

Symmetric Galerkin boundary element method for computing the quantum states of the electron in a piecewise-uniform mesoscopic system

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Abstract. The quantum behavior of charge carriers in semiconductor structures is often described in terms of the effective mass Schrödinger equation, neglecting the rapid fluctuations of the wave function on the scale of the atomic lattice. For systems with piecewise-constant mass and potential energy, this amounts to solving a set of Helmholtz equations with wavenumbers dictated by the physical parameters of each homogeneous subregion. Making use of the Green function method, the system of differential equations can be expressed in boundary integral form to enable efficient numerical solution. In the present study, this strategy is applied in combination with a Galerkin technique to compute the energy spectrum and the wave functions of the electron in a mesoscopic structure composed of two regions. The proposed formulation differs from those presented before for the same scenario in that it implements a symmetric discretization of the four Helmholtz boundary integral operators, which leads to compact expressions and very accurate results.

1. Introduction

In recent years, fundamental and applied research in semiconductor and solid state physics has undergone a significant evolution, with particular emphasis on the study and development of mesoscopic structures and quantum wells [1, 3]. Indeed, the quantum confinement of charge carriers is responsible for a rich variety of phenomena that are of interest in optoelectronics, nanotechnology and quantum computing [4]. As it is well-known, the single-particle electronic properties of mesoscopic structures are dictated by the Schrödinger equation and depend on both the electron energy and the confining potential of the atomic lattice. Since for most geometries the energy levels and wave functions of the electron inside such structures cannot be determined analytically, numerical methods are required for both the analysis and interpretation of the experimental results. Among the various computational techniques, the finite element method (FEM) and the boundary element method (BEM) have been explored in the literature [5, 10]. Whereas the FEM consists in a volume discretization of the original boundary value problem, the BEM leverages the Green function approach to cast the partial differential equations into a boundary integral form which is then projected on finite dimensional trial spaces. In particular, this last step can be addressed by collocation, explicitly imposing the boundary integral equations at a finite set of points, or by the Galerkin approach, where the equations are enforced in a weighted average sense [11]. The main limitation of the BEM is that it requires the knowledge of the Green function of the physical system: for arbitrary confining potentials, the Green

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Symmetric Galerkin Boundary Element Method Alok Sutradhar, Glaucio Paulino, Leonard J. Gray, 2008-09-26 Symmetric Galerkin Boundary Element Method presents an introduction as well as recent developments of this accurate powerful and versatile method The formulation possesses the attractive feature of producing a symmetric coefficient matrix In addition the Galerkin approximation allows standard continuous elements to be used for evaluation of hypersingular integrals FEATURES Written in a form suitable for a graduate level textbook as well as a self learning tutorial in the field Covers applications in two dimensional and three dimensional problems of potential theory and elasticity Additional basic topics involve axisymmetry multi zone and interface formulations More advanced topics include fluid flow wave breaking over a sloping beach non homogeneous media functionally graded materials FGMs anisotropic elasticity error estimation adaptivity and fracture mechanics Presents integral equations as a basis for the formulation of general symmetric Galerkin boundary element methods and their corresponding numerical implementation Designed to convey effective unified procedures for the treatment of singular and hypersingular integrals that naturally arise in the method Symbolic codes using Maple for singular type integrations are provided and discussed in detail The user friendly adaptive computer code BEAN Boundary Element ANalysis fully written in Matlab is available as a companion to the text The complete source code including the graphical user interface GUI can be downloaded from the web site http://www.ghpaulino.com/SGBEM_book The source code can be used as the basis for building new applications and should also function as an effective teaching tool To facilitate the use of BEAN a video tutorial and a library of practical examples are provided A symmetric galerkin boundary element method for multi-domain interface problems Tanjeet Juneja, 2003 *Symmetric Galerkin Boundary Element Method in Elastodynamic Analysis* Weifeng Yuan, 2003 **Boundary Element Advances in Solid Mechanics** D. E. Beskos, Dimitri Beskos, Giulio Maier, 2003-06-12 This volume presents and discusses recent advances in boundary element methods and their solid mechanics applications It illustrates these methods in their latest forms developed during the last five to ten years and demonstrates their advantages in solving a wide range of solid mechanics problems Boundary Element Methods for Soil-Structure Interaction W.S. Hall, G. Oliveto, 2007-05-08 W S HALL School of Computing and Mathematics University of Teesside Middlesbrough TS1 3BA UK G OLIVETO Division of Structural Engineering Department of Civil and Environmental Engineering University of Catania Viale A Doria 6 95125 Catania Italy Soil Structure Interaction is a challenging multidisciplinary subject which covers several areas of Civil Engineering Virtually every construction is connected to the ground and the interaction between the artefact and the foundation medium may affect considerably both the superstructure and the foundation soil The Soil Structure Interaction problem has become an important feature of Structural Engineering with the advent of massive constructions on soft soils such as nuclear power plants concrete and earth dams Buildings bridges tunnels and underground structures may also require particular attention to be given to the problems of Soil

