List of Publications

Nagy Ágnes

Papers in International Journals

1. R. Gáspár–Á. Nagy: $X\alpha$ method with theoretically determined parameter α: calculation of shake–up and multielectron x–ray transition energies. J. Phys. B 19 (1986) 2793.

2. Á. Nagy: Analysis of the r–dependence of self–consistent exchange parameters α_i of different shells in neon, argon and krypton. Phys. Rev. B 34 (1986) 8903.

3. Á. Nagy: Ab initio exchange-correlation parameter in the $X\alpha$ method. Int. J. Quant. Chem. 31 (1987) 269.

4. R. Gáspár–Á. Nagy: Generalized Hellmann–Feynman theorem in the $X\alpha$ method. Int. J. Quant. Chem. 31 (1987) 639.

5. R. Gáspár–Á. Nagy: $X\alpha$ method with theoretically determined parameter α and ionization energies of multiply charged ions. J. Phys. B 20 (1987) 3631.

6. R. Gáspár–Á. Nagy: Local–density–functional approximation for exchange–correlation potential. Application of the self–consistent and statistical exchange–parameters to the calculation of the electron binding energies. Theor. Chim. Acta 72 (1987) 393.

7. Á. Nagy: Molecular $X\alpha$ calculation with theoretically determined statistical parameter α. $X\alpha$ calculation of ionization energies of CO and H_2CO and Auger transition energies of CO. Journal of Molecular Structure (THEOCHEM) 165 (1988) 205.

8. R. Gáspár–Á. Nagy: Electronegativity of several diatomic molecules calculated by the $X\alpha$ method with self–consistent parameter α using the principle of electronegativity equalization. Collection Czechoslovak Chem. Comm., 53 (1988) 2017.

9. Á. Nagy–N.H. March: One–body potential in terms of phase of wave functions for ground–state of the Be atom, Phys. Rev. A 39 (1989) 5512.

10. Á. Nagy: Analysis of the r–dependence of ab initio α_1 parameters of the $X\alpha$–method for different molecular orbitals in the molecule H_2O. Croatica Chemica Acta 62 (1990) 587.

11. Á. Nagy–N.H. March: Exact potential–phase relation for the ground state of the C atom. Phys. Rev. A 40 (1989) 554.

12. Á. Nagy–N.H. March: Asymptotic Behaviour of the Pauli potential for a perfectly screened charge embedded in an almost degenerate dense plasma. Phys. Chem. Liq. 22 (1990) 129.

13. Á. Nagy–N.H. March: Effective potentials for light atoms and ions at zero and finite temperatures. Phys. Lett. A 144 (1990) 241.

14. Á. Nagy–N.H. March: Ground–state energy and one–body virial in density functional theory of atomic ions. Chem. Phys. 140 (1990) 339.

15. Á. Nagy–R.G. Parr: The local virial theorem in density functional theory. Phys. Rev. A 42 (1990) 201.

16. Á. Nagy: Parameter–free exchange potential for excitation in the density functional theory: Application to excitation energies within the fractional–occupation approach. Phys. Rev., A 42 (1990) 4388.

17. Á. Nagy: On the interpretation of the exchange–correlation potential of the density functional theory. Phys. Rev. Lett., 65 (1990) 2608.

18. Á. Nagy–N.H. March: The exact form of the Pauli potential for the ground state of two– and three–level atoms and ions. Int. J. Quantum Chem. 39 (1991) 615.

19. Á. Nagy–N.H.March: Kinetic energy in terms of electron density for atomic s and p shells in a bare Coulumb filed. Chem. Phys. Lett. 181 (1991) 279.

20. Á. Nagy: Excitation energies calculated with parameter–free exchange potential in the density functional theory. J. Phys. B 24 (1991) 4691.

21. Á. Nagy–N.H. March: Relation between total energy and sum of orbital energies for neutral atoms. Chem. Phys., 153 (1991) 141.

22. N.H. March–Á. Nagy: Theory of Inhomogeneous Electron Liquid, Transcending Hartree–Fock. Phys. Chem. Liq. 24 (1992) 183.

23. Á. Nagy: Regional virial theorem in density functional theory. Phys. Rev. A 46 (1992) 5417.

24. Á. Nagy–N.H. March: Relation between the Pauli potential and the Pauli energy density. Phys. Chem. Liquids 25 (1992) 37.

25. Á. Nagy–N.H. March: One–sixth power law for molecular dissociation energies in terms of inhomogeneity kinetic energy. J. Mol. Struct. (Theochem) 277 (1992) 129.

