

Phase space and rotational symmetry  
for molecular vibrational dynamics

V. G. Hartar

Department of Physics, University of Arkansas  
Fayetteville, AR 72401

**TITLES AND ABSTRACTS**

for

**INVITED PRESENTATIONS**

Certain portions of high resolution spectroscopic spectra can be understood and predicted using the phase space approach. The phase space approach can be identified with various representations of a global molecular symmetry induced by local vibrational symmetries of non-integrable trajectories. The dynamics of localized vibrational wavepackets or coherent states may be associated with the spectral line structure in such spectra. Recent ultrahigh resolution spectra of diatomic molecules show rotational symmetry breaking connected with a highly anharmonic potential. Rotational effects are predicted for the isosymmetric asymmetric molecule including the reported carbon cluster  $C_{60}$ .

Models of anharmonic coupled oscillators and local vibrational modes can be treated similarly by expanding in a global phase space associated with the generators of  $SO(2)$  algebra. Dynamical systems associated with local modes is analogous to the rotational symmetry breaking. Also, the coupling between vibrational and rotational modes may be described using a multi-sheeted rotational phase portrait. Such partial quantum level patterns arising in strong harmonic coupling modes can be related to anharmonic phase paths.

1. V. G. Hartar and C. E. Mortenson, *J. Chem. Phys.* **50**, 4361 (1969).
2. V. G. Hartar, *J. West. Phys.* **30**, 749 (1980).
3. Christian Jordan (unpublished).
4. H. W. Kroto, J. K. Manly, R. E. D'Souza, K. V. Carl, and R. F. Smalley, *Nature* **318**, 352 (1985).
5. G. S. van Rooijen, A. Scappia, and R. E. Levine, *J. Chem. Phys.* **81**, 3996 (1984).
6. G. S. van Rooijen, V. Lachelle, R. E. Levine, and A. A. L. D'Amico, *J. Chem. Phys.* **79**, 4335 (1983).
7. H. K. Kallman, *J. Chem. Phys.* **23**, 1043 (1955).

Spin phase space and rotational symmetry  
for molecular rovibrational dynamics

W. G. Harter

Department of Physics, University of Arkansas

Fayetteville, AR 72701

Certain patterns of high resolution molecular spectra can be understood and predicted easily by appealing to rotational phase portraits and coset spaces associated with phase trajectories.<sup>1,2</sup> Different spectral patterns can be identified with various representations of a global molecular symmetry induced by local subgroup symmetries of selected semiclassical trajectories. The dynamics of localized rotational wavepackets or generalized coherent states may be associated with the spectral fine structure in each pattern. Recent ultrahigh resolution spectra<sup>3</sup> of SF<sub>6</sub> show effects of "spontaneous" rotational symmetry breaking connected with a S<sub>6h</sub> ⊃ O<sub>h</sub> ⊃ C<sub>4v</sub> subgroup chain. Related rotational effects are predicted for the icosahedrally symmetric molecules including the reported<sup>4</sup> carbon cluster C<sub>60</sub>.

Models of anharmonic coupled oscillators and local vibrational modes<sup>5,6,7</sup> can be treated similarly by appealing to a quasi-spin phase space associated with the generators of SU(2) algebra. Dynamical symmetry breaking associated with local modes is analogous to the molecular rotational symmetry breaking. Also, the coupling between vibrational and rotational motions may be described using a multi-sheeted rotational phase portrait. Some peculiar quantum level patterns<sup>2</sup> arising in strong Coriolis coupling models can be related to extraordinary phase paths.

1. W. G. Harter and C. W. Patterson, J. Chem. Phys. 80, 4241 (1984).
2. W. G. Harter, J. Stat. Phys. 36, 749 (1984).
3. Christian Bordé (unpublished).
4. H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley, Nature 318, 162 (1985).
5. O. S. van Roosmalen, I. Benjamin, and R. D. Levine, J. Chem. Phys. 81, 5986 (1984).
6. O. S. van Roosmalen, F. Iachello, R. D. Levine, and A. E. L. Dieperink, J. Chem. Phys. 79, 2515 (1983).
7. M. E. Kellman, J. Chem. Phys., 83, 3843 (1985).

spin phase space and rotational symmetry  
for molecular rotational dynamics

W. G. Harter  
Department of Physics, University of Kansas  
Lawrence, KS 66044

Certain patterns of high resolution molecular spectra can be understood  
and predicted easily by appealing to rotational phase portraits and group  
theory associated with phase trajectories. The rotational spectra can  
be identified with various representations of a global molecular symmetry induced  
by local subgroup symmetries of selected semiclassical trajectories. The dynamics  
of localized rotational wavepackets or generalized coherent states may be asso-  
ciated with the spectral line structure in each pattern. Recent highlights  
of rotational spectra of  $H_2$  show effects of "spontaneous" rotational symmetry  
breaking connected with a  $2 \times 2$  subgroup chain. Related rotational effects  
are predicted for the locally nearly symmetric molecules including the reported  
rotational spectra of  $H_2$ .

