Multipacting Analysis and Electromagnetic Field Computation by the Boundary Integral Equation Method in RF Cavities and Waveguides

Pasi Ylä-Oijala

Division of Mathematical Theory and
Applications of Electromagnetic Fields
Rolf Nevanlinna Institute

Faculty of Science
University of Helsinki

Academic Dissertation for the Degree of Doctor of Philosophy

To be presented, with the permission of the Faculty of Science of the University of Helsinki, for public criticism in Small Hall of the Main Building, on November 11th, 1999, at 12 o'clock noon.

Multipacting Analysis and Electromagnetic Field Computation by the Boundary Integral Equation Method in RF Cavities and Waveguides

Pasi Ylä-Oijala

Rolf Nevanlinna Institute
P.O. Box 4 (Yliopistonkatu 5)
00014 University of Helsinki
Finland

Research Reports A29

ISBN 952-9528-55-8
ISSN 0787-8338

YLIOPISTOPAINO
HELSINKI 1999

ISBN 951-45-8728-6 (PDF version)
Helsinki 1999
Helsingin yliopiston verkkojulkaisut

Acknowledgments

I would like to thank my supervisor, Professor Jukka Sarvas, for initially introducing me to work in the area of electromagnetic field computations and for his encouragement and guidance during this work. I also wish to thank Professor Erkki Somersalo and Dr. Dieter Proch for a very fruitful co-operation and for their valuable ideas.

I am grateful to my colleagues in the Division of Mathematical Theory and Applications of Electromagnetic Fields at Rolf Nevanlinna Institute. Without their help this study would have not been possible in the present extent. I also wish to thank the personnel of Rolf Nevanlinna Institute for creating an inspiring and pleasant working atmosphere.

For the financial support I like to thank the Graduate School of Mathematical Analysis and Logic.

Helsinki, October 1999.

Pasi Ylä-Oijala

Contents

Chapter 1

Introduction

1.1 Background

There is a broad agreement within the high energy physics community that the next accelerator facility on the 21th century should be an electron-positron ($e^- e^+$) collider with a center of mass energy of 500 GeV and a luminosity above 10^{33} cm^{-2} s^{-1} [3]. Such a collider would provide a discovery of Higgs particles. Several research groups worldwide are pursuing different linear collider design efforts. One of them is the TESLA (TeV Energy Linear Superconducting Accelerator) collaboration [7]. The fundamental differences of the TESLA approach compared to the other designs are the choices of superconducting accelerator structures and a low frequency.

One of the major problems in the accelerator components operating in vacuum is the *electron multipacting*. Multipacting is a phenomenon of resonant electron multiplication in which a large number of electrons build up an electron avalanche. This avalanche absorbs the rf energy, leading to remarkable power losses and heating of the walls, making it impossible to raise the fields by increasing the input power. Multipacting may cause breakdown in high rf power components such as couplers, cavities and windows. In the superconducting structures a large rise of temperature can eventually lead to a thermal breakdown.

Multipacting starts when certain resonant conditions for electron trajectories are fulfilled and the impacted surface has a secondary yield larger than one. Since there are only a few special cases where the multipacting resonances can be determined analytically, usually numerical methods are applied. Traditionally the numerical methods are based on straightforward Monte-Carlo type electron trajectory simulations. Since the trajectory calculation of a relativistic electron is sensitive even to small perturbations of the electromagnetic field, especially close to the structure walls, the fields must be computed very accurately. This sets a high quality requirement for the accuracy of the field computation algorithm.

The problem of computation of electromagnetic fields in the particle accelerator structures may be mathematically formulated as interior boundary value or eigenvalue problems for time-harmonic Maxwell's equations. Since electromagnetic fields can be found exactly only in few simple cases, in the practical applications usually numerical methods are required. The numerical methods can be divided into two categories, based either on differential equations (finite element method and the method of finite difference) or on integral equations (boundary and volume integral equation method). Traditionally the finite element method has been the most popular method for interior problems with inhomogeneous media. In the integral equation approach the original boundary value problem for partial differential equations is reformulated as integral equations. If the medium is homogeneous, the integral

equations can be transformed to operate on the boundary of the domain. This gives a rise to the *boundary integral equation method*.

1.2 Goals and outline of this thesis

This work has arisen from a practical need to analyze electron multipacting in the TESLA accelerator structures. TESLA is an international linear collider research and development project based on superconducting accelerator components. The project is co-ordinated by Deutsches Elektronen-Synchrotron (DESY), Germany. Although multipacting can be avoided in most $\beta = (v/c) = 1$ cavities, multipacting is still a major problem in many types of vacuum rf components [33]. Hence, it is very important to get information about the possible multipacting resonances and to master various methods to suppress multipacting.

In order to carry out the multipacting analysis, the electromagnetic field map should be available. Since the TESLA accelerator structures include homogeneous, or piece-wise homogeneous, medium only, the boundary integral equation method becomes a considerable choice. Although it might be easier to model complicated 3D structures with the boundary integral equation method than, for example, with the finite element method, the numerical implementation usually becomes much more demanding because of the singularities of the boundary integral operators. For the boundary integral equation method to be effective, the computation of singular integrals requires a special attention.

The goal of this work has been twofold. Firstly, to develop numerically effective and accurate methods for solving (interior) boundary value problems for time-harmonic Maxwell's equations by the boundary integral equation method. Secondly, to develop computational methods for a systematic analysis of electron multipacting. In particular, in this work, these two goals are combined to carry out the multipacting analysis in the TESLA superconducting accelerator cavities and input power couplers. This study have been carried out during the joint research project of Rolf Nevanlinna Institute and DESY in 1993 - 1999. The thesis consists of this overview and five publications. The publications are referred by Roman numerals I-V and they are listed in Section 1.3.

The problem of computation of electromagnetic fields in particle accelerator structures is considered in Publications II and V. Publication II confines to axially symmetric structures, like rf cavities and coaxial input couplers with ceramic windows, whereas in Publication V arbitrary 3-dimensional geometries, like junctions and discontinuities of rectangular and coaxial waveguides, are considered. In both cases, special attention is paid to developing computational methods for the accurate field computation near the boundaries. Furthermore, in Publication III the numerical efficiency and stability of various boundary integral equation formulations is studied in the axisymmetric case. It is found that the accuracy may significantly depend on the type of the formulation and the choice of the test functions.

In Publication I, we present systematic methods to analyze electron multipacting in arbitrary rf structures based on the standard electron trajectory calculations combined with new advanced searching and analyzing methods for multipacting resonances. The developed methods are applied to analyze multipacting in simple geometries like straight and tapered coaxial lines. In straight coaxial lines we have found simple scaling laws for multipacting resonances and studied the effect of biasing DC voltage to multipacting. In particular, we give scaling laws by which one can optimize the biasing voltage to suppress multipacting in any coaxial line. In Publication IV the multipacting analysis of the TESLA superconducting single and multi-cell accelerator cavities and two designs of the TESLA input power coupler with a ceramic window is considered. Because of the complexity of the window geometries and varying field conditions, the multipacting analysis in the input couplers

becomes rather demanding and time consuming.

In addition, to a review of the material presented in Publications I - V, this overview presents a brief theoretical introduction to the boundary integral equation method in nonsmooth domains, so called Lipschitz domains. The presentation is not complete, e.g. the proofs of the theorems are omitted, and it should be seen more as a review of the recent results of the theoretical study of the boundary value problems for Maxwell's equations in Lipschitz domains.

The outline of this overview is the following. In Chapter 2 we consider electromagnetic field computation by the boundary integral equation method. Sections 2.1 - 2.3 review the theoretical background. The required boundary integral equations are derived in Section 2.4 starting from the well-known Stratton-Chu integral representations and the main ideas of the developed numerical algorithms are introduced in Section 2.5. In Chapter 3 we consider multipacting as a dynamical system and present the developed numerical methods. Finally, Chapter 4 reviews the main results of the multipacting analysis and the field computations of the Publications I - V.

Some of the material of this thesis has been also presented in the following reports.

- P. Ylä-Oijala: Analysis of electron multipacting in coaxial lines with traveling and mixed waves, *TESLA Reports 97-20*, pp. 1-21, DESY Print, 1997.
- P. Ylä-Oijala: Suppressing electron multipacting in coaxial lines by DC voltage, *TESLA Reports 97-21*, pp. 1-14, DESY Print, 1997.
- P. Ylä-Oijala: Application of the boundary integral equation method to interior boundary value problems for Maxwell's equations, Licentiates Dissertation, *Rolf Nevanlinna Institute Research Reports C29*, pp. 1-120, Helsinki 1998.

1.3 List of Publications

The thesis consists of this overview and the following five publications.

I. E. Somersalo, P. Ylä-Oijala, D. Proch and J. Sarvas: Computational methods for analyzing electron multipacting in RF structures, *Particle Accelerators*, Vol. **59**, pp. 107-141, 1998.

II. P. Ylä-Oijala and E. Somersalo: Computation of electromagnetic fields in axisymmetric RF structures with boundary integral equations, *Journal of Electromagnetic Waves and Applications*, Vol. **13**, pp. 445-489, 1999.

III. P. Ylä-Oijala: Comparison of boundary integral formulations for electromagnetic field computation in axisymmetric resonators, submitted for publication, preprint in *Rolf Nevanlinna Institute Research Reports A24*, pp. 1-21, Helsinki 1999.

IV. P. Ylä-Oijala: Electron multipacting in TESLA cavities and input couplers, to appear in *Particle Accelerators*, 1999.

V. P. Ylä-Oijala and M. Taskinen: Computation of mixed waves in 3-dimensional waveguide discontinuities by the boundary integral equation method, *Rolf Nevanlinna Institute Research Reports A25*, pp. 1-28, Helsinki 1999.

Chapter 2

Field Computation by Boundary Integral Equations

The boundary integral equation method (BIEM) has been one of the most popular methods for solving various electromagnetic field problems. Especially BIEM has been applied to scattering problems where the advantages compared to the methods based on differential equations (e.g. finite element method, FEM) are obvious. Namely, the radiation conditions are automatically enforced and difficult (3D) mesh generation and truncation problems with some additional absorbing boundary conditions can be avoided. In the BIEM the unknowns are not the electromagnetic fields on the entire space, but some tangential vector fields on the boundaries. Thus, by applying BIEM, the dimensionality of the problem can be reduced by one. The drawbacks of the method are that the numerical treatment of singular integral equations is rather involved and the resulting system matrix is dense.

The problem of computation of electromagnetic fields in the accelerator devices can be mathematically formulated as interior boundary value or eigenvalue problems for Maxwell's equations. In the case of smooth boundaries, the problem can be reduced to weakly singular integral equations, hence giving a rise to compact operators which can be readily handled via classical Fredholm theory [5]. Although the approach based on the Fredholm theory is available for C^1 domains, it no longer works for general nonsmooth (Lipschitz) domains and new techniques are required. In recent years, this topic has received much attention, see e.g. [51], [45], [29], [48], and references therein. As well-known, the theoretical study of boundary value problems using boundary integral equations (often called a layer potential approach) becomes very involved if the boundary of the domain is not smooth. One of the main reasons for this is that some of the resulting integral operators have to be interpreted as principal value integrals. However, the need for a realistic modelling of engineering and physical problems naturally leads to domains with corners and edges, and discontinuous boundary data. This is the case in the present application of the field computation in the particle accelerator structures.

The first numerical applications of the BIEM to electromagnetic scattering problems were rotationally symmetric obstacles, [26], [27], [13], etc. In [39] the authors developed special base functions for solving electromagnetic scattering by arbitrary shaped three dimensional perfectly conducting bodies. More recently the same approach has been applied to dielectric obstacles [50], [40] and to dielectrically coated conducting bodies [41]. The BIEM has been also applied to interior problems, like waveguide discontinuities and waveguide junctions [16], [20]. As well-known, the BIEM is available for homogeneous bodies only. Therefore, in recent years a lot of effort has been put to develop methods for coupling FEM and BIEM, in order to treat inhomogeneous bodies. See e.g. [52] and [42] for the latest developments.

We begin this overview by giving a short review of the main results of the layer potential technique applied to the (interior) boundary value problems for Maxwell's equation in non-smooth domains. The main aim of this thesis is, however, to develop numerical methods for solving various (interior) boundary value problems for Maxwell's equations with boundary integral equations and apply the results to the analysis of electron multipacting.

2.1 Function spaces

When using the layer potential approach, the question of regularity of the tangential components of solutions to Maxwell's equations on the boundary is important. As it has been pointed out in [22], the function space for both electric and magnetic fields must be the same, since the electric and magnetic fields occur in Maxwell's equations in a symmetric fashion. Furthermore, for solutions to Maxwell's equations, the regularity of the fields up to the boundary automatically ensures regularity of the curl of the fields up to the boundary.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded, simply connected region with a connected boundary $\partial\Omega$. A domain Ω is called Lipschitz or C^k, $k \in \mathbb{N}_+$, if $\partial\Omega$ is given locally by the graph of a Lipschitz or C^k function ([46]), respectively. By $L^p(\Omega)$, $1 < p < \infty$, we denote the usual space of functions $f : \Omega \mapsto \mathbb{C}$ with the property $\int_\Omega |f(x)|^p \, dx < \infty$. For vector valued functions $\vec{F} : \Omega \mapsto \mathbb{C}^3$ we denote $\vec{F} \in L^p(\Omega)^3$ if all components of $\vec{F}$ are in $L^p(\Omega)$.

In the case of C^1 and Lipschitz domains with noncontinuous boundary data it is customary to treat the space of tangential L^p functions on the boundary, see e.g. [28] and [46]. Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and let $1 < p < \infty$. Then we define

$$TL^p(\partial\Omega) := \left\{ \vec{F} : \partial\Omega \mapsto \mathbb{C}^3 \,|\, \vec{n} \cdot \vec{F} = 0 \text{ a.e. and } \vec{F} \in L^p(\partial\Omega)^3 \right\}.$$

Here a.e. is an abbreviation for almost everywhere or almost every point, with respect to the surface measure, and $\vec{n}$ denotes the unit normal of $\partial\Omega$ pointing into the exterior of Ω.

Furthermore, in the case of irregular boundary we have to require some boundedness conditions for the nontangential maximal functions $\vec{E}^*$ and $\vec{H}^*$ in order to guarantee the existence of pointwise boundary values for $\vec{E}$ and $\vec{H}$. At every point $x \in \partial\Omega$ we assume that an open right circular, doubly truncated cone $\Gamma(x)$, with vertex at x and two convex components (one in Ω and the other in $\mathbb{R}^3 \setminus \bar{\Omega}$), has been chosen so that the resulting family of such cones is a regular family as described in [51]. The components of such cones are denoted by $\Gamma_- \in \Omega$ and $\Gamma_+ \in \mathbb{R}^3 \setminus \bar{\Omega}$. For a function f defined in Ω (in $\mathbb{R}^3 \setminus \bar{\Omega}$), the nontangential maximal function $f_\mp^*$ is defined as follows [28], [46]

$$f_\mp^*(x) := \sup_{y \in \Gamma_\mp(x)} |f(y)|.$$

The boundary values of functions defined in Ω (in $\mathbb{R}^3 \setminus \bar{\Omega}$) are assumed to be taken as nontangential limits almost everywhere. That is, we define $f_\mp \,|_{\partial\Omega}$ as follows

$$f_\mp(x) := \lim_{y \to x} f(y), \quad y \in \Gamma_\mp(x), \quad \text{for a.e. } x \in \partial\Omega.$$

Similar definitions apply for the partial derivatives of a function, and for each component of a vector-valued function [46].