Structure Interaction Dynamic Soil Structure Interaction is prominent in Earthquake Engineering problems The complexity of the problem due also to its multidisciplinary nature and to the fact of having to consider bounded and unbounded media of different mechanical characteristics requires a numerical treatment for any application of engineering significance The Boundary Element Method appears to be well suited to solve problems of Soil Structure Interaction through its ability to discretize only the boundaries of complex and often unbounded geometries Non linear problems which often arise in Soil Structure Interaction may also be treated advantageously by a judicious mix of Boundary and Finite Element discretizations

2D Cracks Analysis with Symmetric Galerkin Boundary Element Method Kai Xu, 2002 **The Boundary Element Method, Volume 2** M. H. Aliabadi, 2002-04-29 The boundary element method BEM is a modern numerical technique which has enjoyed increasing popularity over the last two decades and is now an established alternative to traditional computational methods of engineering analysis The main advantage of the BEM is its unique ability to provide a complete solution in terms of boundary values only with substantial savings in modelling effort This two volume book set is designed to provide the readers with a comprehensive and up to date account of the boundary element method and its application to solving engineering problems Each volume is a self contained book including a substantial amount of material not previously covered by other text books on the subject Volume 1 covers applications to heat transfer acoustics electrochemistry and fluid mechanics problems while volume 2 concentrates on solids and structures describing applications to elasticity plasticity elastodynamics fracture mechanics and contact analysis The early chapters are designed as a teaching text for final year undergraduate courses Both volumes reflect the experience of the authors over a period of more than twenty years of boundary element research This volume Applications in Solids and Structures provides a comprehensive presentation of the BEM from fundamentals to advanced engineering applications and encompasses Elasticity for 2D 3D and Plates and Shells Non linear Transient and Thermal Stress Analysis Crack Growth and Multi body Contact Mechanics Sensitivity Analysis and Optimisation Analysis of Assembled Structures An important feature of this book is the in depth presentation of BEM formulations in all the above fields including detailed discussions of the basic theory numerical algorithms and where possible simple examples are included as well as test results for practical engineering applications of the method Although most of the methods presented are the latest developments in the field the author has included some simple techniques which are helpful in understanding the computer implementation of BEM Another notable feature is the comprehensive presentation of a new generation of boundary elements known as the Dual Boundary Element Method Written by an internationally recognised authority in the field this is essential reading for postgraduates researchers and practitioners in Aerospace Mechanical and Civil Engineering and Applied Mathematics **Advances in Boundary Element Techniques** James H. Kane, Giulio Maier, Nobuyoshi Tosaka, S.N. Atluri, 2012-12-06 The editors have published a select group of full length papers on boundary element analysis BEA photographed from camera ready manuscripts The articles have been

prepared by some of the most distinguished and prolific individuals in this field More than half of these articles have been submitted by authors that participated in an International Forum on Boundary Element Methods in Melbourne Australia in the Summer of 1991 However this volume is not a conference proceedings as these authors have expanded their accounts to chapter length and or have tailored their expositions more toward the style employed in archival journal publications The authors that did not participate in the International Forum have also adhered to the above mentioned philosophy This work contains a definitive representation of the significant capabilities and applications currently available or under investigation that fall under the general category of advanced boundary element analysis With treatments of mechanical thermal fluid and electromagnetic phenomena this book should thus be of value to graduate students practitioners and researchers in engineering mathematics and the physical sciences wishing to obtain a broader perspective or remain current in these important areas of computational simulation