26. Á. Nagy–N.H. March: Molecular dissociation energies characterized by number of electrons and equilibrium bond length. J. Mol. Struct. (Theochem) 281 (1992) 53.

27. Á. Nagy: Exchange energy in the exact exchange–only density functional theory. J. Phys. B 26 (1993) 43.

28. Á. Nagy: Hierarchy of equations for the energy functional in the density functional theory. Phys. Rev. A 47 (1993) 2715.

29. Á. Nagy: Exact and approximate exchange potentials in the density functional theory. Phil. Mag. 69, (1994) 779.

30. Á. Nagy: Spin virial theorem in the density functional theory. Int. J. Quantum Chem. 49 (1994) 353.

31. Á. Nagy–I. Andrejkovics: Excitation energies in the local density functional theory. J. Phys. B27 (1994) 233.

32. Á. Nagy: Integral and regional virial theorems in the density functional theory. Proceedings of Indian Academy of Sciences (Chemical Sci) 106 (1994) 251.

33. Á. Nagy–R.G. Parr: Density functional theory as thermodynamics. Proceedings of Indian Academy of Sciences (Chemical Sci) 106 (1994) 217.

34. G.J. Laming–Á. Nagy–N.C. Handy–N.H. March: Scaling properties of inhomogeneity kinetic energy in some diatomic molecules, in relation to dissociation energies. Molecular Physics 81 (1994) 1497.

35. Á. Nagy: Relativistic density functional theory for ensembles of excited states. Phys. Rev. A 49 (1994) 3074.

36. Á. Nagy: Coordinate scaling and adiabatic connection formula for ensembles of fractionally occupied excited states, Int. J. Quantum Chem. 56 (1995) 225.

37. R. G. Parr–S. Liu–A.A. Kugler–Á. Nagy: Some identities in density functional theory, Phys. Rev. A 52 (1995) 969.

38. Á. Nagy: Hierarchies of equation for the Legendre transforms of the energy functionals, Phys. Rev. A 52 (1995) 984.

39. P. Süle–O. V. Gritsenko–Á. Nagy–E. J. Baerends : Correlation energy density from ab initio first- and second-order density matrices: A benchmark for approximate functionals, J. Chem. Phys. 103 (1995) 10085.

40. S. Liu–R. G. Parr–Á. Nagy: Cusp relations for local strongly decaying properties in electronic systems, Phys. Rev. A 52 (1995) 2645.

41. Á. Nagy: Exact ensemble exchange potentials for multiplets, Int. J. Quantum Chem.S. 29 (1995) 297.

42. Á. Nagy: Local ensemble exchange potential, J. Phys. B29 (1996) 389.

43. Á. Nagy–R.G. Parr: Information entropy as a measure of the quality of an approximate electronic wave function, Int. J. Quantum Chem. 58 (1996) 323.

44. Á. Nagy–R.G. Parr–S. Liu: Local temperature in an electronic system, Phys. Rev. A 53 (1996) 3117.

45. Á. Nagy–I. Andrejkovics: Pseudopotentials from electron density, Phys. Rev. A 53 (1996) 3656.

46. Á. Nagy: Transition functional method in the density functional theory, Phys. Rev. A 53 (1996) 3660.

47. P. Süle–Á. Nagy: Density functional study of strong hydrogen-bonded systems, J. Chem. Phys. 104 (1996) 8524.

48. S. Liu–P. Süle–R. López-Boada–Á. Nagy: Applications to atoms, ions and molecules of the correlation energy density functional, Chem. Phys. Lett. A 257 (1996) 68.

49. Á. Nagy–N.H. March: Kinetic energy of inhomogeneous electron liquid: form for atom with one p plus s shells. Phys. Chem. Liq. 32 (1996) 319.

50. Á. Nagy–N.H. March: Ratio of density gradient to electron density as a local wavenumber to characterize the ground state of spherical atoms, Molecular Physics 90 (1997) 271.

51. Á. Nagy–N.H. March: Differentional and local virial theorem, Molecular Physics 91 (1997) 597.

52. Á. Nagy: An alternative derivation of the KLI approximation to the OPM potential, Phys. Rev. A 55 (1997) 3465.

53. Á. Nagy: Density functional theory for excited states. Adv. Quant. Chem. 29 (1997) 159.

54. T. Gál–Á. Nagy: Local temperature in molecules, Molecular Physics 91 (1997) 873.

55. Á. Nagy: Kohn-Sham equations for multiplets, Phys. Rev. A 57 (1998) 1672.