Next we define the surface divergence for Lipschitz domains [28]. For the smooth case see e.g. [6].

Definition 2.1.1 *A vector field $\vec{F} \in TL^p(\partial\Omega)$ has a surface divergence, denoted by Div $\vec{F}$, if there exists a (unique) scalar valued function Div $\vec{F}$ in $L^p(\partial\Omega)$ such that for all functions*

$\varphi \in C^\infty(\mathbb{R}^3)$ *it holds*

$$\int_{\partial\Omega} \varphi \, Div\, \vec{F}\, dS = -\int_{\partial\Omega} Grad\, \varphi \cdot \vec{F}\, dS.$$

Here Grad denotes the surface gradient and $1 < p < \infty$.

Now we can state the following lemma [46], which is well-known for smooth domains ([6]).

Lemma 2.1.2 *Let* $\vec{F}$ *be a smooth vector field defined in* Ω, *e.g.* $\vec{F} \in C^2(\Omega)^3$. *If* $\vec{F}$ *and* $\nabla \times \vec{F}$ *have nontangential limits almost at every point* $x \in \partial\Omega$, *and if* $\vec{F}^* \in L^p(\partial\Omega)^3$ *and* $(\nabla \times \vec{F})^* \in L^p(\partial\Omega)^3$ *for some* $1 < p < \infty$, *then* $\vec{n} \times \vec{F}$ *has a surface divergence in* $L^p(\partial\Omega)$. *That is,* $\vec{n} \times \vec{F} \in TL^p_{\mathrm{Div}}(\partial\Omega)$ *and*

$$Div\,(\vec{n} \times \vec{F}) = -\vec{n} \cdot (\nabla \times \vec{F}). \tag{2.1.1}$$

Time-harmonic Maxwell's equations (in a linear, homogeneous and source free medium), with the time-factor $e^{-i\omega t}$,

$$\nabla \times \vec{E} = i\omega\mu\vec{H}, \quad \nabla \times \vec{H} = -i\omega\gamma\vec{E},$$

together with (2.1.1) imply

$$Div\,(\vec{n} \times \vec{E}) = -i\omega\mu\, \vec{n} \cdot \vec{H} \ \text{ and } \ Div\,(\vec{n} \times \vec{H}) = i\omega\gamma\, \vec{n} \cdot \vec{E}. \tag{2.1.2}$$

Hence, the existence of boundary values for the normal components of the fields imply some extra regularity for the tangential components of the fields on the boundary. In particular, the tangential components of $\vec{E}$ and $\vec{H}$ should have a surface divergence in $L^p(\partial\Omega)$. This motivates us to define the following function space. Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and let $1 < p < \infty$, then we define

$$TL^p_{\mathrm{Div}}(\partial\Omega) := \left\{ \vec{F} \in TL^p(\partial\Omega) \,|\, Div\, \vec{F} \in L^p(\partial\Omega) \right\}.$$

It is worth of noticing that in [47] and [48] the author considers electromagnetic transmission problems with the boundary data in $TL^2_{\mathrm{Div}}(\partial\Omega)$.

2.2 Statement of the problem

In this work we consider propagation of time-harmonic electromagnetic fields in a piecewise homogeneous medium. The space dependent parts of the fields satisfy the time-harmonic Maxwell's equations

$$\nabla\times\vec{E}(x) - i\omega\mu(x)\vec{H}(x) = 0 \ \text{ and } \ \nabla\times\vec{H}(x) + i\omega\gamma(x)\vec{E}(x) = 0, \tag{2.2.1}$$

in $\Omega \subset \mathbb{R}^3$, with piecewise constant $\mu(x)$ and $\gamma(x) = \varepsilon(x) + i\sigma(x)/\omega$. First we formulate an interior Maxwell problem in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ with homogeneous interior ([28], [29]).

Problem 2.2.1 *(Interior Maxwell) Find* $\vec{E}$, $\vec{H}$, *with* $\vec{E}^*$, $\vec{H}^* \in L^p(\partial\Omega)^3$, *satisfying Maxwell's equations (2.2.1) in* Ω *with constant* γ *and* μ, *and the boundary condition*

$$\vec{n} \times \vec{E} = \vec{F} \quad on\ \partial\Omega, \tag{2.2.2}$$

where $\vec{F} \in TL^p(\partial\Omega)$ *is a given tangential field and* $1 < p < \infty$.

In a similar fashion as in the smooth case [5], the interior Maxwell problem does not have a unique solution if k is the Maxwell eigenvalue of the domain Ω. A wavenumber $k = \omega\sqrt{\gamma\mu} > 0$ is called a *Maxwell eigenvalue* for domain Ω if for each k there exists nonzero *eigenfields* $\vec{E}$, $\vec{H}$ satisfying Maxwell's equations in Ω and the homogeneous boundary condition $\vec{n}\times\vec{E} = 0$ on $\partial\Omega$. As well-known for each bounded domain there exists a countable set of such eigenvalues accumulating only at infinity. For the interior Maxwell problem we have the following result [29].

Theorem 2.2.1 *If $k > 0$ is not a Maxwell eigenvalue for Ω, then there exists $\epsilon > 0$ depending only on $\partial\Omega$ such that for each $1 < p \leq 2 + \epsilon$ the interior Maxwell problem has a unique solution if and only if $\vec{F} \in TL^p_{\mathrm{Div}}(\partial\Omega)$. In the case in which k is a Maxwell eigenvalue for Ω, the interior Maxwell problem is solvable if and only if $\vec{F} \in TL^p_{\mathrm{Div}}(\partial\Omega)$ and $\vec{F}$ satisfies finitely many linear conditions. In such a case the solution is not unique.*

For the present application of the field computation in the particle accelerators we have to consider more general interior boundary value problems for Maxwell's equations. The medium may be piecewise homogeneous and on the boundary we assume various boundary conditions. Let a bounded domain $\Omega \subset \mathbb{R}^3$ be divided into n open and homogeneous regions

$$\bar{\Omega} = \bigcup_{j=1}^{n} \bar{\Omega}_j, \quad \Omega_i \cap \Omega_j = \emptyset, \ i \neq j. \tag{2.2.3}$$

Here we assume that subdomains Ω_j, $j = 1, \ldots, n$, are Lipschitz domains with constant electromagnetic parameters γ_j and μ_j. We divide the boundary of Ω_j, $\partial\Omega_j$, into three separate regions as follows. Let $\Gamma_j \subset \partial\Omega_j$ denote a portion of $\partial\Omega_j$ where an electric boundary condition $\vec{n}_j \times \vec{E}_j \,|_{\Gamma_j} = \vec{F}_j$ is given. This kind of boundary segment is often called an electric wall. In a similar fashion, a boundary segment $\Lambda_j \subset \partial\Omega_j$ where a magnetic boundary condition $\vec{n}_j \times \vec{H}_j \,|_{\Lambda_j} = \vec{G}_j$ is given, is called a magnetic wall. Functions $\vec{F}_j$ and $\vec{G}_j$ are given (smooth) tangential vector fields defined on the boundary. In practical applications we usually set $\vec{F}_j = 0$ and $\vec{G}_j = 0$, corresponding to physical perfectly conducting electric and magnetic boundary conditions. Furthermore, let us denote the intersections of the subdomains by $\Upsilon_{j,m} = \partial\Omega_j \cap \partial\Omega_m$.

To be more precise, let $\vec{E}_j = \vec{E} \,|_{\Omega_j}$, $\vec{H}_j = \vec{H} \,|_{\Omega_j}$ denote a solution to Maxwell's equations in Ω_j and let $\vec{n}_j$ denote the unit normal of $\partial\Omega_j$ pointing into the exterior of Ω_j. We define the following subboundaries

$$\begin{aligned}
\Gamma_j &= \left\{ x \in \partial\Omega_j \mid \vec{n}_j(x) \times \vec{E}_j(x) = \vec{F}_j(x) \right\} \\
\Upsilon_j &= \bigcup_{m=1,\, m\neq j}^{n} \Upsilon_{j,m} \\
\Lambda_j &= \left\{ x \in \partial\Omega_j \mid \vec{n}_j(x) \times \vec{H}_j(x) = \vec{G}_j(x) \right\},
\end{aligned}$$

for $j = 1, \ldots, n$, so that

$$\partial\Omega_j = \Gamma_j \cup \Upsilon_j \cup \Lambda_j.$$

On $\Upsilon_{j,m}$ we require the transmission conditions

$$\vec{n}_j \times \vec{E}_j = -\vec{n}_m \times \vec{E}_m \ \text{ and } \ \vec{n}_j \times \vec{H}_j = -\vec{n}_m \times \vec{H}_m. \tag{2.2.4}$$

In this work we consider rather complicated interior problems by generalizing Problem 2.2.1 for a piecewise homogeneous domain Ω; Ω defined as in (2.2.3). First we consider a Maxwell eigenvalue problem, see [29]. Physically, such an eigenvalue problem corresponds to a closed cavity resonator (with piecewise homogeneous interior). Here we use $p = 2$ motivated by [47].

Problem 2.2.2 *Let k be a Maxwell eigenvalue for a domain Ω with Ω defined as in (2.2.3). Find the nonzero fields $\vec{E}_j$, $\vec{H}_j$, with $\vec{E}_j^*$, $\vec{H}_j^* \in L^2(\partial\Omega_j)^3$, called Maxwell's eigenfields, satisfying Maxwell's equations (2.2.1) in Ω_j with constant γ_j and μ_j, and the homogeneous boundary conditions*

$$\vec{n}_j \times \vec{E}_j = 0 \text{ on } \Gamma_j, \quad \vec{n}_j \times \vec{H}_j = 0 \text{ on } \Lambda_j, \tag{2.2.5}$$

and the transmission conditions (2.2.4), for all $j, m = 1, \ldots, n$, $m \neq j$.

Obviously, the problem of finding the eigenvalues k for an arbitrary domain is a non-trivial question. In fact, the above problem has non-zero solutions only if k is the Maxwell eigenvalue of Ω. In such a case the solution is not unique.

In addition to the above problem, referred here to a cavity problem, we also consider propagation of electromagnetic fields in waveguides with piecewise homogeneous medium. The waveguide can be open in the sense that after the possible discontinuity, the structure continues (to the infinity) as a uniform waveguide. We assume that the frequency is chosen so that in the regular section only one field mode is propagating. This kind of field problem can be considered by closing the computation domain with properly placed electric or magnetic walls, and treating it as a closed cavity resonator. An other way is to utilize the fact that in the homogeneous sections the field distribution is known up to a constant complex multiplier. In the latter case the waveguide problem is formulated as follows.

Problem 2.2.3 *Let $\vec{E}_j^p$, $\vec{H}_j^p$, be a given incident field in Ω_j, $j = 1, \ldots, n$. Find $\vec{E}_j = \vec{E}_j^p + \vec{E}_j^s$, $\vec{H}_j = \vec{H}_j^p + \vec{H}_j^s$, with $\vec{E}_j^*$, $\vec{H}_j^* \in L^2(\partial\Omega_j)^3$, satisfying Maxwell's equations (2.2.1) in Ω_j with constant γ_j and μ_j, and the boundary conditions (2.2.5) and (2.2.4).*

In practice the computation domain is closed by walls, placed far enough from the discontinuity, and the source terms $\vec{E}_j^p$ and $\vec{H}_j^p$ are generated by the surface currents on these walls.

In the complicated cases of Problems 2.2.2 and 2.2.3, the questions of uniqueness and existence of a solution are open. Thus, this theoretical introduction does not give answers to these questions in the practical situations where the numerical computations are carried out. Motivation to this theoretical section is to show that the boundary integral equation method is applicable to nonsmooth domains, too.

2.3 Layer potential operators

In this section we define appropriate integral operators, so called *layer potential operators*, needed on the formulation of the boundary integral equation method in the context of Maxwell's equations. In particular, we present the nontangential traces of the operators to the boundary (so called jump relations). In the smooth case the classical results with Hölder continuous density functions can be found from [5] (and [59]). See also [22] and [6]. In the Sobolev space setting the results are presented in [14] ([38], [12]).

Let

$$\Phi_k(x-y) := \frac{e^{ik|x-y|}}{4\pi|x-y|}$$

with $k = \omega\sqrt{\gamma\mu}$, denote the fundamental solution of Helmholtz equation in $\mathbb{R}^3$. Often Φ_k is called a free space Green's function. We define the following integral, or potential, operators.

Definition 2.3.1 *Let Ω be a bounded Lipschitz domain, $\vec{F} \in L^p(\partial\Omega)^3$, $\vec{G} \in TL^p(\partial\Omega)$ and $\vec{W} \in TL^p_{\mathrm{Div}}(\partial\Omega)$, $1 < p < \infty$. Then for all $x \in \Omega$ we define*

$$\begin{aligned}
(\mathbf{S}_\Omega \vec{F})(x) &:= \int_{\partial\Omega} \Phi_k(x-y)\, \vec{F}(y)\, dS(y) \\
(\mathbf{K}_\Omega \vec{G})(x) &:= \nabla\times \int_{\partial\Omega} \Phi_k(x-y)\, \vec{G}(y)\, dS(y) \\
(\mathbf{D}_\Omega \vec{W})(x) &:= (\nabla\times)^2 \int_{\partial\Omega} \Phi_k(x-y)\, \vec{W}(y)\, dS(y).
\end{aligned}$$

The next theorem involves the question of the traces of the potential operators to the boundary.

Theorem 2.3.2 *Let Ω be a bounded Lipschitz domain and $\vec{F} \in L^p(\partial\Omega)^3$, $\vec{G} \in TL^p(\partial\Omega)$, $\vec{W} \in TL^p_{\mathrm{Div}}(\partial\Omega)$ with $1 < p < \infty$, then we have the following nontangential boundary traces for almost any point $x_0 \in \partial\Omega$ ($x \in \Omega$)*

$$\begin{aligned}
\lim_{x\to x_0} (\vec{n}(x_0) \times (\mathbf{S}_\Omega \vec{F})(x)) &= (\tilde{\mathbf{S}}\vec{F})(x_0) \\
\lim_{x\to x_0} (\vec{n}(x_0) \times (\mathbf{K}_\Omega \vec{G})(x)) &= (\tilde{\mathbf{K}}\vec{G})(x_0) - \frac{1}{2}\vec{G}(x_0) \\
\lim_{x\to x_0} (\vec{n}(x_0) \times (\mathbf{D}_\Omega \vec{W})(x)) &= (\tilde{\mathbf{D}}\vec{W})(x_0),
\end{aligned}$$

where the boundary integral operators $\tilde{\mathbf{S}}$, $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{D}}$ are defined at $x_0 \in \partial\Omega$ as follows

$$\begin{aligned}
(\tilde{\mathbf{S}}\vec{F})(x_0) &:= \int_{\partial\Omega} \vec{n}(x_0) \times \Big(\Phi_k(x_0-y)\, \vec{F}(y)\Big)\, dS(y) \\
(\tilde{\mathbf{K}}\vec{G})(x_0) &:= p.v. \int_{\partial\Omega} \vec{n}(x_0) \times \nabla_{x_0} \times \Big(\Phi_k(x_0-y)\, \vec{G}(y)\Big)\, dS(y) \\
(\tilde{\mathbf{D}}\vec{W})(x_0) &:= p.v. \int_{\partial\Omega} \vec{n}(x_0) \times (\nabla_{x_0}\times)^2 \Big(\Phi_k(x_0-y)\, \vec{W}(y)\Big)\, dS(y).
\end{aligned}$$

Here p.v. stands for the Cauchy principal value integral.

