Almanasreh, Hasan; **Salomonson, Sten**; **Svanstedt, Nils**
Stabilized finite element method for the radial Dirac equation. (English) Zbl 1286.34119
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Summary: A challenging difficulty in solving the radial Dirac eigenvalue problem numerically is the presence of spurious (unphysical) eigenvalues, among the genuine ones, that are neither related to mathematical interpretations nor to physical explanations. Many attempts have been made and several numerical methods have been applied to solve the problem using the finite element method (FEM), the finite difference method, or other numerical schemes. Unfortunately most of these attempts failed to overcome the difficulty. As a FEM approach, this work can be regarded as a first promising scheme to solve the spuriosity problem completely. Our approach is based on an appropriate choice of trial and test function spaces. We develop a Streamline Upwind Petrov-Galerkin method to the equation and derive an explicit stability parameter.

MSC:

34L40 Particular ordinary differential operators (Dirac, one-dimensional Schrödinger, etc.)
65L60 Finite element, Rayleigh-Ritz, Galerkin and collocation methods for ordinary differential equations
65L20 Stability and convergence of numerical methods for ordinary differential equations
65L15 Numerical solution of eigenvalue problems involving ordinary differential equations

Keywords:

Dirac operator; finite element scheme; spurious eigenvalue; cubic Hermite functions; Petrov-Galerkin; stability parameter

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References:

[1] Ackad, E.; Horbatsch, M., Numerical solution of the Dirac equation by a mapped Fourier grid method, J. Phys. A: Math. Gen., 38, 3157-3171, (2005) · Zbl 1065.81036

[2] Almeida, R. C.; Silva, R. S., A stable Petrov-Galerkin method for convection-dominated problems, Comput. Methods Appl. Mech. Eng., 140, (1997) · Zbl 0899.76258

[3] A.N. Brooks, A Petrov-Galerkin finite element formulation for convection dominated flows, Thesis for the degree of Doctor of Philosophy, California Institute of Technology, California, 1981.

[4] Brooks, A. N.; Hughes, T. J.R., Streamline upwind/petrove-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations, Comput. Methods Appl. Mech. Eng., 32, (1982) · Zbl 0497.76041

[5] Cullin, M. J.P., A finite element method for a non-linear initial value problem, J. Inst. Math. Appl., 13, 233-247, (1974) · Zbl 0279.65090

[6] Dawkins, P. T.; Dunbar, S. R.; Douglass, R. W., The origin and nature of spurious eigenvalues in the spectral tau method, J. Comput. Phys., 147, 441-462, (1998) · Zbl 0924.65077

[7] De Sampaio, P. A.B., A Petrov-Galerkin/modified operator formulation for convection-diffusion problems, Int. J. Numer. methods Eng., 30, (1990) · Zbl 0714.76077

[8] Fisher, C. F.; Zatsarinny, O., A B-splines Galerkin method for the Dirac equation, Comput. Phys. Commun., 180, 879-886, (2009) · Zbl 1198.81036

[9] Griesemer, M.; Lutgen, J., Accumulation of discrete eigenvalues of the radial Dirac operator, J. Funct. Anal., 162, (1999) · Zbl 0926.34074

[10] Idelsohn, S.; Nigro, N.; Storti, M.; Buscaglia, G., A Petrov-Galerkin formulation for advection-reaction-diffusion problems, Comput. Methods Appl. Mech. Eng., 136, (1996) · Zbl 0896.76042

[11] Lindgren, I.; Salomonson, S.; Åsén, B., The covariant-evolution-operator method in bound-state QED, Phys. Rep., 389, 161-261, (2004)

[12] P.E. Lony, W.A. Shaffer, Some physical and numerical aspects of boundary layer modeling, in: Presented at the Second Conference on Numerical Prediction, Montrey, Calif, 1973, 37pp. (Available as NOAA Tech. Memo. NWS TDL-56, Silver Spring, MD).

[13] P.E. Lony, W.A. Shaffer, Boundary layer modeling experiments of the techniques development laboratory, in: Presented at the First Conference on Regional and Mesoscale Modeling, Analysis and Prediction, Las Vegas, Nev, 1975 (Abstract in Bull. Amer. Meteor. Soc., 56, 103).

[14] Mur, G., On the causes of spurious solutions in electromagnetics, Electromagnetic, 22, 357-367, (2002)

[15] Müller, C.; Grün, N.; Scheid, W., Finite element formulation of the Dirac equation and the problem of fermion doubling, Phys. Lett. A, 242, 245-250, (1998)

[16] Pestka, G., Spurious roots in the algebraic Dirac equation, Chem. Phys. Lett., 376, 659-661, (2003) · Zbl 1055.81016

[17] Rosenberg, L., Virtual-pair effects in atomic structure theory, Phys. Rev. A, 39, 4377-4386, (1989)

[18] Schroeder, W.; Wolf, I., The origin of spurious modes in numerical solutions of electromagnetic field eigenvalue problems, IEEE Trans. Microw. Theory Tech., 42, 644-653, (1994)

[19] Shabaev, V. M.; Tupitsyn, I. I.; Yerokhin, V. A.; Plunien, G.; Soff, G., Dual kinetic balance approach to basis-set expansions for the Dirac equation, Phys. Rev. Lett., 93, (2004)

[20] Thaller, B., The Dirac equation, (1993), Springer-Verlag Berlin · Zbl 0881.47021

[21] Tupitsyn, I. I.; Shabaev, V. M., Spurious states of the Dirac equation in a finite basis set, Opt. Spektrosk., 105, 203-209, (2008)

[22] Salomonson, S.; Öster, P., Relativistic all-order pair functions from a discretized single-particle Dirac Hamiltonian, Phys. Rev. A, 40, 5548-5558, (1989)

[23] Zhao, S., On the spurious solutions in the high-order finite difference methods for eigenvalue problems, Comput. Methods Appl. Mech. Eng., 196, 5031-5046, (2007) · Zbl 1173.74462