Chapter 2

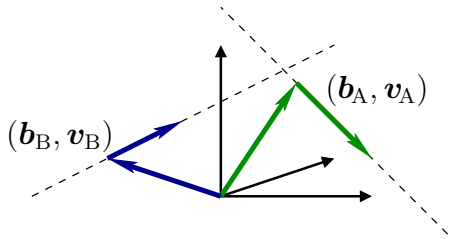
Semiclassical Approximation

In collision experiments with heavy-ion accelerators the laboratory frame is frequently identical to the target frame of reference, in which the initial electronic state is at rest. In the literature, the two-centre Dirac equation has only been considered in the target, collider or projectile frames of reference, with the direction of relative motion chosen as the $\boldsymbol{e}_3$-axis. However, with the aim of formulating a relativistically invariant theory, it is necessary to start with the most general inertial frame, in which the colliding nuclei move in arbitrary directions. Furthermore, this approach provides general insight into the theory. The scattering theory, presented in the next chapter, refers to this general approach.

On the other hand, for numerical calculations, as those presented later in this work, a specific frame of reference must be chosen. Again, in the literature only the target and collider frames have been used for numerical calculations. In this work numerical calculations are presented, which have been done in various different reference frames, thereby showing the influence of the choice of the reference frame on the numerical results.

2.1 Relativistic kinematics

We start by considering an arbitrary frame of reference, where the centres of force A and B move with constant velocities along straight line trajectories. These trajectories will



be written in the following form,

$$\begin{aligned} \boldsymbol{R}_\mathrm{A}(t) &= \boldsymbol{b}_\mathrm{A} + t\boldsymbol{v}_\mathrm{A}, \\ \boldsymbol{R}_\mathrm{B}(t) &= \boldsymbol{b}_\mathrm{B} + t\boldsymbol{v}_\mathrm{B}, \end{aligned} \tag{2.1}$$

with three-velocities $\boldsymbol{v}_\mathrm{A}$ and $\boldsymbol{v}_\mathrm{B}$ that satisfy $|\boldsymbol{v}_\mathrm{A}|, |\boldsymbol{v}_\mathrm{B}| < 1$, and arbitrary three-vectors $\boldsymbol{b}_\mathrm{A}$ and $\boldsymbol{b}_\mathrm{B}$. The world-line corresponding to the trajectory of centre A is given by the four-vector,

$$\mathfrak{X}^\mu_\mathrm{A}(s) = \Big(\gamma_\mathrm{A} s, \boldsymbol{b}_\mathrm{A} + \gamma_\mathrm{A} s\, \boldsymbol{v}_\mathrm{A}\Big),$$

Here, the proper time is denoted by s. The definition of $\mathfrak{X}^\mu_\mathrm{B}(s)$ is analogous. The Lorentz factors, corresponding to the velocities $\boldsymbol{v}_\mathrm{A}$ and $\boldsymbol{v}_\mathrm{B}$, are denoted by γ_A and γ_B

respectively:

$$\gamma_\Gamma = \frac{1}{\sqrt{1-\boldsymbol{v}_\Gamma^2}},$$

with $\Gamma = \mathrm{A}, \mathrm{B}$. The world-line representation $\mathfrak{X}^\mu_\Gamma(s)$ of the trajectories is useful for the computation of Lorentz transformed trajectories, since $\mathfrak{X}^\mu_\Gamma(s)$ transforms like a Lorentz four-vector.

2.1.1 Lorentz invariants. The relative motion of the centres A and B is described entirely by two Lorentz invariant quantities, namely the collision energy and the impact parameter. Their relation to the parameters of the trajectories is discussed next.

Since the modulus $|\boldsymbol{v}_\mathrm{B} - \boldsymbol{v}_\mathrm{A}|$ is not invariant with respect to Lorentz boosts, it is not suitable for a characterisation of the collision energy of the centres. One may, therefore, consider the modulus v of the relative velocity of A and B in a rest frame either of centre A or equivalently of centre B. This velocity v is a Lorentz invariant, as well as the corresponding Lorentz factor $\gamma = (1-v^2)^{-1/2}$, which in terms of $\boldsymbol{v}_\mathrm{A}$ and $\boldsymbol{v}_\mathrm{B}$ is given by:

$$\gamma = \gamma_\mathrm{A}\gamma_\mathrm{B}(1 - \boldsymbol{v}_\mathrm{A}\cdot\boldsymbol{v}_\mathrm{B}). \tag{2.2}$$

As mentioned in the introduction, it is customary to indicate the collision energy, associated with the trajectories (2.1), by this Lorentz factor γ.