For the proof of the jump relations of the scalar and vector layer potentials in Lipschitz domains see e.g. [51], [45], [28], [29] and [47], and references therein.

Let $\mathbf{S}$, $\mathbf{K}$ and $\mathbf{D}$ denote the operators $\tilde{\mathbf{S}}$, $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{D}}$ without taking the vector products with $\vec{n}$. In the sequel, we will need the following lemma [46].

Lemma 2.3.3 *Let Ω be a bounded Lipschitz domain and let $1 < p < \infty$. Then for a vector field $\vec{G} \in TL^p_{\mathrm{Div}}(\partial\Omega)$ it holds*

$$\nabla \cdot (\mathbf{S}_\Omega \vec{G}) = \mathbf{S}_\Omega(Div\, \vec{G}).$$

The identity is valid on $\partial\Omega$ by interpreting the operator $\nabla \cdot \mathbf{S}_\Omega$ in the principal value sense.

By this lemma, we may write

$$(\tilde{\mathbf{D}}\vec{F}) = \vec{n} \times \Big(\nabla \mathbf{S}(Div\, \vec{F})\Big) + k^2 \tilde{\mathbf{S}}(\vec{F}), \tag{2.3.1}$$

where $\nabla\mathbf{S}$ has to be interpreted in the sense of principal value. Next we give the mapping properties of the potential operators [28], [29].

Theorem 2.3.4 *Let Ω be a bounded Lipschitz domain. Then*

$$\tilde{\mathbf{S}} \quad : \quad L^p(\partial\Omega)^3 \mapsto L^p(\partial\Omega)^3$$

is compact and

$$\begin{aligned}
\tilde{\mathbf{K}} \quad &: \quad TL^p(\partial\Omega) \mapsto TL^p(\partial\Omega) \\
\tilde{\mathbf{K}} \quad &: \quad TL^p_{\mathrm{Div}}(\partial\Omega) \mapsto TL^p_{\mathrm{Div}}(\partial\Omega) \\
\tilde{\mathbf{D}} \quad &: \quad TL^p_{\mathrm{Div}}(\partial\Omega) \mapsto TL^p_{\mathrm{Div}}(\partial\Omega)
\end{aligned}$$

are bounded, for all $1 < p < \infty$. If Ω is a C^1 domain, then $\tilde{\mathbf{K}}$ is actually compact in $TL^p(\partial\Omega)$.

In the case of transmission problems the original boundary value problem is usually reduced to a set of boundary integral equations involving differences of the layer potential operators ([31], [48]). Therefore, it is also important to know the properties of these difference operators. The next theorem is a straightforward corollary of the corresponding results given in [47] for the operators $\tilde{\mathbf{K}} - \tilde{\mathbf{K}}_0$ and $\tilde{\mathbf{D}} - \tilde{\mathbf{D}}_0$. Here $\tilde{\mathbf{K}}_0$ and $\tilde{\mathbf{D}}_0$ denote $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{D}}$ with $k = 0$.

Theorem 2.3.5 *Let Ω be a bounded Lipschitz domain and let $\tilde{\mathbf{K}}_j$ and $\tilde{\mathbf{D}}_j$ denote operators $\tilde{\mathbf{K}}$ and $\tilde{\mathbf{D}}$ with wave numbers k_j, $j = 1, 2$, $k_1 \neq k_2$. Then*

$$\begin{aligned}
\tilde{\mathbf{K}}_1 - \tilde{\mathbf{K}}_2 \quad &: \quad TL^2(\partial\Omega) \mapsto TL^2(\partial\Omega) \\
\tilde{\mathbf{D}}_1 - \tilde{\mathbf{D}}_2 \quad &: \quad TL^2(\partial\Omega) \mapsto TL^2(\partial\Omega).
\end{aligned}$$

are compact.

2.4 Boundary integral equations

The boundary integral equation method is based on certain integral representations. A usual method of representing fields is to express them as integrals over sources or fields on surfaces or volumes. Typical sources, for instance, are electric and magnetic currents and electric and magnetic charges. Integral equations can be obtained by various methods, such as using Green's theorem, the reciprocity theorem or field expressions in the terms of vector potentials or Hertz vectors [30]. Here we apply the method based on the (vector) Green's theorem. This method yields the well-known *Stratton-Chu representation formulas.*

In the sequel we will apply the fact that the electromagnetic fields can be represented in a bounded, homogeneous and source free domain by certain integral operators operating on the boundary of the domain. Let us first define the *equivalent electric and magnetic surface currents*[1] as

$$\vec{J} = -\vec{n} \times \vec{H} \mid_{\partial\Omega} \quad \text{and} \quad \vec{M} = \vec{n} \times \vec{E} \mid_{\partial\Omega} .$$

Then the Stratton-Chu representation formulas can be written as follows (for the smooth case see [5]). Here, and in the sequel, $\vec{n}$ is always the outward unit normal of $\partial\Omega$.

Theorem 2.4.1 *Let Ω be a bounded Lipschitz domain and let $\vec{E}$ and $\vec{H}$ be smooth fields defined in Ω, e.g. in $C^2(\Omega)^3$, with $\vec{J}$, $\vec{M} \in TL^p_{\mathrm{Div}}(\partial\Omega)$, $1 < p < \infty$. Assume that $\vec{E}$, $\vec{H}$ and*

[1] Note that in Publications II and III, and in [59] we defined $\vec{J} = -\vec{n} \times \vec{H}$ and $\vec{M} = -\vec{n} \times \vec{E}$.

$\nabla \times \vec{E}$, $\nabla \times \vec{H}$ exist a.e. on $\partial\Omega$ and $\vec{E}^*$ and $\vec{H}^*$ are in $L^p(\partial\Omega)^3$. If $\vec{E}$, $\vec{H}$ is a solution to homogeneous Maxwell's equations in Ω, then we have

$$-\frac{1}{i\omega\gamma}\left(\mathbf{D}_\Omega \vec{J}\right)(x) - \left(\mathbf{K}_\Omega \vec{M}\right)(x) = \begin{cases} \vec{E}(x), & \text{if } x \in \Omega, \\ 0, & \text{if } x \in \mathbb{R}^3 \setminus \bar{\Omega}, \end{cases} \tag{2.4.1}$$

$$\left(\mathbf{K}_\Omega \vec{J}\right)(x) - \frac{1}{i\omega\mu}\left(\mathbf{D}_\Omega \vec{M}\right)(x) = \begin{cases} \vec{H}(x), & \text{if } x \in \Omega, \\ 0, & \text{if } x \in \mathbb{R}^3 \setminus \bar{\Omega}. \end{cases} \tag{2.4.2}$$

The representation formulas for Maxwell's equations follow from the corresponding formulas for the vector Helmholtz equation when proper conditions for $\vec{E}$ and $\vec{H}$ are required, because divergence free solutions to the vector Helmholtz equation satisfies Maxwell's equations, and vice versa [5], [46]. The representation formula for the vector Helmholtz equation in the Lipschitz domains is given e.g. in [46].

Next the boundary value problems introduced in Section 2.2, i.e., Problems 2.2.2 and 2.2.3, are reduced to a set of boundary integral equations by applying the boundary conditions to the Stratton-Chu representation formulas. There are several alternative ways to derive the equations [11], [25]. The method based on the field representations is called a direct method, or a field formulation.

Let $\mathbf{K}_{\Omega_j}$ and $\mathbf{D}_{\Omega_j}$ denote the operators $\mathbf{K}_\Omega$ and $\mathbf{D}_\Omega$ with

$$\Phi_{k_j}(x-y) := \frac{e^{ik_j|x-y|}}{4\pi|x-y|}, \quad k_j = \omega\sqrt{\mu_j\,\gamma_j}.$$

Suppose that in Ω the total electromagnetic field consists of a known primary field $\vec{E}^p$, $\vec{H}^p$, and an unknown secondary field $\vec{E}^s$, $\vec{H}^s$. Furthermore, we define

$$\vec{E}^p_j = \vec{E}^p\,|_{\Omega_j}, \quad \vec{H}^p_j = \vec{H}^p\,|_{\Omega_j}, \quad \vec{E}^s_j = \vec{E}^s\,|_{\Omega_j} \quad \text{and} \quad \vec{H}^s_j = \vec{H}^s\,|_{\Omega_j}\ .$$

Since in the case of the eigenvalue problem, Problem 2.2.2, we have no primary field, the following equations hold for the eigenvalue problem too, when the primary field is omitted.

Let us introduce a notation $\tilde{F} = \vec{n} \times \vec{F}$ and define the following surface currents

$$\vec{J}^s_j = -\tilde{H}^s_j, \ \vec{M}^s_j = \tilde{E}^s_j, \ \vec{J}^p_j = -\tilde{H}^p_j \ \text{ and } \ \vec{M}^p_j = \tilde{E}^p_j.$$

Then the total surface currents are given by

$$\vec{J}_j := \vec{J}^p_j + \vec{J}^s_j \quad \text{and} \quad \vec{M}_j := \vec{M}^p_j + \vec{M}^s_j.$$

We represent both the scattered and primary fields by the Stratton-Chu formulas in Ω_j as follows

$$-\frac{1}{i\omega\gamma_j}\left(\mathbf{D}_{\Omega_j}\vec{J}^p_j\right)(x) - \left(\mathbf{K}_{\Omega_j}\vec{M}^p_j\right)(x) = \begin{cases} 0, & \text{if } x \in \Omega_j, \\ \vec{E}^p_j(x), & \text{if } x \in \Omega \setminus \bar{\Omega}_j, \end{cases}$$

$$\left(\mathbf{K}_{\Omega_j}\vec{J}^p_j\right)(x) - \frac{1}{i\omega\mu_j}\left(\mathbf{D}_{\Omega_j}\vec{M}^p_j\right)(x) = \begin{cases} 0, & \text{if } x \in \Omega_j, \\ \vec{H}^p_j(x), & \text{if } x \in \Omega \setminus \bar{\Omega}_j, \end{cases}$$

and

$$-\frac{1}{i\omega\gamma_j}\left(\mathbf{D}_{\Omega_j}\vec{J}^s_j\right)(x) - \left(\mathbf{K}_{\Omega_j}\vec{M}^s_j\right)(x) = \begin{cases} \vec{E}^s_j(x), & \text{if } x \in \Omega_j, \\ 0, & \text{if } x \in \Omega \setminus \bar{\Omega}_j, \end{cases}$$

$$\left(\mathbf{K}_{\Omega_j}\vec{J}^s_j\right)(x) - \frac{1}{i\omega\mu_j}\left(\mathbf{D}_{\Omega_j}\vec{M}^s_j\right)(x) = \begin{cases} \vec{H}^s_j(x), & \text{if } x \in \Omega_j, \\ 0, & \text{if } x \in \Omega \setminus \bar{\Omega}_j. \end{cases}$$

Then by adding the above equations together, we get in Ω_j

$$
\begin{aligned}
-\frac{1}{i\omega\gamma_j}\left(\mathbf{D}_{\Omega_j}\vec{J}_j\right)(x) - \left(\mathbf{K}_{\Omega_j}\vec{M}_j\right)(x) &= \vec{E}_j^s(x), \\
\left(\mathbf{K}_{\Omega_j}\vec{J}_j\right)(x) - \frac{1}{i\omega\mu_j}\left(\mathbf{D}_{\Omega_j}\vec{M}_j\right)(x) &= \vec{H}_j^s(x).
\end{aligned} \tag{2.4.3}
$$

Letting $x \to \partial\Omega_j$, taking the vector product with $\vec{n}_j$ on the both sides of equations (2.4.3), and by applying the (nontangential) traces of the tangential components of $\mathbf{K}$ and $\mathbf{D}$, we get the following set of boundary integral equations

$$
-\frac{1}{i\omega\gamma_j}(\tilde{\mathbf{D}}_j\vec{J}_j)(x) - \left(\tilde{\mathbf{K}}_j + \frac{1}{2}\mathbf{I}_{M_j}\right)(\vec{M}_j)(x) = -\tilde{E}_j^p(x), \quad \text{a.e. } x \in \partial\Omega_j, \tag{2.4.4}
$$

$$
\left(\tilde{\mathbf{K}}_j + \frac{1}{2}\mathbf{I}_{J_j}\right)(\vec{J}_j)(x) - \frac{1}{i\omega\mu_j}(\tilde{\mathbf{D}}_j\vec{M}_j)(x) = -\tilde{H}_j^p(x), \quad \text{a.e. } x \in \partial\Omega_j, \tag{2.4.5}
$$

for all $j = 1, \ldots, n$. Here

$$
\mathbf{I}_{M_j}(x) = \begin{cases} \mathbf{I}, & \text{if } x \in \partial\Omega_j \setminus \Gamma_j, \\ 0, & \text{if } x \in \Gamma_j, \end{cases} \quad \text{and} \quad \mathbf{I}_{J_j}(x) = \begin{cases} \mathbf{I}, & \text{if } x \in \partial\Omega_j \setminus \Lambda_j, \\ 0, & \text{if } x \in \Lambda_j, \end{cases}
$$

and $\mathbf{I}$ denotes the identity operator. Equation (2.4.4) is called an *electric field integral equation* (EFIE) and (2.4.5) is called a *magnetic field integral equation* (MFIE).

From (2.4.4) and (2.4.5) we find that on the perfectly conducting portion of the boundary, i.e, as $\vec{M}_j = 0$, EFIE leads to an integral equation of the first kind, whereas MFIE leads to an integral equation of the second kind. Obviously a converse result holds on the magnetic wall Λ_j. On the transmission boundary $\Upsilon_{j,m}$, on the other hand, both EFIE and MFIE lead to integral equations of the second kind.

