Chapter 1

Introduction

1.1 Relativistic ion-atom collisions

The aim of this thesis is to contribute to the theory of relativistic atomic collisions. In relativistic as well as nonrelativistic ion-atom and ion-ion collisions nuclear interactions of the ionic nuclei are of no importance for physical processes. Electromagnetic interactions prevail. Principal physical phenomena occurring in such collisions are, e.g., electronic excitation, ionisation, nonradiative and radiative electron transfer. In relativistic collisions another process, the electromagnetic creation of electron-positron pairs, has been observed as well.

There are two principal features each of which can make an atomic collision relativistic in character. First, large nuclear charge numbers of the colliding ions render a relativistic description of bound states of inner atomic shells mandatory. Second, a relativistic theory for the exchange of an electron is required in collisions with a relative velocity of the collision partners that is comparable to the speed of light. Moreover, for such relativistic collision velocities the retardation of electromagnetic fields of moving charges, neglected in nonrelativistic theories, must be taken into account. In this work collision systems are considered, for which the nuclear charge numbers of the ions are very large and also the collision velocities are comparable to the speed of light, but not approaching the latter.

The acceleration of heavy-ions to relativistic velocities requires large-scale experimental facilities. Table 1.1 lists the main laboratories that are capable of providing beams of highly charged heavy-ions with particle velocities exceeding 75% of the speed of light. As common practice in the field of relativistic atomic collisions, beam energies are given in terms of a Lorentz factor γ corresponding to a Lorentz boost from the laboratory frame to a rest frame of the accelerated ions. Collision experiments with heavy and highly-charged ions are usually performed with solid or gas targets, at rest in the laboratory. Only recently, when the Relativistic Heavy Ion Collider (RHIC) in Brookhaven started operating in July 2000, experiments with counter-propagating colliding beams of heavy ions have become feasible, yielding much higher collision energies compared to fixed target experiments.

The main purpose of investigating high-energy collisions of heavy ions is the study of nuclear interactions and nuclear matter under extreme conditions. The search for new phenomena in nuclear and particle physics has led to the construction of more and more powerful heavy-ion accelerators. However, due to the availability of these experimental facilities also the experimental and theoretical investigation of electromagnetic, or atomic, processes in these high-energy collisions has been revived during the last two decades. It should be mentioned that not only the physics of relativistic atomic collisions has become experimentally accessible by the advent of these accelerator facilities, but also other branches of atomic physics, like spectroscopic and recombination experiments with highly-charged few-electron ions [Mok94]. For

TABLE 1.1. Heavy-ion accelerators, storage rings, and colliders that are able to provide heavy-ion beams with relativistic particle velocities. Some typical accelerated ions are listed as well as typical *beam energies*. The latter are given in terms of the corresponding Lorentz factor γ. Accelerators and storage rings allow for fixed target experiments and the *collision energy* is, hence, characterised by the Lorentz factor γ given in the table. For colliding beam machines the collision energy instead corresponds to a Lorentz factor $2\gamma^2 - 1$, where γ is the Lorentz factor of the counter-propagating beams given in the table.

Accelerators and storage rings		
Schwerionen-Synchrotron (SIS), GSI, Darmstadt, Germany	$C^{6+} \ldots U^{73+}$ ($\gamma \approx 3$)	
Experimentier-Speicherring (ESR), GSI, Darmstadt, Germany	U^{92+} ($\gamma = 1.6$)	
BEVALAC (shut down in 1993), LBNL, Berkeley, U.S.A.	La^{57+} ($\gamma = 2.4$)	U^{92+} ($\gamma = 2.0$)
Alternating Gradient Synchrotron (AGS), BNL, Brookhaven	Au^{79+} ($\gamma = 12.6$)	
Super Proton Synchrotron (SPS), CERN, Geneva, Switzerland	O^{8+}, S^{16+} ($\gamma = 215$)	Pb^{82+} ($\gamma = 170$)
Colliders		
Relativistic Heavy-Ion Collider (RHIC), BNL, Brookhaven, U.S.A.	Au^{79+} ($\gamma = 108$)	
Large Hadron Collider (LHC), CERN, Geneva, Switzerland (under construction)	Pb^{82+} ($\gamma \approx 3000$)	

example, fully stripped uranium ions U^{92+} have been produced first using the BEVALAC at Berkeley. Today, the electron beam ion trap is a competing source of highly charged ions, but for spectroscopic studies of highly charged few-electron systems heavy ion accelerators are still important.