Moreover, as opposed to nonrelativistic kinematics, the distance of closest approach of the centres may be different in reference frames which are moving with respect to each other. Hence, the impact parameter b must be defined as the distance of closest approach of the centres in a rest frame of either centre A or centre B. In terms of the parameters $\boldsymbol{b}_\mathrm{A}, \boldsymbol{b}_\mathrm{B}, \boldsymbol{v}_\mathrm{A}$ and $\boldsymbol{v}_\mathrm{B}$ of the pair of trajectories (2.1), the Lorentz invariant impact parameter b is given by the relation:

$$b^2 = \boldsymbol{d}^2 - \frac{\left((\boldsymbol{d}\cdot(\boldsymbol{v}_\mathrm{B}-\boldsymbol{v}_\mathrm{A})\right)^2 - \left((\boldsymbol{d}\cdot\boldsymbol{v}_\mathrm{A})\,\boldsymbol{v}_\mathrm{B} - (\boldsymbol{d}\cdot\boldsymbol{v}_\mathrm{B})\,\boldsymbol{v}_\mathrm{A}\right)^2}{\left(\boldsymbol{v}_\mathrm{B}-\boldsymbol{v}_\mathrm{A}\right)^2 - \boldsymbol{v}_\mathrm{A}^2\boldsymbol{v}_\mathrm{B}^2 + (\boldsymbol{v}_\mathrm{A}\cdot\boldsymbol{v}_\mathrm{B})^2}. \tag{2.3}$$

Here, the abbreviation $\boldsymbol{d} = \boldsymbol{b}_\mathrm{B} - \boldsymbol{b}_\mathrm{A}$ was used. In the limit $|\boldsymbol{v}_\mathrm{A}|, |\boldsymbol{v}_\mathrm{B}| \ll 1$ the nonrelativistic expression for the impact parameter is recovered.

2.1.2 Lorentz scalars. In the following, some Lorentz scalars associated with the pair of trajectories (2.1) are defined for later reference. Let primed quantities refer to a rest frame of centre A, such that the transformed trajectory $\boldsymbol{R}'_\mathrm{A}(t')$ of A satisfies,

$$\boldsymbol{R}'_\mathrm{A}(t') = 0.$$

We define r'_A in the primed coordinate system as the radial distance from the spatial origin, i.e.:

$$r'_\mathrm{A}(t', \boldsymbol{x}') = |\boldsymbol{x}'|.$$

Transforming this quantity back to the unprimed reference frame one obtains,

$$\begin{aligned} r_\mathrm{A}(t,\boldsymbol{x}) &= \left|(\boldsymbol{x}-\boldsymbol{b}_\mathrm{A}) + (\gamma_\mathrm{A}-1)(\hat{\boldsymbol{v}}_\mathrm{A}\cdot(\boldsymbol{x}-\boldsymbol{b}_\mathrm{A}))\,\hat{\boldsymbol{v}}_\mathrm{A} - \gamma_\mathrm{A} t\boldsymbol{v}_\mathrm{A}\right| \\ &= \sqrt{(\boldsymbol{x}_\perp - \boldsymbol{b}_{\mathrm{A}\perp})^2 + \gamma_\mathrm{A}^2\left(\boldsymbol{x}_\parallel - \boldsymbol{b}_{\mathrm{A}\parallel} - t\boldsymbol{v}_\mathrm{A}\right)^2}, \end{aligned} \tag{2.4}$$

which is a Lorentz scalar by definition. Here, the subscripts $\parallel$ and $\perp$ indicate components parallel and perpendicular to the velocity $\boldsymbol{v}_{\mathrm{A}}$. The corresponding scalar with reference to centre B will be denoted by $r_{\mathrm{B}}(t, \boldsymbol{x})$. The Lorentz scalars $r_\Gamma(t, \boldsymbol{x})$ are related to the trajectories $\boldsymbol{R}_\Gamma(t)$ by the following inequality:

$$|\boldsymbol{x} - \boldsymbol{R}_\Gamma(t)| \;\leq\; r_\Gamma(t, \boldsymbol{x}) \;\leq\; \gamma_\Gamma \, |\boldsymbol{x} - \boldsymbol{R}_\Gamma(t)| \,, \tag{2.5}$$

with $\Gamma = \mathrm{A}, \mathrm{B}$.