56. Á. Nagy: Density functional theory and applications, Physics Reports 298 (1998) 1.

57. Á. Nagy–E. Bene: Total electron density from s-electron density, Phys. Rev. A 57 (1998) 3458.

58. N.H. March–A. Holas–Á. Nagy: Self-Cosistent Thomas-Fermi-Dirac Theory, Extended by Gell-Mann and Brueckner Correlation, in Terms of Density n and Its Two Reduced Gradients $\nabla^2 n/n$ and $\nabla n/n$, Int. J. Quantum. Chem. 69 (1998) 145.

59. Á. Nagy: Optimized potential method for ensembles of excited states Int. J. Quantum Chem. 69 (1998) 247.

60. N.H. March–T. Gál–Á. Nagy: Differential Equation for Ground-State Electron Density in Hookean Atom with Two Electrons Repelling Coulombically, Chem. Phys. Lett. A 292 (1998) 384.

61. Á. Nagy - M. Levy: Test for new ionization formula in density functional theory, Chem. Phys. Lett. A 296 (1998) 313.

62. I. Andrejkovics–Á. Nagy: Excitation energies in density functional theory: comparison of several methods for the H_2O, N_2, CO and C_2H_4 molecules, Chem. Phys. Lett. A 296 (1998) 489.

63. Á. Nagy: Excited states in density functional theory, Int. J. Quantum Chem. 70 (1998) 681.

64. S. Liu - Á. Nagy–R. G. Parr: Expansion of the density functional energy components E_c and T_c in terms of moments of the electron density, Phys. Rev. A 59 (1999) 1131.

65. M. Levy - Á. Nagy: Excited state Koopmans theorem for ensembles Phys. Rev. A 59 (1999) 1687.

66. S. Liu - F. De Proft -Á. Nagy–R. G. Parr: Exchange energy of density functionals as linear combinations of homogeneous functionals of density Adv. Quant. Chem. 36 (1999) 77.

67. Á. Nagy–S. Liu –R. G. Parr: Density functional formulas for atomic electronic energy components in terms of moments of the electron density, Phys. Rev. A 59 (1999) 3349.

68. Á. Nagy: Kohn-Sham Potentials for Atomic Multiplets, J. Phys. B 32 (1999) 2841.

69. T. Gál - N. H. March - Á. Nagy: Differential equation for ground-state electron density of He-like ions for large atomic number, Chem. Phys. Lett. 305 (1999) 429.

70. T. Gál - N. H. March - Á. Nagy: Generalized local density approximation in an inhomogeneous electron liquid, Phys. Chem. Liq. 37 (1999) 641.

71. Á. Nagy - N. H. March: Exchange-only theory: Relation between exchange energy, its functional derivative and eigenvalue sums in an inhomogeneous electron liquid, Phys. Chem. Liq. 37 (1999) 671.

72. M. Levy - Á. Nagy: Variational density functional theory for an individual excited state, Phys. Rev. Lett. 83 (1999) 4361.

73. C. Amovilli - T. Gál - N. H. March - Á. Nagy: Force-balance and differential equation for the ground-state electron density in atoms and molecules, Int. J. Quantum Chem. 77 (1999) 716.

74. Á. Nagy - K. D. Sen: Higher-order cusp of the density in certain highly excited states of atoms and molecules, J. Phys. B 33 (2000) 1745.

75. E. Bene - Á. Nagy: The correlation energy in terms of density moments along the adiabatic connection in the density functional theory, Chem. Phys. Lett. 324 (2000) 475.

76. Á. Nagy - N. H. March: Homogeneity properties of kinetic energy in the density functional theory of an inhomogeneous electron liquid, Phys. Chem. Liq. 38 (2000) 345.

77. Á. Nagy - R. G. Parr: Remarks on density functional theory as thermodynamics, J. Mol. Struct. (Theochem) 501 (2000) 101.

78. E. Bene - Á. Nagy: Determination of the total electron density from its l-shell contribution, J. Mol. Struct. (Theochem) 501 (2000) 107.

79. T. Gál - Á. Nagy: A method to get analytical expression for the non-interacting kinetic energy density functional, J. Mol. Struct. (Theochem) 501 (2000) 167.

80. Á. Nagy -H. Adachi: Total energy versus one-electron energy differences in the excited-state density functional theory, J. Phys. B 33 (2000) L585.

81. Á. Nagy - N. H. March: Homogeneity properties of Pauli energy in the density functional theory of an electron liquid, Phys. Chem. Liq. 38 (2000) 759.