In heavy-ion collisions without nuclear, or strong, interaction between the ionic nuclei, the nuclei remain intact in the course of a collision (except for Coulomb dissociation of the nuclei [BB88, VGS93, BRBW96, NW98]). Such processes are physically possible due to the short-range nature of the strong interaction. The colliding nuclei pass each other at a distance that does not allow for strong interaction, the colliding nuclei exhibit no overlap. Therefore, these collisions are often referred to as *peripheral* or distant heavy-ion collisions. In such collisions all physical processes are of electromagnetic origin.

Moreover, in peripheral collisions with relativistic beam energies the Coulomb deflection of projectile nuclei by target nuclei is typically less than a few mradians [EM95]. Therefore, the marginal Coulomb scattering of the nuclei in high-energy collisions is not important for a theoretical description. An undisturbed linear motion of the ionic nuclei, without momentum transfer between the nuclei during a collision, is an assumption widely adopted in relativistic and even nonrelativistic theoretical approaches to ion-atom collisions [BM92, EM95].

The physics of atomic collisions has been an intensely studied branch of both experimental and theoretical physics at least since the early days of quantum physics. The first theoretical description of charge exchange in atomic collisions, discovered by Henderson in 1923, was given by Thomas (1927) using a classical model. Oppenheimer (1928), and Brinkmann and Kramers (1930) published the first quantum mechanical calculations. Today, even the literature on relativistic peripheral collisions of heavy ions has become very extensive, since the investigation of high-energy peripheral collisions of highly charged nuclei provides a unique physical system to study quantum electrodynamics in the presence of the strongest electromagnetic fields experimentally accessible to date [Tel87]. For general reviews we mainly refer to [BM92], for the nonrelativistic theory, and to [Eic90, EM95], regarding relativistic collisions.

1.2 Survey of experiments

In the following, we want to describe briefly some experiments investigating peripheral heavy-ion collisions, in order to sketch the experimental status of the field.

The experimental investigation of relativistic charge transfer has been carried out since the mid 1980's using the most powerful heavy-ion accelerator at that time, the BEVALAC at the Lawrence Berkeley Laboratory. Cross sections for electron capture by 82, 140, and 200 MeV/u Xe^{54+}, Xe^{53+}, and Xe^{52+} ions incident on thin solid targets from Be to Au have been measured and reported in [MAE$^+$85].[1] In [AMX$^+$87] single electron capture has been investigated also for higher projectile charge numbers and collision energies, e.g., U^{92+} ions with collision energy of 430 and 955 MeV/u, with targets up to Au. In these experiments total capture cross sections have been measured, not differentiating between the various final states of the projectile electron. Two different processes contribute to this total cross section, nonradiative electron capture (NRC) and capture of an electron with the simultaneous emission of a photon, referred to as radiative electron capture (REC). The theoretical understanding of the measured cross sections, based on the relativistic eikonal theory of electron capture [Eic85] and photoelectric cross sections, has been regarded satisfactory. Electron capture measurements in relativistic collisions of bare ions, U^{92+} and La^{57+}, in the 1 GeV/u energy range impinging on solid targets of Cu, Ag and Au have been reported in [BGF$^+$97] as well. Again, the theoretical understanding was found to be satisfactory except for the heavy collision system U^{92+}+Au, where the measured cross section was found to be larger than theoretically predicted by perturbative theories. Using the ESR in Darmstadt, Stöhlker and collaborators have performed electron capture measurements with 223 MeV/u Helium-like U^{90+} impinging on gaseous targets of N_2, Ar, Kr and Xe. They investigated the distribution of final states of the captured electron by means of x-ray spectroscopy of radiation

[1]The collision energy is given here in terms of the kinetic energy of the projectile in the target frame divided by the projectile nuclear mass in atomic mass units (cf. appendix C).

emitted by decaying excited projectile states. Their results, which are not published yet, partly lack theoretical understanding, in particular for the high-Z targets [Stö].

