integrable case parameters are

$$\alpha = 2/3,\ \beta = 1 \tag{20}$$

(see Ref. [39,41]). The situation realizing a chaotic Y-M dynamics is suitably described by the set [39]:

$$\alpha = 0,\ \beta = 1. \tag{21}$$

With these sets we will also examine the quantum curvature indices.

Let us briefly outline some computational details. For solving the spectral problem generated by the two-degrees-of-freedom Hamiltonian

$$H = (p_x{}^2 + p_y{}^2)/2 + U(x, y) \tag{22}$$

(p_x is the momentum of the *x*-component) we used the common finite-dimensional technique. The direct products

$$\{|m \otimes n\rangle\}_{\substack{0 \le m \dim -1 \\ 0 \le n \dim -1}}$$

of the eigenstates $\{|m\rangle\}_{0 \le m \dim -1}$ of the harmonic oscillator is chosen as an appropriate basis set, such that the finite-size solution were

$$|\Psi\rangle = \sum_{m,n=0}^{\dim -1} C_{mn} |m \otimes n\rangle. \tag{23}$$

Typically we took the basis size $\dim = 50 \div 60$, thereby dealing with the eigenvalue problem for the matrix

$$\left\| \langle m \otimes n | \hat{H} | m' \otimes n' \rangle \right\|_{\substack{0 \le m \le \dim, 0 \le m' \le \dim \\ 0 \le n \le \dim, 0 \le n' \le \dim}} \tag{24}$$

of size ≈ 3000. As a rule, we selected only a small reliable part ($\approx 10\%$) of the computed spectrum having an admissible variance value $\approx 10^{-4}$ (for correct estimations of accuracy the consistent evaluation of the average $\langle \hat{H}^2 \rangle$ was performed for each eigenvectors). For arbitrary power value ν, the matrix elements $\langle m | \hat{x}^\nu | n \rangle$ etc were easily calculated recurrently starting from the known result for $\langle m | \hat{x} | n \rangle$.

The typical results are shown in Figs. 1-4 and 6-9. In all figures the curvature indices (the abscissa) are presented as a function of the energy (the coordinate) calculated for individual eigenstates. All the quantities are given in atomic units. Apart from the curvature indices (3), (4), (9), and (12) we also present the quantum Shannon entropy (Figs. 5 and 10) for which the corresponding probability distribution was taken from the squared set of the expansion coefficients C_{mn}, Eq. (23). Similar entropy measures are frequently used in the analysis of quantum chaos [36, 42].

From the presented plots we see that the quantum results behave rather differently in the integrable Hamiltonian systems and non-integrable ones. We also see a poorer distinction between these cases for the Yang-Mills systems (17). It is interesting that in this case the quantum *E*-curvature (9) provides

a clearer difference between the two types of dynamics. . We also see that the fluctuations provide a more clear distinction of the dynamical systems and it is in accordance with the behaviour of the classical fluctuations reported in [17]. At the same time, in both examples (the H-H and Y-M systems) the behaviour of the Shannon entropy seems to be visually less obvious.

