

Publications of Jiří Čížek

1. J. Koutecký and J. Čížek: Korrektur auf die spährische Diffusion bei polarographischen kinetischen Strömen. *Coll. Czech. Chem. Commun.* **21**, 836-843 (1956).
2. J. Koutecký and J. Čížek: Korrektur auf die spärische Diffusion bei katalytischen polarographischen Strömen. *Coll. Czech. Chem. Commun.* **21**, 1063-1066 (1956).
3. J. Koutecký and J. Čížek: Anwendung der Methode der dimensionslosen Parameter für die Lösung von Transportproblemen bei der Elektrolyse mit konstantem Strom an flacher und kugelförmiger Elektrode. *Coll. Czech. Chem. Commun.* **22**, 914-928 (1957).
4. J. Čížek, J. Koryta and J. Koutecký: Polarographische Ströme, die durch die Dissoziation einer elektroinaktiven Verbindung in einen elektroaktivten Stoff und in einen elektroinaktiven Stoff bedingt sind. *Coll. Czech. Chem. Commun.* **24**, 633-677 (1959).
5. J. Čížek, J. Koryta and J. Koutecký: Polarographische Ströme, die durch die Geschwindigkeit der Bildung eines elektroaktivten Stoffes aus zwei elektroinaktiven Stoffen, wovon keiner im Überschuss ist, bestimmt sind. *Coll. Czech. Chem. Commun.* **24**, 3844-3860 (1959).
6. J. Koutecký, R. Zahradník and J. Čížek: Relationship between Quantum-Chemical Indices of Reactivity of Polycyclic Alternant Hydrocarbons. *Trans. Faraday Soc.* **57**, 169-182 (1961).
7. A.V. Kiselev, J. Koutecký and J. Čížek: O prirode vzaimodejstvija molekuly benzola s gidroksilnoj gruppou. *Akad. Nauk. URSS* **137**, 638-641 (1961).
8. J. Koutecký and J. Čížek: Rascot energii vzaimodejstveja molekuly benzola s dipolem, metodom molekuljarnych orbit. *Zhur. Phys. Chem.* **36**, 1508-1518 (1962).
9. J. Koutecký and J. Čížek: A remark on the General Perturbation Theory. *Czech. J. Phys.* **B12**, 567-570 (1962).
10. J. Čížek: A New Method of Approximative Calculation of Polycentric Integrals Used in the Quantum Mechanical Study of Molecular Structure. *Molecular Physics* **6**, 19-31 (1963).
11. J. Čížek and J. Koutecký: Two Notes on the Theory of Kinetic and Catalytic Polarographic Currents. *Coll. Czech. Chem. Commun.* **28**, 2808-2810 (1963).
12. J. Koutecký, J. Čížek, J. Dubský and K. Hlavatý. The Effect of the Choice of Parameters on the Order of Energy Levels of Benzene Calculated in the π -Electron Approximation by the Configuration Interaction Method Including Double- and Triple-Excited Configurations. *Theoret. Chim. Acta (Berl.)* **2**, 462-467 (1964).
13. J. Čížek: Polycentric $2p\pi$ Repulsion Integrals for the Benzene Molecule, *Molecular Physics* **10**, 83-84 (1965).
000. J. Čížek, Příspěvek ke studiu korelačních efektů u atomů a molekul. Kandidátská disertační práce. Ústav fyzikální chemie ČSAV, 1965. PhD. dissertation written in Czech.

000. J. Čížek, Contribution au calcul de l'énergie de correlation dans les atomes et les molécules. Traduction de quelques chapitres de la thèse, CMOA, CNRS, Paris 1965.
14. J. Čížek and K. Holub: Beitrag zur Theorie der Folgereaktionen bei der Elektrolyse mit konstanter Stromdichte. *Coll. Czech. Commun.* **31**, 689-694 (1966).
15. I. Kössler and J. Čížek: Mischungen als Standards für die Infrarot-Spektroskopie. *Zeitschrift für analytische Chemie* **4**, 272-279 (1966).
16. J. Čížek: Eléments matriciels de l'hamiltonien entre les états monoexcités et biexcités singulets. *Theoret. chim. Acta (Berlin)* **6**, 292-298 (1966).
17. J. Čížek: On the Correlation Problem in Atomic and Molecular Systems. Calculation of Wavefunction Components in Ursell-Type Expansions Using Quantum-Field Theoretical Methods. *J. Chem. Phys.* **45**, (11), 4256-4266 (1966).

Reprinted in Three Approaches to Electron Correlation in Atoms, O. Sinanoglu and K.A. Brueckner, Eds. (Yale University Press, New Haven and London 1970), pp. 350-360.

This paper was discussed in the collection "A new century of theoretical chemistry" which was published in Theoretical Chemistry Accounts **103**, issue 3-4 (2000). In this collection 66 of the most influential papers in quantum chemistry of 20-th century were evaluated. See R. J. Bartlett "Perspective on 'On the correlation problem...'", *Theor. Chem. Acc.* **103**, 273-275 (2000).

