

PUBLICATIONS

"Zero-temperature properties of matter and the quantum theorem of corresponding states: The liquid-to-crystal phase transition for Fermi and Bose systems," with L.H. Nosanow and L.J. Parish, Phys. Rev. B11, 191 (1975).

"Depolarization of light and pair-pair correlations of Argon gas," with C.E. Campbell, Chem. Phys. Lett. 56, 156 (1978).

"Integrated Raman intensity of ^4He ," Correlation Function and Quasiparticle Interactions in Condensed Matter, J.W. Halley, Editor, NATO Advanced Study Institute Series, Vol. 35 (B Physics), 469 (Plenum, NY 1978).

"Electron-phonon contributions to electrical resistivity and superconducting 'p-wave' transition temperature of Pd," with P. Allen and W. Butler, Phys. Rev. Lett. 41, 431 (1978).

"Theory of fourth order structure and Raman scattering in liquid ^4He ," with C.E. Campbell, J. of Phys. (Paris), 390, C6, 233 (1978).

"Calculated electron-phonon coupling and superconducting T_c of transition metals: Mo and Pd," with P. B. Allen and W. H. Butler, J. of Phys. (Paris) 39, C6, 472 (1978).

"Functional optimization of the Jastrow wave function for liquid ^4He ," with C. E. Campbell, Phys. Lett. 79B, 23 (1978).

"Phonon line widths and electron-phonon interaction in Nb," with P. B. Allen and W. H. Butler, Phys. Rev. B19, 3708 (1979).

"Calculated phonon linewidths and electronic mass enhancement in Pd." with W. H. Butler, Phys. Rev. B19, 6010 (1979).

"The structure of the ground state and low excited states of quantum fluids," with C. E. Campbell, Nucl. Phys. A328, 210 (1979).

"Exotic pairing in metals: formalism and application to Nb and Pd," with P. B. Allen and W. H. Butler, Superconductivity in d-and f-bands metals, H. Suhl and M.B. Maple, Editors, 215 (Academic Press, New York, 1980).

"Integrated polarized light scattering from liquid ^4He ," with C. E. Campbell and J. W. Halley, Phys. Rev. B21, 1323 (1980).

"Solutions to the Boltzmann equation for electrons in a metal: Energy dependence," Phys. Rev. B21, 4380(1980).

"Calculated ideal electrical and thermal conductivity of Pd and Nb," with P. B. Allen and W. H. Butler, Phys. Rev. B23, 5080 (1981).

"Low-field Hall coefficient of Cu and Nb," with P. B. Allen and T. P. Beaulac, Phys. Rev. B23, 3617 (1981).

"Test of interparticle potentials for liquid ^4He ," with C. E. Campbell and L. R. Whitney, J. Low Temp. Phys. 44, 367 (1981).

"Electron-phonon effects in copper. I. Electron scattering rate and mass enhancement," with P. B. Allen, W. H. Butler, and F. S. Khan, Phys. Rev. B26, 1538 (1982).

"Electron-phonon effects in copper. II. Electrical and thermal resistivities and Hall coefficient," with P.B. Allen and T.P. Beaulac, Phys. Rev. B26, 1549 (1982).

"Ideal thermal conductivity of Pd and Nb," with P. B. Allen and W. H. Butler, Thermal Conductivity 16, D.C. Larsen, Editor, 155 (Plenum, New York, 1983).

"A fast method for calculating the self-consistent electron structure of random alloys," with D. D. Johnson and G. M. Stocks, Phys. Rev. B10, 5508 (1984).

"The one electron Schrodinger equation and the single scatter S matrix in the complex energy plane," Ψ_K -Newsletter of the Collaborative Computation Project No. 9 on the Electronic Structure of Solids (England), No. 8, p. 27, August, 1984.

Self-consistent electronic structure of disordered $\text{Fe}_{0.65}\text{Ni}_{0.35}$," with D. D. Johnson and G. M. Stocks, J. Appl. Phys. 57, 3018 (1985).

"A fast method for calculating the self-consistent electronic structure of random alloys. II. Optimal use of the complex plane," Phys. Rev. B32, 4204 (1985).