Moreover, consider the distance between centres A and B at time t' in the primed frame, the rest frame of centre A, and define,

$$d'_{\mathrm{A}}(t', \boldsymbol{x}') = |\boldsymbol{R}'_{\mathrm{B}}(t')|.$$

By substituting $t' = \gamma_{\mathrm{A}}(t - \boldsymbol{v}_{\mathrm{A}} \cdot (\boldsymbol{x} - \boldsymbol{b}_{\mathrm{A}}))$ the Lorentz scalar $d_{\mathrm{A}}(t, \boldsymbol{x})$ in the unprimed frame is obtained. A purely algebraic calculation shows that $d_{\mathrm{A}}(t, \boldsymbol{x})$ is given by:

$$d_{\mathrm{A}}(t, \boldsymbol{x})^2 = b^2 + \left\{ \frac{\gamma_{\mathrm{B}} \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{d}}{\gamma v} - \frac{\gamma_{\mathrm{A}} \boldsymbol{v}_{\mathrm{A}} \cdot \boldsymbol{d}}{\gamma^2 v} + v \gamma_{\mathrm{A}} \Big(t - \boldsymbol{v}_{\mathrm{A}} \cdot (\boldsymbol{x} - \boldsymbol{b}_{\mathrm{A}}) \Big) \right\}^2 . \tag{2.6}$$

Here, the quantities b, v, γ and $\boldsymbol{d}$ are defined as above. Similarly, the scalar $d_{\mathrm{B}}(t, \boldsymbol{x})$ is derived from the distance between the centres A and B in a rest frame of centre B. Contrary to nonrelativistic kinematics d_{A} and d_{B} differ.

2.2 Static charge distributions

With each of the centres A and B we may associate a spherically symmetric electric charge distribution $\rho_\Gamma(r)$ that is time-independent in the respective rest frame of each centre $\Gamma = \mathrm{A}, \mathrm{B}$. The two charge distributions model the moving nuclei in a peripheral heavy ion collision, and possibly a mean field of their bound electrons as well. These charge distributions $\rho_\Gamma(r)$ shall refer to the respective rest frames of their centres: the primes, usually employed to indicate this fact, are omitted here for simplicity of the notation.[1] A Lorentz boost of these static charge distributions to an arbitrary unprimed frame of reference yields a four-current, which is time-dependent.

In principle, the charge distributions do not have to be spherically symmetric in their respective rest frames. However, spherical symmetry considerably simplifies the following discussion. In this case, the relative orientation of the rest frame coordinates does not matter and the discussion is not complicated by the necessity for rotations in coordinate transformations. Furthermore, the most simple charge distribution, the point charge, occurring most often in the literature and applied in numerical calculations of this work, has spherical symmetry. For the presentation of the scattering theory in the next chapter, it is mandatory to consider more general spherical charge distributions than the point charge only.

The radially symmetric electrostatic potential $V_\Gamma(r)$ in the rest frame of centre Γ (again omitting primes) and the charge distribution $\rho_\Gamma(r)$ are related by the Poisson

[1] This convention allows us to refer unambiguously to the charge distributions $\rho_\Gamma(r)$, and also their spherically symmetric electrostatic potentials $V_\Gamma(r)$, in contexts in which primed coordinates do not denote rest frame coordinates of these entities.

equation, which is given in the spherically symmetric case by:

$$-\frac{1}{4\pi r}\,\frac{\partial^2}{\partial^2 r}\,rV_\Gamma(r) = \rho_\Gamma(r) \qquad (\text{for } r \neq 0). \tag{2.7}$$

We use Gaussian units for the electrical charge everywhere in this thesis, because they are usually preferred in atomic physics (cf. appendix C).

The time-dependent electromagnetic field in the unprimed reference frame, originating from the moving charge distribution $\rho_\Gamma(r)$, time-independent only in a rest frame of centre Γ, is given by the following electromagnetic four-potential:

$$\Big({A_\Gamma}^0(t,\boldsymbol{x}), \boldsymbol{A}_\Gamma(t,\boldsymbol{x})\Big) = \gamma_\Gamma\, V_\Gamma(r_\Gamma(t,\boldsymbol{x}))\,(1,\boldsymbol{v}_\Gamma)\,. \tag{2.8}$$

This four-potential satisfies the Lorenz gauge condition [Jac99]. It is obtained by a Lorentz boost of the electrostatic potential $V_\Gamma(r)$ from a rest frame of centre Γ to the unprimed reference frame. In the case of a moving point charge it is usually referred to as a Liénard–Wiechert potential [Jac99, EM95].