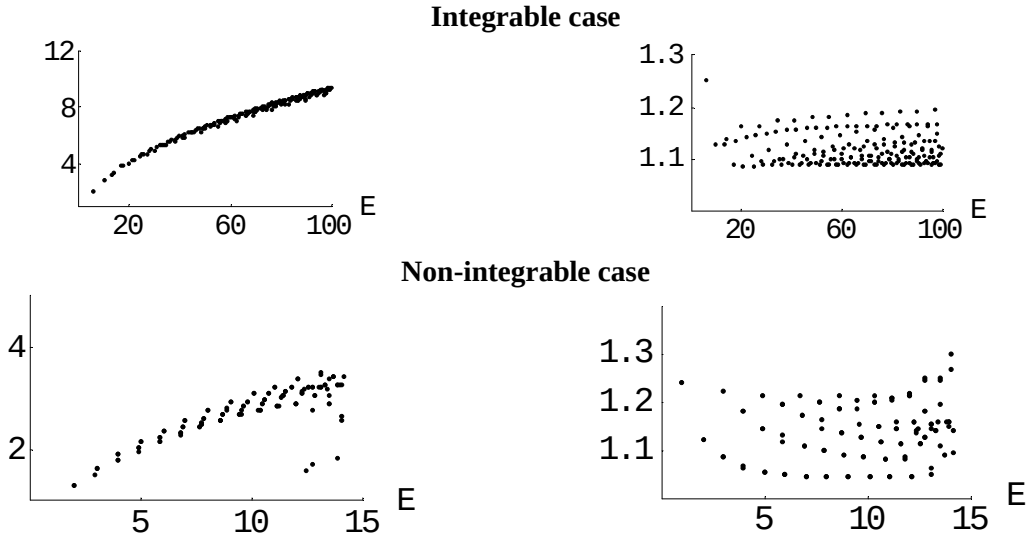

Fig. 1. Quantum length (3) and its fluctuation (14) for the H-H integrable (18) and nonintegrable (19) cases.

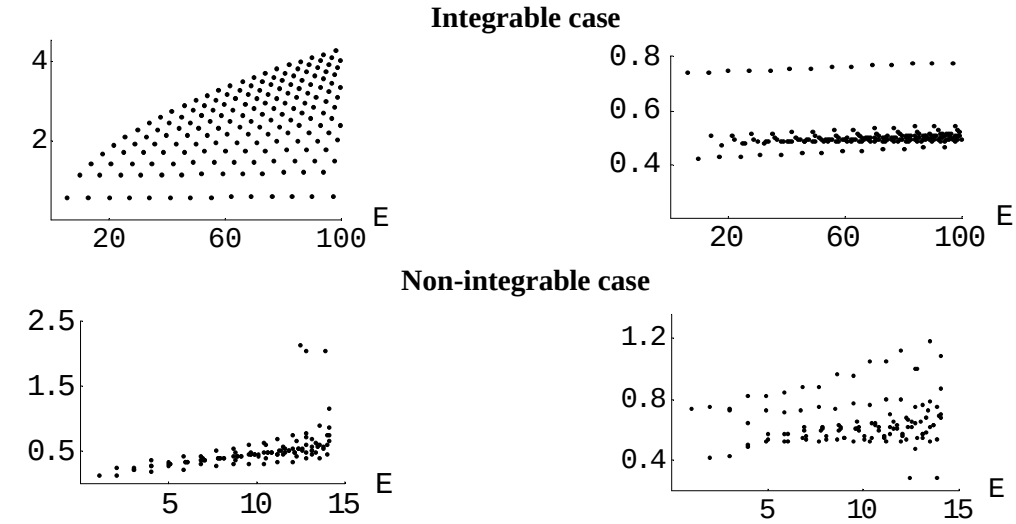

Fig. 2. Quantum 1-curvature (4) and its fluctuation (15) for the H-H integrable (18) and nonintegrable (19) cases.

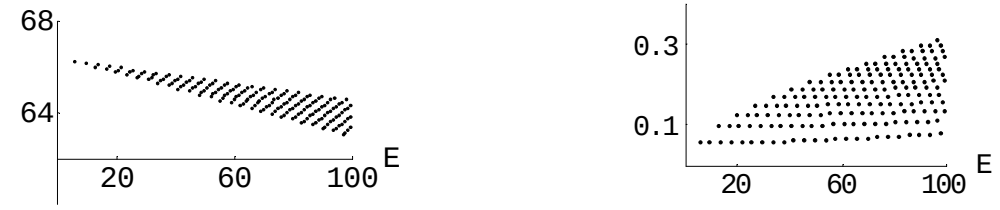

Fig. 3. Quantum E-curvature (9) and its fluctuation for the H-H integrable (18) case (in the H-H non-integrable (19) case the E-curvature is zero).

Fig. 4. Quantum U-curvature (12) for the H-H integrable (18) and non-integrable (19) cases.

Fig. 5. The quantum Shannon entropy for the H-H integrable (18) and non-integrable (19) cases.