18. J. Čížek, G. Biczo and J. Ladik: Some Comments on the Band Structure Calculations of Linear Chains in the semiempirical SCF LCAO Crystal Orbital Approximation. *Theoret. chim. Acta (Berl.)* **8**, 175-177 (1967).
19. O. Sinanoglu and J. Čížek: Reducible and Irreducible Pair Correlations in Benzene. *Chem. Phys. Letters* **1**, 337-339 (1967).
Reprinted in Sigma Molecular Orbital Theory, O. Sinanoglu and K.B. Wiberg, Eds. (Yale University Press, New Haven and London 1970), pp. 378-380.
20. J. Čížek and A. Pellegatti: Calcul de l'Énergie de Corrélation pour l'État Fondamental de la Molécule d'Acétylene. *Intern. J. Quantum Chem.* **1**, 653-655 (1967).
21. J. Čížek and J. Paldus: Stability Conditions for the Solution of the Hartree-Fock Equations for Atomic and Molecular Systems. Application to the Pi-Electron Model of Cyclic Polyenes. *J. Chem. Phys.* **47** (10), 3976-3985 (1967).
22. J. Koutecký, P. Hochmann, J. Paldus, R. Polák and J. Čížek: Quantum Chemical Treatment of Both Weak and Strong Intermolecular Interactions. (First conference on the theoretical problems of the adsorption, USSR Academy of Sciences, Moskva, 1968 - Nauka, Moskva 1968 p. 1-32).
23. J. Čížek: On the Use of the Cluster Expansion and the Technique of Diagrams in Calculations of Correlation Effects in Atoms and Molecules. *Adv. Chem. Phys.* **14**, 35-89 (1968).

24. M. Benard, J. Čížek, A. Pellegati and R. Polák: Structure Électronique du Styrolène et du Phénylacétylène. Méthode L.C.A.O. amelioree. *Annales de la Faculté des Sciences de Marseille* **41**, 51-58 (1968).
25. J. Čížek, J. Paldus and L. Šroubková: Cluster Expansion Analysis for Delocalized Systems. *Intern. J. Quantum Chemistry* **3**, 149-167 (1969).
26. J. Paldus and J. Čížek: Stability Conditions for the Solutions of the Hartree-Fock Equations for the Simple Open-Shell Case. *Chem. Phys. Letters* **3** (1), 1-3 (1969).
27. J. Paldus and J. Čížek: A Comment on the Paper by Hidio Fukatome: Spin Density Wave and Charge Transfer Wave in Long Conjugated Molecules. *Progress Theoretical Physics (Kyoto)* **42** (4), 769-774 (1969).
28. J. Paldus and J. Čížek: Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems II. Simple Open-Shell Case. *J. Chem. Phys.* **52**, 2919-2936 (1970).
29. J. Paldus and J. Čížek: The Instabilities of the Hartree-Fock Solutions for Cyclic Polyenes with Respect to the Spin and Charge Density Fluctuations. (Proceedings of the International Symposium on Organic Superconductors, Honolulu 1969). *J. Polymer Sci. Part C, No. 29*, 199-210 (1970).
30. J. Čížek and J. Paldus: Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems. III. Rules for the Singlet Stability of Hartree-Fock Solutions of π -Electronic Systems. *J. Chem. Phys.* **53** (2), 821-829 (1970).
31. J. Paldus and J. Čížek: Comment on the paper by Harris and Falicov: Self-Consistent Theory of Bond Alternation in Polyenes: Normal States, Charge-Density Waves, and Spin-Density Waves. *J. Chem. Phys.* **53** (4), 1619-1620 (1970).
32. J. Paldus and J. Čížek: Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems IV. A Study of Doublet Stability for Odd Linear Polyenic Radicals. *J. Chem. Phys.* **54** (6), 2293-2303 (1971).
33. J. Čížek and J. Paldus: Correlation Problems in Atomic and Molecular Systems III. Rederivation of the Coupled-Pair Many-Electron Theory Using the Traditional Quantum Chemical Methods. *Intern. J. Quantum Chemistry* **5**, 359-379 (1971).
34. J. Čížek and J. Paldus: Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems V. The Non-Analytic Behavior of the Broken-Symmetry Solutions at the Branching Point. *Phys. Rev. A* **3** (2), 525-527 (1971).
35. J. Paldus and J. Čížek: Stability Conditions for the Solutions of the Hartree-Fock Equations for Atomic and Molecular Systems VI. Singlet-Type Instabilities and Charge-Density-Wave Hartree-Fock Solutions for Cyclic Polyenes. *Phys. Rev. A* **2** (6), 2268-2283 (1970).