A particular class of radially symmetric charge distributions will be important in the subsequent presentation, especially serving as an example in chapter 3. Consider the static charge distribution,

$$\rho_\Gamma(r) = -\frac{eZ_\Gamma\,\mu_\Gamma^2\exp(-\mu_\Gamma r)}{4\pi r} + eZ_\Gamma \begin{cases} \frac{3}{4\pi}\varrho_\Gamma^{-3} & \text{if } r \leq \varrho_\Gamma, \\ 0 & \text{otherwise,} \end{cases} \tag{2.9}$$

leading to the following electrostatic potential, vanishing at spatial infinity:

$$V_\Gamma(r) = \frac{eZ_\Gamma\exp(-\mu_\Gamma r) - eZ_\Gamma}{r} + \frac{eZ_\Gamma}{r} \begin{cases} \frac{3}{2}\frac{r}{\varrho_\Gamma} - \frac{1}{2}\left(\frac{r}{\varrho_\Gamma}\right)^3 & \text{if } r \leq \varrho_\Gamma, \\ 1 & \text{otherwise.} \end{cases} \tag{2.10}$$

Here e denotes the unit charge. This electrostatic potential depends on three parameters, namely Z_Γ, ϱ_Γ and μ_Γ. In the limit $\rho_\Gamma \to 0$ we obtain the Yukawa potential. The case where only $\mu_\Gamma = 0$ corresponds to the potential of a homogeneously charged sphere. If both $\mu_\Gamma = 0$ and $\rho_\Gamma = 0$ the potential $V_\Gamma(r)$ is identical to the Coulomb potential of a point charge with charge number Z_Γ. Clearly, the charge distribution (2.9) is a sum of a homogeneously charged sphere, with radius $\rho_\Gamma \geq 0$ and total charge eZ_Γ, and an infinitely extended screening charge distribution, with inverse screening length $\mu_\Gamma \geq 0$ (also known as the Debye screening parameter [Jac99]) and total charge $-eZ_\Gamma$. The total charge q_Γ corresponding to the charge distribution (2.9) is given by:

$$q_\Gamma = 4\pi\int_0^\infty r^2\rho_\Gamma(r)\;\mathrm{d}r = \begin{cases} eZ_\Gamma & \text{if } \mu_\Gamma = 0, \\ 0 & \text{if } \mu_\Gamma > 0. \end{cases}$$

In particular Z_Γ is not the charge number of the total charge in the case of the Yukawa potential, but represents its field strength near the origin.

Such a potential is not unphysical, it is used as a simple model for an atomic potential, describing the finite nuclear size and the screening of the nuclear charge by the electrons of an atom. The nuclear radius then determines ϱ_Γ and the screening length μ_Γ is obtained by a rough fit to the Thomas–Fermi atomic potential [Jac99, 13.5]. In some situations the idealisation of the atomic nucleus as a point charge

is an over-simplification: a proper finite nuclear radius is essential, for example, in quantum electrodynamical calculations [MPS98].

2.3 Two-centre Dirac equation

We shall now introduce the Dirac equation for particles that are subject to the external electromagnetic field of the two linearly moving classical charge distributions presented in the previous section. This Dirac equation reads:

$$[H_0 + W_\mathrm{A}(t,\boldsymbol{x}) + W_\mathrm{B}(t,\boldsymbol{x}) - \mathrm{i}\partial_t]\ \Psi(t,\boldsymbol{x}) = 0. \tag{2.11}$$

Here, the following abbreviations have been used, which will be used throughout this thesis:

$$H_0 = -\mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta, \tag{2.12}$$

$$W_\mathrm{A}(t,\boldsymbol{x}) = -eV_\mathrm{A}(r_\mathrm{A}(t,\boldsymbol{x}))\,\gamma_\mathrm{A}(1-\boldsymbol{v}_\mathrm{A}\cdot\boldsymbol{\alpha}), \tag{2.13}$$

$$W_\mathrm{B}(t,\boldsymbol{x}) = -eV_\mathrm{B}(r_\mathrm{B}(t,\boldsymbol{x}))\,\gamma_\mathrm{B}(1-\boldsymbol{v}_\mathrm{B}\cdot\boldsymbol{\alpha}). \tag{2.14}$$

Here $\boldsymbol{\alpha} = \alpha_1, \alpha_2, \alpha_3$ and β denote Dirac matrices. For the numerical calculations of this thesis the standard Dirac–Pauli representation has been used (cf. appendix C). However, all subsequent analytical considerations hold for an arbitrary, unitarily equivalent representation of the Dirac matrices, if not indicated otherwise.