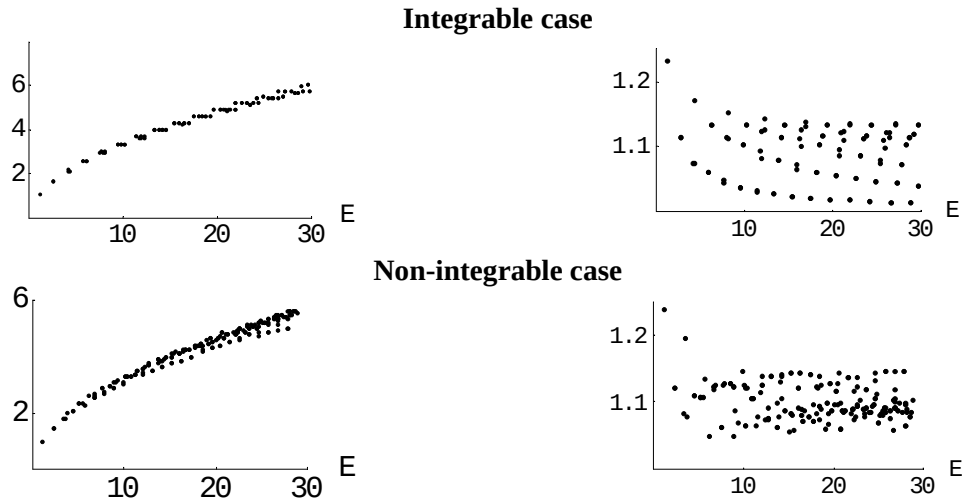

Fig. 6. Quantum length (3) and its fluctuation (14) for the Y-M integrable (20) and non-integrable (21) cases.

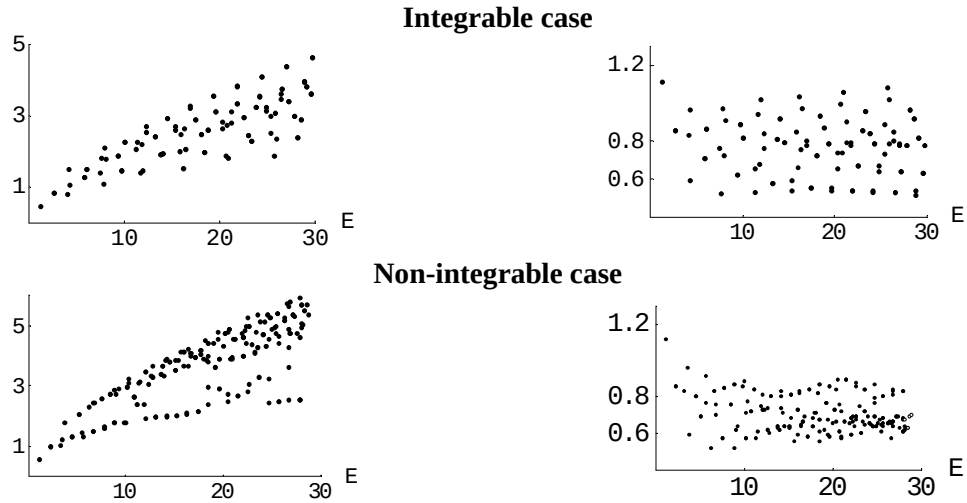

Fig. 7. Quantum 1-curvature (4) and its fluctuation (15)) for the Y-M integrable (20) and non-integrable (21) cases.

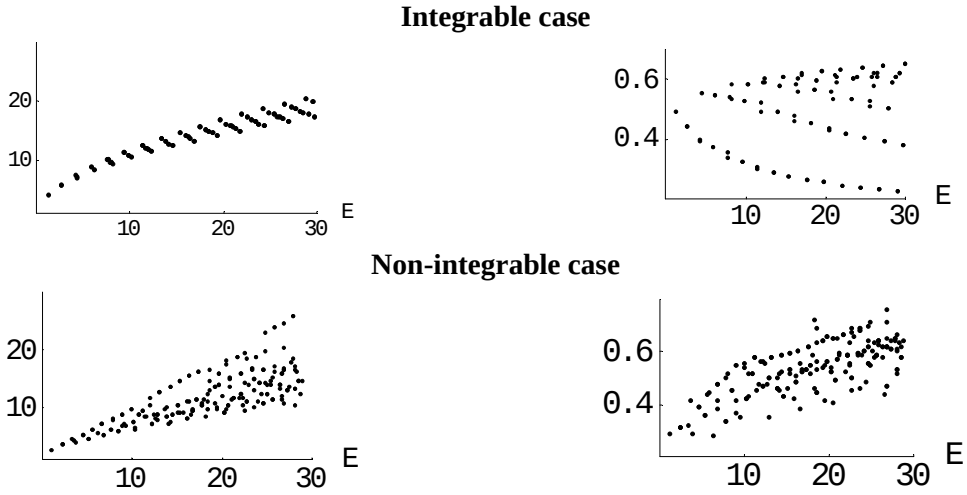

Fig. 8. Quantum E-curvature (9) and its fluctuation (15) for the Y-M integrable (20) and non-integrable cases (21).