Finite Element and Boundary Element Techniques from Mathematical and Engineering Point of View E. Stein, W. Wendland, 2014-05-04 Traditional FEM and the more recent BEM underlie many engineering computational methods and corresponding software Both methods have their merits and also their limitations The combination of both methods will provide an improved numerical tool in the future The aim of this book is to present significant basic formulations of FEM and BEM and to show their common practical and mathematical foundations their differences and possibilities for their combination These include variational foundations FEM and BEM for linear and non linear elasticity and potential problems the combination of FEM BEM asymptotic error analysis modifications due to corner and crack singularities and corresponding improvement of convergence plastic analysis numerical algorithms and engineering applications

Computational Methods in Fracture Mechanics Ferri M.H. Aliabadi, A.P. Ciolino, 2010-12-06 Special topic volume with invited peer reviewed papers only

The hybrid boundary element method applied to symmetric and antisymmetric problems, 2002 Este trabalho trata o Mtodo Hbrido dos Elementos de Contorno com vista anlise de problemas que envolvam simetria ou antissimetria Nestes casos apenas uma parte da estrutura que pode ser a metade um quarto ou um oitavo deve ser discretizada e capaz de representar o todo Os mtodos de contorno apresentam a vantagem quando comparados com os de domnio de no ser necessrio nenhum tipo de discretiza o ao longo dos eixos ou planos de simetria sem a introdu o de mais aproxima es visto que apenas o contorno discretizado Embora estas simplifica es venham a restringir alguns deslocamentos de corpo rgido para problemas de elasticidade no Mtodo dos Elementos de Contorno convencional coloca o ou Galerkin a ausncia de tais deslocamentos no acarreta altera es na sistem tica do m todo Nos Mtdos Hbridos de Elementos de Contorno por outro lado os deslocamentos de corpo rgido so necessrios direta ou indiretamente para a aplica o de condi es de ortogonalidade e avalia o das propriedades espectrais que so essenciais na obten o da diagonal principal de certas matrizes inerentes ao m todo tais como de flexibilidade de deslocamentos e de tens es Esta necessidade de avalia o uma caracter stica de suma importncia do m todo e quando no houver possibilidade de faz-la

deve se procurar uma forma substituta conceitualmente equivalente. Verifica-se que apesar de este método ser baseado em funções singulares de Green capaz de representar estados simples de tensões tanto por trabalhos virtuais quanto por interpolações no domínio. Como objetivo principal deste trabalho ser demonstrado que para cada deslocamento de corpo rígido perdido devido a restrições impostas pela simetria ou antissimetria poder ser utilizado um estado simples de tensões constantes na maioria dos casos que permitir o estabelecimento de propriedades espectrais apropriadas. De forma a se garantir uma sistemática estruturada para o trabalho faz-se uma abordagem de conceitos fundamentais aplicados a problemas da elastostática e potencial estacionário na formulação variacional do Método dos Elementos de Contorno com posteriores considerações especiais de estados simples de tensões representados polinomialmente para elasticidade tridimensional em geral visto que para problemas bidimensionais o caso se torna uma particularização. Todas as combinações de simetria e antissimetria são avaliadas com a implementação numérica. Diversos exemplos de problemas bidimensionais ilustram a formulação teórica.