In this thesis, equation (2.11) is referred to as the *two-centre Dirac equation*. The uppercase Greek letter Ψ usually denotes solutions of this two-centre Dirac equation. Note that the external electromagnetic field is minimally coupled to the Dirac field. We denote the unitary time-evolution operator of the two-centre Dirac equation by $U(t,s)$. It satisfies:

$$U(t,t) = 1, \quad U(t,s_0) = U(t,s)U(s,s_0), \quad U(t,s)^{-1} = U(t,s)^* = U(s,t), \tag{2.15}$$

and

$$[H_0 + W_\mathrm{A}(t,\boldsymbol{x}) + W_\mathrm{B}(t,\boldsymbol{x}) - \mathrm{i}\partial_t]\,U(t,s) = 0. \tag{2.16}$$

2.3.1 Note on the unitary time-evolution. If the external fields $W_\mathrm{A}(t,\boldsymbol{x})$ and $W_\mathrm{B}(t,\boldsymbol{x})$ are bounded functions, then it is well-known that the time-evolution operator is given by a Dyson series [RS75, Tha92]. However, the Coulomb and Yukawa potentials (and their corresponding Liénard-Wiechert potentials) are not bounded. Therefore, the existence of a unitary time-evolution is a more complicated mathematical problem, since the self-adjointness of the time-dependent Hamilton operator $H(t)$ is not sufficient. The existence has been proved for the Dirac equation with moving point charges by Kato and Yajima using the technique of local pseudo-Lorentz transformations [KY91].

2.4 Symmetry

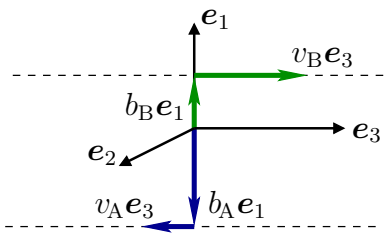
In this section, symmetries of the two-centre Dirac equation are discussed. Recall that a symmetry is a transformation of a solution $\Psi_1(t,\boldsymbol{x})$ of the time-dependent

Dirac equation into another time-dependent wave function $\Psi_2(t, \boldsymbol{x})$, such that both, Ψ_1 and Ψ_2, solve the same two-centre Dirac equation,

$$[H_0 + W_\mathrm{A}(t, \boldsymbol{x}) + W_\mathrm{B}(t, \boldsymbol{x}) - \mathrm{i}\partial_t]\, \Psi_i(t, \boldsymbol{x}) \qquad \text{for } i = 1, 2.$$

Such transformations must commute with the external field operator $W(t, \boldsymbol{x})$ and, therefore, they reflect the symmetries of the external field. In common text book presentations of invariance properties of the Dirac equation, the transformation of wave functions is always accompanied by a transformation of the external field. Occasionally, this form invariance of the Dirac equation, namely that a transformed Dirac spinor solves the transformed Dirac equation, is also called a symmetry of the Dirac equation [Sch95]. We shall stress that this is not meant by symmetry here. Instead the symmetries, described below, establish conserved quantities and the corresponding symmetry operators commute with the unitary time evolution $U(t, s)$ of the two-centre Dirac equation.

In order to facilitate the discussion of the symmetries of the two-centre Dirac equation it is useful to chose a particular frame of reference. In this section unprimed



coordinates $(t, \boldsymbol{x})$ exclusively refer to a reference frame for which the trajectories $\boldsymbol{R}_\mathrm{A}(t)$ and $\boldsymbol{R}_\mathrm{B}(t)$ are given by:

$$\begin{aligned} \boldsymbol{R}_\mathrm{A}(t) &= b_\mathrm{A}\boldsymbol{e}_1 + t v_\mathrm{A}\boldsymbol{e}_3, \\ \boldsymbol{R}_\mathrm{B}(t) &= b_\mathrm{B}\boldsymbol{e}_1 + t v_\mathrm{B}\boldsymbol{e}_3. \end{aligned} \tag{2.17}$$