36. J. Čížek, J. Paldus, L. Šroubková and J. Vojtík: Full Configuration Interaction for the π -Electron Model of Benzene. I. General Expressions for Singlets. *Coll. Czech. Chem. Commun.* **36**, 599-617 (1971).
37. J. Paldus, J. Čížek and L. Šroubková: Full Configuration Interaction for the π -Electronic Model of Benzene II. Correlation Energy and Low Lying Singlet Excitation Energies. *Coll. Czech. Chem. Commun.* **36**, 618-624 (1971).
38. J. Paldus, J. Čížek and S. Sengupta: Geminal Localization in the Separated Pair π -Electronic Model of Benzene. *J. Chem. Phys.* **55** (5), 2452-2462 (1971).
39. J. Paldus, J. Čížek and I. Shavitt: Correlation Problem in Atomic and Molecular Systems IV. Extended Coupled-Pair Many-Electron Theory and its Application to the BH_3 Molecule. *Phys. Rev. A5* (1), 50-67 (1972).
40. S. Sengupta, J. Paldus and J. Čížek: Geminal Localization in the Separated-Pair Model. II. Excited States of π -Electronic Model of Benzene. *Intern. J. Quantum Chem.* **6**, 153-169 (1972).
41. J. Paldus, S. Sengupta and J. Čížek: Diagrammatical Method for Geminals II. Applications. *J. Chem. Phys.* **57** (2), 652-666 (1972).
42. J. Čížek and J. Paldus: A Direct Calculation of the Excitation Energies of Closed-Shell Systems Using the Green Function Technique. *Intern. J. Quantum Chem.* **6**, 435-438 (1972).
43. J. Čížek and J. Paldus: A Novel Approach to a Diagonalization of the PPP Hamiltonian, Proceedings of the Summer Conference in Theoretical Chemistry, University of Colorado, (J. Wiley & Sons), 389-390 (1973).
44. J. Paldus and J. Čížek: Relation of the Coupled-Pair Theory, CI and Some Other Many-Body Approaches. Proceedings of the Summer Research Conference in Theoretical Chemistry, University of Colorado, (J. Wiley & Sons), 198-209 (1973).
45. J. Paldus, J. Čížek and B.A. Keating: Stability Conditions for Maximum-Overlap (Brueckner) Independent Particle Wave Functions. *Phys. Rev. A8* (2), 640-649 (1973).
46. A. Laforgue, J. Čížek and J. Paldus: Study of the Correlation Effects in a Three-Electron Model System Using the Projected Hartree-Fock Method and the Natural Spinorbital Formalism. *J. Chem. Phys.* **59** (5), 2560-2571 (1973).
47. J. Paldus and J. Čížek: Green's Function Approach to the Direct Perturbation Calculation of the Excitation Energies of Closed Shell Fermion Systems. *J. Chem. Phys.* **60**, 149-163 (1974).
48. A. Pellegatti, J. Čížek and J. Paldus: Convergence of the Rayleigh-Schrödinger Perturbation Expansions for the Energy Levels of the Pariser-Parr-Pople Model of the Benzene Molecule. *J. Chem. Phys.* **60** (12), 4825-4829 (1974).

49. J. Čížek, J. Paldus and I. Hubač: Correlation Effects in the Low Lying Excited States of the PPP Models of Alternant Hydrocarbons. I. Qualitative Rules for the Effect of Limited Configuration Interaction. *Intern. J. Quantum Chem.* **8**, 951-970 (1974).
50. J. Paldus, J. Čížek and I. Hubač: Correlation Effects in the Low Lying Excited States of the PPP Models of Alternant Hydrocarbons II. State Correlation Diagrams. *Intern. J. Quantum Chem.* **S8**, 293-303 (1974).
51. J. Paldus and J. Čížek: Time-independent Diagrammatic Approach to Perturbation Theory of Fermion Systems. *Advances in Quantum Chemistry* **9**, 105-197 (1975).
52. J. Čížek, A. Pellegatti and J. Paldus: Correlation Effects in the PPP Model of Alternant π -Electronic Systems: Two-Point Padé Approximant Approach. *Intern. J. Quantum Chem.* **9**, 987-1007 (1975).
53. J. Paldus, B.G. Adams and J. Čížek: Applications of Graphical Methods of Spin Algebras to Limited CI Approaches. I. Closed Shell Case. *Intern. J. Quantum Chem.* **11**, 813-848 (1977).
54. B.G. Adams, J. Paldus and J. Čížek: Application of Graphical Methods of Spin Algebras to Limited CI Approaches. II. A Simple Open Shell Case. *Intern. J. Quantum Chem.* **11**, 849-867 (1977).
55. J. Čížek and E.R. Vrscay: On the Use of SO(4,2) Dynamical Group for the Study of the Ground State of a Hydrogen Atom in a Homogeneous Magnetic Field: Proceedings of the NATO Symposium. “Group Theoretical Methods in Theoretical Physics”, Montreal, (Academic Press, New York), 155-160 (July 1976).
56. J. Paldus, J. Čížek and A. Laforgue: The Relationship Between the Unrestricted and Projected Hartree-Fock Methods in a Simple Three-Electron Model System. *Intern. J. Quantum Chem.* **13**, 41-65 (1978).
57. J. Čížek and J. Paldus: An Algebraic Approach to Bound States of Simple One-Electron Systems. *Intern. J. Quantum Chem.* **12**, 875-896 (1977).
58. J. Paldus, J. Čížek, M. Saute and A. Laforgue: Correlation Problems in Atomic and Molecular Systems - VI. Coupled Cluster Approach to Open Shell Systems. *Phys. Rev.* **A17** (3), 805-815 (1978).
59. M. Saute, J. Paldus and J. Čížek: Correlation Problems in Atomic and Molecular Systems. VII. Application of the Open-Shell Coupled-Cluster Approach to Simple π -Electronic Model Systems. *Intern. J. Quantum Chem.* **15**, 463-479 (1979).
60. J. Čížek: Coupled Cluster Many-Electron Theory and the Cohesive Energy of Large Systems Consisting of Weakly Interacting Subsystems. *Quantum Theory of Polymers*, (Reidel, Dordrecht), 103-116 (1978).