Selected Topics in Boundary Integral Formulations for Solids and Fluids Vladimir Kompiš, 2014-05-04 The book outlines special approaches using singular and non singular multi domain and meshless BEM formulations hybrid and reciprocity based FEM for the solution of linear and non linear problems of solid and fluid mechanics and for the acoustic fluid structure interaction Use of Trefftz functions and other regularization approaches to boundary integral equations BIE boundary contour and boundary node solution of BIE sensitivity analysis shape optimization error analysis and adaptivity stress and displacement derivatives in non linear problems smoothing using Trefftz polynomials and other special numerical approaches are included Applications to problems such as noise radiation from rolling bodies acoustic radiation in closed and infinite domains 3D dynamic piezoelectricity Stefan problems and coupled problems are included *Singular Integrals in Boundary Element Methods* Vladimír Sládek, Ján Sládek, 1998 A text in singular integrals in boundary element methods Topics covered include treatment in crack problems regularization of boundary integral equations by the derivative transfer method regularization and evaluation of singular domain integrals in boundary element methods and others **Boundary Element Methods** Stefan A. Sauter, Christoph Schwab, 2010-11-01 This work presents a thorough treatment of boundary element methods BEM for solving strongly elliptic boundary integral equations obtained from boundary reduction of elliptic boundary value problems in \mathbb{R}^3 The book is self contained the prerequisites on elliptic partial differential and integral equations being presented in Chapters 2 and 3 The main focus is on the development analysis and implementation of Galerkin boundary element methods which is one of the most flexible and robust numerical discretization methods for integral equations For the efficient realization of the Galerkin BEM it is essential to replace time consuming steps in the numerical solution process with fast algorithms In Chapters 5-9 these methods are developed analyzed and formulated in an algorithmic way Boundary Element Methods Masataka Tanaka, Zhenhan Yao, 1996 This volume contains research topics on the boundary element methods of both basic mathematical schemes and engineering applications It aims to provide

research workers in computational mechanics and engineering with up to date information on applied research in the field

Development of a Computational Procedure for Three-dimensional, Linear, Second Order, Elliptic Boundary Value Problems Involving a Surface of Discontinuity with a Weakly Singular, Symmetric Galerkin Boundary Element Method (SGBEM) ,2009 **Fourier BEM** Fabian M.E. Duddeck,2002-08-07 Like FEM the Boundary Element Method BEM provides a general numerical tool for the solution of complex engineering problems In the last decades the range of its applications has remarkably been enlarged Therefore dynamic and nonlinear problems can be tackled However they still demand an explicit expression of a fundamental solution which is only known in simple cases In this respect the present book proposes an alternative BEM formulation based on the Fourier transform which can be applied to almost all cases relevant in engineering mechanics The basic principle is presented for the heat equation Applications are taken from solid mechanics e g poroelasticity thermoelasticity Transient and stationary examples are given as well as linear and nonlinear Completed with a mathematical and mechanical glossary the book will serve as a comprehensive text book linking applied mathematics to real world engineering problems Meshless Standard and Hypersingular Boundary Node Methods - Applications in Three-dimensional Potential Theory and Linear Elasticity Mandar Kalidas Chati,1999 **Mathematical and Computational Aspects** C. A. Brebbia,Wolfgang L. Wendland,G. Kuhn,1987-09 This book contains the edited versions of most of the papers presented at the 9th International Conference on Boundary Elements held at the University of Stuttgart Germany from August 31st to September 4th 1987 which was organized in co operation with the Computational Mechanics Institute and GAMM Society for Applied Mathematics and Mechanics This Conference as the previous ones aimed to review the latest developments in technique and theory and point out new advanced future trends The emphasis of the meeting was on the engineering advances versus mathematical formulations in an effort to consolidate the basis of many new applications Recently engineers have proposed different techniques to solve non linear and time dependent problems and many of these formulations needed a better mathematical understanding Furthermore new approximate formulations have been proposed for boundary elements which appeared to work in engineering practice but did not have a proper theoretical background The Conference also discussed the engineering applications of the method and concentrated on a link between BEM practitioners industrial users and researchers working on the latest development of the method The editors would like to express their appreciation and thanks to Ms Liz Newman and Mr H Schmitz for their unstinting work in the preparation of the Conference The Fast Solution of Boundary Integral Equations Sergej Rjasanow,Olaf Steinbach,2007-04-17 Boundary Element Methods BEM play an important role in modern numerical computations in the applied and engineering sciences These methods turn out to be powerful tools for numerical studies of various physical phenomena which can be described mathematically by partial differential equations The most prominent example is the potential equation Laplace equation which is used to model physical phenomena in electromagnetism gravitation theory and in perfect fluids A further application