"Self-consistent electronic structure of α -phase Hume-Rothery electron compound alloys $\text{Cu}_c\text{Zn}_{1-c}$, $\text{Cu}_c\text{Ga}_{1-c}$ and CuGe_{1-c} ," with G.M. Stocks, A.M Boring, D.M. Nicholson, D.D. Johnson, J.S. Faulkner, and B.L. Gyorffy, invited contribution, A.I.M.E. Symposium on Nobel Metal Alloys (AIME, New York, 1985).

"Density functional theory for random alloys: Total energy within the coherent potential approximation," with D.D. Johnson, D.M. Nicholson, B.L. Gyorffy and G.M. Stocks, Phys. Rev. Lett, 56, 2088 (1986).

"Three and four body correlation functions in simple fluids," with C.E. Campbell, Phys. Rev. A 33, 4232 (1986).

"Calculations of resistivity and superconducting T_c in transition metals," with P.B. Allen, T.P. Beaulac, F.S. Khan, W.H. Butler and J.C. Swihart, MRS Symposium Proceedings: Computer based microscopic description of the Structure and Properties of Materials, J.Q. Broughton, W. Krakow and S.T. Pantelides, Editors (MRS, Boston, 1986).

"Ferromagnetism versus antiferromagnetism in face centered cubic iron," with J. Staunton, B.L. Gyorffy, D.D. Johnson and G.M. Stocks, Phys. Rev. Letts., 56, 2096 (1986).

"DC transport in metals," with P.B. Allen, T.P. Beaulac, F.S. Khan, W.H. Butler, and J.C. Swihart, Phys. Rev. B34, 4331 (1986).

"The Slater-Pauling curve: First principles calculations of the moments of $Fe_{1-c}Ni$ and $V_{1-c}Fe_c$," with D.D. Johnson and J.B. Staunton, J. Appl. Phys. 61, 3715 (1987).

"The electronic structure of the disordered-local-moment state of face-centered-cubic iron," with W.A. Shelton, Jr., G.M. Stocks, D.M. Nicholson and B.L. Gyorffy, J. Appl. Phys. 61, 3712 (1987).

"Electron-phonon interaction effects in tantalum," with A. Al-Lehaibi, J.C. Swihart, and W.H. Butler, Phys.Rev. B36, 4103 (1987)

"Ab initio theory of the ground state properties of ordered and disordered alloys and the theory of ordering processes in alloys," with G.M. Stocks, D.M. Nicholson, W.H. Butler, P. Sterne, W.M. Temmerman, D.D. Johnson, B.L. Gyorffy, A. Gonis, X.-G Zhang, and P.E.A. Turchi, MRS Symp. Proc., Vol. 81 (MRS, Pittsburgh, 1987).

"Magnetism in alloys," with B.L. Gyorffy, D.D. Johnson, and J.B. Staunton, in Electronic Band Structure and Its Applications, Vol. 283, Lecture Notes in Physics (Springer-Verlag, New York 1987).

"Theoretical study of the environmental effects on the hyperfine fields of Ni and Fe in $Ni_{0.75}Fe_{0.25}$ " with H. Ebert, H. Winter, B. Gyorffy, and D.D. Johnson, Solid State Commun., 64, 1011 (1987).

"Electronic structure of random alloys and the theory of ordering processes," with G.M. Stocks, D.M. Nicholson, D.D. Johnson and A. Gonis, Proceedings of the U.S.-Japan Seminar on Electronic Structure and Lattice Defects in Alloys, Honolulu, May, 1987.

"Theoretical study of the hyperfine fields of Ni and Fe in FCC Ni_xFe_{1-x} alloys," with H. Ebert, H. Winter, B. Gyorffy, and D.D. Johnson, J. Phys. F. 18, 719 (1988).

"Effects of chemical and magnetic disorder in $Fe_{.50}Mn_{.50}$," with D.D. Johnson and G.M. Stocks, J. Appl. Phys., 63, 3490 (1988).

"Rare gas impurities in alkali metals - relation to optical absorption," with D.E. Meltzer and G.M. Stocks, Phys. Rev. B. 37 6011 (1988).

"Correlation between bandstructure and magneto-optical properties of BCC $\text{Fe}_x\text{Co}_{1-x}$," D. Weller, W. Reim, H. Ebert, D.D. Johnson, F.J. Pinski, Journal de Physique 49, NC-8, 41-41 (1988).