W. G. Harter and G. W. Patterson, *J. Chem. Phys.* **90**, 4241 (1989).  
W. G. Harter, *J. Stat. Phys.* **58**, 749 (1984).  
J. Gruber and G. W. Patterson (unpublished).  
R. W. Krotz, J. R. Heath, S. C. O'Brien, R. V. Goff, and R. E. Smalley,  
*Science* **218**, 105 (1982).  
D. E. von Rosenberg, I. Benjamine, and R. D. Levine, *J. Chem. Phys.* **81**, 3586  
(1984).  
D. E. von Rosenberg, F. Iachello, R. D. Levine, and A. E. L. Dieperink, *J.  
Chem. Phys.* **79**, 1315 (1983).  
A. E. L. Dieperink, *J. Chem. Phys.* **81**, 3843 (1985).

INVITED PRESENTATIONS  
MONDAY, OCT. 20, MANDELL THEATER

**Review of Recent Developments in the Use of  
Symmetries in Reactions  
F. Iachello  
Yale University**

Algebraic Methods for Medium Energy  
Scattering from Nuclei and  
Molecules  
R. D. Amado  
The Ohio State University  
The Ohio State University, Columbus, OH 43210

Algebraic Methods in Medium Energy  
Scattering from Nuclei and  
Molecules. R. D. AMADO,  
University of Pennsylvania.  
The eikonal approximation  
combined with an algebraic  
treatment of target dynamics  
permits a description of medium  
energy scattering from complex  
targets including channel  
coupling to all orders.  
Representation matrices of the  
underlying target dynamical  
symmetry are used to obtain simple  
closed form expressions for  
scattering amplitudes for proton-  
nucleus and for electron-diatomic  
and electron-triatomic molecule  
scattering that agree well with  
experiment.

INVITED PRESENTATIONS  
MONDAY, OCT. 20, MANDELL THEATER

2:30 PM

CHAIRMAN: E. H. LIEB

Algebraic Method for Molecular Structure and Dynamics

R.D. Levine

The Fritz Haber Research Center for Molecular Dynamics  
The Hebrew University, Jerusalem 91904, Israel

There is considerable current experimental interest in the spectroscopy of highly excited molecules and in the intra- and inter-molecular dynamics of such energy rich species. It is thus no longer sufficient to employ the harmonic, small amplitude approximation for the vibration nor the rigid rotor for the rotation. An algebraic approach where even in the zeroth order the motion is anharmonic will be discussed and compared with the conventional, geometrical, approach. Current trends, future perspectives and open problems will be summarized.

*The dynamics of rotating structures*, J. E. Marsden, *University of California, Berkeley*.  
The methods of Hamiltonian dynamics are applied to the problem of coupled rigid bodies and rigid bodies with attached rods and plates. In particular, the hamiltonian structure is found using the methods of group theoretical reduction, and stability of equilibria is determined by the energy casimir method and some bifurcation results are obtained using the theory of bifurcation with symmetry. Some comments on chaotic dynamics are given and remarks are made about the applicability to fluid and plasma systems.

INVITED PRESENTATIONS  
TUESDAY, OCT. 21, MANDELL THEATER  
9:00 AM  
CHAIRMAN: J. L. BIRMAN

## Icosahedral Alloys: Crystals, Quasicrystals, or Glasses?

Paul Heiney

University of Pennsylvania

### "DAS PENTAGRAMMA MACHT DIR PEIN?" \*) VIOLATION OF PERIODIC SYMMETRY IN QUASI- CRYSTALS \*\*)

P. KRAMER, Institut für Theoretische Physik der  
Universität Tübingen, F.R.G.

In November 1984, D. Shechtman, I. Blech, D.  
Gratias and J.W. Cahn /1/

reported on a phase of the alloy Al-Mn which  
shows a sharp diffraction pattern of icosaha-  
dral point symmetry. This result excludes per-  
iodic symmetry and implies a new type of non-  
periodic order. Theoretical studies on non-per-  
iodic space fillings were reported before this  
discovery by Kramer and Neri /2,3/. The basic  
concepts of the theory are reviewed, and pro-  
gress in the theoretical and experimental work  
on quasicrystals is reported.