leading to the Laplace equation is the model of steady state heat flow One of the most popular applications of the BEM is the system of linear elastostatics which can be considered in both bounded and unbounded domains A simple model for a fluid flow the Stokes system can also be solved by the use of the BEM The most important examples for the Helmholtz equation are the acoustic scattering and the sound radiation The Fast Solution of Boundary Integral Equations provides a detailed description of fast boundary element methods which are based on rigorous mathematical analysis In particular a symmetric formulation of boundary integral equations is used Galerkin discretisation is discussed and the necessary related stability and error estimates are derived For the practical use of boundary integral methods efficient algorithms together with their implementation are needed The authors therefore describe the Adaptive Cross Approximation Algorithm starting from the basic ideas and proceeding to their practical realization Numerous examples representing standard problems are given which underline both theoretical results and the practical relevance of boundary element methods in typical computations

Reviewing **Symmetric Galerkin Boundary Element Method**: Unlocking the Spellbinding Force of Linguistics

In a fast-paced world fueled by information and interconnectivity, the spellbinding force of linguistics has acquired newfound prominence. Its capacity to evoke emotions, stimulate contemplation, and stimulate metamorphosis is actually astonishing. Within the pages of "**Symmetric Galerkin Boundary Element Method**," an enthralling opus penned by a very acclaimed wordsmith, readers set about an immersive expedition to unravel the intricate significance of language and its indelible imprint on our lives. Throughout this assessment, we shall delve into the book's central motifs, appraise its distinctive narrative style, and gauge its overarching influence on the minds of its readers.

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Table of Contents Symmetric Galerkin Boundary Element Method

1. Understanding the eBook Symmetric Galerkin Boundary Element Method
 - The Rise of Digital Reading Symmetric Galerkin Boundary Element Method
 - Advantages of eBooks Over Traditional Books
2. Identifying Symmetric Galerkin Boundary Element Method
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Symmetric Galerkin Boundary Element Method
 - User-Friendly Interface
4. Exploring eBook Recommendations from Symmetric Galerkin Boundary Element Method
 - Personalized Recommendations
 - Symmetric Galerkin Boundary Element Method User Reviews and Ratings
 - Symmetric Galerkin Boundary Element Method and Bestseller Lists

5. Accessing Symmetric Galerkin Boundary Element Method Free and Paid eBooks
 - Symmetric Galerkin Boundary Element Method Public Domain eBooks
 - Symmetric Galerkin Boundary Element Method eBook Subscription Services
 - Symmetric Galerkin Boundary Element Method Budget-Friendly Options
6. Navigating Symmetric Galerkin Boundary Element Method eBook Formats
 - ePub, PDF, MOBI, and More
 - Symmetric Galerkin Boundary Element Method Compatibility with Devices
 - Symmetric Galerkin Boundary Element Method Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Symmetric Galerkin Boundary Element Method
 - Highlighting and Note-Taking Symmetric Galerkin Boundary Element Method
 - Interactive Elements Symmetric Galerkin Boundary Element Method
8. Staying Engaged with Symmetric Galerkin Boundary Element Method
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Symmetric Galerkin Boundary Element Method
9. Balancing eBooks and Physical Books Symmetric Galerkin Boundary Element Method
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Symmetric Galerkin Boundary Element Method
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Symmetric Galerkin Boundary Element Method
 - Setting Reading Goals Symmetric Galerkin Boundary Element Method
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Symmetric Galerkin Boundary Element Method
 - Fact-Checking eBook Content of Symmetric Galerkin Boundary Element Method
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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