Dynamical study of quantum systems

(résumé anglais du memoire présenté pour l'obtention du titre d'habilité à diriger des recherches)

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to Ms Bimmer and Mr Marinoni, friends on a lonely journey who didn't quite make it ...
to my wife and sons, who were far and yet so close
to mom, dad, and Granny

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He didn't say any more, but we've always been unusually communicative in a reserved way, and I understood that he meant a great deal more than that.

F. Scott Fitzgerald, The Great Gatsby

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Dmitrií Sadovskií, Dunkerque, June 8, 1998

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This résumé summarizes the work carried out by the author on the various aspects of the quantum theory of molecular and atomic systems, and on applications of this theory. It is part of the presentation for the title *habilité à diriger des recherches*.

CONTENTS

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Abstract

As part of the presentation for the title *habilité à diriger des recherches*, we summarize our work on various aspects of quantum and classical theory of molecular and atomic systems, and on applications of this theory. Our central idea is to use the results obtained in the classical dynamical theory of such systems for the analysis of the corresponding quantum systems. To study classical dynamics we rely extensively on the normal form transformation methods, which we apply both near equilibria and near periodic orbits. The normalization, especially in the presence of symmetries, involves construction of polynomial integrity bases and thus the relevant aspects of the theory of invariants. Group theory and basic topology are used extensively in the qualitative analysis of the reduced classical problems obtained by the normal form methods, and the results are then transferred to quantum theory. Quantum problems are studied independently and the results of the two approaches are compared. Several concrete systems: hydrogen atom in external magnetic and electric fields, electronic Rydberg states of diatomic molecules, notably rare gas hydrides, and rotation-vibration states of spherical top molecules are considered in detail. A number of qualitative phenomena in these systems: crossover of rotational multiplets and of Rydberg n shells, "organized" bifurcations of periodic orbits, diabolic points, and others is analyzed. Other important results include the normal form reconstruction of nonlinear normal modes and the first successful spectroscopic analysis of the rotation-vibration structure of the spherical top molecule SnH_4, and of electron-rotation structure of Rydberg excimers ArD and KrD.

Key words: *dynamical theory, periodic orbit, reduced phase space, relative equilibria, normal form, reduction, Lie transformation, integrity basis, generating function, Morse theory, group theory, finite group, isotropy group, orbit space, irreducible tensor, contact transformation, hydrogen atom in external fields, n shell, Kustaanheimo-Stiefel regularization, Hénon-Heiles oscillator, Rydberg states, excimer, Rydberg diatomic molecules, ArD, KrD, spherical top molecules, vibrational polyad, rotation-vibration states*

Résumé français

Comme partie de la présentation pour l'obtention du titre d'habilité à diriger des recherches, nous résumons notre travail sur différents aspects de la théorie quantique et classique des systèmes moléculaires et atomiques, et sur les applications de cette théorie. Notre idée centrale est d'utiliser les résultats obtenus pour ces systèmes en théorie dynamique classique dans l'analyse des systèmes quantiques correspondants. Pour étudier la dynamique classique, nous appliquons largement les méthodes de transformation en forme normale au voisinage d'un équilibre aussi bien que d'une orbite périodique. La normalisation, surtout en présence de symétries, implique la construction des bases polynômiales d'intégrité et par conséquent, les aspects pertinents de la théorie des invariants. La théorie des groupes et la topologie élémentaire sont utilisées en grande mesure dans l'analyse qualitative des problèmes classiques réduits qui sont déduits par les méthodes des formes normales. Ensuite, les résultats sont transférés vers la théorie quantique. Les problèmes quantiques sont étudiés indépendemment et les résultats des deux approches sont comparés. Plusieurs systèmes concrets: l'atome d'hydrogène soumis aux champs magnétique et électrique extérieures, états électroniques de Rydberg des molécules diatomiques, notamment des hydrides des gaz rares, et états de rotation-vibration des molécules de type toupie sphérique sont considérés en détail. Un nombre des phénomènes qualitatifs ayant lieu dans ces systèmes: le croisement des multiplets rotationnels et des couches n de Rydberg, bifurcations "organisées" d'orbites périodiques, points diaboliques, et autres sont analysés. Parmi les autres résultats importants, il y a la reconstruction des modes normaux nonlinéaires et la première analyse spectroscopique successive de la structure rovibrationnelle de la molécule de type toupie sphérique SnH_4 et de la structure électronique-rotationnelle des excimers de Rydberg ArD et KrD.

Mots clés: *théorie dynamique, orbite périodique, espace des phases réduit, équilibres relatifs, forme normale, réduction, transformation de Lie, base d'intégrité, fonction génératrice, théorie de Morse, théorie des groupes, groupe fini, groupe d'isotropie, espace des orbites, tenseur irréductible, transformation de contact, atome d'hydrogène soumis aux champs extérieurs, n-couche, régularisation de Kustaanheimo-Stiefel, oscillateur de Hénon-Heiles, états de Rydberg, excimer, molécules de Rydberg diatomiques, ArD, KrD, molécules de type toupie sphérique, polyade vibrationnelle, états de rotation-vibration*

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