Usually the fundamental integral equations (2.4.4) and (2.4.5) are combined on the transmission boundaries $\Upsilon_{j,m}$ in order to get as many equations as unknowns. Let us multiply the equations arising from $\partial\Omega_j$ by complex constants a_j and b_j, and the equations arising from $\partial\Omega_m$ by constants a_m and b_m, respectively. Next we subtract the equations from each other. The transmission conditions on $\Upsilon_{j,m}$ imply

$$
\vec{J}_j\,|_{\Upsilon_{j,m}} = -\vec{J}_m\,|_{\Upsilon_{j,m}} \quad \text{and} \quad \vec{M}_j\,|_{\Upsilon_{j,m}} = -\vec{M}_m\,|_{\Upsilon_{j,m}}\,.
$$

Let $\vec{J} := \vec{J}_j\,|_{\Upsilon_{j,m}}$ and $\vec{M} := \vec{M}_j\,|_{\Upsilon_{j,m}}$. Then the combined equations on $\Upsilon_{j,m}$ read

$$
-\frac{1}{i\omega}\left(\frac{a_j}{\gamma_j}\tilde{\mathbf{D}}_j - \frac{a_m}{\gamma_m}\tilde{\mathbf{D}}_m\right)(\vec{J}) - \left(a_j\tilde{\mathbf{K}}_j - a_m\tilde{\mathbf{K}}_m + \frac{1}{2}(a_j - a_m)\mathbf{I}_M\right)(\vec{M}) = 0 \tag{2.4.6}
$$

$$
\left(b_j\tilde{\mathbf{K}}_j - b_m\tilde{\mathbf{K}}_m + \frac{1}{2}(b_j - b_m)\mathbf{I}_J\right)(\vec{J}) - \frac{1}{i\omega}\left(\frac{b_j}{\mu_j}\tilde{\mathbf{D}}_j - \frac{b_m}{\mu_m}\tilde{\mathbf{D}}_m\right)(\vec{M}) = 0. \tag{2.4.7}
$$

There are a lot of possible choices for the coefficients a_j, a_m, b_j and b_m, see e.g. [11] and [25].

2.5 Numerical solution to the integral equations

There are various alternative ways to solve boundary integral equations (see e.g. [21] and [30]). The most popular methods in 3D are the point-matching and Galerkin methods. Here we apply the Galerkin method. By the Galerkin method the degree of the singularity of the operator $\tilde{\mathbf{D}}$ can be decreased by integrating by parts. Furthermore, we assume that the base and test functions are piecewise linear functions. Since various axisymmetric structures are very common in the particle accelerators, we consider separately axisymmetric and arbitrary 3D geometries.

2.5.1 The Galerkin method

In this work we find nonzero solutions to the equations of the following form

$$\mathbf{L}f = 0, \quad \text{and} \quad \mathbf{L}f = g, \tag{2.5.1}$$

where $\mathbf{L}$ is a linear integral operator, f is an unknown function and g is a known function. The operator $\mathbf{L}$ is either an *integral operator of the first kind*

$$(\mathbf{L}f)(x) = \int_{\partial\Omega} K(x,y)\, f(y)\, dSy \tag{2.5.2}$$

or an *integral operator of the second kind*

$$(\mathbf{L}f)(x) = f(x) - \int_{\partial\Omega} K(x,y)\, f(y)\, dSy. \tag{2.5.3}$$

Generally $\mathbf{L}$ can be a combination of (2.5.2) and (2.5.3). The kernel K is a function involving Green's function (Φ_k) or derivatives of Green's function, or both. The method for solving equations (2.5.1) in Hilbert spaces via orthogonal projection into finite dimensional subspaces leads to the method called *Galerkin method* [21].

Let us consider more precisely how the Galerkin method is applied in the present situation. In order to simplify the notations we drop out the subindex j. The unknown surface currents $\vec{J}$ and $\vec{M}$ are expanded by base functions $\vec{j}_l$ and $\vec{m}_l$ as

$$\vec{J}(x) = \sum_{l=1}^{N} \alpha_l\, \vec{j}_l(x) \tag{2.5.4}$$

$$\vec{M}(x) = \sum_{l=1}^{M} \beta_l\, \vec{m}_l(x). \tag{2.5.5}$$

Let

$$\vec{\varphi}_k,\ k = 1,\dots,P \quad \text{and} \quad \vec{\psi}_k,\ k = 1,\dots,Q$$

denote the electric and magnetic test functions (not necessarily equal with $\vec{j}_l$ and $\vec{m}_l$)[2]. At this point the choice of base and test functions is arbitrary. They are fixed later in Sections 2.5.2 and 2.5.3. The testing procedure is carried out through the following lines. The EFIE (2.4.4) is multiplied by the electric test functions via a symmetric scalar product, or a bi-linear form, defined by

$$\left\langle \vec{F}, \vec{G} \right\rangle_S = \int_S \vec{F}\cdot\vec{G}\, dx,$$

where S is the area of integration. This gives the following equations for $k = 1,\dots,P$,

$$-\frac{1}{i\omega\gamma}\sum_{l=1}^{N}\alpha_l \left\langle \vec{\varphi}_k, (\tilde{\mathbf{D}}\vec{j}_l)\right\rangle_{S_k} - \left(\sum_{l=1}^{M}\beta_l \left\langle \vec{\varphi}_k, (\tilde{\mathbf{K}}\vec{m}_l)\right\rangle_{S_k} + \frac{1}{2}\sum_{l=1}^{M}\beta_l \left\langle \vec{\varphi}_k, \vec{m}_l\right\rangle_{S_k}\mathbf{I}_M\right) = -\left\langle \vec{\varphi}_k, \tilde{E}^p\right\rangle_{S_k}.$$

Here $S_k \subset \partial\Omega$ is the support of $\vec{\varphi}_k$, so that $S = \cup_{k=1}^{P} S_k$ is the portion of $\partial\Omega$ where the testing procedure is carried out (either Γ, Υ or Λ). In a similar fashion the MFIE (2.4.5) is tested by the magnetic test functions. This leads to the following equations for $k = 1,\dots,Q$,

$$\left(\sum_{l=1}^{N}\alpha_l \left\langle \vec{\psi}_k, (\tilde{\mathbf{K}}\vec{j}_l)\right\rangle_{S_k} + \frac{1}{2}\sum_{l=1}^{N}\alpha_l \left\langle \vec{\psi}_k, \vec{j}_l\right\rangle_{S_k}\mathbf{I}_J\right) - \frac{1}{i\omega\mu}\sum_{l=1}^{M}\beta_l \left\langle \vec{\psi}_k, (\tilde{\mathbf{D}}\vec{m}_l)\right\rangle_{S_k} = -\left\langle \vec{\psi}_k, \tilde{H}^p\right\rangle_{S_k},$$

[2] In the literature there are various definitions for the Galerkin method. In the electromagnetic engineering community above method is called a Galerkin method if the test and base functions are identical, otherwise the method is called the method of moments. Here we follow the definition of [21].

where $S_k = \mathrm{supp}(\vec{\psi}_k)$.

The above discretized EFIE and MFIE can be written shortly by the following matrix equations

$$-\frac{1}{i\omega\gamma}A^{(E,J)}\alpha - \left(B^{(E,M)} + \frac{1}{2}C^{(E,M)}\,I_M\right)\beta = -e^E, \tag{2.5.6}$$

$$\left(B^{(H,J)} + \frac{1}{2}C^{(H,J)}\,I_J\right)\alpha - \frac{1}{i\omega\mu}A^{(H,M)}\beta = -h^H, \tag{2.5.7}$$

where (after integrating by parts twice)

$$\begin{aligned} A^{(E,J)}_{k,l} &= \int\limits_{\partial S_k} \vec{\nu}_k\cdot(\vec{\varphi}_k\times\vec{n})\;(\mathbf{S}_{S_l}\,Div\,\vec{j}_l)\,dl - \int\limits_{S_k} Div\;(\vec{\varphi}_k\times\vec{n})\;(\mathbf{S}_{S_l}\,Div\,\vec{j}_l)\,dS, \\ &\quad - \int\limits_{\partial S_k}\vec{\nu}_k\cdot(\vec{\varphi}_k\times\vec{n})\int\limits_{\partial S_k}\Phi\,\vec{\nu}_k\cdot\vec{j}_l\,dl\,dl + \int\limits_{S_k} Div\;(\vec{\varphi}_k\times\vec{n})\int\limits_{\partial S_k}\Phi\,\vec{\nu}_k\cdot\vec{j}_l\,dl\,dS \\ &\quad + k^2\int\limits_{S_k}(\vec{\varphi}_k\times\vec{n})\cdot(\mathbf{S}_{S_l}\,\vec{j}_l)\,dS, \quad k=1,\dots,P,\ l=1,\dots,N \end{aligned} \tag{2.5.8}$$

$$\begin{aligned} B^{(E,M)}_{k,l} &= \int\limits_{S_k}\vec{\varphi}_k\cdot\int\limits_{S_k}\vec{n}\times(\nabla\Phi\times\vec{m}_l)\;dS\,dS \\ &= \int\limits_{S_k}(\vec{\varphi}_k\times\vec{n})\cdot(\mathbf{K}_{S_l}\,\vec{m}_l)\,dS, \quad k=1,\dots,P,\ l=1,\dots,M, \end{aligned} \tag{2.5.9}$$

$$\begin{aligned} C^{(E,M)}_{k,l} &= \int\limits_{S_k}\vec{\varphi}_k\cdot\vec{m}_l\,dS, \quad k=1,\dots,P,\ l=1,\dots,N, \\ e^E_k &= \int\limits_{S_k}\vec{\varphi}_k\cdot\tilde{E}^p\,dS, \quad k=1,\dots,P, \end{aligned}$$

I_j and I_m are unit matrices, and the coefficient vectors are

$$\alpha = [\alpha_1,\dots,\alpha_N]^T, \quad \beta = [\beta_1,\dots,\beta_M]^T.$$

Above $\vec{\nu}_k$ stands for a unit outward normal of ∂S_k. In order to apply the integration by parts, we have to assume that the surface divergence of functions $\vec{\varphi}_k\times\vec{n}$ and $\vec{j}_l$ ($\vec{\psi}_k\times\vec{n}$ and $\vec{m}$, respectively) exists. In the operators $\mathbf{S}_{S_l}\vec{F}$ and $\mathbf{K}_{S_l}\vec{F}$ the integration is extended over the support of $\vec{F}$, which we have denoted by S_l. The other matrix and vector elements are obtained with obvious modifications. In a similar fashion we may write the matrix equations due to the combined equations (2.4.7) and (2.4.7) ([59]).

Repeating this procedure for all integral equations in each homogeneous region leads to a homogeneous (block-)matrix equation (Problem 2.2.2)

$$S\,c = 0, \tag{2.5.10}$$

or to a nonhomogeneous (block-)matrix equation (Problem 2.2.3)

$$S\,c = b. \tag{2.5.11}$$

Here S is a block matrix whose components are $A^{(E,J)}$, $B^{(E,M)}$, etc., and c is a vector containing the coefficients of the piecewise linear base functions. We find that the original problem is reduced to the problem of finding a nonzero c satisfying one of the above matrix equations. How to find a solution to the latter equation is obvious. Let us consider the

former case. Obviously, if S is nonsingular, the only solution of the homogeneous matrix equation is $c = 0$. Thus, the matrix S must be singular for a nonzero solution. At resonance, i.e., when S is singular, the condition number of S explodes, and the solution $c \neq 0$ of the equation (2.5.10) is a constant times the eigenvector of S corresponding to the least singular value of the matrix S. The resonances of a given structure may be found by studying the condition number of $S(\xi)$, denoted by $cond\, S(\xi)$, depending on a free parameter ξ. The parameter ξ can be either the frequency of the field or the length (or size) of the resonator.

Once the coefficients c are found, the fields $\vec{E}$ and $\vec{H}$ can be evaluated using the Stratton-Chu representations (2.4.1) and (2.4.2). Because of the singularities of the integral operators, the field computation near the boundaries requires a special attention. Note that at the boundary the fields are determined by the surface currents as follows

$$\begin{aligned} \vec{E}\,|_{\partial\Omega} &= \vec{n} \times (\vec{E} \times \vec{n}) + (\vec{n} \cdot \vec{E})\,\vec{n} = -\vec{n} \times \vec{M} - \frac{1}{i\omega\gamma} Div\,(\vec{J})\,\vec{n} \\ \vec{H}\,|_{\partial\Omega} &= \vec{n} \times \vec{J} - \frac{1}{i\omega\mu} Div\,(\vec{M})\,\vec{n}. \end{aligned}$$

In the following two sections we briefly recall the essential features of the numerical computation of the matrix elements (2.5.8) and (2.5.9), and the computation of the fields. In particular, we consider the questions of the choice of the test and base functions as well as numerical implementation of the singular integral equations. These questions are essential in order to get a numerically efficient algorithm.

2.5.2 Axisymmetric case

The problem of electromagnetic field computing in axisymmetric structures with dielectric windows is considered in Publication II. In this section we shortly recall the main features of the developed numerical methods.

For the boundary surface of an axisymmetric domain with the z axis of the cylindrical coordinate system (r, θ, z) coinciding with the symmetry axis of the domain we have the following parameter representation

$$u(s,\theta) = \{(x_1, x_2, x_3)\,|\,x_1 = r(s)\cos\theta,\ x_2 = r(s)\sin\theta,\ x_3 = z(s)\}, \tag{2.5.12}$$

where (x_1, x_2, x_3) are the Cartesian coordinates in $\mathbb{R}^3$, s is the arc length along the boundary curve $\theta = 0$, i.e., $r'(s)^2 + z'(s)^2 = 1$, $0 \leq s \leq S$ and $0 \leq \theta \leq 2\pi$.

The tangential unit vector $\vec{e}_s$ and the azimuthal unit vector $\vec{e}_\theta$ of the boundary $\partial\Omega$ are given by

$$\begin{aligned} \vec{e}_s(s,\theta) &= \frac{\partial u(s,\theta)}{\partial s} \Big/ \left|\frac{\partial u(s,\theta)}{\partial s}\right| = (r'(s)\cos\theta, r'(s)\sin\theta, z'(s)) \\ \vec{e}_\theta(s,\theta) &= \frac{\partial u(s,\theta)}{\partial \theta} \Big/ \left|\frac{\partial u(s,\theta)}{\partial \theta}\right| = (-\sin\theta, \cos\theta, 0). \end{aligned}$$

Typically the boundary of an axisymmetric domain is divided into conical elements and the surface currents are approximated in angular direction by Fourier series expansions and along the boundary profile of the domain by some low order polynomials. For example, in [26] and [27] the following approximation is used

$$\vec{F}(y) \approx \sum_{l=1}^{P_s} \sum_{k=1}^{P_t} (\alpha_{k,l}\,\vec{e}_s + \beta_{k,l}\,\vec{e}_\theta)\,u_l(s)\,e^{-ik\theta}, \tag{2.5.13}$$

where $\vec{F}$ stands for $\vec{J}$ or $\vec{M}$, and u_l is a scalar valued piecewise linear base function defined on the boundary profile of the domain. However, for the present application of the field computation in the axisymmetric particle accelerator structures it is sufficient to confine the discussion to the fields in TM_{0ml}-mode. This implies that the fields are independent of the θ-variable and can be written in the cylindrical coordinates as

$$\begin{aligned} \vec{E}(r,\theta,z) &= E_r(r,z)\,\vec{e}_r + E_z(r,z)\,\vec{e}_z \\ \vec{H}(r,\theta,z) &= H_\theta(r,z)\,\vec{e}_\theta . \end{aligned}$$

Thus, we may choose the base functions as $\vec{j}_l(x) = j_l(s)\vec{e}_s$ and $\vec{m}_l(x) = \eta_0 m_l(s)\vec{e}_\theta$ and have the following approximations for the currents

$$\begin{aligned} \vec{J}(s,\theta) &\approx \sum_{l=1}^{P} \alpha_l\, j_l(s)\,\vec{e}_s \\ \vec{M}(s,\theta) &\approx \eta_0 \sum_{l=1}^{Q} \beta_l m_l(s)\,\vec{e}_\theta . \end{aligned} \tag{2.5.14}$$

Here $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$ is the wave impedance in vacuum, j_l and m_l are scalar valued piecewise linear roof-top functions. Constant η_0 is included to improve the balance of the numerical computations. Thereafter, the test functions are chosen as follows

$$\vec{\varphi}_k = \vec{n} \times \vec{j}_k \quad \text{and} \quad \vec{\psi}_k = \vec{n} \times \vec{m}_k .$$

It is essential to test with $\vec{n} \times \vec{j}_k$ and $\vec{n} \times \vec{m}_k$ instead of $\vec{j}_k$ and $\vec{m}_k$, because the boundary integral equations are derived by applying $\vec{n}\times$ to the integral representations.