82. Á. Nagy - K. D. Sen: Exact results on the curvature of the electron density at the cusp in certain highly excited states of atoms Chem. Phys. Lett. 332 (2000) 154.

83. Á. Nagy - N. H. March: Legendre transform of the non-interacting kinetic energy: especially from March-Murray perturbation theory based on plane waves Int. J. Quantum Chem. 82 (2001) 138.

84. Á. Nagy- M. Levy: Variational density-functional theory for degenerate excited states, Phys. Rev. A 63 (2001) 052502.

85. Á. Nagy: An alternative optimized potential method for ensembles of excited states, J. Phys. B 34 (2001) 2363.

86. Á. Nagy: Effective potential of a single excited state along the adiabatic path, Adv. Quant. Chem. 39 (2001) 35.

87. Á. Nagy - K. D. Sen: Ground- and excited-state cusp conditions for the electron density, J. Chem. Phys. 115 (2001) 6300.

88. P. W. Ayers- R. G. Parr -Á. Nagy: Local kinetic energy and local temperature in the density functional theory of electronic structure, Int. J. Quantum Chem. 90 (2002) 309.

89. Á. Nagy: Density Matrix Functional Theory, Phys. Rev. A 66 (2002) 022505.

90. T. Gál- N.H. March - Á. Nagy: Differential equation for the determination of a first-degree homogeneous noninteracting kinetic-energy functional for two-level systems, Phys. Lett. A 302 (2002) 55.

91. F. Tasnádi - Á. Nagy: Local self-interaction-free approximate exchange-correlation potentials in the variational density functional theory for individual excited states, Chem. Phys. Lett. 366 (2002) 496.

92. I. A. Howard - N. H. March - Á. Nagy: Ten-electron central field problem: An inhomogeneous electron liquid, Phys. Chem. Liq. 20 (2002) 47.

93. Á. Nagy: Exact energy expressions for energy functional in the time-dependent density functional theory Int. J. Quantum Chem. 92 (2003) 229.

94. F. Tasnádi - Á. Nagy: Study of Subspace Density-Functional Theory. Application of LSDA to Excited States of Atoms Int. J. Quantum Chem. 92 (2003) 234.

95. Á. Nagy: Theories for excited states, Adv. Quant. Chem. 42 (2003) 363.

96. I. A. Howard - N. H. March - Á. Nagy: Local density of states $N(r, E)$ for central fields,with energy E in the continuum: especially the Coulomb potential, J. Phys. A 36 (2003) 6473.

97. C. Amovilli - Á. Nagy - N. H. March: Approximate ansatz for the expansion of the spherically averaged wave function in terms of interelectronic separation r_{12} for the Hookean atom, atomic ions and the H_2 molecule, Int. J. Quantum Chem. 95 (2003) 21.

98. F. Tasnádi - Á. Nagy: Ghost and self-interaction free ensemble calculations for atoms with local exchange-correlation potential, J. Phys. B 36 (2003) 4073.

99. F. Tasnádi - Á. Nagy: An approximation to the ensemble Kohn-Sham exchange potential for excited states of atoms, J. Chem. Phys. 119 (2003) 4141.

100. Á. Nagy: Spin virial theorem in the time-dependent density functional theory, Phys. Rev. A 68 (2003) 042503.

101. Á. Nagy: Fisher Information in Density Functional Theory J. Chem. Phys. 119 (2003) 9401.

102. Á. Nagy: Theories for individual excited states, Int. J. Quantum Chem. 99 (2004) 256.

103. Á. Nagy - C. Amovilli, Effective Potential in Density Matrix Functional Theory: J. Chem. Phys. 121 (2004) 6640.

104. I. A. Howard - D. J. Klein - N. H. March - C. Van Alsenoy - S. Suhai - Zs. Janosfalvi - Á. Nagy: Change in Electronic Structure of Polyenes Due to Interaction with Polyacenes and with Graphitic Strips, J. Phys. Chem. B108 (2004) 14870.

105. Á. Nagy - I. A. Howard - N. H. March - Zs. Jánosfalvi: Subspace density of the first excited state for two harmonically interacting electrons with isotropic harmonic confinement, Phys. Lett. A 335 (2005) 347.

106. Á. Nagy - S. Liu - L. Bartolotti: Generalized density functional theory for degenerate states. J. Chem. Phys. 122 (2005) 134107.

107. Á. Nagy: A generalized Kohn-Sham scheme, Chem. Phys. Lett. 411 (2005) 492.