/1/ Shechtman, D., et al. Phys.Rev.Lett. 53  
(1984)1951-1953 /2/ P. Kramer and R. Neri,  
Int.Coll. on Group Theor. Methods in Physics,  
Trieste 1983 /3/ P. Kramer and R. Neri, Acta  
Cryst. A40(1984)580-587

- \*) J.W. von Goethe, Faust, part 1, verse 1396  
\*\*) Work supported by the Deutsche Forschungs-  
gemeinschaft

## The Growth of Quantum Crystals

Viet Elser

AT&T Bell Laboratories

### INTRODUCTION TO THE PHYSICS OF QUASICRYSTALS

Abstract of Invited Talk for XV International Colloquium on Group

Theoretical Methods in Physics

Paul J. Steinhardt

Department of Physics

University of Pennsylvania

Philadelphia, PA 19104

Quasicrystals are solids which exhibit long range quasiperiodic translational order and long range orientational order with symmetry that is disallowed for conventional crystals. Recently, new metallic alloys have been discovered which appear to be examples of icosahedral quasicrystals. The defining structural and symmetry properties of quasicrystals will be briefly introduced. In particular, broken translational symmetry will be shown to lead to extra degeneracy of the ground state and extra hydrodynamic degrees of freedom (phasons) compared with conventional crystals. The physical interpretation of the phasons and their predicted effects on the growth, atomic structure and elastic properties of quasicrystals will be discussed and compared with recent experimental results.

The Growth of Quantum Crystals  
Vik Bieri  
AT&T Bell Laboratories

INTRODUCTION TO THE PHYSICS OF QUASICRYSTALS  
Abstract of invited talk for XV International Colloquium on Group  
Theoretical Methods in Physics  
Paul J. Steinhardt  
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dynamic degrees of freedom (phonons) compared with conventional crystals.  
The physical interpretation of the phonons and their predicted effects on  
the growth, atomic structure and elastic properties of quasicrystals will be  
discussed and compared with recent experimental results.

INVITED PRESENTATIONS  
TUESDAY, OCT. 21, MANDELL THEATER  
2:30 PM  
CHAIRMAN: P. CVITANOVIC

Rationalization Approach to Chaos  
P. Cvitanovic  
Nordita

Number of Periodic Windows in One-Dimensional Mappings and Group Theory. Bai-Lin Hao, Institute of Theoretical Physics. The number of periodic windows in one dimensional mappings, or the number of zeros of some set of composite functions in a certain range, is related to a combinatorial problem solved by mathematicians long ago. However, to apply their results one must be careful in choosing the correct group, as is shown in the example of the antisymmetric cubic map.

INVITED PRESENTATIONS  
WEDNESDAY, OCT. 22, MANDELL THEATER

9:00 AM

CHAIRMAN: B.-L. HAO

**Renormalization Approach to Chaos**

**P. Cvitanovic**

**Nordita**

**CHAOS IN THE TRANSITION FROM CLASSICAL TO QUANTUM MECHANICS**

Martin C. Gutzwiller

IBM T.J. Watson Research Center, Yorktown Heights, N.Y. 10598

Conservative dynamical systems with few degrees of freedom come in four varieties all of which are represented by variations of hydrogen. The isolated atom is superregular in complete analogy to the geodesics on a sphere. The positive ion of the hydrogen molecule is simply regular (integrable, separable) as the geodesics on an ellipsoid. In a magnetic field, the H-atom becomes mildly chaotic as the motion of the moon around the earth. For a donor impurity in a semiconductor, however, with an anisotropic mass-tensor, chaos becomes harsh as for the geodesics on a surface of negative curvature. The connection between classical and quantum behavior can be established only through the trace formula which relates the energy spectrum to the collection of periodic orbits. Group theory is essential in proving the trace formula to be an identity. In the Anisotropic Kepler Problem, one has to settle for less; but the problem now becomes to understand why a sensible spectrum should result from the sum over periodic orbits. The detailed statistical distribution of their lengths seems to be responsible, a property which one could call their third entropy, in addition to their metric and topological entropies.



INVITED PRESENTATIONS  
WEDNESDAY, OCT. 22, MANDELL THEATER  
9:00 AM  
CHAIRMAN: B.-L. HAO

Renormalization Approach to Chaos  
P. Cvitanovic  
Notas

CHAOS IN THE TRANSITION FROM CLASSICAL TO QUANTUM MECHANICS  
Martin C. Gutzwiller  
IBM T.J. Watson Research Center, Yorktown Heights, N.Y. 10598

Conservative dynamical systems with few degrees of freedom come in four varieties: all of which are represented by variations of hydrogen. The isolated atom is superregular in complete analogy to the geodesics on a sphere. The positive ion of the hydrogen molecule is simply regular (integrable, separable) as the geodesics on an ellipsoid. In a magnetic field, the H-atom becomes mildly chaotic as the geodesics on the moon around the earth. For a donor impurity in a semiconductor, however, with an anisotropic mass tensor, chaos becomes harsh as for the geodesics on a surface of negative curvature. The connection between classical and quantum behavior can be established only through the trace formula which relates the energy spectrum to the collection of periodic orbits. Group theory is essential in proving the trace formula to be an identity. In the Anisotropic Ising Problem, one has to settle for less; but the problem now becomes to understand why a renormalized spectrum should result from the sum over periodic orbits. The detailed statistical distribution of their lengths seems to be responsible, a property which one would call their third entropy, in addition to their metric and topological entropies.