After applying the parameter representation (2.5.12) and dividing the boundary into conical segments at points $s_1 < \ldots < s_P$, on the boundary profile, we observe from (2.5.8) and (2.5.9) that we have to calculate the following integrals (the possible boundary terms are omitted here)

$$\int_{s_p}^{s_{p+1}} \int_{s_q}^{s_{q+1}} \int_0^{2\pi} \Phi_k(t,s,\theta)\, Div\, \vec{v}_j(t)\, Div\, \vec{u}_l(s,\theta)\, d\theta\, ds\, dt$$

$$\int_{s_p}^{s_{p+1}} \int_{s_q}^{s_{q+1}} \int_0^{2\pi} \Phi_k(t,s,\theta)\, \vec{v}_j(t) \cdot \vec{u}_l(s,\theta)\, d\theta\, ds\, dt$$

$$\int_{s_p}^{s_{p+1}} \int_{s_q}^{s_{q+1}} \int_0^{2\pi} \vec{v}_j(t) \cdot \left(\nabla_x \Phi_k(t,s,\theta) \times \vec{u}_l(s,\theta)\right)\, d\theta\, ds\, dt,$$

and

$$\int_{s_p}^{s_{p+1}} \vec{v}_j(s) \cdot \vec{u}_l(s)\, ds,$$

for all p, $q = 1, 2, \ldots$. Here $\vec{v}_j$ and $\vec{u}_l$ are piecewise linear functions (either of electric or magnetic type). Obviously the first three integrals have singularities at $x(t) = y(s,\theta)$. Note that the test point x can be assumed to be independent of the angular variable, since in the TM_{0ml}-mode the fields and, thus, also the surface currents are independent of the angular coordinate. Above singular integrals are considered in two parts by writing

$$\Phi_k = (\Phi_k - \Phi_0) + \Phi_0 \quad \text{and} \quad \nabla\Phi_k = \nabla\,(\Phi_k - \Phi_0) + \nabla\Phi_0,$$

where $\Phi_0(x-y) = 1/(4\pi|x-y|)$. We readily see by the series expansion of the exponential function that the kernels involving differences $\Phi_k - \Phi_0$ are weakly singular and allow a straightforward numerical integration. Hence, it remains to consider the integrals with the static kernel Φ_0. We have shown in Publication II that the following θ integrals

$$\int_0^{2\pi} \Phi_0(t,s,\theta)(1+\cos\theta)\,d\theta \quad \text{and} \quad \int_0^{2\pi} \nabla\Phi_0(t,s,\theta)(1+\cos\theta)\,d\theta,$$

can be efficiently evaluated by elliptic integrals of the first and second kind, $\mathcal{K}$ and $\mathcal{E}$. When integrating with respect to t and s variables the elliptic integral of the first kind, $\mathcal{K}$, is logarithmically singular as $|t-s| \to 0$. This singularity can be, however, extracted and computed analytically.

Furthermore, we have developed accurate numerical quadratures with special weight functions for calculating the fields close to the boundaries. After integrating the θ direction by elliptic integrals and extracting the singular terms, we need to calculate the following singular integrals

$$\int_0^S f(s)\ln(d_0^2+s^2)\,ds \quad \text{and} \quad \int_0^S \frac{f(s)}{d_0^2+s^2}\,ds,$$

where d_0 is the distance from the boundary and f is a regular function. Here s is a (normalized) arc length along the boundary at $\theta = 0$. These integrals are evaluated using Gaussian quadrature with the weight functions

$$\ln\frac{1}{x^2+d^2} \quad \text{and} \quad \frac{1}{x^2+d^2}.$$

The evaluation of the weights and quadrature points is discussed in Publication II.

2.5.3 3D case

In Publication V we consider the problem of electromagnetic field computation in 3-dimensional waveguide discontinuities. In this section we introduce the used base and test functions and shortly consider the numerical computation of the singular integral equations.

The boundary of an arbitrary 3D domain is usually divided into flat or curved patches of triangular or rectangular shape. Thereafter, the unknown surface currents are expanded by some low order polynomial approximations. For various applications of different base and test functions, see e.g. [39], [15] and [44]. In this work the surface is divided into flat triangular elements and the surface currents are presented by so called Whitney face functions, or RWG (Rao-Wilton-Glisson) base functions [39]. See also [50], [40] and [41] for other applications of the RWG functions. In a recent paper [10], the authors develop more general higher order base functions.

An RWG function is defined on a triangle pair T^+, T^- having a common edge as follows

$$\vec{f}(y) = \begin{cases} \dfrac{l}{2A^+}(y-p^+), & y \in T^+, \\ -\dfrac{l}{2A^-}(y-p^-), & y \in T^-, \\ 0, & \text{otherwise.} \end{cases}$$

Here $A^\pm$ is the area of the triangle $T^\pm$, l is the length of the common edge and $p^\pm$ is the "free" vertex of $T^\pm$. These base functions have two important features. Firstly, the surface diverge is constant ($\pm l/A^\pm$) on each triangle and secondly the normal component of the

current is continuous across the common edge vanishing on the other edges. Naturally an RWG function is tangential on the boundary.

Let $\mathcal{T}$ denote the triangularization of the boundary. In a similar fashion as in the axisymmetric case we have to evaluate the following integrals

$$\int_{T_p}\int_{T_q} \Phi_k(x-y)\, Div\, \vec{v}_j(x)\, Div\, \vec{u}_l(y)\, dSy\, dSx$$

$$\int_{T_p}\int_{T_q} \Phi_k(x-y)\, \vec{v}_j(x)\cdot\vec{u}_l(y)\, dSy\, dSx$$

$$\int_{T_p}\int_{T_q} \vec{v}_j(x)\cdot(\nabla_x \Phi_k(x-y)\times\vec{u}_l(y))\; dSy\, dSx,$$

and

$$\int_{T_p} (\vec{n}_j(x)\times\vec{v}_j(x))\cdot\vec{u}_l(x)\, dS(x),$$

for all triangles $T_p,\ T_q \in \mathcal{T}$. Here both $\vec{v}_j$ and $\vec{u}_l$ are RWG functions (possibly multiplied by constant η_0). The boundary terms vanish if we expand both $\vec{J}$ and $\vec{M}$ by the RWG functions and choose the test functions as $\vec{n}\times\vec{f}_k$. Obviously the first three integrals have singularities if $T_p \cap T_q \neq \emptyset$. As in the axisymmetric case we first add and subtract the static kernel Φ_0. Then we have applied the formulas presented in [54], [9] and [8] to evaluate the integrals with the static kernel Φ_0 over the triangles. For instance, it has been shown that the following integrals

$$\int_T \psi(y)\,\Phi_0(x-y)\, dy \quad \text{and} \quad \int_T \psi(y)\,\nabla_x\Phi_0(x-y)\, dy,$$

where ψ is a constant function or a linear shape function of T, can be evaluated analytically. This permits a very effective numerical evaluation of the system matrix elements, since only the outer integration of the Galerkin method has to be treated numerically. Also the field computation becomes accurate even very close to the boundaries. Again the remaining terms including kernels

$$\Phi_k - \Phi_0 \quad \text{and} \quad \nabla_x\,(\Phi_k - \Phi_0)$$

are weakly singular and can be evaluated numerically.

2.5.4 Generating mixed waves

For a complete analysis of electron multipacting in input power couplers it is essential to consider a large number of different field distributions, because during the operation of the system, i.e., while filling the accelerator cavity, the reflection conditions on the coupler vary. Next we shortly consider how arbitrary wave forms can be obtained in irregular waveguides by combining two field solutions which are found by the techniques explained in the previous sections. We assume that outside the possible irregularity the structure continues as a homogeneous waveguide with a uniform cross section, either coaxial or rectangular, to the infinity. Generally we may consider a junction of n regular waveguides, but here in order to simplify the notations we consider only a junction of two waveguides, or more precisely, a discontinuity of a single waveguide.

Suppose first that outside the discontinuity the waveguide is uniform in z direction and that the wave propagation along the z-axis is of the form $e^{i\beta z}$, where β is the propagation

constant. We consider a superposition of the waves propagating into positive and negative z directions with amplitudes A and B. Such a wave is called a mixed wave. The electromagnetic fields can then be written in the rectangular coordinates (x, y, z) as ([36])

$$\vec{E}(x,y,z) = E_t(x,y)\,\vec{e}_t\,(A\,e^{i\beta z} + B\;e^{-i\beta z}) + E_z(x,y)\,\vec{e}_z\,(A\,e^{i\beta z} - B\;e^{-i\beta z})\,, \tag{2.5.15}$$

$$\vec{H}(x,y,z) = H_t(x,y)\,\vec{e}_t\,(A\,e^{i\beta z} - B\;e^{-i\beta z}) + H_z(x,y)\,\vec{e}_z\,(A\,e^{i\beta z} + B\;e^{-i\beta z})\,. \tag{2.5.16}$$

Here E_t and H_t represent the transverse electric and magnetic field components, while E_z and H_z are the longitudinal electric and magnetic field components. We want to get an electromagnetic field whose z dependence in the regular waveguide section is of the form

$$\begin{aligned} \vec{E}(z) &= E_t\,\vec{e}_t\,(e^{i\beta z} + R\,e^{-i\beta z}) + E_z\,\vec{e}_z\,(e^{i\beta z} - R\,e^{-i\beta z}) \\ \vec{H}(z) &= H_t\,\vec{e}_t\,(e^{i\beta z} - R\,e^{-i\beta z}) + H_z\,\vec{e}_z\,(e^{i\beta z} + R\,e^{-i\beta z})\,, \end{aligned} \tag{2.5.17}$$

where $R \in \mathbb{C}$, $R = B/A$, $B \leq A > 0$, is a given *reflection coefficient*. Actually, we want to generate an entire family of mixed waves with given $R \in \mathbb{C}$, $|R| \leq 1$.

We have applied two methods. In the first method, applied in Publications II, III and IV, we close the waveguide by properly placed electric walls. The positions of these "pseudo-walls" have to be chosen so that the reflected electromagnetic wave, generated by the discontinuity, has settled down to the fundamental waveguide mode (TEM-mode in coaxial lines and TE_{10}-mode in rectangular waveguides) at the walls. Furthermore, we require that the given frequency, in addition to be chosen so that only the fundamental mode is propagating in the regular waveguide sections, is also a resonant frequency of the resulting cavity. The resonance state of the system is found by studying the condition number of the system matrix as a function of the location of the "pseudo-walls". By this procedure we get standing waves (SW) in a waveguide. By shifting the electric walls (so that the resonance condition is still satisfied) we may model several different SW field patterns in irregular waveguides. The traveling waves (TW) and partially reflected waves, or mixed waves, MW, can be obtained by combing two SW solutions as follows. Let $\vec{E}^{(1)}$, $\vec{H}^{(1)}$ and $\vec{E}^{(2)}$, $\vec{H}^{(2)}$ denote the SW field solutions with electric walls at $z = 0, L_1$ and at $z = L_0, L_2$, where $0 < L_0 < L_1 < L_2$. We calibrate and normalize the fields so that $\vec{E}^{(1)}$, $\vec{H}^{(1)}$ and $\vec{E}^{(2)}$, $\vec{H}^{(2)}$ have the same peak voltage of 1 V. We look for a MW, in the region $z \leq L_0$ or $z \geq L_1$, with a given R as a linear combination of the SW fields as follows

$$\begin{aligned} \vec{E} &= c_1\,\vec{E}^{(1)} + c_2\,\vec{E}^{(2)}, \\ \vec{H} &= c_1\,\vec{H}^{(1)} + c_2\,\vec{H}^{(2)}. \end{aligned} \tag{2.5.18}$$

Here c_1 and c_2 are complex constants, depending on R. The coefficients c_1 and c_2 are solved by substituting the representations of the fields $\vec{E}^{(j)}$, $\vec{H}^{(j)}$, $j = 1, 2$, ((2.5.15) and (2.5.16)) with $A = 1, B = -1$ for $\vec{E}^{(1)}$, $\vec{H}^{(1)}$ and $A = e^{-i\beta L_0}, B = -e^{i\beta L_0}$ for $\vec{E}^{(2)}$, $\vec{H}^{(2)}$ into (2.5.18) and by requiring that the z-dependence of the fields $\vec{E}$ and $\vec{H}$ outside the discontinuity is of the form (2.5.17).

The second method is to apply the fact that the electromagnetic fields are known up to a complex multiplier in the regular sections of the structure. We again close the waveguide, far enough from the discontinuity so that the field is settled down to the fundamental field mode, but now the field form is not fixed at the ends. Rather we suppose that the electromagnetic fields at the ends (numbered by 1 and 2) are given by formulas (2.5.15) and (2.5.16), where constants A_j (input amplitudes) and B_j (output amplitudes), $j = 1, 2$, are unknown. Then we set $A_1 = 1$ and $A_2 = 0$ and find the coefficients B_1 and B_2 by solving the waveguide problem, Problem 2.2.3. Let $B_1^{(1)}$ and $B_2^{(1)}$ denote the found coefficients and $\vec{E}^{(1)}$, $\vec{H}^{(1)}$ the corresponding fields. Next we set $A_1 = 0$ and $A_2 = 1$, and solve the

coefficients $B_1^{(2)}$, $B_2^{(2)}$ and the fields $\vec{E}^{(2)}$, $\vec{H}^{(2)}$. The wanted field is obtained as in the first method above by substituting the representations of the fields $\vec{E}^{(j)}$, $\vec{H}^{(j)}$, $j = 1, 2$, (2.5.15) and (2.5.16) with $A_1 = 1$, $A_2 = 0$, $B_1 = B_1^{(1)}$, $B_2 = B_2^{(1)}$, and thereafter, with $A_1 = 0$, $A_2 = 1$, $B_1 = B_1^{(2)}$, $B_2 = B_2^{(2)}$, into (2.5.18) and by requiring that (2.5.17) holds outside the discontinuity. Now the (unnormalized) scattering matrix of a two port system can be given as follows

$$S = \begin{bmatrix} B_1^{(1)} & B_2^{(1)} \\ B_1^{(2)} & B_2^{(2)} \end{bmatrix}.$$

In order to get a unitary scattering matrix, the matrix elements S_{ij}, $i, j = 1, 2$, are normed by factors $\sqrt{P_j/P_i}$, where P_j is the power flow in the waveguide number j. Thus, we may conclude that solving the coefficients $B_j^{(l)}$ is identical with the computation of the scattering matrix.