108. Á. Nagy: Density Scaling and Exchange-Correlation Energy, J. Chem. Phys. 123 (2005) 044105.

109. Á. Nagy: Hardness and excitation energy, Journal of Chemical Sciences (formerly Proceedings of the Indian Academy of Sciences, Chemical Sciences) 117 (2005) 437.

110. Á. Nagy - Zs. Jánosfalvi: Exact Energy Expression in the Strong-Interaction Limit of the Density Functional Theory, Phil. Mag. A 86 (2006) 2101-2114.

111. Zs. Jánosfalvi - K. D. Sen - Á. Nagy: Cusp conditions for non-interacting kinetic energy density of the density functional theory, Phys. Lett. A 344 (2005) 1.

112. N. H. March - Á. Nagy: Formally exact integral equation theory of the exchange-only potential in density functional theory: refined closure approximation, Phys. Lett. A348 (2006) 374.

113. N. H. March - Á. Nagy: Non-relativistic binding energies of heavy neutral atoms: dependence of correlation energy on atomic number, Chem. Phys. Lett. 416 (2005) 104.

114. Á. Nagy:Hierarchy of Equations in the Generalized Density Functional Theory, Int. J. Quantum Chem. 106 (2006) 1043.

115. I.A. Howard - F. Bartha - N. H. March - Á. Nagy: Electron densities of the He-like sequence of atomic ions, and associated physical properties, Phys. Lett. A .350 (2006) 236.

116. N. H. March - Zs. Jánosfalvi - Á. Nagy - S. Suhai: Kinetic and exchange energy related non-locally in Hartree-Fock theory of an inhomogeneous electron liquid, Phys. Chem. Liq. 44 (2006) 493

117. Á. Nagy: Fisher Information in a Two-electron Entangled Artificial Atom, Chem. Phys. Lett. 425 (2006) 157.

118. Á. Nagy - K. D. Sen: Atomic Fisher information versus atomic number, Phys. Lett. A 360 (2006) 291.

119. Á. Nagy: Spherically and System-Averaged Pair Density Functional Theory J. Chem. Phys. 125 (2006) 184104.

120. I. Hornyák - Á. Nagy: Phase-space Fisher information Chem. Phys. Lett. 437 (2007) 132.

121. P. W. Ayers - Á. Nagy: Alternatives to electron density for describing Coulomb systems J. Chem. Phys. 126 (2007) 144108.

122. R. C. Morrison - P. W. Ayers - Á. Nagy: Density scaling and relaxation of the Pauli principle J. Chem. Phys. 126 (2007) 124111.

123. Á. Nagy: Fisher Information and Steric Effect Chem. Phys. Lett. 449 (2007) 212.

124. Á. Nagy - S. B. Liu: Local wave-vector, Shannon and Fisher Information Phys. Lett. A Phys. Lett. A 372 (2008) 1654.

125. I.A. Howard - N. H. March - Á. Nagy: Exact asymptotic solution of the Della Sala-Görling integral equation for the exchange-only potential for Be-like atomic ions at large Z, Phys. Lett. A .372 (2008) 3256.

126. Á. Nagy - C. Amovilli, Electron-electron Cusp Condition and Asymptotic Behaviour for the Pauli Potential in Pair Density Functional Theory: J. Chem. Phys. 128 (2008) 114115.

127. J. B. Szabó - K. D. Sen - Á. Nagy: The Fisher-Shannon information plane for atoms, Phys. Lett. A .372 (2008) 2428.

128. N. H. March - Á. Nagy - C. Amovilli: Asymptotic form at large r of a third-order linear homogeneous differential equation for the ground-state electron density of the He atom, Phys. Rev. A 77 (2008) 034501.

129. E. Romera - Á. Nagy: Rényi information of atoms Phys. Lett. A .372 (2008) 4918.

130. Á. Nagy: Alternative descriptors of Coulomb systems and their relationship to the kinetic energy Chem. Phys. Lett. 460 (2008) 343.

131. C. Amovilli - N. H. March - I.A. Howard - Á. Nagy: Exact Hamiltonian for an analytic correlated ground-state wave function for He-like ions, Phys. Lett.372 (2008) 4053.

132. E. Romera - Á. Nagy: Fisher-Rényi entropy product and information plane, Phys. Lett. A .372 (2008) 6823-6825.

133. N. H. March -Á. Nagy: Exact integral constraint requiring only the groun d-state electron density as input on the exchange-correlation force $-\partial V_{xc}(r)/\partial r$ for spherical atoms, J. Chem. Phys. 129 (2009) 194114.