"The theory of random alloys," with D.M. Nicholson, G.M. Stocks, W.H. Butler, D.D. Johnson and B.L. Gyorffy, invited contribution, Proceedings of the Third International Conference on Supercomputing, Boston, (International Supercomputing Institute, 1988).

"Magnetism in metals and alloys," with J.B. Staunton, B.L. Gyorffy, D.D. Johnson and G.M. Stocks, in Physics of metals, E.S. Guiliano and C. Rizzuot, editors (World Scientific, New Jersey, 1988), p.431.

"The electronic structure and the state of compositional order in metallic alloys," with B.L. Gyorffy, D.D. Johnson, D.M. Nicholson, and G.M. Stocks, in Alloy Phase Stability, NATO ASI, G.M. Stocks and A. Gonis, editors (Kluwer, Norwell, Mass, 1989), pp. 421-468.

"Local density theory of magnetism and its interrelation with compositional order in alloys," with J.B. Staunton, B.L. Gyorffy, D.D. Johnson and G.M. Stocks in Alloy Phase Stability, NATO ASI, G.M. Stocks and A. Gonis editors, (Kluwer, Norwell, Mass, 1989), pp. 469-508.

"A theoretical study of the hyperfine fields of Fe and Co in ferromagnetic bcc $\text{Fe}_x\text{Co}_{1-x}$," Hyperfine Interactions, 51, 925 (1989).

"NiFe Invar Alloys: Theoretical insights into the underlying mechanisms responsible for their physical properties," with D.D. Johnson, J.B. Staunton, B.L. Gyorffy, and G.M. Stocks, in Physical Metallurgy of Controlled Expansion "Invar-Type" Alloys, K.C. Russell and D. Smith editors, (The Metals Society, 1989).

"Pair-pair correlations and collision induced light scattering," with C.E. Campbell, B.E. Clements and P. Samsel, Condensed Matter Theories, vol 4, Jamine Keller, editor, Plenum, New York, (1989), p. 17.

"Investigation of magnetic and compositional order in alloys and multilayers," with D.D. Johnson, J.B. Staunton, B.L. Gyorffy, and G.M. Stocks, invited contribution, Proceedings of the Fourth International Conference on Supercomputing, Santa Clara, (International Supercomputing Institute, 1989), p. 72.

"Correlations between bandstructure and magneto-optical properties of BCC $\text{Fe}_x\text{Co}_{1-x}$ " with D. Weller, W.Reim, H. Ebert, D.D. Johnson, J. Phys. (Paris) C8, 42 (1989).

"A theoretical study of the hyperfine fields in BCC $\text{Fe}_x\text{Cr}_{1-x}$ and FeCo_{1-x} alloys," with H. Ebert, H. Winterand D.D. Johnson, J. Phys.: Condens. Matter 2, 433, (1990).

"Ordering mechanism in Ni-Cr alloys: theory and experiment," with P.E.A. Turchi, R.H. Howell, A.L. Wachs, M.J. Fluss, D.D. Johnson, G.M. Stocks and D.M. Nicholson, *Mat. Res. Soc. Symp.*, **166**, 231, (1990).

"A first-principles study of short-range order in Cu-Zn," with M. Sluiter, P.E.A. Turchi, D.D. Johnson, D.M. Nicholson and G.M. Stocks, *Mat. Res. Soc. Symp.*, **166**, 225, (1990).

"Total energy and pressure calculations for random substitutional alloys," with D.D. Johnson, D.M. Nicholson, G.M. Stocks and B.L. Gyorffy, *Phys. Rev.* **B41**, 9701, (1990).

"Theory of compositional and magnetic correlations in alloys-interpretation of a diffuse neutron scattering experiment on an iron-vanadium single crystal," with J.B. Staunton and D.D. Johnson, *Phys. Rev. Lett.* **65**, 1259 (1990).

"Modeling high-temperature superconductors and metallic alloys on the Intel iPSc/860," with G.A. Geist, B.W. Peyton, W.A. Shelton and G.M. Stocks, *Proceedings of the 5th Distributed Memory Computing Conference*, David Walker, editor (IEEE, 1990).

"The electronic structure and phase stabilities of metallic alloys" with B.L. Gyorffy, A. Barbieri, D.D. Johnson, D.M. Nicholson, W.A. Shelton, and G.M. Stocks, *Alloy Phase Stability and Design*, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors (MRS, 1991) **186**, 3.