A general feature of the capture of target electrons is the decrease of the total cross section with increasing projectile kinetic energy. Another atomic process has been experimentally confirmed in 1993 [BGF+93], namely 'capture from the vacuum' or bound-electron free-positron pair creation. Regarding the detection of a down-charged projectile ion, this process is appearing like an ordinary electron capture process. But it can be distinguished from the latter by the presence of an emitted positron. An important difference of 'capture from the vacuum' as compared to capture of target electrons is the increase of the cross section with increasing collision energy. In collision experiments, performed closely before the final shutdown of the BEVALAC accelerator, 0.96 GeV/u bare uranium ions (U^{92+}) have been used to observe this process, incident on various solid targets from Mylar foils up to Au. Down-charged U^{91+} have been measured in coincidence with positrons created in the collision. Cross sections have been determined not only for bound-electron free-positron pair production, but also for the creation of free electron-positron pairs in peripheral collisions. It was found that both cross sections are of the same order of magnitude for the U^{91+}+Au collision system. After a series of measurements had been carried out, it was concluded in [BGF+97] that unlike capture and ionisation, bound-free pair creation at collision energies around 1 GeV/u is not reproduced well by any of the existing theoretical approaches.

Gould emphasized in 1984 that the bound-free pair creation process is of importance for the construction of heavy-ion colliders, since it can occur also in peripheral collisions of bare nuclei and its cross section increases with collision energy. The latter fact has been verified experimentally [BGF+94] after it had been theoretically predicted. This capture mechanism limits the lifetime of stored beams of colliding bare ions in heavy-ion colliders, since lower charge-state projectiles are lost from the beam circulating in a ring. Therefore, the experimental and theoretical investigation of bound-free pair creation was stimulated starting in the late 1980's, when the design of the RHIC and LHC colliders began.

Cross sections of capture and pair creation in peripheral collisions have been measured also at higher energies using the 10.8 GeV/u Au^{79+} beam of the Alternating Gradient Synchrotron at Brookhaven [CBD+97, BCD+98]. For this collision energy the perturbative theories well describe experimental data, i.e. the absolute value of the cross section for the Au^{79+}+Au collision as well as the Z_T^2-dependence of the total cross section on the target charge number Z_T.

Electron capture measurements with Pb^{82+} ions at 160 GeV/u, available from the Super Proton Synchrotron at CERN, are reported in [KVD+98, VKD+00, KVD+01]. In peripheral heavy-ion collisions at this energy, the highest used to date in atomic physics experiments, bound-free pair creation becomes the most important mechanism for electron capture. This has been confirmed experimentally.

Many related experiments have been done for similar collision systems and energies, investigating processes like ionisation, free electron-positron pair production, spectra and angular distributions of emitted electrons and positrons, etc.. Here we have sketched briefly the development of relativistic electron-capture experiments during the last fifteen years, since this process is of principal interest in the present work.

1.3 General theoretical approach

Generally, ion-atom collisions are processes involving many particles which mutually interact and which are coupled to the electromagnetic radiation field. It is clear that such many-particle theories are prohibitively complicated for practical calculations. Therefore, suitable idealisations of the physical situation are necessary in order to allow for theoretical investigations. Here, we want to describe briefly the main theoretical background of this work.

The principal model which has been studied theoretically by many authors is the three-particle system comprising two nuclei and a single electron. In fact, this system can be realised in experiments in which, for example, protons or alpha-particles impinge on hydrogenic targets. However, the three-particle model has proved to be extremely useful for understanding other, more complicated collision experiments as well. Today, beams of hydrogenic and bare heavy-ions are available. For the description of collision experiments with such beams and atomic targets, the passive target electrons are usually neglected or enter a theoretical description only indirectly. Qualitatively, it is comprehended that electron motion is primarily governed by the strong electromagnetic field of the heavy and highly charged nuclei.

In a relativistic atomic collision to a good approximation the nuclear motion can be described by classical mechanics while the motion of the electron must be described by quantum theory. This approach is highly successful also in nonrelativistic collisions, although in some circumstances, which are not discussed in this thesis, quantum interference effects are not negligible [BM92]. Moreover, not only the quantum character of the nuclei is simplified, but it is assumed as well that the motion of the nuclei is not influenced by the much lighter electrons. Taking this point of view, a simplified model of an atomic collision is given by the equation of motion of a single quantum-mechanical electron subject to the field of classical point charges moving along prescribed trajectories. As indicated above the Coulomb deflection of the colliding nuclei can often be neglected successfully in theoretical descriptions, in particular of collisions of heavy-ions at high collision energies.