61. V. Bonacic-Koutecký, J. Čížek, D. Döhnert and J. Koutecký: On the Nature of the “Sudden Polarization” Effect in Low Lying Singlet Excited States. *J. Chem. Phys.* **69** (3), 1168-1176 (1978).
62. J. Koutecký, V. Bonacic-Koutecký, J. Čížek and D. Döhnert: Nature of the “Sudden Polarization” Effect and its Role in Photochemistry. *Intern. J. Quantum Chem.* **S12**, 357-369 (1978).
63. J. Čížek and J. Paldus: Coupled Cluster Approach. *Physica Scripta* **21**, 251-254 (1980).
64. J. Čížek, B.G. Adams and J. Paldus: The Use of Algebraic Methods in Perturbation Theory. *Physica Scripta* **21**, 364-365 (1980).
65. H.J. Silverstone, B.G. Adams, J. Čížek and P. Otto: Stark Effect in Hydrogen: Dispersion Relation, Asymptotic Formulas, and Calculation of the Ionization Rate via High-Order Perturbation Theory. *Phys. Rev. Letters* **43** (20), 1498-1502 (1979).
66. J.E. Avron, B.G. Adams, J. Čížek, M. Clay, M.L. Glasser, P. Otto, J. Paldus and E.R. Vrscay: The Bender Wu Formula, SO(4,2) Dynamical Group and the Zeeman Effect in Hydrogen. *Phys. Rev. Letters* **43**, 691-693 (1979). **Reprinted** in Large-Order Behaviour of Perturbation Theory, edited by J.C. Le Guilon and J. Zinn-Justin, North Holland, p. 247-249.
67. J. Ladik and J. Čížek: A Proposal for the Calculation of the Correlation Energy Using a One Centre Expansion in Larger Molecules. *J. Chem. Phys.* **73** (5), 2357-2359 (1980).
68. J.W. Downing, J. Michl, J. Čížek and J. Paldus: Multidimensional Interpolation by Polynomial Roots. *Chem. Phys. Letters* **67** (2,3), 377-379 (1979).
69. B.G. Adams, J.E. Avron, J. Čížek, P. Otto and J. Paldus: Bender Wu Formulas for Degenerate Eigenvalues. *Phys. Rev.* **A21** (6), 1914-1916 (1980). **Reprinted** in Large-Order Behaviour of Perturbation Theory, edited by J.C. Le Guilon and J. Zinn-Justin, North Holland, p. 256-258.
70. J. Paldus, K. Jankowski, B.G. Adams and J. Čížek: Quasi-Degeneracy Effects in Coupled-Pair Theories, Proceedings of Conference in Daresbury, England (1979).
71. J. Čížek, M.R. Clay and J. Paldus: Asymptotic Behavior of the Ground-State Energy Expansion for H_2^+ in Terms of Internuclear Separation. *Phys. Rev.* **A22** (3), 793-796 (1980).
72. J. Čížek and E.R. Vrscay: Large Order Perturbation Theory in the Contact of Atomic and Molecular Physics - Interdisciplinary Aspects. *Intern. J. Quantum Chem.* **21**, 27-68 (1982).
73. B.G. Adams, J. Čížek and J. Paldus: Representation of SO(4,2) for the Perturbation Treatment of Hydrogenic type Hamiltonians by Algebraic Methods. *Intern. J. Quantum Chem.* **21**, 153-171 (1982).
74. A. Pellegatti, J. Čížek and J. Paldus: Numerical Estimates of the Rayleigh-Schrödinger Perturbation Expansions for the Energy Levels of Various Models of the Benzene Molecule. *Intern. J. Quantum Chem.* **21**, 147-151 (1982).

75. J. Ladik, J. Čížek and P.K. Mukherjee: Relativistic HF Theories for Molecules and Crystals in LCOA Form. (NATO Advanced Study Institute “Relativistic Effects in Atoms, Molecules and Solids”), ed. G. Malli, Plenum Press, p. 305 (1983).
76. J. Čížek and E.R. Vrscay: Asymptotic Estimation of the Coefficients of the Continued Fraction Representing the Binet Function. *C.R. Math. Rep. Acad. Sci. Canada* **4**, 201-206 (1982).
In this paper a conjecture about asymptotic behavior of the coefficients of continued fractions representing the Binet function. The Binet function is very important for the asymptotic expansion of Gamma function. this conjecture was finally proved in W. B. Jones and W. van Asschler, pp. 257-274, Orthogonal Functions, Moment Theory and Continuous Fractions, ed. by W. B. Jones and A. Sri Ranga, Publisher M. Dekker, New York, 1998.
77. J. Čížek, R. Pauncz and E.R. Vrscay: The Concept of Quasispin and its Use for the Study of Physical and Chemical Properties of Alternant Conjugated Hydrocarbons. *J. Chem. Phys.* **78** (5), 2468-2475 (1983).
78. J. Čížek, W. Forner and J. Ladik: Localization of the Filled and Virtual Orbitals in the Nucleotide Bases. *Theoret. Chimica Acta* **64**, 107-116 (1983).
79. A. Laforgue, J. Čížek, J. Paldus and A. Pelléatti: Trigonometric Polynomial Interpolation of Quantum Mechanical Properties by Mutual Perturbation Approach. *J. Chem. Phys.* **80** (1), 372-379 (1984).
80. M. Takahashi, J. Paldus and J. Čížek: Perturbation Theory and Electron Correlation in Extended Systems: Cyclic Polyene Model. *Intern. J. Quantum Chem.* **24**, 707-727 (1983).
81. J. Ladik and J. Čížek: Probable Physical Mechanisms of the Activation of Oncogenes through Carcinogens. *Intern. J. Quantum Chem.* **26**, 955-964 (1984).
82. J. Čížek and E.R. Vrscay: Continued Fractions for the Stirling Expansion Revisited. *Intern. J. Quantum Chem.* **24**, 521-522 (1983).
83. J. Koutecký, D. Döhnert, P.E.S. Wormer, J. Paldus and J. Čížek: Spin Properties of Radicaloid Alternant Hydrocarbons. Exact Solutions for Representative Pariser-Parr-Pople Model Systems. *J. Chem. Phys.* **80** (5), 2244-2246 (1984).
84. R.J. Damburg, R.Kh. Propin, S. Graffi, V. Grecchi, E.M. Harrell II, J. Čížek, J. Paldus and H.J. Silverstone: 1/R Expansion for H_2^+ : Analyticity, Summability, Asymptotics, and Calculation of Exponentially Small Terms. *Phys. Rev. Lett.* **52** (10), 1112-1115 (1984). **Reprinted** in Large-Order Behaviour of Perturbation Theory, edited by J.C. Le Guilon and J. Zinn-Justin, North Holland, p. 297-300.
85. J. Paldus, J. Čížek and M. Takahashi: Approximate Account of the Connected Quadruply Excited Clusters in the Coupled-Pair Many-Electron Theory. *Physical Review A* **30**, 2193-2209 (1984).
86. J. Koutecký, J. Paldus and J. Čížek: Alternancy Symmetry: A Unified Viewpoint. *J. Chem. Phys.* **83** (4), 1722-1735 (1985).