This method is applied in Publication V in the case of 3-dimensional waveguides. The method is also applied in the axisymmetric case with ceramic windows (but is not reported).

Chapter 3

Electron Multipacting

The mechanism for multipacting can be described as follows [33]. An electron is spontaneously emitted from the surface of an rf structure and driven by the electromagnetic field. When the electron impacts the wall, it may release one or more electrons from the surface of the wall. The number of the secondary electrons depends on the impact energy of the impacting electron and the wall material characteristics at the location of the impact. These secondary electrons are again accelerated by the field, yielding new impacts and possibly new secondary electrons. In appropriate conditions the process repeats and the number of electrons may increase exponentially, leading to an electron avalanche - multipacting. The conditions for multipacting can be summarized as follows:

1. An electron emitted from the cavity wall is driven by the electromagnetic field and returns back after an integer number of rf cycles to the same point of the cavity wall.

2. The impacting electron produces more than one secondary electron.

Multipacting phenomena can be divided into two categories. In the first case multipacting is predominantly due to the electric field [55], [56], [43]. The electrons are accelerated by a high electric field in the region of a low magnetic field. This kind of multipacting is called *electric multipacting*. In the second category, so called *magnetic multipacting*, the electrons are again primarily accelerated by the electric field, but the shape of the multipacting trajectories is mostly due to a high magnetic field [1], [17], [34]. Typically similar multipacting processes of different order repeat on discrete field levels. The order of the multipacting process is defined as the number of full rf periods needed for a complete trajectory cycle.

In the past, up to late 70's, multipacting was a major performance limitation especially in the superconducting cavities so that it was impossible to increase the cavity fields by rising the incident power [1], [24]. The accelerating gradient was practically limited up to a couple of MV/m. A significant step towards higher gradients was the finding that multipacting can be overcome by changing the cavity shape from a cylindrical to a spherical or elliptical one [17]. Nowadays multipacting can be avoided in most $\beta = v/c = 1$ cavities by choosing a proper cavity shape. However, multipacting still plays a significant and unpleasant role in many types of rf vacuum structures, such as low β cavities, couplers, transmission lines and rf windows [33]. Especially, it is crucial for the input couplers to avoid such rf operation conditions which lead to multipacting.

A general cure against multipacting is to avoid the resonant conditions by either a proper choice of the geometry or by coating the critical areas by a material with a lower secondary yield [32], [37]. In many cases, however, it might not be possible to change the rf geometry

sufficiently and the coating, which is typically used to reduce the secondary yield of a ceramic window, does not suppress completely multipacting and the success rate of the reduced secondary yield is often unsatisfactory. In those cases, other suppressing methods must be applied, like static electric [49] or magnetic perturbations, or grooving [35] the surfaces.

3.1 Multipacting and dynamics

Let Ω denote a void cavity with the boundary $\partial\Omega$ and with the time-harmonic rf field given by

$$\vec{E}(x,\varphi) = \vec{E}(x)\sin\varphi \quad \text{and} \quad \vec{B}(x,\varphi) = \vec{B}(x)\cos\varphi,$$

where $x \in \Omega$ and $\varphi = \omega t \in [0, 2\pi]$ is the phase of the field. Let us define a *phase space* as

$$X = \partial\Omega \times [0, 2\pi[.$$

An electron may escape the wall only if the electric field $\vec{E}$ points against the wall. Therefore, we divide X into an electron emitting and non-emitting part by writing $X = G \cup W$, where

$$G = \{\, p = (x,\varphi) \in X \,|\, \vec{n}(x)\cdot\vec{E}(x,\varphi) > 0 \,\} \quad \text{and} \quad W = X \setminus G.$$

Here $\vec{n}$ is the unit normal of $\partial\Omega$ pointing into the exterior of Ω. The set G is called a *bright set* and W is called a *shadow set*. Consider an electron emitted from G at position $x_0 \in \partial\Omega$, the phase at the time of emission being $\varphi_0 \in [0, 2\pi[$. A relativistic electron is accelerated by the rf field $\vec{E}$, $\vec{B}$, according to the following system [23] (assuming that the field of the electron itself is neglected)

$$\text{(3.1.1)} \qquad \begin{cases} \dfrac{d\vec{v}}{dt} = -\dfrac{e}{m}\left(1 - \left(\dfrac{v}{c}\right)^2\right)^{1/2}\left(\vec{E} + \vec{v}\times\vec{B} - \dfrac{1}{c^2}(\vec{v}\cdot\vec{E})\vec{v}\right), \\ \dfrac{d\vec{x}}{dt} = \vec{v}\,, \end{cases}$$

where $e(>0)$ is the charge of the electron, m is the rest mass of the electron, $\vec{v}$ is the velocity of the electron, $v = |\vec{v}\,|$ and c is the speed of light in vacuum. Let $p_1 = (x_1, \varphi_1)$ denote the first impact point in X. We define the following mapping

$$\mathcal{P} : p_0 \mapsto p_1.$$

This mapping defines a dynamical system in the phase space X; each point $p_0 \in X$ generates a discrete trajectory $\{p_0, \mathcal{P}(p_0), \mathcal{P}^2(p_0), \ldots\}$. The process stops at step k if $\mathcal{P}^k(p_0) \in W$.

For each impact $k = 1, 2, \ldots$, let $\delta(x_k, E_k)$ be the number of new secondary electrons emitted. Here δ is the *secondary yield function* depending on the wall material characteristics at the location of the impact x_k and the impact energy E_k of the impacted electron. The function δ is strongly material dependent, but for most materials it is larger than one in the range from a few tens of electron-volts to a few thousand electron-volts [33]. Even for the same material δ may vary significantly, depending on the treatment and contamination of the surface.

In suitable conditions the procedure repeats leading to new impacts and new secondary electrons. The number of secondary electrons due to a single electron launched at $p_0 = (x_0, \varphi_0)$ after n impacts is given by

$$N_n(p_0) = \prod_{k=1}^{n} \delta(x_k, E_k(p_{k-1})).$$

For multipacting we require that the number of secondary electrons explodes, that is

$$N_n \to \infty \quad \text{as} \quad n \to \infty.$$

Obviously this is satisfied if the electron stays at the bright set and if $\delta > 1$ for all impacts.

3.2 Numerical methods for analyzing multipacting

The basis of our method consists of standard trajectory calculations in relativistic dynamics. The novel feature is to analyze nearly periodic structures of the resonant trajectories by using special counter and distance functions defined in a multidimensional phase space X. The method has been successfully applied in several structures with various field patterns, such as straight coaxial lines, superconducting cavities, ceramic windows and rectangular waveguides (Publications I and III).

Suppose that the electromagnetic field map is available. Then the electron trajectories can be calculated by integrating the equations of motion (3.1.1), e.g. by the Runge-Kutta method. For a fixed field level $|\vec{E}|$ we send a sufficiently large number of electrons from different points in G and calculate the electron trajectories. The initial velocity is typically a few eV and perpendicular to the wall. Let $p_0^{(j)} = (x_0^{(j)}, \varphi_0^{(j)})$, $j = 1, \ldots, N_0$, denote the initial sites and $p_1^{(j)} = (x_1^{(j)}, \varphi_1^{(j)}) = \mathcal{P}(p_0^{(j)})$ the corresponding points of the first impact in X. If $p_1^{(j)} \in G$ the trajectory calculation is continued. Let n be a given maximum number of impacts. The trajectory calculation is continued up to n impacts, if $\mathcal{P}^k(p_0^{(j)}) \in G$ for all $k \leq n$, otherwise we stop the calculation. In other words, we compute the discrete trajectories

$$\{p_0^{(j)}, \mathcal{P}(p_0^{(j)}), \mathcal{P}^2(p_0^{(j)}), \ldots, \mathcal{P}^n(p_0^{(j)})\},$$

and the corresponding impact energies $E_1^{(j)}, \ldots, E_n^{(j)}$, for all $j = 1, \ldots, N_0$.

After n impacts (usually 20 or 30 impacts are calculated), the number of electrons in the bright set is counted. Depending on whether the secondary yield is taken into account, we call this total number of electrons as a *counter function* (no secondary yield included), given by

$$c_n(|\vec{E}|) = \#\{p_0^{(j)} \in G \,|\, \mathcal{P}^n(p_0^{(j)}) \in G,\ j = 1, \ldots, N_0\},$$

or the *enhanced counter function* (secondary yield included),

$$e_n(|\vec{E}|) = \sum_{j=1}^{N_0} N_n(p_0^{(j)}). \tag{3.2.1}$$

Note that we naturally define

$$N_n(p_0^{(j)}) = 0, \quad \text{if } \mathcal{P}^k(p_0^{(j)}) \in W \text{ for some } k \leq n,$$

i.e., the secondary yield of the shadow set is zero.

We repeat the trajectory calculations with several fixed field levels. The scanning of $|\vec{E}|$ must be sufficiently dense so that none of the multipacting resonances is missed. The maxima of the counter function c_n are the potential multipacting field levels, however, it is not necessary that multipacting occurs at those field levels, because the secondary yield is not yet taken into account. Rather c_n indicates the stability of the process. The enhanced counter function e_n is a good indicator whether the conditions for multipacting are fulfilled.

Basically multipacting occurs at the field level $|\vec{E}|$, if the number of secondary electrons is (much) larger than the number of initial electrons, i.e., if

$$e_n(|\vec{E}|) \gg N_0, \tag{3.2.2}$$

with a sufficiently large n. Usually multipacting occurs on discrete field levels, or rather at field level bands, which might be rather broad. The broadness of the multipacting field levels may be explained by the stability of the process with respect to the perturbations of the field (variation of the field level and phase of the field), rather than by the variation of the initial velocity. In our computations the initial velocity is fixed. Also other factors, such as stability of the rf field, contamination of the surface and multipacting itself, effect to the multipacting. These aspects are, however, not taken into account in our model.

After the possible multipacting field levels are found, we locate the multipacting processes in the phase space X by measuring the distance between the initial and nth impact point in the phase space by the following *distance function*

$$d_n(p_0) = \sqrt{|x_0 - x_n|^2 + \kappa |e^{i\varphi_0} - e^{i\varphi_n}|^2}, \tag{3.2.3}$$

where κ is an appropriately chosen scaling factor (e.g. $\kappa = \lambda/(2\pi)$). Obviously, the minima of the function d_n point out the starting points and phases of those resonant trajectories that survive n impacts and are able to multipact. By recalculating the electron trajectories by using these minima as initial points we may identify the multipacting processes. In other words, we can determine the order of the process and whether multipacting is due to the electric or magnetic field.

Chapter 4

Numerical Results and Multipacting Analysis

In this section we review the main results of our multipacting analysis and field computations in the TESLA particle accelerator structures. We begin by considering the analysis of electron multipacting in a simple geometry where the electromagnetic fields allow analytical expressions, but the multipacting resonances cannot be solved analytically, namely in a straight coaxial line. This simple case is considered in Publications I and further results are presented in reports [57] and [58]. A coaxial line is of a great interest since many of the present input couplers include long straight coaxial sections. Thereafter, we consider the electromagnetic field computation and multipacting analysis in the TESLA accelerator cavities and input power couplers with ceramic windows. The results are presented in Publications II, III, V (field computations) and in Publication IV (multipacting analysis). In rf cavities multipacting has been analyzed by numerous authors, see e.g. [1], [2], [17] and [24], but the input couplers with ceramic windows were not systematically analyzed before.

4.1 Multipacting in coaxial lines

In the coaxial lines with the standing wave (SW) operation, i.e., $R = 1$, we have found that both one-point multipacting on the outer conductor and two-point multipacting between the conductors appear always close to the maxima of the electric field (electric multipacting). Outside the maxima the electrons tend to drift away from the maxima due to the magnetic field, eventually drifting into shadow regions. Thus, the processes are defocusing in the spatial direction. Furthermore, we have found that the electric multipacting is focusing in the phase direction.

In the traveling wave (TW) operation, i.e., when $R = 0$, we have found that the distribution of the multipacting power levels and the multipacting processes resemble the SW case, but the electrons are traveling along with the wave as the wave form moves. This traveling is, however, rather slow; the distance between successive wall impacts is typically a couple of mm. This tells that, the magnetic field must play a crucial role in the process and multipacting is due to both electric and magnetic fields. The wall impacts of the stable trajectories appear still close to the maximum of the electric field. In addition, we have found that the corresponding SW and TW multipacting power levels of different order satisfy the following simple scaling law

$$P_{TW} = 4P_{SW}. \tag{4.1.1}$$

For more general waves, $0 < R < 1$, we have found two families of multipacting processes, which clearly have a different behavior. The first one appears close to the electric field maxima (electric multipacting) and the multipacting power levels allow the follow scaling law

$$P_R^{\text{electric}} \sim \frac{1}{(1+R)^2} P_{TW} = \frac{4}{(1+R)^2} P_{SW}, \tag{4.1.2}$$

as the reflection coefficient R is varied. The other processes appear close to the maxima of the magnetic field (magnetic multipacting). Magnetic multipacting is found to be focusing in both phase and spatial directions. In the TW operation ($R = 0$) these two families are merged together, but they start to separate as the reflection coefficient is increased.

By varying the dimensions of the line and the field frequency, we have found the following scaling laws for the multipacting power levels

$$P_{\text{one-point}} \sim (f\,d)^4\, Z, \quad P_{\text{two-point}} \sim (f\,d)^4\, Z^2, \tag{4.1.3}$$

where f is the frequency, d is the outer diameter and Z is the impedance of the line. These scaling laws are valid for all wave forms with $0 \leq R \leq 1$. However, if the impedance is very low, $Z < 20$, the situation starts to resemble the case of parallel electrodes (see Publication I) and the one-point multipacting processes disappear.

It is worth of noticing that in homogeneous geometries where the fields are translation invariant, like in straight coaxial lines and rectangular waveguides, the multipacting analysis may be confined to the real values of the reflection coefficient R. Actually, a complex R shifts the wave by $arg(R)/(4\pi)\lambda$, where $arg(R)$ is the argument, or phase, of R and λ is the wavelength.