If the motion of electrons and nuclei is not relativistic, the electrons may be treated as spinless particles and the Schrödinger equation can be used. The retardation of the electromagnetic fields of the classical nuclei and magnetic fields are not taken into account. This model is Galilean invariant and referred to as the *impact parameter model*, *semiclassical approximation* or charge-transfer model. The relation between nonrelativistic quantum-mechanical three-particle scattering and the charge-transfer model is described in more detail for example in [BM92]. Recently a precise mathematical discussion has appeared as well [Ito95].

A refined description, necessary for high collision velocities, must take into consideration the magnetic field induced by a moving point nucleus and the retardation of a time-dependent electromagnetic field. In addition, the electronic spin can be described by the Pauli–Schrödinger equation. Note, however, that such quantum theories are neither Galilean nor Lorentz invariant.

Since the present work is concerned with high-energy ion-atom collisions of heavy ions the dynamical equation for electrons must be the Dirac equation with an external electromagnetic field. The electromagnetic field originates from the moving nuclei and includes both electric and magnetic field components and retardation effects. This description allows for Lorentz invariance. In the rest frame of one of the point nuclei, which is denoted by A in the following, this time-dependent Dirac equation reads:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(t,\boldsymbol{x}) = \left[-\mathrm{i}\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + m_{\mathrm{e}}c^2\beta + \frac{-e^2 Z_{\mathrm{A}}}{|\boldsymbol{x}|} + \frac{-e^2 Z_{\mathrm{B}}}{|\boldsymbol{x}'|}\gamma\left(1-\frac{v}{c}\alpha_3\right)\right]\Psi(t,\boldsymbol{x}), \quad (1.1)$$

with

$$\boldsymbol{x}' = \boldsymbol{x} + (\gamma-1)(x^3 - tv)\boldsymbol{e}_3 - \boldsymbol{b}.$$

Gaussian units have been used for the electrical charge. The quantities Z_{A} and Z_{B} denote the charge numbers of the nuclei and m_{e} the electron mass. The $\boldsymbol{e}_3$-axis of the spatial coordinate system has been chosen in the direction of linear motion of nucleus B. The latter moves with velocity v, corresponding to a Lorentz factor γ. The impact parameter of the trajectory is $\boldsymbol{b}$, with $\boldsymbol{b} \perp \boldsymbol{e}_3$, and $\alpha_1, \alpha_2, \alpha_3$ and β denote Dirac matrices. Clearly, in equation (1.1) the Dirac particle is subject to a stationary Coulomb potential of nucleus A and the time-dependent Liénard–Wiechert potential of the moving nucleus B. The numerical solution of equation (1.1), and corresponding Lorentz-transformed equations, is a major topic of this work.

Charge transfer. In the literature equation (1.1) has been used as a model to describe charge transfer in relativistic atomic collisions. The Dirac equation(1.1) has solutions which represent bound states of nucleus A or of nucleus B, as $t \to -\infty$ or as $t \to +\infty$ (cf. chapter 3). Denote by $a_{\mathrm{fi}}(\boldsymbol{b})$ the impact-parameter-dependent amplitude for the transition from an incoming configuration i, say a bound state of nucleus A, to an outgoing configuration f, say a bound state of nucleus B. As shown, e.g., in [EM95] the total cross section σ_{fi} for the nonradiative charge-transfer process i→f is then obtained by integrating the probability $|a_{\mathrm{fi}}(\boldsymbol{b})|^2$ over the entire impact-parameter plane:

$$\sigma_{\mathrm{fi}} = \int |a_{\mathrm{fi}}(\boldsymbol{b})|^2 \,\mathrm{d}^2 b. \quad (1.2)$$

The calculation of the transition amplitudes $a_{\mathrm{fi}}(\boldsymbol{b})$ is accordingly the principal task for the theoretical determination of NRC cross sections. Many different perturbative approaches have been used for that in the literature (see [EM95]). In addition, two-centre coupled channel calculations have been performed, prior to this work, in order to obtain transition amplitudes nonperturbatively [TE88b, TE88a, TE89]. In these numerical calculations the two-centre Dirac equation has been solved numerically using the coupled channel ansatz. They are reproduced and extended in the present work.