87. J. Paldus and J. Čížek: Hartree-Fock Stability and Symmetry Breaking: Oxygen Doubly Negative Ion. *Can. J. Chem.* **63** (7), 1803-1811 (1985).
88. J. Paldus and J. Čížek: Comment on the Derivation of Coupled Cluster Equations. *Can. J. Phys.* **63**, 151-153 (1985).
90. J. Čížek and F. Vinette: Prolegomena to the study of divergent Series, Lecture Notes, University of Waterloo, 1985
89. J. Čížek, R.J. Damburg, S. Graffi, V. Grecchi, E.M. Harrell II, J.G. Harris, S. Nakai, J. Paldus, R. Kh. Propin and H.J. Silverstone: I/R Expansion of H_2^+ : Calculation of Exponentially Small Terms and Asymptotics. *Phys. Rev. A* **33**, 12-33 (1986).
90. H.J. Silverstone, J.G. Harris, J. Čížek and J. Paldus: Asymptotics of High-Order Perturbation Theory for the One-Dimensional Anharmonic Oscillator by Quasi-Semiclassical Methods. *Phys. Rev. A* **32** (14), 1965-1980 (1985).
91. J. Čížek and E.R. Vrscay: Continued Fractions and Quantum-Mechanical Large-Order Perturbation Theory: The Anharmonic Oscillator Revisited. *Phys. Rev. A* **30** (3), 1550-1553 (1984).
92. W. Förner, J. Čížek, P. Otto and J. Ladik. Coupled-Cluster Studies I. Application to Small Molecules, Basis Set Dependences. *Chem. Phys.* **97**, 235-249 (1985).
93. W. Förner, J. Ladik, P. Otto and J. Čížek: Coupled-Cluster Studies II. The Role of Localization in Correlation Calculations on Extended Systems. *Chem. Phys.* **97**, 251-262 (1985).
94. B.G. Adams, J. Čížek and J. Paldus: Lie Algebraic Methods and Their Applications to Simple Quantum Systems. *Adv. Quantum Chem.* **19**, 1-85 (1988). **Reprinted** in Dynamical Groups and Spectrum Generating Algebras, A.O. Barut, A. Böhm and Y. Neeman, Eds. (World Scientific, Singapore 1988) pp. 1-85.
95. E.R. Vrscay and J. Čížek: Continued Fractions and Rayleigh-Schrödinger Perturbation Theory at Large Order. *J. Math. Phys.* **27** (1), 185-201 (1986).
96. J. Čížek and E.R. Vrscay. Inner Projection With and Without Perturbation Theory: The Anharmonic Oscillator Revisited and the Quadratic Zeeman Effect in Ground-State Hydrogen. *Intern. J. Quantum Chem.* **28**, 665-686 (1985).
97. M. Takahashi, J. Čížek and J. Paldus: Determination of the Radius of Convergence of the Perturbation Expansion Using Padé Approximants: Application to the Hückel limit of the Hubbard Model for Finite Cyclic Polyenes. *Phys. Rev. B* **33** (2), 1203-1205 (1986).
98. Y. Smeyers, P. Otto, J. Ladik, J. Čížek and E.O. Steinborn: Valence-Shell Correlation Calculation of the CO Molecule in One-Center Expansion. *Chem. Phys. Letters* **126**, 314-318 (1986).
99. J. Čížek and Giuseppe Del Re: C.A. Coulson and the Surface Energy of Metals: the Distribution of Eigenvalues as a Difficult Problem in Number Theory. *Intern. J. Quantum Chem.* **31**, 287-293 (1987).

