

RESEARCH GROUP: MOLECULAR DYNAMICS OF COMPLEX SYSTEMS

Publications in peer review Journals

1. AGAPITO, F.; NUNES, P.A.; CABRAL, B.J.C.; et al. – Energetic differences between the five- and six-membered ring hydrocarbons: Strain energies in the parent and radical molecules, *Journal of Organic Chemistry*, Vol. 73, Issue 16 (2008), 6213-6223.
2. ALMEIDA, T.S.; COUTINHO, K.; CABRAL, B.J.C.; et al. - Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach, *Journal of Chemical Physics*, Vol. 128, Issue 1 (2008), 014506.
3. COUTO, N.; RAMOS, M.J.; FERNANDEZ, M.T.; et al. - Study of doubly charged alkaline earth metal and 3-azidopropionitrile complexes by electrospray ionization mass spectrometry, *Rapid Communications in Mass Spectrometry*, Vol. 22, Issue 4 (2008), 582-590.
4. ESTÁCIO, S.G.; CABRAL, B.J.C. - Born-Oppenheimer molecular dynamics of phenol in a water cluster, *Chemical Physics Letters*, Vol. 456, Issue 4-6 (2008), 170-175.
5. GALAMBA N.; CABRAL B.J.C. - The Changing Hydrogen-Bond Network of Water from the Bulk to the Surface of a Cluster: A Born-Oppenheimer Molecular Dynamics Study, *Journal of the American Chemical*, Vol. 130, Issue 52 (2008), 17955-17960.
6. MATA R.A.; CABRAL, B.J.C.; MILLOT, C.; et al. - Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach, *Journal of Chemical Physics*, Vol. 130, Issue 1 (2009), 014505.
7. MILLOT, C.; CABRAL, B.J.C. - Electronic properties of liquid water by sequential molecular dynamics/density functional theory, *Chemical Physics Letters*, Vol. 460, Issue 4-6 (2008), 466-469.
8. NUNES, P.M.; ESTÁCIO, S.G.; LOPES, G.T.; et al. - C-H bond dissociation enthalpies in norbornane. An experimental and computational study, *Organic Letters*, Vol. 10, Issue 8 (2008), 1613-1616.

Other Publications

(Include books, chapters or full papers published in conference proceedings)

1. ESTÁCIO, S.G.; MARTINIANO, H.F.M.C.; DO COUTO, P.C.; CABRAL, B.J.C. - Electronic properties of hydrogen bond networks: implications for solvent effects in polar liquids, Chapter 5 in *Solvation effects on Molecules and Biomolecules*, 115-133. Editor: S. Canuto, Springer Science 2008.

RESEARCH GROUP: ANALYSIS AND GEOMETRY IN MATHEMATICAL PHYSICS

Publications in peer review Journals

1. ABREU, M.; DRYDEN, E.B.; FREITAS, P.; GODINHO, L. - Hearing the weights of weighted projective planes, *Ann. Global Anal. Geom.* 33 (2008), 373-395.
2. ANEVA, B.; CHAICHIAN, M.; KULISH, P.P. - From Quantum Affine Symmetry to Boundary Askey-Wilson Algebra and Reflection Equation, *J. Phys. A: Math. Theor.* 41 (2008), 135201 (18pp).
3. ANTUNES, P.; FREITAS, P. - A numerical study of the spectral gap, *J. Phys. A* 41 (2008), 055201.
4. BASTOS, C.; BERTOLAMI, O.; DIAS, N.C.; PRATA, J.N. - Phase-space noncommutative quantum cosmology, *Phys. Rev. D* 78 (2008), 023516.
5. BASTOS, C.; BERTOLAMI, O.; DIAS, N.C.; PRATA, J.N. - Weyl-Wigner formulation of non commutative quantum mechanics, *J. Math. Phys.* 49 (2008), 072101.
6. COUTINHO, R.; FERNANDEZ, B.; GUIRAUD, P. - Symbolic dynamics of two coupled Lorenz maps: from uncoupled regime to synchronisation, *Physica D* 237 (2008), 2444-2462.
7. DIAS, N.C.; PRATA, J.N. - A multiplicative product of distributions and a global formulation of the confined Schrodinger equation, *Journal of Generalized Lie Theory and Applications* 2 (2008), 137.
8. EKHOLM, T.; FRANK, R.L. - Lieb-Thirring inequalities on the half-line with critical exponent, *J. Eur. Math. Soc.* 10 (2008), 739-755.
9. FARIA MARTINS, J.; MIKOVIC, A. - Invariants of spin networks embedded in 3-manifolds, *Comm. Math. Phys.* 279 (2008), 381-399.
10. FREITAS, P.; KREJCIRIK, D. - A sharp upper bound for the first Dirichlet eigenvalue and the growth of the isoperimetric constant of convex domains, *Proc. Amer. Math. Soc.* 136 (2008), 2997-3006.
11. FREITAS, P.; KREJCIRIK, D. - Location of the nodal set for thin curved tubes, *Indiana Univ. Math. J.* 57 (2008), 343-376.
12. KULISH, P.P.; MANOJLOVIC, N.; NAGY, Z. - Quantum symmetry algebras of spin systems related to Temperley-Lieb R-matrices, *J. Math. Phys.* 49 (2008), 023510.
13. MIKOVIC, A. - Spin network wavefunction and nonperturbative graviton propagator, *Fortschr. Phys.* 56 (2008), 475-479.