We note that the Dirac equation allows for an unambiguous interpretation only in a multi-particle theory, i.e. the framework of quantum field theory, as multiply

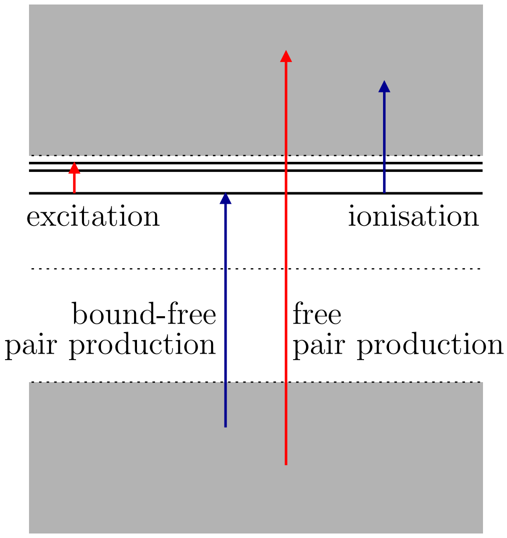

FIGURE 1.1. Furry picture of pair creation by an external perturbation.

discussed in the literature. Therefore, it is not surprising that multi-particle phenomena like pair creation have to be dealt with, as soon as a relativistic description of electron motion is sought.

Pair creation. The description of pair creation in peripheral heavy-ion collisions clearly requires a multi-particle theory. Frequently, pair creation is viewed as a transition from the negative energy continuum of a time-independent Dirac Hamiltonian to a state of positive energy. Consider the electron-positron field in the presence of a static external field, for example the Coulomb potential of nucleus A. The energy spectrum of the corresponding Dirac Hamiltonian is sketched in figure 1.1. Energy eigenvalues in the gap between the negative and positive energy continua correspond to bound states of the static external field, i.e. bound states of classical nucleus A. A time-dependent perturbation, as, e.g., the Liénard–Wiechert potential of nucleus B, leads to transitions between the eigenstates of the time-independent Dirac Hamiltonian of nucleus A,

$$H_{\mathrm{A}} = -\mathrm{i}\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + m_{\mathrm{e}}c^2\beta + \frac{-e^2 Z_{\mathrm{A}}}{|\boldsymbol{x}|}. \tag{1.3}$$

Transitions from the negative energy continuum to the positive energy continuum correspond to the creation of free electron-positron pairs, whereas transitions from states of negative energy to discrete eigenstates of nucleus A represent bound-free pair creation. Note that this theory also describes ionisation, but not charge transfer.

Assuming that the time-dependent perturbation vanishes as $t \to \pm\infty$ (which can be achieved technically by using the adiabatic switching formalism [THA92]) a proper multi-particle interpretation of the seemingly ‘single-particle’ transition amplitudes is obtained by second quantisation. Second quantisation is the construction of a multi-particle Fock space based on the spectral decomposition of the state-space of the classical ‘single-particle’ Dirac equation. For the spectral decomposition, and, therefore, the particle interpretation, reference to a time-independent

Hamilton operator is necessary. The relation between quantum field theory subject to external classical sources and the classical Dirac equation has been discussed in the literature for a long time, starting with the early works of Feynman, Dyson and others (e.g. [Sch58]). It is a mathematically well-established theory (e.g. [SM53, Cap69, Sei72, Rui77a, Rui77b, Rui77c]) discussed in many text books (e.g. [RS79, FGS91, Tha92, Sch95]). We do not review this formalism in the present work but take the 'single-particle' point of view right from the beginning. For a few important remarks we refer to section 3.6.

As an alternative to the Furry picture, in which the particle interpretation refers to the Dirac Hamiltonian with a stationary external Coulomb potential (1.3), the external fields of nuclei A and B may be regarded both as perturbations of the free Dirac Hamiltonian,

$$H_0 = -\mathrm{i}\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + m_{\mathrm{e}}c^2\beta. \tag{1.4}$$

This point of view corresponds to the Feynman–Dyson approach to quantum electrodynamics, in which all particles are asymptotically free. This approach does not allow for particles bound to either classical nucleus A or B. Therefore, the description of the elementary bound-free pair creation process is not feasible in this picture.