100. W. Förner, L. Pylypow and J. Čížek: Coupled Cluster Studies. III. Comparison of the Numerical Behaviour of Coupled Cluster Doubles with Configuration Interaction and Perturbation Theory, Basis Set and Geometry Optimizations. *J. Chem. Phys.* **110**, 355 (1986).
101. M. Jeziorska, B. Jeziorski and J. Čížek: Direct Calculation of the Hartree-Fock Interaction Energy via Exchange-Perturbation Expansion. The He-He Interaction. *Intern. J. Quantum Chem.* **32**, 149-164 (1987).
102. J. Čížek and E.R. Vrscay: Lower Bounds to Ground State Eigenvalues of the Schrödinger Equation via Optimized Inner Projection: Application to Quartic and Sextic Anharmonic Oscillators. *Intern. J. Quantum Chem., Quantum Chem. Symposium* **20**, 65-72 (1986).
103. F. Vinette, J. Čížek and E.R. Vrscay: Renormalized Inner Projection. A Case Study: The Octic Oscillator. *I.J.Q.C.* **32**, 663-667 (1987); French version in *Comptes rendus de l'Académie des Sciences*, **306**, 21-25 (1988).
104. J. Čížek, F. Vinette and E.R. Vrscay: Renormalized Inner Projection, Symbolic Computation and Löwdin Rational Approximants in Explicit Form. *Intern. J. Quantum Chem., Quantum Chem. Symposium* **21**, 757-758 (1987).
000. J. Čížek, J. Paldus and S.G. Davison: A Tribute to Professor Jaroslav Koutecký. *Prog. Sur. Sciences* **25**, 1-15 (1987).
000. J. Čížek and J. Paldus. J. Koutecký. *T.C.A.* **72**, 335-336 (1987).
105. J. Čížek and F. Vinette: *N*-Dimensional Hydrogen Atom in an External Spherically Symmetric Field. Symbolic Computation and Explicit Expressions Derived from Rayleigh-Schrödinger-Type Perturbation Theory. *T.C.A.* **72**, 497-506 (1987).
106. N. March and J. Čížek: Dimensionality Dependence of Total Energy of Closed Shells in a Bare Coulomb Field for Large Atomic Number. *Intern. J. Quantum Chem.* **33**, 301-304 (1988).
107. J. Čížek and F. Vinette: The Application of Inner Projection Technique to Many Electron Systems as Compared with the Coupled Cluster Expansion. A Study of the Pariser-Parr-Pople Model of the Benzene Molecule”, *Collection of Czechoslovak Chemical Communications* **53**, 1910-1918 (1988).
108. J. Čížek, J. Paldus, U.W. Ramgulam and F. Vinette: Two-Point Padé Approximants in Electrochemical Kinetic Currents. *Progress in Surface Science* **25**, 17-39 (1988).
109. J. Čížek and F. Vinette: Symbolic Computation in Quantum Mechanics; Several Simple Examples. *Intern. J. Quantum Chem., Quantum Chem. Symposium* **S22**, 537-548 (1988).
110. K. Hashimoto, J. Čížek and J. Paldus: Convergence Radii of the Perturbation Expansions for the Ground-State Energies of Finite Hubbard Models. *Intern. J. Quantum Chem.* **34**, 407-415 (1988).
111. J. Čížek and F. Vinette: Lower Bounds for the Ground State Energy for the PPP and Hubbard Models of the Benzene Molecule. *Chemical Physics Letters* **149**, 516-520 (1988).

112. F. Vinette and J. Čížek: Perturbation Energy Expansion using Hypervirial Theorem and Symbolic Computation for the N-Dimensional Hydrogen Atom in an External Spherically Symmetric Field. *Computer Physics Communications* **52**, 35-41 (1988).
113. F. Vinette and J. Čížek. The Use of Symbolic Computation in Solving Some Non-Relativistic Quantum Mechanical Problems. Proceedings of The 1988 International Symposium on Symbolic and Algebraic Computation. *Lecture Notes in Computer Science* **385**, Springer Verlag, 85-95.
114. J. Čížek, F. Vinette and J. Paldus. “Diagrammatic Approach to the Calculation of the Lower Bounds using Optimized Inner Projection Technique. Application to the Cyclic Polyene Model”, Proceedings of the Symposium on Many-Body Methods in Quantum Chemistry, held in Tel Aviv-Israel, August 1988, Springer-Verlag, ed. U. Kaldor, p. 23-42.
115. J. Paldus, J. Čížek and B. Jeziorski: Coupled Cluster Approach or Quadratic Interaction? *J. Chem. Phys.* **90**, 4356-4562 (1989).
116. R. Pauncz and J. Čížek: Comparison of GVB and AMO Approaches to the Study of the PPP Model of Butadiene. *Intern. J. Quantum Chem.* **37**, 509-516 (1990).
117. J. Paldus, J. Čížek and B. Jeziorski: Coupled Cluster Approach or Quadratic Configuration Interaction?: Reply to Comment by Pople, Head-Gordon and Raghavachari. *J. Chem. Phys.* **90**, 4356-4362 (1989).
118. E.J. Weniger and J. Čížek: Rational Approximations for the Modified Bessel Function of the Second Kind. *Computer Physics Communications* **59**, 471-493 (1990).
119. J. Čížek, F. Vinette and J. Paldus: Explicit Algebra Form of Coupled Cluster Equations for the PPP Model of Benzene with an Approximate Inclusion of Triexcited Clusters. *Intern. J. Quantum Chem.* **38**, 831-851 (1990).
120. P. Piecuch, S. Zarrabian, J. Paldus and J. Čížek: Coupled-cluster Approaches with an Approximate Account of Triexcitations and the Optimized-Inner-Projection Technique. II. Coupled-cluster Results for Cyclic-polyene Model Systems. *Phys. Rev. B* **42**, 3351-3379 (1990).
121. P. Piecuch, S. Zarrabian, J. Paldus and J. Čížek: Coupled-cluster Approaches with an Approximate Account of Triexcitations and the Optimized Inner Projection Technique. III. Lower Bounds to the Ground State Correlation Energy of Cyclic Polyene Model Systems. *Phys. Rev. A* **42**, 5155-5167 (1990).
122. E.J. Weniger, J. Čížek and F. Vinette: Very Accurate Summation for the Infinite Coupling Limit of the Perturbation Series Expansions of Anharmonic Oscillators. *Phys. Letters A* **156**, 169-174 (1991).
123. E.J. Weniger, J. Čížek and F. Vinette: The Summation of the Ordinary and Renormalized Perturbation Series for the Ground State Energy of the Quartic, Sextic, and Octic Anharmonic Oscillators Using Nonlinear Sequence Transformations. *J. Math. Phys.* **34**, 571-609 (1993).