INVITED PRESENTATIONS  
THURSDAY, OCT. 23, MANDELL THEATER  
9:00 AM  
CHAIRMAN: P. KRAMER

Quasiperiodicity, Chaos and Turbulence in Mercury and Helium Experiments  
A. J. Libchaber  
University of Chicago

Characterization of Strange Sets  
M. J. Feigenbaum  
Cornell University

Generalized symmetries, also known as Liouville integrability, were introduced by E. Noether in 1918. Conservation laws, however, have only recently come to the fore in research into the symmetry properties of partial differential equations. This talk will survey the basic theory of generalized symmetries and their application to the theory of conservation laws. It will include a discussion of the generalization of Noether's theorem to non-Lagrangian systems and methods for constructing explicit solutions of systems of partial differential equations, including separation of variables and partial invariance. Recent applications to the equations of elasticity, Maxwell's equations, the equations of gas dynamics, etc. will be touched on.

**INVITED PRESENTATIONS  
THURSDAY, OCT. 23, MANDELL THEATER**

**9:00 AM**

**CHAIRMAN: P. KRAMER**

Generalized Symmetries

Peter J. Olver  
University of Minnesota

Abstract:

Generalized symmetries (also known as "Lie-Bäcklund transformations") were introduced by E. Noether in her seminal paper on conservation laws, but have only recently come to the forefront of research into the symmetry properties of partial differential equations. This talk will survey the basic theory of generalized symmetries and recursion operators, and discuss a number of their applications to the differential equations of mathematical physics. These will include connections with soliton equations, conservation laws and the general form of Noether's theorem, Hamiltonian systems, and methods of constructing explicit solutions to systems of partial differential equations, including separation of variables and partial invariance. Recent applications to the equations of elasticity, Maxwell's equations, the equations of gas dynamics, etc. will be touched on.

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Peter J. Olver  
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INVITED PRESENTATIONS  
FRIDAY, OCT. 24, MANDELL THEATER  
9:00 AM  
CHAIRMAN: J. KAMRICH

Title to be Announced  
A. Deprit  
National Bureau of Standards

New Results in the Application of Group Theory to  
Differential Equations  
P. Winternitz  
University of Montreal

Dynamical Symmetries in  
Collective Nuclear Structure Physics  
C.-L. Wu  
Jilin University

Title to be announced  
L. Suss  
Boston University

Title to be announced  
C. N. Yang  
S. U. N. Y., Stony Brook

INVITED PRESENTATIONS  
FRIDAY, OCT. 24, MANDELL THEATER  
9:00 AM  
CHAIRMAN: J. MANDULA

**Title to be announced**  
**E. Witten**  
**Institute for Advanced Study**

Approximate Global Symmetries of the Electroweak Interactions, H. Georgi, Harvard University and Boston University. I discuss and exemplify a simple explanation for the approximate symmetries of the electroweak interactions that arises naturally in models in which the quarks, leptons, and Higgs particles are all composite states of strongly interacting fermions.

**Title to be announced**  
**L. Sulak**  
**Boston University**

**Title to be announced**  
**C. N. Yang**  
**S. U. N. Y., Stony Brook**

INVITED PRESENTATIONS  
FRIDAY, OCT. 24, MANDELL THEATER  
9:00 AM  
CHAIRMAN: J. MANDULA

This to be announced  
E. Wilson  
Institute for Advanced Study

Approximate Global Symmetries of the  
Electron-Positron Interaction, H. Georgi,  
Harvard University and Boston University.  
I discuss and exemplify a simple extension  
of the approximate symmetries of  
the electron-positron interaction that arises  
naturally in models in which the quarks,  
leptons, and other particles are all com-  
posites of strongly interacting  
fermions.

This to be announced  
J. Suk  
Boston University

This to be announced  
C. H. Yang  
S. U. N. Y., Stony Brook

**Boğaziçi Üniversitesi**

**Arşiv ve Dokümantasyon Merkezi**

**Kişisel Arşivlerle İstanbul'da Bilim, Kültür ve Eğitim Tarihi**

**Feza Gürsey Arşivi**



**FGASCI0500105**