In both approaches, the Furry picture and the Feynman–Dyson interaction picture, pair creation cross sections are calculated by the determination of transition amplitudes of the 'single-particle' theory. This has been done using many different approximations. Principally perturbation theory has been used, in combination with a variety of initial and final states (reviewed in [EM95, Ion97]). Moreover, several attempts to solve the two-centre Dirac equation (1.1) numerically using a variety of different techniques have been published (e.g. [MGS91, TBM+92, WOU+92, RSG93, THGS95, MBS96, MGS98, IB99]). These numerical solutions are generally very demanding with respect to computing time and, therefore, their reliability is still more or less limited by this fact. However, for peripheral collisions at small impact parameters of heavy and highly charged nuclei these nonperturbative calculations are regarded to be more appropriate than perturbation theory, due to the very strong electromagnetic interaction in this case.

Finally, let us mention briefly another theoretical approach to describe ionisation and pair creation in peripheral collisions. It makes use of the equivalent-photon method developed by Fermi, von Weizsäcker and Williams [Jac99, EM95], replacing the Liénard–Wiechert potential of nucleus B by a pulse of linearly polarised electromagnetic radiation. This is a suitable approximation for high collision velocities and can be applied to describe many different electromagnetic processes in atoms and nuclei induced by passing charged projectiles [BB88]. The Fermi–Weizsäcker–Williams method has been the basis of the first calculations of electron-positron pair creation in the 1930's, published by Landau and Lifshitz, Bhabha, Racah, Nishina, Tomonaga and Kobayashi. However, we will not encounter this approach in this work again.

1.4 Aim and context

In view of the presumed necessity of a nonperturbative description of bound-free pair creation in peripheral collisions of highly charged nuclei, several different attempts to