"First-Principles study of phase stability of Pd-Rh alloys," with D.D. Johnson, P.E.A. Turchi, M. Sluiter, D.M. Nicholson, and G.M. Stocks, *Alloy Phase Stability and Design*, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors (MRS, 1991) **186**, 21.

"Ground state properties and magnetism in substitutionally disorderd $\text{Fe}_{1-x}\text{Cr}_x$ alloys," with W.A. Shelton, D.D. Johnson, D.M. Nicholson, and G.M. Stocks, *Alloy Phase Stability and Design*, MRSSymposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors (MRS, 1991) **186**, 27.

"A comparative first-principles study of Phase Stability in Ni-Ti and Ni-Al alloys around equiatomic composition," with P.E.A. Turchi, M. Sluiter, D.D. Johnson, *Alloy Phase Stability and Design*, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors, (MRS, 1991) **186**, 59.

"Electronic structure and phase stability properties of Al-Li alloys," with A. Gonis, P.E.A. Turchi, M. Sluiter, D.D. Johnson, *Alloy Phase Stability and Design*, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors (MRS, 1991) **186**, 89.

"Ordering energy of B2 alloys calculated in the frozen potential and Harris approximations," with W.A. Shelton, D.M. Nicholson, G.M. Stocks, D.D. Johnson, P. Sterne, and W.M. Temmerman, Alloy Phase Stability and Design, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors, (MRS, 1991), **186**, 113.

"Photoemission measurements from nickel-iron alloys," with R.G. Jordan, M.A. Hoyland, D.D. Johnson, and J.B. Staunton, Alloy Phase Stability and Design, MRS Symposium Proceedings, G.M. Stocks, D.P. Pope, and A.F. Giamei, editors (MRS, 1991) **186**, 199.

"Order and disorder in metallic alloys," with B.L. Gyorffy, G.M. Stocks, B. Ginatempo, D.D. Johnson, D.M. Nicholson, and J.B. Staunton, Phil. Trans. R. Soc. Lond. A, **334**, 515, (1991).

"The origins of compositional order in PtNi Alloys," with B. Ginatempo, D.D. Johnson, J.B. Staunton, G.M. Stocks, and B.L. Gyorffy, Phys. Rev. Lett. **66**, 766 (1991).

"Molecular-dynamic simulation of the static pair-pair correlation function for classical fluids," with B.E. Clements, C.E. Campbell and P.J. Samsel, Phys. Rev. A, **44**, 1139 (1991).

"First-principles study of phase stability in Cu-Zn substitutional alloys," with P.E.A. Turchi, M. Sluiter, D.D. Johnson, D.M. Nicholson, G.M. Stocks, and J.B. Staunton, Phys. Rev. Lett. **67**, 1779 (1991).

Reply to Comment on "The Origins of Compositional Order in NiPt alloys," with B. Ginatempo, D.D. Johnson, J.B. Staunton, G.M. Stocks, and B.L. Gyorffy, Phys. Rev. Lett. **68**, 1962, (1992).

"On the causes of compositional Order in NiPt alloys," with B.L. Gyorffy, B. Ginatempo, G.M. Stocks, D.M. Nicholson, D.D. Johnson, J.B. Staunton, W.A. Shelton, D.M. Nicholson in Structural and Phase Stability of Alloys, J.L. Moran-Lopez, F. Mejialira, and J.M. Sanchez, editors, (Plenum, New York, 1992), pp. 167180.

"First principles theory of alloy phase stability--Ordering and premartensitic phenomena in beta-phase NiAl," with G.M. Stocks, W.A. Shelton, D.M. Nicholson, B. Ginatempo, A. Barbieri, B.L. Gyorffy, D.D. Johnson, J.B. Staunton, P.E.A. Turchi, and M. Sluiter in Ordered Intermetallics--Physical Metallurgy and Mechanical Behavior, NATO ASI, C.T. Liu, R.W. Cahn, and G. Sauthoff, editors, (Kluwer, Norwell, Mass, 1992) pp.15-36.

"Inclusion of charge correlations in calculations of the energetics and electronic structure for random-substitutional alloys," with D.D. Johnson, Phys. Rev. B **48**, 11553 (1993).