124. F. Vinette and J. Čížek: Renormalized Inner Projection Applied to the Quartic, Sextic and Octic Anharmonic Oscillators. *J. Math. Phys.* **32**, 3392-3404 (1991).
125. P. Piecuch, J. Čížek and J. Paldus: Behavior of the Coupled Cluster Energy in the Strongly Correlated Limit of the Cyclic Polyene Model. Comparison with the Exact Results. *Intern. J. Quantum Chem.* **42**, 165-191 (1992).
126. J. Čížek: Origins of Coupled Cluster Technique for Atoms and Molecules. *Theoretica Chimica Acta* **80**, 91-94 (1991).
127. J. Čížek, K. Hashimoto, J. Paldus and M. Takahashi: Relationship between Lieb and Wu Approach and Standard Configuration Interaction Method for the B_{2u}^- State of the Hubbard Model of Benzene. *Israel Journal of Chemistry* **31**, 423-426 (1991).
128. J. Čížek, F. Vinette and E.J. Weniger: Symbolic Computation in Physics and Chemistry: Applications of the Inner Projection Technique and of a New Summation Method for Divergent Series. *Intern. J. Quantum Chem.* **S25**, 209-223 (1991).
129. J. Čížek, V. Špirko and O. Bludsky: On the Use of Divergent Series in Vibrational Spectroscopy. *J. Chem. Phys.* **99**, 7331-7336 (1993).
130. J. Čížek, F. Vinette and E.J. Weniger: On the Use of Maple in Physics and Chemistry. *Int. Journal of Modern Physics* **C4**, 257-270 (1993).
131. M.D. Gould, J. Paldus and J. Čížek: Quasispin and the Pseudo-Orthogonal Group in the Hubbard Model. *Intern. J. Quantum Chem.* **50**, 207-231 (1994).
132. P. Bracken and J. Čížek: Construction of Interpolant Polynomials for Approximating Eigenvalues of a Hamiltonian which is Dependent on a Coupling Parameter. *Physics Letters A* **194**, 337-342 (1994).
133. J. Delhalle, J. Čížek, I. Flamant, J.L. Calais and J.G. Fripiat: Fourier Representation Method for Accurate Evaluation of the Coulomb and Exchange Lattice Sums in Extended Chains, *J. Chem. Phys.* **101** (12), 10717-10729 (1994).
134. M. Takahashi, P. Bracken, J. Čížek and J. Paldus: Perturbation Expansion of the Ground State Energy for the One-Dimensional Cyclic Hubbard System in the Hückel Limit. *Intern. J. Quantum Chem.* **53**, 457-466 (1995).
135. P. Bracken and J. Čížek: Investigation of the ${}^1E_{2g}^-$ States in Cyclic Polyenes. *Intern. J. Quantum Chem.* **53**, 467-471 (1995).
136. J. Delhalle and J. Čížek: Momentum Space and Zeeman Effect, *Intern. J. Quantum Chem.* **56**, 9-17 (1995).
137. O. Bludský, V. Špirko and J. Čížek: Solution of the One-Dimensional Schrödinger Equation by the Combined Use of Symbolic and Numerical Computation, *J. Phys. Chem.* **99**, 15608-15610 (1995).

138. V. Špirko and J. Čížek: Non-adiabatic Corrections for Coupled Oscillators Using Rayleigh-Schrödinger Perturbation Theory of Very High Orders, *J. Chem. Phys.* **102** (22), 8906 (1995).
139. V. Špirko, J. Čížek and L. Skála, Non-adiabatic Corrections for Coupled Morse Oscillators Using Hutson and Howard Perturbation Theory, *J. Chem. Phys.* **102** (22), 8916 (1995).
140. P. Bracken and J. Čížek, Interpolant Polynomial Technique Applied to the PPP Model. I. Asymptotics for Excited States of Cyclic Polyenes in the Finite Cyclic Hubbard Model, *Intern. J. Quantum Chem.* **57**, 1019-1032 (1996).
141. J. Čížek and P. Bracken, Interpolant Polynomial Technique Applied to the PPP Model. II. Testing the Interpolant Technique on the Hubbard Model, *Intern. J. Quantum Chem.* **57**, 1033-1048 (1996).
142. P. Bracken and J. Čížek, Analytic Calculation of Second-Order Perturbation Energy for the One-Dimensional Hubbard Model in the Hückel Limit, *Journal of Mathematical Chemistry* **18**, 217-235 (1996).
143. L. Skála, J. Čížek, J. Dvořák and V. Špirko, A Method for Calculating Analytical Solutions of the Schrödinger Equation. Analytical Results for Anharmonic Oscillators and Generalized Morse Oscillators, *Physical Review A* **53**, 2009-2020 (1996).
144. L. Skála and J. Čížek, A New Efficient Method for Calculating Perturbation Energies Using Functions which are not Quadratically Integrable, *J. Phys. A* **29**, L129-L132 (1996).
145. L. Skála and J. Čížek, Reply to Comments on “A New Efficient Method for Calculating Perturbation Energies Using Functions which are not Quadratically Integrable”, *J. Phys. A* **29**, 6467-6470 (1996).
146. R. Knab, W. Förner, J. Čížek and J. Ladik, Optimal Localization of Warnier Functions and the Correlation Energy in Different Approximations, *J. Mol. Structure* **366**, 11-33 (1996).
147. J. Čížek, E.J. Weniger, P. Bracken and V. Špirko, Effective Characteristic Polynomials and Two-Point Padé Approximants as Summation Techniques for the Strongly Divergent Perturbation Expansions of the Ground State Energies of Anharmonic Oscillators, *Physical Review E* **53**, 2925-2939 (1996).
148. J. Čížek and P. Bracken, Transformation of Bethe Equations for Finite Cycles into Secular Polynomials in Energy, *Physical Review Letters* **77**, 211-214 (1996).
149. V. Špirko and J. Čížek, Rayleigh-Schrödinger Perturbation Theory for Coupled Oscillators III. Curve-crossing Problems, *J. Chem. Phys.* **106**, 6338-6345 (1997).
150. P. Bracken and J. Čížek, Reconstruction of Secular Polynomials for Hubbard Model from Energy Perturbation Series for Weak and Strong Coupling, *J. Math. Phys.* **38**, 5493-5504 (1997).