Fig. 9. Quantum U-curvature (12) for the Y-M integrable case (20) and non-integrable case (21).

Fig. 10. The quantum quantum Shannon entropy for the Y-M integrable case (20) and non-integrable case (21).

Note that for the H-H model the dissociation energy is equal to $1/6\alpha^2 \approx 13.3$ and the critical energy (the rough estimation of the onset of the developed dynamical chaos) is ≈ 8.7 [43]. Figs. 1-5 show that a more irregular distribution of the curvatures appears only near $E = 10$. Thus, in the curvature approach the quantum stochasticity emerges with a more developed dynamic nonlinearity than in its classical counterpart. A similar situation is observed for the non-integrable Y-M problem where the graphs show irregularity above $E = 5 \div 7$. It is worth to mention the previous study of the same problem in Ref. [39] where not as clear distinction of the quantum chaos was obtained using quite different approach based on the level-spacing distribution analysis.

4. Concluding remarks

The specific results given in the preceding section have to be regarded as preliminary, first phase of the implementation of the quantum curvature analysis to dynamic Hamiltonian systems. Further studies are required in order to understand a connection of the scheme with other techniques. In the majority of current approaches an emphasis is made on the properties of the selected wave functions with the energy in the range of the developed classical chaos. In our scheme we analyze the whole set of the relevant dynamic averages in the range of their quantum variation. When studying further examples

we could encounter unpredictable situations, however, we hope that at the qualitative level the method will be able to make a distinction between two kinds of quantum regimes, the chaotic and the regular ones.

In this paper we examined only two-dimensional Hamiltonian systems with polynomial potential. It is especially intriguing to apply the curvature analysis to many-degree-of-freedom systems such as the quantum Toda chain and the related many-particle nonlinear models. Incorporating a more extended statistical technique such as cumulant analysis etc., is also desirable. We are planning to investigate such the problems in the nearest future.