4.2 Suppressing multipacting in coaxial lines by DC voltage

Usually multipacting is avoided by a proper choice of the geometry. In many cases, however, it is not possible to sufficiently change the design. Thus, it is important to know the effect of various suppressing methods to multipacting. In Publication I we have considered the suppressing method where the electric field is perturbed by a DC biasing voltage between the conductors of a coaxial line as follows

$$\tilde{E}(r,z,\varphi) = \vec{E}(r,z,\varphi) + \frac{V}{r\ln(b/a)}\,\vec{e}_r, \tag{4.2.1}$$

with a constant biasing voltage V. By varying the voltage V and computing the multipacting field levels, we have found that in the straight coaxial lines the biasing DC voltage scales according to the following scaling laws, for one-point and two-point multipacting,

$$V_{\text{one-point}} \sim (f\,d)^2\, Z, \quad V_{\text{two-point}} \sim (f\,d)^2\, Z^2. \tag{4.2.2}$$

These scaling laws are valid for all wave forms with $0 \leq R \leq 1$. However, because the impact energy scales differently, the DC voltage which is required to suppress multipacting satisfies roughly the following rule [58]

$$V \sim f\,d\,Z.$$

4.3 Field computation and multipacting in cavities

A key component of a particle accelerator is the device which imparts energy to the beam. This is an electromagnetic cavity resonating at a certain resonant or eigen frequency. When

the particle beam passes through the accelerating cavity, the beam absorbs the energy increasing the velocity of the particles. Typically accelerating cavities consist of a chain of coupled single-cell cavities. The dimensions of the cavity must be chosen so that the rf electric field is inverted in the time a particle needs to travel from one cell to the next one [33]. Thus, for $\beta = 1$ cavities the length of the cavity cells must be $\lambda/2$.

In order to carry out the multipacting analysis in the axisymmetric TESLA cavities the electromagnetic fields must be calculated. The superconducting TESLA cavities consist of nine cells made of niobium. Due to the symmetry of the accelerating field mode, TM_{010}-mode (or π-mode), there are magnetic walls between the cavity cells. The field computation problem in a single-cell cavity can be formulated as follows.

Problem 4.3.1 *Let Ω denote a single-cell cavity with a superconducting ($\sigma = \infty$) conducting wall Γ and let Λ_1 and Λ_2 denote the magnetic ends so that the boundary of Ω is given by $\partial\Omega = \Gamma \cup \Lambda_1 \cup \Lambda_2$. Find the non-zero electromagnetic fields $\vec{E}$ and $\vec{H}$ satisfying the time-harmonic Maxwell's equations*

$$\nabla \times \vec{E} = i\omega\mu_0 \vec{H} \quad \textit{and} \quad \nabla \times \vec{H} = -i\omega\varepsilon_0 \vec{E}, \quad \textit{in } \Omega,$$

with the boundary conditions

$$\vec{n} \times \vec{E} = 0 \quad \textit{on } \Gamma \quad \textit{and} \quad \vec{n} \times \vec{H} = 0 \quad \textit{on } \Lambda_j, \quad j = 1, 2. \tag{4.3.1}$$

Here ε_0 and μ_0 are the electromagnetic parameters in vacuum.

The unknowns are the electric surface current $\vec{J} = -\vec{n} \times \vec{H} \mid_\Gamma$ on Γ and the magnetic surface currents $\vec{M}_j = \vec{n} \times \vec{E} \mid_{\Lambda_j}$ on Λ_j, $j = 1, 2$. The resonance state of the system with a fixed geometry is found by studying the condition number of the system matrix while varying the frequency. The eigen frequency of the TESLA cavity is 1.3 GHz.

In a similar fashion we may consider multi-cell cavities, too. In the multi-cell cavities the situation is however more involved. A chain of n coupled cells has n different eigen modes with n different amplitude relations [33]. In Publication IV we consider a 3-cell cavity with so called 0, $\pi/2$ and π-modes, according to the different amplitude relations. In the case of a 3-cell cavity, the field computation problem is identical with Problem 4.3.1 when Γ denotes the conducting surface of all three cells, Λ_1 denotes the left end of the first cell and Λ_2 denotes the right end of the third cell. In a typical accelerator cavity only the π-mode, i.e., all cells are excited to the same field level, is used for acceleration. However, the existence of the other modes is possible because of the different excitation of the individual cells.

The boundary integral equations are derived by applying the boundary conditions (4.3.1) to the integral representations as explained in Section 2.4. In the numerical experiments we have applied two integral equations, EFIE (Electric Field Integral Equation) and MFIE (Magnetic Field Integral Equation), on both conducting boundaries and magnetic walls. This leads to four formulations, referred to EE, EH, HE and HH-formulations. The first letter in the pair stands for the conducting boundary Γ and the second one stands for the magnetic walls Λ_j, $j = 1, 2$. Furthermore, E stands for EFIE and H stands for MFIE. In Publication III we show that the solution is rather sensitive to the type of an integral formulation on the magnetic walls. Actually, MFIE on the magnetic walls, becomes numerically unstable as the discretization gets denser. This is due to the fact that in the axisymmetric case $Div\, \vec{M}_j = 0$ and the MFIE on Λ_j leads to an integral equation of the first kind

$$i\omega\varepsilon_0(\tilde{\mathbf{S}}\vec{M}_j)(x) = 0, \quad x \in \Lambda_j.$$

As well-known, the integral equations of the first kind (with a compact operator) are numerically unstable [21]. More details about the field computations are given in Publications II and III.

Once the electromagnetic field distribution is known and given in a sufficiently fine grid inside the cavity, we can start the multipacting analysis, see Publication IV. The field values at a given point are evaluated by a (bi-)linear interpolation. In the case of a single-cell cavity with TM_{010}-mode, the analysis reveals a broad field level region where the number of secondary electrons is increased. This finding corresponds to a well-known two-point (side-to-side) magnetic multipacting of order one close to the cavity equator [53], [18], [19]. The electrons will drift towards the cavity equator due to the shape of the cavity, eventually ending up to a region with a very low electric field, where the impact energy is not strong enough for electron multiplication. Thus, although the electrons start to repeat resonant trajectories the process does not usually lead to multipacting, because the secondary yield is rather low.

The single-cell case contains the π mode in the multicell cavities, since all cells are excited to the same field level. Furthermore, in the 3-cell cavities with π and 0-modes the field distribution in each individual cell is almost identical, therefore multipacting resonances can be reliably predicted by the single-cell case. In the $\pi/2$-mode, on the other hand, the field distribution in the midmost cell, called an empty cell, is different. Thus, this case needs a special treatment. The analysis finds an one-point multipacting of different order clearly outside the equator of the empty cell. Also in this case the shape of the multipacting trajectories is predominantly due to the magnetic field and the secondary yield is rather low.

4.4 Field computation and multipacting in coaxial couplers with windows

The input power coupler transfers the rf field to the cavity and to the beam. The input coupler must also provide a match between the generator impedance and the combined impedance of the cavity-beam system, so as to minimize the wasted reflected power. The input coupler design for TESLA has been developed at DESY and Fermi National Accelerator Laboratory (FNAL), USA. Both designs consist of two windows, one at 70 K (cold window) and one at room temperature (warm window), bellows, coaxial line and waveguide to coaxial transition. In the FNAL design the cold window has a conical shape, while in the DESY design the cold window is cylindrical. Also the designs for the waveguide to coaxial transitions are different.

In this section we consider the cylindrically symmetric coaxial sections of the coupler designs (Publications II, III and IV). The coaxial to waveguide transitions are typically 3D geometries and so called doorknob transition is discussed in the following section (Publication V). The most critical components in the sense of multipacting are the ceramic windows, which may be broken by a heavy bombing of multipacting electrons. Therefore, the multipacting analysis is especially confined to the surfaces of the (cold) windows. The primary function of the window is to protect the cavity vacuum. The two-window solution is chosen to give a better protection for the cavity against window failures during the operation of the accelerator. Because a pure ceramic (made of aluminum oxide, Al_2O_3) would have a very high secondary yield coefficient [33], it is essential to reduce the secondary emission coefficient of the ceramic by a thin coating of special material. The most usual coating is titanium nitride (TiN). Here, we assume that the ceramic window has the same secondary

yield function as a metallic (niobium) surface.

During the operation of the rf pulse, i.e., while filling the accelerator cavity, the reflection conditions on the input coupler vary. This leads to operating with the mixed waves, and for a complete multipacting analysis we have to consider a large number of electron trajectory simulations with changing reflection conditions. The various wave forms (mixed waves) can be obtained by combining two SW solutions as explained in Section 2.5.4.

For the field computation the input coupler, which in reality is an open ended waveguide with a discontinuity (the window), is modelled as a closed cavity resonator by properly placed electric walls. The resonance state of the system is found by varying the location of the "pseudo"-walls while keeping the frequency fixed (1.3 GHz). The computation domain consists of three homogeneous regions so that the region in the middle is the ceramic window with $\varepsilon_r = 9$ and $\mu_r = 1$. The other regions are assumed to be vacuum. We formulate the field computation problem as the following boundary value, or eigenvalue, problem.

Problem 4.4.1 *Let Ω_j, $j = 1,2,3$, denote the homogeneous regions of the input coupler with constant electromagnetic parameters γ_j and μ_j so that*

$$\gamma_j = \begin{cases} \varepsilon_0, & \text{if } = 1 \text{ or } 3 \\ 9\varepsilon_0, & \text{if } j = 2 \end{cases} \qquad \text{and} \quad \mu_j = \mu_0 \quad \text{for all} \quad j = 1,2,3.$$

Let Γ_j, $j = 1,2,3$, denote the conducting walls of $\partial\Omega_j$ and $\Upsilon_j = \partial\Omega_j \cap \partial\Omega_{j+1}$, $j = 1,2$, denote the interfaces of the homogeneous regions (surfaces of the window). Find the non-zero electromagnetic fields $\vec{E}_j$ and $\vec{H}_j$ satisfying the time-harmonic Maxwell's equations

$$\nabla \times \vec{E}_j = i\omega\mu_j \vec{H}_j \quad \text{and} \quad \nabla \times \vec{H}_j = -i\omega\varepsilon_j \vec{E}_j, \quad \text{in } \Omega_j, \quad j = 1,2,3,$$

with the boundary conditions

$$\vec{n}_j \times \vec{E}_j = 0 \quad \text{on } \Gamma_j, \; j = 1,2,3, \tag{4.4.1}$$

$$\vec{n}_j \times \vec{E}_j = -\vec{n}_{j+1} \times \vec{E}_{j+1} \quad \text{on } \Upsilon_j, \; j = 1,2, \tag{4.4.2}$$

$$\vec{n}_j \times \vec{H}_j = -\vec{n}_{j+1} \times \vec{H}_{j+1} \quad \text{on } \Upsilon_j, \; j = 1,2. \tag{4.4.3}$$

Here $\vec{n}_j$ denotes the exterior unit normal of $\partial\Omega_j$.

The unknowns are the electric surface currents $\vec{J}_j$ on $\partial\Omega_j$, $j = 1,2,3$, i.e., on the conducting and dielectric surfaces, and the magnetic surface currents $\vec{M}_j$ on the dielectric surfaces Υ_m, $j = 1,2,3$, $m = 1,2$. The boundary integral equations are derived by applying the boundary conditions (4.4.1) - (4.4.3) to the integral representations, see Section 2.4.

On the conducting surfaces we have applied both EFIE and MFIE. On the surfaces of the window, we have used the following choices for the coefficients of the combined equations (2.4.7) and (2.4.7)

$$\begin{aligned} a_j = 1, \;\; a_m = 1, \;\; b_j = 1, \;\; b_m = 1, & \qquad (\mathrm{CFF}^+) \\ a_j = 1, \;\; a_m = -1, \;\; b_j = 1, \;\; b_m = -1, & \qquad (\mathrm{CFF}^-) \\ a_j = \varepsilon_j^r, \;\; a_m = -\varepsilon_m^r, \;\; b_j = \mu_j^r, \;\; b_m = -\mu_m^r, & \qquad (\text{Müller}) \end{aligned}$$

where $j = 1,2$, $m = j+1$ and $\varepsilon_j^r = \varepsilon_j/\varepsilon_0$ and $\mu_j^r = \mu_j/\mu_0$. Furthermore, we have applied an additional formulation where the equations due to the transmission conditions are not combined. This gives overdetermined equations on Υ_j. In Publication III we show that by this overdetermation we can improve the numerical stability of the equations. Especially CFF^+ and CFF^- turn out to be rather sensitive to the choice of the test functions at the

singular junctions of the metallic and dielectric surfaces, and to the perturbations of the resonance conditions as the discretization gets denser.

The multipacting analysis (Publication IV) finds the following main features. In the DESY design we have found one-point multipacting of different order on the inner surface of the window on the cold side (the section from the cold window to the cavity). On the warm side (the section from the cold window to the waveguide) we have found one-point multipacting of different order on the outer conductor. These multipacting processes, however, appear on rather small areas on the reflection chart, and may be avoided by a proper optimization of the design. For example, by placing the window at the right distance from the coupler end.

In the FNAL design we have found two-point multipacting of order one on the cold side between the inner conductor and the surface of the window, and on the warm side between the outer conductor and the surface of the window. In this geometry multipacting appears on a very broad area on the reflection chart and it is not possible to avoid multipacting by optimizing the design. Therefore, other methods such as DC voltage are required to suppress multipacting. However, the effect of biasing DC voltage to multipacting in ceramic windows is still an open question.

4.5 Field computation in doorknob transition

In this section we consider field computation in a special waveguide to coaxial transition, so called doorknob design, see Publication V. In this geometry the multipacting analysis has not yet been carried out. The doorknob transition is a 3-dimensional waveguide to coaxial transition that incorporates a cylindrical knob as the impedance transformation device.

Because the computation of the singular values and vectors is a very time consuming task, especially for large dense matrices, we do not close the design by electric walls and find the resonance state by studying the condition number of the system matrix as a function of the distance between the ends, but we apply another idea, which is introduced in the latter part of Section 2.5.4. The field computing problem can be formulated as follows.

Problem 4.5.1 *Let Ω denote the doorknob design and let Γ denote the conducting wall of Ω. Suppose that the domain Ω is closed by walls Γ_1 and Γ_2 and let $\vec{E}_p$, $\vec{H}_p$ denote a (primary) field generated by the surface currents at the walls Γ_1 and Γ_2. Find the non-zero electromagnetic fields $\vec{E} = \vec{E}_p + \vec{E}_s$ and $\vec{H} = \vec{H}_p + \vec{H}_s$ satisfying the time-harmonic Maxwell's equations*

$$\nabla \times \vec{E} = i\omega\mu\,\vec{H} \quad \textit{and} \quad \nabla \times \vec{H} = -i\omega\varepsilon\,\vec{E}, \quad \textit{in } \Omega,$$

with the boundary condition

$$\vec{n} \times \vec{E} = 0 \quad \textit{on } \Gamma. \tag{4.5.1}$$

For the unknown surface current $\vec{J}$ we derive an EFIE by applying the integral representation of the electric field (2.4.1) and requiring that condition (4.5.1) holds. The derived equation is solved by applying the methods reviewed in Sections 2.5.1 and 2.5.3.

The walls, often called ports, [36], Γ_1 on the waveguide side, and Γ_2 on the coaxial side, are placed far enough from the doorknob area so that the electromagnetic field is settled down to the fundamental field mode. This implies that the source currents $\vec{J}_j$ and $\vec{M}_j$, $j = 1, 2$ are known up to a constant complex multiplier. These constants can be found by computing the scattering matrix of the system.