134. C. Amovilli -Á. Nagy: Modelling the Pauli Potential in the Pair Density Functional Theory, J. Chem. Phys. 129 (2009) 204108.

135. N. H. March -Á. Nagy: Differential virial theorem in DFT in terms of the Pauli potential for spherically symmetric electron densities: illustrative exam ple for the family of Be-like atomic ions, Phys. Rev. A 78 (2009) 044501.

136. Á. Nagy - C. Amovilli: Exact differential and integral constraints for the Pauli potential in the pair density functional theory, Chem. Phys. Lett. 469 (2009) 353.

137. C. Amovilli - N. H. March -Á. Nagy: Exact integral relation between the triplet correlation function in the ground state of the completely polarized homogeneous electron fluid and the pair function: comparison with the classical liquid argon result, Phys. Chem. Liq. 47 (2009) 5.

138. Á. Nagy - E. Romera: Maximum Rényi entropy principle and the generalized Thomas-Fermi model Phys. Lett. A 373 (2009) 844-846.

139. Á. Nagy - M. Levy - P. W. Ayers: Time-independent theories for a single excited state, in *Theory of Chemical Reactivity* ed. by P. K. Chattaraj (Taylor and Francis, London, 2009)p. 121-136.

140. Á. Nagy - E. Romera: Relative Rényi entropy for atoms, Int. J. Quant. Chem. 109 (2009) 2490-2494.

141. V. G. Tsirelson - Á. Nagy: Binding entropy and its application to solids, J. Phys. Chem. A 113 (2009) 9022-9029.

142. Á. Nagy - K. D. Sen - H. E. Montgomery: LMC complexity for the ground states of different quantum systems, Phys. Lett. A .373 (2009) 2552-2555.

143. E. Romera, R. López-Ruiz -J. Sanudo and Á. Nagy: A generalized statistical complexity and Fisher-Rényi product in the H-atom, Int. Rev. Phys. 3 (2009) 207-211.

144. R. López-Ruiz- Á. Nagy- E. Romera and J. Sanudo: A generalized statistical complexity measure: Applications to quantum sysytems J. Math. Phys. 50 (2009) 123528 -10.

145. N. H. March -Á. Nagy: The Pauli potential in terms of kinetic energy density and electron density in t he leading Coulombic term of the non-relativistic $1/Z$ expansion of spherical a tomic ions Phys. Rev. A 81 (2010) 014502.

146. N. H. March -Á. Nagy: Proposed approximate relation in inhomogeneous ele ctron liquids between exchange-only potential and its Slater conterpart, Phys. Chem. Liq. 48 (2010) 648-651.

147. Á. Nagy: Time-dependent density functional theory as thermodynamics, J. Mol. Struct Theochem 943 (2010) 48-52.

148. Á. Nagy: The Pauli potential from the differential virial theorem, Int. J. Quant. Chem. 110 (2010) 2117-2120.

149. Á. Nagy and E. Romera: Relation between Fisher measures of information coming from pair distribution functions, Chem. Phys. Lett. 490 (2010) 242-244.

150. C. Amovilli -Á. Nagy: Erratum: "Modelling the Pauli Potential in the Pair Density Functional Theory" [J. Chem. Phys. 129 204108(2008)]. J. Chem. Phys. 132 (2010) 109902.

151. Á. Nagy - C. Amovilli: Ground- and excited-state cusp conditions for the pair density, Phys. Rev. A 82 (2010) 042510.

152. Á. Nagy: Density and pair-density scaling for deriving the Euler equation in density-func tional and pair-density-functional theory Phys. Rev. A 84 (2011) 032506.

153. E. Romera - K. Sen - Á. Nagy: A generalized relative complexity measure, J. Stat. Mech. P09016 doi:10.1088/1742-5468/2011/09/P09016

154. Á. Nagy: Functional derivative of the kinetic energy functional for spherically symmetric systems, J. Chem. Phys. 135 (2011)044106.

155. E. Romera - Á. Nagy: Rényi entropy and quantum phase transition in the Dicke model, Phys. Lett. A, 375 (2011) 3066-3069.

156. Á. Nagy: Density Scaling for Multiplets, J. Phys. B 44 (2011) 035001.

157. N. H. March - Á. Nagy: Scaling of some chemical properties of tetrahedral and octahedral molecules plus almost spherical C and B cages, J. Math. Chem. 49 (2011) 2268.