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References

1. Hadamard J. Journal de Math´ematiques Pures et Appliqu´ees. 1898. V. 4. P. 27 - 73.
2. Krylov N.S. Works on the foundations of statistical physics. Princeton: Princeton University Press, 1979. 283 p.
3. Anosov D.V. Soviet Math. Dokl. 1962, 3. P.1068–1069; Proc. Steklov Inst. Math. 1969. V. 90. P. 1-235.
4. Moser J. J. Diff. Eq. 1969. V. 5. P. 411 - 440.
5. Franks J. Anosov diffeomorphisms. Proceedings of Symposia in Pure Mathematics, American Mathematical Society .1970. P. 1461-1493.
6. Manning A. In Ergodic Theory, Symbolic Dynamics and Hyperbolic Spaces. Eds.: Bedford T., Keane M. Series C. Oxford: Oxford University Press, 1991.
7. Casetti L., Livi R. C, Pettini M. Phys. Rev. Lett. 1996. V. 74: P. 375-378.
8. Brin M., Stuck G. Introduction to Dynamical Systems. Cambridge: Cambridge University Press, 2002.
9. Krivoshei I.V. J. Struct. Chem. 1984. V. 24. P. 926 -928.
10. Synge J.L. Phil. Trans. Roy. Soc. 1927. V. 226. P. 31-106.
11. Pin O. C. Adv. Math. 1975. V. 12. P. 269 - 311.
13. Savvidy G K. Nucl. Phys. 1984. V. B 246. P. 302-334.
14. Szydlowski M., Szczesny J. Phys. Rev. 1994. V. D 50. P. 819-840.
15. Pettini M Phys. Rev. 1996. V. E 47. P. 828-850.
16. Casetti L., Clementi C, Pettini M. Phys. Rev. 1996. V. E 54. P. 5969-5984.
17. Casetti L., C, Pettini M., Cohen E. G. D. Phys. Rep. 2000. V. 337. P. 237-341.
18. Krivoshei I.V., Luzanov A.V. J. Struct. Chem. 1983. V. 23. P.489-494.
19. Alabiso C., Casartelli M. J. Phys. 2001. V. A 34. P. 1223–1230.
20. Zaslavsky G. M. Phys. Rep. 1981. V. 80. P. 159 – 250.
21. Tabor. M. Chaos and Integrability in Nonlinear Dynamics: An Introduction. New York: Wiley, 1989. 364 p.
22. Gutswiller M. C. Chaos in Classical and Quantum Mechanics. New York: Springer-Verlag, , 1990. 432 p.
23. Chaos and Quanum Physics, Editors: Giannoni M-J, Voros A., Zinn-Justin J. Amsterdam: North-Holland, 1991. 759 p.
24. Ott E. Chaos in Dynamic Systems. Cambridge: Cambridge University Press, 1993. 385 p.
25. Haake F. Quantum Signatures of Chaos 2nd ed. New York: Springer-Verlag, 2001. 479 p.
26. Bolotin Yu. L., Tur A.V., Yanovsky V.V. Costructive Chaos. Kharkov: Institute for Single Crystals, 2005.
27. Gnutzmann S, Smilansky U. Advances in Physics. 2006. V. 55. P. 527-625.
28. Luzanov A.V, Babich E.N. Struct. Chem. 1992. V. 3. P.175-181.
29. Luzanov A.V., Babich E J. Mol Struct.(Theochem). 1995. V. 333. P. 279-290.
30. Luzanov A.V., Nerukh D. Functional Materials. 2005. V.12. No 1. P. 55–64.
31. Luzanov A.V., Nerukh D. .J. Math. Chem. 2007. V.41. P. 417–435.
32. Nerukh D., Karvounis G., Glen R.C. J. Chem. Phys. 2002. V. 117. P. 9611-9617.
33. Szydlowski M.J. Math. Phys. 1999. V. 40. P. 3519-3539.
34. Brumer P. Adv. Chem. Phys. 1981. V. 47. 201-237.

35. Krivoshei I.V., Luzanov A.V., Litinski G.B. Khim Fiz. 1985. V. 45. P.759-769.
36. Berezovoj V.P., Bolotin Yu.L.,.Gonchar V.Yu., Granovsky M. Fiz. Elem. Chast. At. Yad. 2003. V. 34. P. 388-447.
37. Henon M., Heiles C. Astron. J. 1964. V. 69. P. 73-79.
38. Pullen R.A., Edmons A.R. J. Phys. 1981. V. A 14. P. L477 - L484.
39. Vorobyev P.A., Zaslavsky G. M. Zh. Eksp. Teor. Fiz. 1987. V. 92. P. 1564-1572.
40. Salasnich L. Mod. Phys. Lett. 1997. V. 12. P. 1473-1480.
41. Nakagawa K., Yoshida H. J. J. Phys. 2001. V. A 34. P. 8611–8630.
42. Zyczkowski K. J. Phys. 1990. V. A 23. P. 4427-4438.
43. Hose G., Taylor H.S. J. Chem. Phys. 1982. V. 76. P. 5356-5364.
44. Lichtenberg, A. and Lieberman, M. Regular and Stochastic Motion. 2-nd Edition. New York: Springer-Verlag, 1994. 499 p.
45. Nerukh D., Karvounis G., Glen R.C. Complexity. 2004. V. 10. P. 40-46.

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Kharkov University Bulletin 2007. № 770. Chemical Series Issue 15(38). А.В. Лузанов. Анализ квантовых кривизн в простых колебательных системах.

Вводятся квантовомеханические аналоги кривизн линий и поверхностей для оценки степени нелинейности и сложности квантовых состояний соответствующих динамических систем. Введенные меры используются для выявления особенностей систем в контексте проблемы квантового хаоса. На примере модельных задач Хенона-Хейлиса и Янга–Миллса продемонстрировано использование флуктуаций кривизн для различения регулярного и хаотического режима поведения.