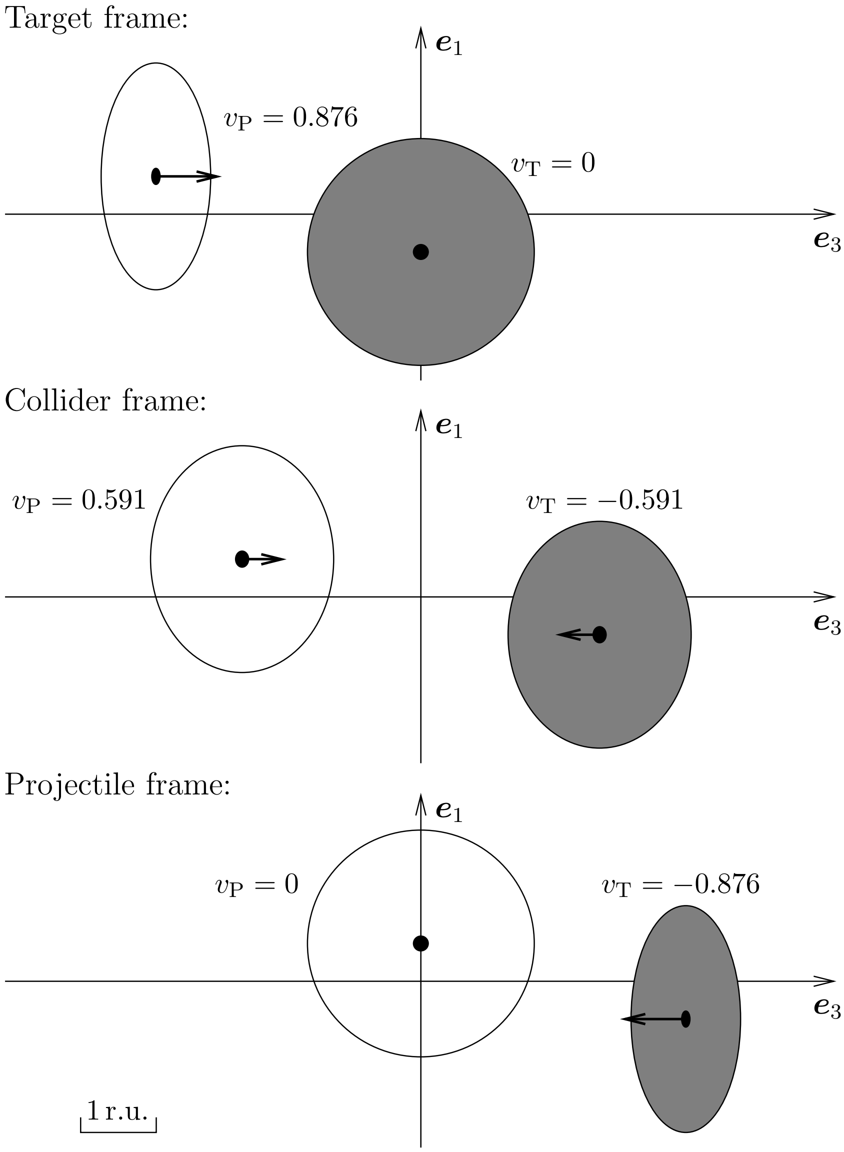

FIGURE 1.2. Three different frames of reference are depicted which have been studied numerically in this work. The Lorentz contraction of moving bound states is shown for a collision energy of 1 GeV/u in all three cases. One centimetre of the drawing corresponds to one relativistic unit of both length and velocity. In relativistic natural units $\hbar = c = m_e = 1$ holds. The Lorentz-contracted circles have the size of the K-shell of uranium (≈ 1.5 r.u.). In all three cases, the impact parameter is 1 r.u. and the time is 4 r.u. before the closest approach of the nuclei.

solve the time-dependent Dirac equation (1.1) numerically have been published. Due to the more or less successful explanation of experimental data at collision energies above 10 GeV/u, or equivalently $\gamma \geq 12$, the energy regime of interest for the present work is 1 GeV/u. By contrast to higher energies, the cross sections of the first experiments observing bound-free pair creation at this intermediate relativistic collision energy have not been reproduced reliably by theoretical calculations [BGF+97].

In particular, single-centre coupled channel calculations have been done to determine probabilities of bound-free pair creation at intermediate relativistic collision energies. In such single-centre calculations the solution $\Psi(t,\boldsymbol{x})$ of equation (1.1) is approximated by a finite linear combination of eigenstates $\Phi_{\mathrm{A},k}(t,\boldsymbol{x})$ of the Coulomb–Dirac Hamiltonian (1.3),

$$\Psi(t,\boldsymbol{x}) = \sum_k c_{\mathrm{A},k}(t)\Phi_{\mathrm{A},k}(t,\boldsymbol{x}), \tag{1.5}$$

and the coefficients $c_{\mathrm{A},k}(t)$ are determined numerically. Some authors have found that a strong nonperturbative enhancement of pair creation is exhibited by these calculations [RMS+91, RSG93] others have argued later that this could not be reproduced if larger coupled channel bases are used [BRBW93, BRBW94].

A principle objection against single-centre expansions as in equation (1.5) is that it does not allow for the description of the charge transfer process. Moreover, the representation of the free-particle states is asymmetrical with respect to the nuclei. In [Eic95] a 'transfer-like' bound-free pair creation description by perturbative means has been proposed. In this approach, the electron bound state and the positron states are referred to different nuclei.

Apart from single-centre coupled channel calculations, also relativistic two-centre coupled channel calculations have been reported [TE88b, TE88a, TE90]. The latter make use of the two-centre expansion,

$$\Psi(t,\boldsymbol{x}) = \sum_k c_{\mathrm{A},k}(t)\Phi_{\mathrm{A},k}(t,\boldsymbol{x}) + \sum_k c_{\mathrm{B},k}(t)\Phi_{\mathrm{B},k}(t,\boldsymbol{x}), \tag{1.6}$$

using bound-state wave functions $\Phi_{\mathrm{A},k}(t,\boldsymbol{x})$ and $\Phi_{\mathrm{B},k}(t,\boldsymbol{x})$ of the nuclei A and B respectively. These calculations allowed for the determination of charge transfer amplitudes and have been carried out as well for the 1 GeV/u collision-energy range. Attempts to describe ionisation in such two-centre calculations as well, by using so-called pseudo-states, have been made [TE89]. Although this approach is very successful in nonrelativistic coupled channel calculations, the use of pseudo-states in relativistic calculations, however, gave rise to serious problems.

A two-centre coupled channel treatment of the Dirac equation (1.1) with a suitable description of free-particle states has not been attempted before this work. However, only such a coupled channel expansion allows for the investigation of two-centre effects in the process of bound-free pair creation. The question arose whether two-centre effects could be a reason for the remaining discrepancies between existing 'excitation-like' descriptions of bound-free pair creation and experimentally determined cross sections.