RESEARCH GROUP: STOCHASTIC ANALYSIS, PATH INTEGRALS AND APPLICATIONS

Publications in peer review Journals

1. ALVES, C.J.S.; CRUZEIRO, A.B - Monte-Carlo simulation of stochastic differential systems - a geometrical approach. *Stoch. Processes Appl.*, 118, nº 3 (2008), 346-367.
2. CHAARI, S; CIPRIANO, F.; GHERYANI, S.; OUERDIANE, H. - Sanov's theorem for white noise distributions and application to the Gibbs conditioning principle. *Acta Appl. Math.* 104, no. 3 (2008), 313-324.
3. CRUZEIRO, A.B.; MALLIAVIN, P. - Non-existence of infinitesimally invariant measures on loop groups. *J. Funct. Anal.* 254, nº7 (2008), 1974-1987.
4. CRUZEIRO, A.B.; MALLIAVIN, P. - Nonergodicity of Euler fluid dynamics on tori versus positivity of the Arnold-Ricci tensor. *J. Funct. Anal.* 254, nº 7 (2008), 1903-1925.
5. DRAGOVIC, V.; GAJIC, B. - Hirota-Kimura Type Discretization of the Classical Nonholonomic Suslov Problem, *Regul. Chaotic Dyn.* vol. 13, no. 4 (2008), 250-256.
6. DRAGOVIC, V.; RADNOVIC, M. - Hyperelliptic Jacobians as billiard algebra of pencils of quadrics: Beyond Poncelet porisms, *Advances in Mathematics*, vol. 219 (2008), 1577-1607.
7. HAHN, A. - An analytic approach to Turaev's Shadow Invariant. *J. Knot Th. Ram.* 17(11) (2008), 1327-1385.
8. HAHN, A. - Chern-Simons models on $S^2 \times S^1$, torus gauge fixing, and link invariants II, *J. Geom. Phys.* 58 (2008), 1124-1136.
9. MENDES, R.V.; CIPRIANO, F. - A stochastic representation for the Poisson-Vlasov equation. *Comm. Nonlinear Sci. Numer. Simul.* 13, nº1 (2008), 221-226.

Other Publications

(Include books, chapters or full papers published in conference proceedings)

1. BEN AROUS, G.; CRUZEIRO, A.B.; LE JAN, Y.; ZAMBRINI, J.-C. (Editors) - *Stochastic Analysis in Mathematical Physics* (Proceedings of the conference held in Lisbon, 2006), World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2008.
2. CRUZEIRO, A.B.; MALLIAVIN, P. - Stochastic parallel transport on the d-dimensional torus. *Stochastic Analysis in Mathematical Physics*, World Sci. Publ., Hackensack, NJ, 2008, 1-18.

3. CRUZEIRO, A.B.; MALLIAVIN, P. - Stochastic evolution of inviscid Burgers fluid. *Probability, Geometry and Integrable Systems* (Ed. Mark Pinsky, Björn Birnir, Henry P. McKean), Math. Sci. Res. Inst. Publ., Cambridge Univ. Press, 2008, 167-183.
4. HAHN, A. - Two Hida distributions appearing in the study of Chern-Simons theory in the torus gauge. In L. Accardi et al., editors, *Infinite Dimensional Stochastic Analysis*, volume XXI, *Quantum Probability and White Noise Analysis*, World Scientific, 2008, 85-96.
5. HAHN, A. - White noise analysis in the theory of three-manifold quantum invariants. In A.N. Sengupta and P. Sundar (editors), *Infinite Dimensional Stochastic Analysis*, volume XXII of *Quantum Probability and White Noise Analysis*, World Scientific, 2008, 201-225.
6. LESCOT, P.; ZAMBRINI, J.C. - Probabilistic deformation of contact geometry, diffusion processes and their quadratures, *Seminar on Stochastic Analysis, Random Fields and Applications V*, *Prog. Probab.* 59, Birkhäuser, Basel, 2008, 203-226.