"First-principles theory of disordered alloys and alloy phase stability," with G.M. Stocks, D.M. Nicholson, W.A. Shelton, B.L. Gyroffy, D.D. Johnson, J.B. Staunton, B. Ginatempo, P.E.A. Turchi, and M. Sluiter in *Statistics and Dynamics of Alloy Phase Transformations*, NATO ASI, A. Gonis and P.E.A. Turchi editors, (Plenum, New York, 1994), p. 305.

"Including charge correlations in the calculation of the total energy and electronic structure of random alloys," with D.D. Johnson in *Metallic Alloys: Experimental and Theoretical Perspectives*, NATO ASI, J.S. Faulkner and R.G. Jordan, editors, (Kluwer, Norwell, Mass, 1994), pp. 149-158.

"The origins of ordering in CuPt," with J.F. Clark, P.A. Sterne, D.D. Johnson, J.B. Staunton, and B. Ginatempo in *Metallic Alloys: Experimental and Theoretical Perspectives*, NATO ASI, J.S. Faulkner and R.G. Jordan, editors (Kluwer, Norwell, Mass, 1994), pp. 159-166.

"Concentration waves, itinerant electrons and Onsager cavity fields," with J.B. Staunton, M.F. Ling, and D.D. Johnson in *Metallic Alloys: Experimental and Theoretical Perspectives*, NATO ASI J.S. Faulkner and R.G. Jordan, editors (Kluwer, Norwell, Mass, 1994), pp. 1349-357.

"Thermodynamics of the fully frustrated quantum Josephson-junction array: A hybrid Monte Carlo study," with J. Mikalopas, M. Jarrell, W. Chung, and M.A. Novotny, *Rapid Communications*, Phys. Rev. B50, 1321 (1994).

"Compositional short-range ordering in metallic alloys: Band-filling, charge-transfer, and size effects from a first-principles all-electron Landau-type theory," with J.B. Staunton and D.D. Johnson, Phys. Rev. B50, 1450 (1994).

"First-principles all-electron theory of atomic short-range ordering in metallic alloys: DO_{22} - versus $L1_1$ -like correlations," with D.D. Johnson and J.B. Staunton, Phys. Rev. B50, 1473 (1994).

"First-principles simulation of materials properties," with W.A. Shelton, G.M. Stocks, R.G. Jordan, Y. Liu, L. Qui, D.D. Johnson, J.B. Staunton, and B. Ginatempo, invited contribution to Scalable High-Performance Computing Conference, (IEEE, 1994), in press.

"Commensurate and incommensurate ordering in the ternary Cu-Ni-Zn system," with J.D. Althoff and D.D. Johnson, Phys. Rev. Lett. **74**, 138 (1995).

"van Hove singularity induced $L1_1$ ordering in CuPt," with J.F. Clark, D.D. Johnson, P.A. Sterne, J.B. Staunton, and B. Ginatempo, Phys. Rev. Lett. **74**, 3225 (1995).

"Origins of the $\langle 1, 1/2, 0 \rangle$ atomic short-range order in Au-rich AuFe alloys," with M.F. Ling, J.B. Staunton, and D.D. Johnson, Phys. Rev. **B52**, R3816 (1995).

"Competing mechanisms for ordering tendencies in BCC CuAuZn₂ and FCC AuFe alloys," with D.D. Johnson, J.D. Althoff, J.B. Staunton, M.F. Ling, Proceedings of a NATO Summer School, A. Gonis, et al., Editors, in Press (June 1995).

"Commensurate and incommensurate ordering tendencies in the ternary FCC Cu-Ni-Zn system," with J.D. Althoff, D.D. Johnson, Phys. Rev. Lett. **74** 138-141 (1995).

"Electronic origins of ordering in multicomponent metallic alloys: Application to the Cu-Ni-Zn system," with J.D. Althoff and D.D. Johnson, Phys. Rev. B **53**, 10610-10625 (1996).

"First-principles theory of magnetocrystalline anisotropy of disordered alloys: Application to cobalt platinum," with S.S.A. Razee, J.B. Staunton, Phys. Rev. B **56**, 8082-8090 (1997).

"Ordering tendencies in alloys and their microscopic origins from a first-principles theory of concentration waves," with D.D. Johnson, J.D. Althoff, J.B. Staunton, M.F. Ling, J. Phase Equilibria **18**, 598-607 (1997).