Because the doorknob design is a complicated 3D structure, a lot of unknowns are required to get an accurate field solution. In the computer used here, the maximum number of unknowns is about 3200. It is not clear whether 3200 is enough for an accurate solution. Thus, some additional methods are required to increase the number of unknowns, for instance, the multipole method [4].

Chapter 5

Conclusions

Electron multipacting is a serious problem in many high power rf structures operating in vacuum. The knowledge of the possible multipacting resonances may be crucial when planning new rf designs and when struggling against multipacting in already existing structures. To this end, we have developed systematic methods to analyze multipacting in arbitrary rf structures. The methods have been applied in various rather complicated structures, such as straight and tapered coaxial lines, ceramic windows, input power couplers, superconducting cavities and rectangular waveguides.

In straight coaxial lines we have found simple scaling laws for the multipacting field levels with respect to the dimensions and frequency of the line. By these laws one can shift the multipacting resonances by appropriately altering the design of the line. However, in many cases it is not possible to change the design sufficiently and other methods are required to avoid multipacting. Therefore, in straight coaxial lines we have studied the effect of a biasing DC voltage to multipacting. In particular, we have found simple scaling laws by which one can optimize the biasing voltage to suppress multipacting in any coaxial line.

In the past, multipacting was the major performance limitation in rf cavities. Therefore, multipacting simulations in rf cavities have received a lot of attention. Eventually it was found that in most $\beta = 1$ cavities multipacting can be overcame by a proper choice of the cavity geometry. In more complicated structures, such as input couplers and ceramic windows, it is more difficult to reliably predict multipacting resonances. In this work we the first time systemically study multipacting in two special window geometries. Because of the complexity of the coupler and window geometries and of the varying field conditions during the operation of the system it is not possible to give any general rules for multipacting. Therefore, in each new design the multipacting resonances have to be recalculated. An interesting open question is how the biasing DC voltage effect to multipacting in ceramic windows.

An important requirement for a reliable multipacting analysis is that the electromagnetic fields are known accurately, especially close to the surfaces, since even small errors in the rf field may destroy the trajectory calculation of a relativistic electron. Therefore, in this work a special emphasis has been given to the development of numerical methods to improve the accuracy of the electromagnetic field computation near the boundaries. We have applied the boundary integral equation method with special integration quadratures and analytical formulas for computing singular integral equations.

Furthermore, in the axisymmetric geometries we have studied the numerical efficiency of various boundary integral equations used frequently in the literature. We have found that in certain cases the choices of an integral formulation and test functions are critical in order

to maintain the numerical stability of a solution as the discretization is made denser. To overcome this instability, we derived an overdetermined formulation which turns out to be sufficiently robust and always leads to a stable solution.

Bibliography

[1] I. Ben-Zvi, J.F. Crawford and J.P. Turneature: Electron multipacting in cavities, *IEEE Trans. Nuclear Science*, Vol. **NS-22**, pp. 54-58, 1973.

[2] R. Boni, V. Chimenti, P. Fernandes, R. Paroni, B. Spataro and F. Tazzioli: Reduction of multipacting in an accelerator cavity, *IEEE Trans. Nuclear Science*, Vol. **NS-32**, No. 5, pp. 2815-2817, 1985.

[3] R. Brinkmann, G. Materlik, J. Rossbach and A. Wagner (Editors): Conceptual design of a 500 GeV e^+e^- linear collider with integrated X-ray laser facility, Volume I, DESY 1997-048, ECFA 1997-182.

[4] W.C. Chew, J.M. Lin, C.C. Lu, E. Michielssen and J.M. Song: Fast solution methods in electromagnetics, *IEEE Trans. Antennas and Propagation*, Vol. **45**, No. 3, pp. 533-543, 1997.

[5] D. Colton and R. Kress: *Integral Equation Methods in Scattering Theory*, John Wiley & Sons, New York, 1983.

[6] D. Colton and R. Kress: *Inverse Acoustic and Electromagnetic Scattering Theory*, Applied Mathematical Sciences 93, Springer Verlag, Berlin Heidelberg, 1992.

[7] D.A. Edwards (editor): TESLA test facility Linac - Design report, *TESLA Reports 95-01*, DESY Print 1995.

[8] T. Eibert and V. Hansen: Calculation of unbounded field problems in free space by a 3D FEM/BEM-hybrid approach, *Journal of Electromagnetic Waves and Applications*, Vol. **10**, No. 1, pp. 61-78, 1996.

[9] R.D. Graglia: On the numerical integration of the linear shape functions times the 3-D Green's function or its gradient on a plane triangle, *IEEE Trans. Antennas and Propagation*, Vol. **41**, No. 10, pp. 1448-1455, 1993.

[10] R.D. Graglia, D.R. Wilton and A.F. Peterson: Higher order interpolatory vector bases for computational electromagnetics, *IEEE Trans. Antennas and Propagation*, Vol. **45**, No. 3, pp. 329-342, 1997.

[11] R.F. Harrington: Boundary integral formulations for homogeneous material bodies, *Journal of Electromagnetic Waves and Applications*, Vol. **3**, No. 1, pp. 1-15, 1989.

[12] C.C. Hsiao and R.E. Kleinman: Mathematical foundations for error estimation in numerical solutions of integral equations in electromagnetics, *IEEE Trans. on Antennas and Propagation*, Vol. **45**, No. 3, pp. 316-328, 1997.

[13] P.L. Huddleston, L.N. Medgyesi-Mitschang and J.M. Putnam: Combined field integral equation formulation for scattering by dielectrically coated conducting bodies, *IEEE Trans. on Antennas and Propagation*, Vol. **AP-34**, No. 4, pp. 510-520, 1986.

[14] P. Hähner: An exterior boundary-value problem for the Maxwell's equations with boundary data in a Sobolev space, *Proc. of the Royal Society of Edinburgh*, Vol. **109A**, pp. 213-224, 1988.

[15] M.S. Ingber and R.H. Ott: An application of the boundary element method to the magnetic field integral equation, *IEEE Trans. on Antennas and Propagation*, Vol. **39**, No. 5, pp. 606-611, 1991.

[16] S. Kagami and I. Fukai: Application of boundary-element method to electromagnetic field problems, *IEEE Trans. Microwave Theory and Techniques*, Vol. **MTT-32**, No. 4, pp. 455-461, 1984.

[17] U. Klein and D. Proch: Multipacting in superconducting RF structures. *Proc. of the Conference of Future Possibilities for Electron Accelerators*, Charlottesville, (1979), WU B 78-34.

[18] J. Knobloch, W. Hartung and H. Padamsee: Multipacting in 1.5-GHz superconducting niobium cavities of the CEBAF shape, *8th Workshop on RF Superconductivity*, Padova, Italy (1997), (SRF 981012-09, Cornell Report).

[19] J. Knobloch: Advanced thermometry studies of superconducting radio-frequency cavities, *PhD Thesis*, Cornell University, CLNS 97-3, 1997.

[20] M. Koshiba and M. Suzuki: Application of the boundary-element method to waveguide discontinuities, *IEEE Trans. Microwave Theory and Techniques*, Vol. **MTT-34**, No. 2, pp. 301-307, 1986.

[21] R. Kress: *Linear Integral Equations*, Applied Mathematical Sciences 82, Springer-Verlag, Berlin Heidelberg, 1989.

[22] R. Kress: On the boundary operator in electromagnetic scattering, *Proc. of the Royal Society of Edinburgh*, Vol. **103A**, pp. 91-98, 1986.

[23] L.P. Landau and E.M. Lifshitz: *Course of Theoretical Physics*, Volume 2. Pergamon 1976.

[24] C.M. Lyneis, H.A. Swettman and J.P. Turneaure: Elimination of electron multipacting in superconducting structures for electron accelerators, *Appl. Phys. Lett.*, Vol. **31**, No. 8, pp. 541-543, 1977.

[25] P.A. Martin and P. Ola: Boundary integral equations for the scattering of electromagnetic waves by a homogeneous dielectric obstacle, *Proc. of the Royal Society of Edinburgh*, Vol. **123A**, pp. 185-208, 1993.

[26] J.R. Mautz and R.F. Harrington: H-field, E-field and combined-field solutions for conducting bodies of revolution, *Arch. Elektron. Übertragungstechn.* (Electron. Commun.), Vol. **32**, pp. 157-164, 1978.

[27] J.R. Mautz and R.F. Harrington: Electromagnetic scattering from a homogeneous material body of revolution, *Arch. Elektron. Übertragungstechn.* (Electron. Commun.), Vol. **33**, pp. 71-80, 1979.

[28] M. Mitrea: The method of layer potentials in electromagnetic scattering theory on nonsmooth domains, *Duke Mathematical Journal*, Vol. **77**, No. 1, pp. 111-133, 1995.

[29] D. Mitrea, M. Mitrea and J. Pipher: Vector potential theory on nonsmooth domains in $\mathbb{R}^3$ and applications to electromagnetic scattering, *The Journal of Fourier Analysis and Applications*, Vol. **3**, No. 2, pp. 131-192, 1997.

[30] N. Morita, N. Kumagai and J.R. Mautz: *Integral Equation Methods for Electromagnetics*, Artech House, London, 1990.

[31] C. Müller: *Foundations of the Mathematical Theory of Electromagnetic Waves*, Springer, Berlin, 1969.

[32] A.R. Nayaiesh, E.L. Garwin, F.K. King and R.E. Kirby: Properties of thin anti-multipactor coatings for klystron windows, *SLAC-PUB-3760*, 1985.

[33] H. Padamsee, J. Knobloch and T. Hays: *RF Superconductivity for Accelerators*, John Wiley & Sons, Inc., New York 1998.

[34] H. Padamsee and A. Joshi: *Journal of Applied Physics*, Vol. **50**, No. 2, pp. 1112- , 1979.

[35] H. Padamsee, D. Proch, P. Kneisel and J. Mioduszewski: Field strengh limitations in superconducting cavities - multipacting and thermal breakdown, *IEEE Trans. Magnetics*, Vol. **17**, No. 1, pp. 947-950, 1981.

[36] D.M. Pozar: *Microwave engineering*, Addison-Wesley, New York, 1990.

[37] D. Proch, D. Einfeld, R. Onken and N. Steinhauser: Measurement of multipacting currents of metal surfaces in RF fields, *WPQ24, IEEE Proceedings, PAC 95*, pp. 1776-1778, 1996.

[38] P. Ola, L. Päivärinta and E. Somersalo: An inverse boundary value problem in electrodynamics, *Duke Mathematical Journal*, Vol. **70**, No. 3, pp. 617-653, 1993.

[39] S.M. Rao, D.R. Wilton and A.W. Glisson: Electromagnetic scattering by surfaces of arbitrary shape, *IEEE Trans. Antennas and Propagation*, Vol. **AP-30**, No. 3, pp. 409-418, 1982.

[40] S.M. Rao and D.R. Wilton: E-field, H-field, and combined field solution for arbitrarily shaped three-dimensional dielectric bodies, *Electromagnetics*, Vol. **10**, pp. 407-421, 1990.

[41] S.M. Rao, C.C. Cha, R.L. Cravey and D. Wilkes: Electromagnetic scattering from arbitrary shaped conducting bodies coated with lossy materials of arbitrary thickness, *IEEE Trans. on Antennas and Propagation*, Vol. **39**, No. 5, pp. 627-631, 1991.

[42] X-Q. Sheng, J-M. Jin, J. Song, C-C. Lu and W.C. Chew: On the formulation of hybrib finite-element and boundary-integral methods for 3-D scattering, *IEEE Trans. on Antennas and Propagation*, Vol. **46**, No. 3, pp. 303-311, 1998.

[43] E. Somersalo, P. Ylä-Oijala and D. Proch: Analysis of multipacting in coaxial lines, *FAE08, IEEE Proceedings, PAC 95*, pp. 1500-1502, 1996.

[44] J.M. Song and W.C. Chew: Moment method solutions using parametric geometry, *Journal of Electromagnetic Waves and Applications*, Vol. **9**, No. 1/2, pp. 71-83, 1995.

[45] R.H. Torres and G.V. Welland: The Helmholtz equation and transmission problems with Lipschitz interfaces, *Indiana University Mathematics J.*, Vol. **42**, No. 4, pp. 1457-1485, 1993.

[46] R.H. Torres and G.V. Welland: Layer potential operators and a space of boundary data for electromagnetism in nonsmooth domains, *Michigan Mathematics J.*, Vol. **43**, pp. 189-206, 1996.

[47] R.H. Torres: A transmission problem in the scattering of electromagnetic waves by a penetrable object, *SIAM J. Mathematical Analysis*, Vol. **27**, No. 5, pp. 1406-1423, 1996.

[48] R.H. Torres: Maxwell's equations and dielectric obstacles with Lipschitz boundaries, *J. London Mathematical Society*, Vol. **57**, pp. 157-169, 1998.

[49] J. Tückmantel: Multipacting calculations for a power DC-biased 75 Ω coupler, *Technical Report 94-26, CERN LEP-2 Notes*, Geneva, Switzerland, 1994.

[50] K. Umashankar, A. Taflove and S.M. Rao: Electromagnetic scattering by arbitrary shaped three-dimensional homogeneous lossy dielectric objects, *IEEE Trans. Antennas and Propagation*, Vol. **AP-34**, No. 6, pp. 758-766, 1986.

[51] G. Verchota: Layer potential and regularity for the Dirichlet problem for Laplace's equation in Lipschitz domains, *J. Functional Analysis*, Vol. **59**, pp. 572-611, 1984.

[52] J.L. Volakis, T. Özdemir and J. Gong: Hybrid finite-element methodologies for antennas and scattering, *IEEE Trans. Antennas and Propagation*, Vol. **45**, No. 3, pp. 493-507, 1997.

[53] W. Weingarten: Electron loading, *Proceedings of the 2nd workshop on RF superconductivity*, edited by H. Lengeler, CERN, Geneva, Switzerland, CERN, pp. 551-582, 1984.

[54] D.R. Wilton, S.M. Rao, A.W. Glisson, D.H. Schaubert, O.M. Al-Bundak and C.M. Butler: Potential integrals for uniform and linear source distributions on polygonal and polyhedral domains, *IEEE Trans. Antennas and Propagation*, Vol. **AP-32**, No. 3, pp. 276-281, 1984.

[55] R. Woo: Multipacting discharges between coaxial electrodes, *J. Appl. Phys.*, Vol. **39**, No. 3, pp. 1528-1533, 1968.

[56] A. Woode and J. Petit: Investigations into multipactor breakdown in satellite microwave payloads. *ESA Journal 1990*, Vol. **14**, pp. 467-477.

[57] P. Ylä-Oijala: Analysis of electron multipacting in coaxial lines with traveling and mixed waves, *TESLA Reports 97-20*, DESY Print, 1997.

[58] P. Ylä-Oijala: Suppressing electron multipacting in coaxial lines by DC voltage, *TESLA Reports 97-21*, DESY Print, 1997

[59] P. Ylä-Oijala: Application of the boundary integral equation method to interior boundary value problems for Maxwell's equations, Licentiates Dissertation, *Rolf Nevanlinna Institute research reports C29*, Helsinki 1998.