158. N. H. March - Á. Nagy: Some model inhomogeneous electron liquid in D dimens ions: relation between energy and chemical potential and a spatial generalizatio n of Kato's nuclear cusp theorem, Phys. Chem. Liq. 2011(2011) 1

159. Á. Nagy - E. Romera: Fisher entropy, Rényi entropy power and quantum phase transition in the Dicke model, Phys. A. doi: 10.1016/j.physa.2012.02.024

160. H. Iwasaki - J. Kawai - K. Yuge- Á. Nagy: Similarity between blackbody and sy nchrotron radiation analyzed by Tsallis entropy, X-Ray Spectrom. **41**, 125 (2012). doi: 10.1002/xrs.2362

161. E. Romera - M. Calixto - Á. Nagy: Entropic uncertainty and the quantum phase transition in the Dicke model, Europh ys. Lett. **97** (2012). doi:10.1209/0295-5075/97/2011.

162. I. Hornyák - Á. Nagy: Inequalities for Phase-Space Rényi entropies, Int. J. Quantum. Chem. 112 (2012) 1285.

Papers in journals published in Hungary

1. R. Gáspár–Á. Nagy: On the calculation of ionization energies of methane by universal potential. Acta Phys. et Chim. Debr., 21 (1978) 13.

2. R. Gáspár–Á. Nagy: A new valence exchange potential. Acta Phys. et Chim. Debr., 23 (1980) 89.

3. R. Gáspár–Á. Nagy: $X\alpha$ method of calculating the electronic structure of atoms, molecules and solids II. Acta Phys. et Chim. Debr., 23 (1980) 97.

4. R. Gáspár–Á. Nagy: Ionization energies of N_2, CO, CO_2, N_2O, C_2H_2 and SiH_4 molecules calculated by universal model potential. Acta Phys. Hung., 50 (1981) 359.

5. R. Gáspár–Á. Nagy: Statistical determination of exchange parameter α in the $X\alpha$ method. Acta Phys. et Chim. Debr. 24 (1982) 37.

6. R. Gáspár–Á. Nagy: Comparison of orbitals of neon, argon and krypton calculated by the Hartree–Fock and the $X\alpha$ methods with several values of α. Acta Phys. Hung. 53 (1982) 247.

7. R. Gáspár–Á. Nagy: Pseudopotential and valence exchange in the multiple scattering method. Acta Phys. Hung., 55 (1984) 45.

8. R. Gáspár–G. Erdős–Gyarmati–Á. Nagy: Ab initio relativistic $X\alpha$ calculations of the ionization energies of multiply charged ions. Acta Phys. et Chim. Debr., 25 (1984) 59.

9. R. Gáspár–Á. Nagy: Self–interaction and interelectronic exchange. An extension of the $X\alpha$ method. The F^- negative ion. Acta Phys. et Chim. Debr., 25 (1984) 39.

10. R. Gáspár–Á. Nagy: The $X\alpha$ method with ab initio exchange parameters. Diamagnetic susceptibility and nuclear magnetic shielding constants for several atoms. Acta Phys. Hung., 58 (1985) 107.

11. R. Gáspár–Á. Nagy: Spin orbitals and total energy calculated by the $X\alpha$ method including ab initio self consistent exchange parameters α. Acta Phys. Hung., 62 (1987) 131.

12. R. Gáspár–Á. Nagy: The first ionization energy, electron affinity and electronegativity calculated by the $X\alpha$ method with ab initio self–consistent exchange parameter Acta Phys. Hung., 64 (1988) 405.

13. Á. Nagy: The hyperfine interaction parameter $\rho(0)$ calculated by the $X\alpha$ method with ab initio self–consistent exchange parameter α. Acta Phys. Hung., 65 (1989) 55.

14. R. Gáspár–Á. Nagy: Self–interaction correction in the local density functional and the $X\alpha$ methods. Acta Phys. et Chim. Debr., 26 (1989) 7.

15. R. Gáspár–Á. Nagy: Electronegativities and hardnesses of several atoms and ions calculated with the $X\alpha$ method having self–consistent parameter α. Acta Phys. Hung., 65 (1989) 159.

16. Á. Nagy: An investigation on spin orbitals of several singly ionized positive ions by the $X\alpha_{SCF}$ method. Acta Phys. et Chim. Debr., 26 (1989) 33.

17. Á. Nagy: Ab initio exchange–correlation potentials in the local density approximation. The r–dependence of parameters α_1 for different shells in isoelectronic ions (N=18). Acta Phys. et Chim. Debr. 27 (1990) 31.