151. W. Föerner, R. Knab, J. Čížek and J. Ladik, Numerical Application of the Coupled Cluster Theory with Localized Orbitals to Polymers. IV. Band Structure Corrections in Model Systems and Polyacetylene, *J. Chem. Phys.* **106**, 10248-10264 (1997).
152. L. Skála, J. Čížek, V. Kapsa and E.J. Weniger, Large Order Analysis of the Convergent Renormalized Strong Coupling Perturbation Theory for the Quartic Anharmonic Oscillator, *Phys. Rev. A* **56**, 4471-4476 (1997).
153. L. Skála, J. Čížek and J. Zamastil, Large-Order Behavior of the Strong Coupling Perturbation Expansion for Anharmonic Oscillators, *J. Phys. A* **32**, L123-L127 (1999).
154. L. Skála, J. Čížek, E.J. Weniger and J. Zamastil, Large-Order Behavior of the Convergent Perturbation Theory for Anharmonic Oscillators, *Phys. Rev. A* **59** (1), 102-106 (1999).
155. J. Zamastil, J. Čížek and L. Skála, Renormalized Perturbation Theory for Quartic Anharmonic Oscillator, *Ann. Phys. (NY)* **276**, 39-63 (1999).
156. L. Skála, J. Čížek and J. Zamastil, Strong Coupling Perturbation Expansions for Anharmonic Oscillators. Numerical Results, *J. Phys. A* **32**, 5715-5734 (1999).
157. R. Polak and J. Čížek, On the VB Adiabatic-Diabatic Picture of Bonding CO^{2+} , *J. Mol. Struct. (Theochem)* **547**, 17 (2001).
158. V. Špirko, M. Rozložník and J. Čížek, Brillouin-Wigner Perturbation Methods for Coupled Oscillators, *Phys. Rev. A* **61**, 14102-14106 (1999).
159. J. Zamastil, L. Skála and J. Čížek, WKB Approach to Calculating Lifetime of Quasistationary States, *Phys. Rev. Lett.* **84**, 5683-5686 (2000).
160. J. Zamastil, L. Skála, and J. Čížek, Large-order strong coupling perturbation coefficients for anharmonic oscillators, *Int. J. Theor. Phys.* **39**, 2427-2434 (2000).
161. J. Zamastil, J. Čížek, and L. Skála, WKB approach to calculating lifetime of quasistationary states. Harmonic oscillator in polynomial perturbation, *Phys. Rev. A* **63**, 022107 (2001)
162. J. Zamastil, V. Špirko, J. Čížek, L. Skála, and O. Bludský, Multidimensional WKB approximation and lifetime calculation, *Phys. Rev. A* **64**, 042101 (2001).
163. L. Skála, M. Kalhous, J. Zamastil, and J. Čížek, Perturbation theory using functions that are not quadratically integrable, *J. Phys. A* **35**, L167 (2002).
164. P. Bracken and J. Čížek, Evaluation of quantum mechanical perturbative sums in terms of quadratic surds and their use in the approximation of $\zeta(3)/\pi^3$, *Int. J. Quantum Chem.* **90**, 42-53 (2002).
165. M. Kalhous, L. Skála, J. Zamastil and J. Čížek, New version of the Rayleigh-Schrodinger perturbation theory, *Collect. Czech. Chem. Commun.* **68**, 295-306 (2003).

166. J. Čížek, J. Zamastil and L. Skála, New summation technique for rapidly divergent perturbation series. Hydrogen atom in magnetic field, *J. Math. Phys.* **44**, 962-968 (2003).
167. J. Čížek, A. Martinez and J. Ladik, A note on the mechanism of charge transport at different temperatures in aperiodic nucleotide base-stacks, *J. Mol. Struct.-Theochem* **626**, 77-80 (2003).
168. J. Zamastil, J. Čížek, M. Kalhous, L. Skála and M. Šimánek, Algebraic approach to the evaluation of the atomic integrals. Study of two-electron atoms. *J. Math. Phys.* **45**, 2674 (2004).
169. M. Kalhous, L. Skála, J. Zamastil and J. Čížek, New version of the Rayleigh-Schrödinger perturbation theory: Examples, *Int. J. Quantum Chem.* **99**, 325 (2004).
170. J. Zamastil, M. Šimánek, J. Čížek and L. Skála, Method of variation of constants for difference equations and its application to the calculation of atomic integrals, *J. Math. Phys.* **46**, 033504 (2005).
171. J. Zamastil, J. Čížek, L. Skála, M. Šimánek, Convergence study of the $1/Z$ expansion for the energy levels of two-electron atoms, *Phys. Rev. A* **81**, 032118 (2010).
172. L. Skála, J. Čížek and V. Kapsa, Quantum mechanics as applied mathematical statistics, *Annals of Physics* **326** (2011), 1174-1188.
173. L. Skála, J. Čížek and V. Kapsa, Quantum mechanics and mathematical statistics, in *Quantum Mechanics*, Ed.: Jonathan P. Groffe, Nova Science Publishers, New York 2012, ISBN 978-1-61728-966-8-2.