Another problem, which has not been paid much attention in the literature before this work, is the Lorentz frame dependence of numerical results obtained by means of relativistic coupled channel calculations. Since finite expansions of the form (1.5) and (1.6) respectively can only be approximations to exact solutions of the two-centre Dirac equation, Lorentz invariance is not guaranteed. Such a problem does not exist for nonrelativistic coupled channel calculations, since Galilean boosts do not transform the time axis. A quantitative study of the frame dependence of numerical results has been carried out in the present work. Previous numerical calculations only considered the frame of reference in which the initial electronic configuration before the collision is at rest (top subfigure of figure 1.2). Two other reference frames, which have been used for numerical calculations of the present work, are also shown in figure 1.2. Note that this figure depicts the same collision system as viewed in different reference frames. In fact, the problem of frame dependence of numerical calculations has not been considered in the literature for any of the approaches to solve the time-dependent Dirac equation until now.

For the coupled channel calculations of this work a new computer code had to be written. Owing to the availability of this numerical code it became feasible to extend existing nonperturbative studies of the relativistic charge transfer process. In particular coupled channel calculations for the determination of parametric dependencies of the electron transfer cross section on the charge numbers Z_A and Z_B of the nuclei and the collision energy γ have not been done prior to this work. Such parametric dependencies had been theoretically derived by perturbative approaches only. However, the applicability of perturbation theories is doubtful for collisions of two heavy ions at intermediate relativistic collision energies.

1.5 Outline of this work

Chapter 2 gives a detailed exposition of the semiclassical approximation, i.e. the impact parameter model in which colliding nuclei are represented by classical charge distributions moving along prescribed trajectories. Particular emphasis is put onto the choice of the frame of reference with the aim of formulating a relativistically invariant theory. Symmetries of the two-centre Dirac equation are presented. In *chapter 3* a multi-channel scattering theory for the classical two-centre Dirac equation is formulated. Transition amplitudes are defined, and the asymptotic convergence and orthogonality of the Møller wave operators are proved, provided the charges of the nuclei are screened. A similar presentation of the scattering theory of the two-centre Dirac equation is not available in the literature. In particular we demonstrate the Lorentz invariance of the excitation and transfer amplitudes. The aspects regarding second quantisation are discussed, furthermore, Coulomb boundary conditions are explained. The latter have been used previously to deal with the problem of the long-range nature of the unscreened Coulomb potential in coupled channel and perturbative calculations.

The coupled channel method, employed in the present work for the approximate, but nonperturbative numerical solution of the two-centre Dirac equation, is presented in *chapter 4*. Properties of the fundamental solution of the coupled channel equations and its relation to transition amplitudes are discussed. In *chapter 5* we describe the specific two-centre coupled channel ansatz that was used for the numerical calculations of this work. The basis functions for asymptotically bound and asymptotically free particles are presented and motivation for their choice is given. Numerical results are shown that demonstrate the proper numerical implementation of the coupled channel ansatz. These results not only represent an important test of the software, but also, for the first time, reproduce some existing numerical data found in the literature.

In *chapter 6* we present the new numerical results of this thesis, together with their discussion and comparison with literature. Heavy-ion collision systems with charge numbers ranging from $Z = 66$ to $Z = 92$ are considered at collision energies in the $1\,\mathrm{GeV/u}$ range. In the first sections of the chapter, we discuss coupled channel calculations that use a basis of bound state functions only. Such calculations allow for the theoretical investigation of the relativistic charge transfer process. The frame dependence of such numerical calculations is demonstrated and analysed in this work for the first time. Furthermore, parametric dependencies are studied nonperturbatively, which has likewise not been done before. In the last two sections of chapter 6 results from two-centre coupled channel calculations using bound-state and free-particle basis functions are presented. Such calculations have neither been published nor attempted before. We show results of calculations which have been performed to assess the importance of two-centre effects for the process of bound-free pair creation in peripheral collisions. The problem of frame dependence of the results is discussed, as well as the influence of the free-particle channels on the charge transfer process.

The technical details of the numerical calculations are not described in the main part of the thesis but in *appendix A*. In that appendix not only numerical methods are explained but also some aspects of the implementation of the calculations. In *appendix B* we state and prove some mathematical results referred to in the main chapters, but which are not easily found in literature. *Appendix C* states some conventions and definitions used in this work, in particular it comprises a table of notation and symbols. Finally, relativistic natural units (r.u.) for which $\hbar = c = m_\mathrm{e} = 1$ are used throughout this work, unless specified explicitly.

> **collide, collision.** *It is sometimes asserted that these two words are 'properly' restricted to circumstances involving a violent impact between two moving objects. There is no basis for such a belief. [. . .]*
>
> H. W. Fowler and R. W. Burchfield, *Modern English Usage*