18. Á. Nagy: Analysis of the Pauli potential of atoms and ions. Acta Phys. Hung., 70 (1991) 33.

19. Á. Vibók–Á. Nagy: BSSE–free SCF method with local density functional correlation correction. Application to $(H_2)_2$ dimer, Acta Phys. Chim. Debr. 28, 7 (1993).

20. I. Andrejkovics–Á. Nagy: Excitation in the local spin density functional theory, Acta Phys. Chim. Debr., XXIX (1994) 7.

21. P. Süle–Á. Nagy: Comparative test of local and nonlocal Wigner-like correlation energy functionals, Acta Phys. Chim. Debr., XXIX (1994) 31.

22. Á. Nagy: Potentials from electron density, Acta Phys. et Chim. Debr. 30 (1995)47.

23. E. Bene - Á. Nagy: Generalized KLICS Calculations for Atomic Multiplets, Acta Phys. et Chim. Debr.

    33 (2000) 7.

24. Á. Nagy: Virial theorem in the density functional ensemble theory, Acta Phys. et Chim. Debr. 34-35 (2002) 99.

25. J. B. Szabó - Á. Nagy: Gáspár's universal potential as an external potential dependent function, Acta Phys. et Chim. Debr. 36 (2003) 45.

26. Á. Nagy - J. B. Szabó, A Simple Approximate Pauli Potential in Density Matrix Functional Theory, Acta Phys. et Chim. Debr. 37 (2004) 81.

27. Á. Nagy - J. B. Szabó: Universal Exchange Charge Density, Acta Phys. et Chim. Debr. 38-39 (2005) 269.

28. J. B. Szabó and Á. Nagy: Atomic Shannon information versus atomic number Acta Phys. et Chim. Debr. 40 (2006) 131.

29. Á. Nagy: Entropic uncertainty relations, Acta Physica Debrecina 43 (2009) 37-43

30. Á. Nagy - K. D. Sen: Fisher information from the pair density, Acta Physica Debrecina 45 (2011) 105.

Book chapters

1. R. Gáspár–Á. Nagy: The chemical bond and model exchange–corellation potentials. in Molecules in Physics, Chemistry and Biology, Vol. III. 93., ed. Jean Maruani (Kluver 1989).

2. Á. Nagy: Exact relations for the electron density and the energy functionals, in Recent Advances in Comp. Chemistry, Vol. 1. Recent advances in the density functional methods, ed. by D. P. Chong (World Scientific, 1996) Part I. p. 1

3. Á. Nagy: Density functional theory for a single excited state, in Electron Correlations and Materials Properties eds. A. Gonis, N. Kioussis and M. Ciftan (Kluwer, New York, 1999) p. 451.

4. Á. Nagy: Theory of exact exchange relations for a single excited state, in New Trends in Quantum Systems in Chemistry and Physics (Progress in Theoretical Chemistry and Physics Vol. 6), eds. J. Maruani, C. Minot, R. McWeeny Y. G. Smeyers and S. Wilson, (Kluwer, Dordrecht, 2001) Vol. 1, p. 13.

5. Á. Nagy: Theory for a single excited state. Differential virial theorem, in Recent Advances in Comp. Chemistry, Vol. 1; Recent advances in the density functional methods, ed. by V. Barone, A. Bencini and P. Fantucci (World Scientific, 2002) Part III. p. 247.

6. Á. Nagy: Density-Functional Theory as Thermodynamics, in Reviews of Modern Quantum Chemistry, ed. by K. D. Sen (World Scientific, 2002) Vol.I, p.413.

7. Á. Nagy: Pair Density Functional Theory, in The Fundamentals of Electron Density, Density Matrices and Density Functional Theory in Atoms, Molecules and Solid State, Eds. N. I. Gidopoulos and S. Wilson (Kluwer, 2003) p. 79.

8. Á. Nagy - M. Levy - P. W. Ayers: Time-independent theories for a single excited state, in *Chemical Reactivity Theory, A Density Functional View* ed. by P. K. Chattaraj (Taylor and Francis, London, 2009)p. 121-136.

9. Á. Nagy and E. Romera: Rényi entropy and complexity, in *Statistical Complexity* ed. K. D. Sen, (Springer, Berlin, 2011) pp 215.

10. Á. Nagy: Density Scaling for Excited States, in *Progress in Theoretical Chemistry and Physics* ed. P. Hoggan, (Springer, Berlin, 2011) p 185.