"Magnetic correlations in gamma-Mn and a Mn-10 at %Cu alloy," with M.F. Ling, J.B. Staunton, D.D. Johnson, J. Magnetism and Mag. Materials **177**, 1399-1400 Part 2 (1998).

"Magnetic anisotropies of Ni-Pt and Co-Pt alloys," with S.S.A. Razee, J.B. Staunton, J. Appl. Phys. **83**, 7097-7099 Part 2 (1998).

"Charge fluctuations in alloys: a coarse-grained model," Phys. Rev. B **57**, 15140-15143 (1998).

"Charge-correlation effects in calculations of atomic short-range order in metallic alloys," with J.B. Staunton, D.D. Johnson, Phys. Rev. B **57**, 15177-15182 (1998).

"Magnetic alloys, their electronic structure and micromagnetic and microstructural models," with J.B. Staunton, S.S.A. Razee, M.F. Ling, J. Phys. D Appl. Phys. **31**, 2355-2375 (1998).

"The nature and extent of paramagnons in palladium: A 'First-Principles' theoretical description," with J.B. Staunton, J. Poulter, B. Ginatempo, and E. Bruno, Proceedings of the 2nd Annual National Symposium on Computational Science and Engineering, Thailand, (1998)

"Electronic and crystal structure of NiTi martensite," with M. Sanati, R.C. Albers, Phys. Rev. B **58**, 13590-13593 (1998).

"Effect of atomic short-range order on magnetic anisotropy," with S.S.A. Razee, J.B. Staunton, Philos. Mag B **78**, 611-615 (1998).

“An *ab initio* theoretical description of the interrelation between magnetocrystalline anisotropy and atomic short-range order,” with S.S.A. Razee, J.B. Staunton, B. Ginatempo, E. Bruno, *Phys. Rev. Lett.* **82**, 53695372 (1999).

“Computation of Diffuse Intensities in Alloys,” with D.D. Johnson and J.B. Staunton, *Methods in Materials Research*, Unit 2b.3, John Wiley & Sons (2000).

“Importance of Temperature-Induced Configurational Excitations for Predicting Thermodynamic and Mechanical Properties of Alloys,” with D.D. Johnson, A.V. Smirov, J.B. Staunton, W.A. Shelton, Rapid Communication, *Phys. Rev. B*, R11917-R11920, (2000).

“Magnetism in Alloys,” with D.D. Johnson J.B. Staunton and S.S.A. Razee, *Methods in Materials Research*, Unit 2a.8, John Wiley & Sons (2001).

“Ab initio theoretical description of the dependence of magnetocrystalline anisotropy on both compositional order and lattice distortion in transition metal alloys,” with S.S.A. Razee, J.B. Staunton, B. Ginatempo, and E. Bruno, *Phys. Rev. B* **64**, 014411 (2001).

“The effects of magnetic annealing of transition metal alloys deduced from *ab initio* electronic structure calculations,” with S.S.A. Razee, J.B. Staunton, B. Ginatempo, and E. Bruno, *J. Phys: Condens. Matter* **13**, 8565-8572 (2001).

“ ω -phase Formation in NiAl and Ni₂Al Alloys,” with M. Sanati and R. Albers, *J. Phys: Condens. Matter*, **13**, 5387-5398 (2001).

“Classical density functional theory of freezing in simple fluids: Numerically induced false solutions,” M. Valera, F.J. Pinski, D.D. Johnson, *Phys. Rev. E* **64**, 062501 (2001).

“Reply to Comment on ‘Classical density functional theory of freezing in simple fluids: Numerically induced false solutions,’ ” M. Valera, F.J. Pinski, D.D. Johnson, *Phys. Rev. E* **67**, 063502 (2003).

“Transition paths in molecules at finite temperature,” F. J. Pinski and A. M. Stuart, *J. Chem. Phys.* **132**, 184104 (2010).

“Hybrid Monte Carlo on Path Spaces,” A. Beskos, F.J. Pinski, J.-M. Sanz-Serna and A.M. Stuart, Hybrid Monte-Carlo on Hilbert. Spaces, *Stoch. Proc. Applic.* **121**, 2201–2230 (2011).

“Gamma-Limit for Transitions Paths of Maximal Probability,” F.J. Pinski, F. Theil and A.M. Stuart, *J. Stat. Phys.* **146**, 955–974 (2012).