In such frames of reference the trajectories are invariant under a reflection at the $\boldsymbol{e}_1$-$\boldsymbol{e}_3$-plane. Another symmetry transformation is time-reversal in combination with a reflection in the $\boldsymbol{e}_1$-$\boldsymbol{e}_2$-plane. In order to construct operators representing these transformations on Dirac four-spinors, recall that an active rotation by some angle φ around an axis, which is given in terms of the unit three-vector $\boldsymbol{n}$, is generally represented by the following spinor transformation matrix [Tha92, eq. (2.172)]:

$$\exp\left(-\frac{\mathrm{i}\varphi}{2}\, \boldsymbol{n} \cdot \gamma_5 \boldsymbol{\alpha}\right).$$

Here the matrix γ_5 is defined as $\gamma_5 = \mathrm{i}\gamma_0\gamma_1\gamma_2\gamma_3$, in agreement with the phase conventions in [BD66, Tha92, Sch95]. In the particular case of a rotation by an angle π around one of the coordinate axes the previous expression simplifies to:

$$\exp\left(-\frac{\pi\mathrm{i}}{2}\, \boldsymbol{e}_i \cdot \gamma_5\gamma^0\boldsymbol{\gamma}\right) = \exp\left(-\frac{\pi\mathrm{i}}{2}\, \gamma^i\gamma_5\gamma^0\right) = -\mathrm{i}\gamma^i\gamma_5\gamma^0.$$

A reflection at the plane that is perpendicular to $\boldsymbol{e}_i$ and passes through the origin can be obtained by a space inversion $\mathcal{P}$ (cf. section C.2 of the appendix) followed by

a rotation by π around $\boldsymbol{e}_i$. Therefore, the reflection of a Dirac wave function $\Psi(t, \boldsymbol{x})$ at the $\boldsymbol{e}_1$-$\boldsymbol{e}_3$-plane is accomplished by an operator $\mathcal{P}_2$ defined as follows:

$$(\mathcal{P}_2\Psi)(t, \boldsymbol{x}) = \gamma^2\gamma^5\Psi(t, \boldsymbol{x} - 2x^2\boldsymbol{e}_2). \tag{2.18}$$

Correspondingly the operators $\mathcal{P}_1$ and $\mathcal{P}_3$ may be defined by substituting all indices 2 with 1 and 3 respectively.

The operator $\mathcal{T}_3$ implementing the other transformation described above, namely a time reversal followed by a reflection at the $\boldsymbol{e}_1$-$\boldsymbol{e}_2$-plane, may be defined as,

$$\mathcal{T}_3 = \mathcal{P}_3\mathcal{T}.$$

Here $\mathcal{T}$ denotes the time-reversal operator (cf. appendix C.2). In the following, C shall denote the unitary 4×4 matrix which satisfies $\gamma^{\mu T} = -C^{-1}\gamma^\mu C$ and $C^T = -C$, and which is employed in the standard definition of the time-reversal operator $\mathcal{T}$ for Dirac spinor-fields. With reference to C the operator $\mathcal{T}_3$ is then given explicitly by:

$$(\mathcal{T}_3\Psi)(t, \boldsymbol{x}) = \gamma^3 C\Psi^*(-t, \boldsymbol{x} - 2x^3\boldsymbol{e}_3), \tag{2.19}$$

The operators $\mathcal{T}_i$, where $i = 1, 2$, may again be defined similarly by $\mathcal{T}_i = \mathcal{P}_i\mathcal{T}$.

In the definitions (2.18) and (2.19) the phases have been chosen such that the operators $\mathcal{P}_i$ and $\mathcal{T}_i$ are involutions:

$$(\mathcal{P}_i{}^2\Psi)(t, \boldsymbol{x}) = \gamma^i\gamma^5\gamma^i\gamma^5\Psi(t, \boldsymbol{x}) = \Psi(t, \boldsymbol{x}),$$

$$(\mathcal{T}_i{}^2\Psi)(t, \boldsymbol{x}) = \gamma^i CK\gamma^i CK\Psi(t, \boldsymbol{x}) = \gamma^i C\gamma^{i*}C^*\Psi(t, \boldsymbol{x}) = \gamma^i\gamma^{i\dagger}\Psi(t, \boldsymbol{x}) = \Psi(t, \boldsymbol{x})$$

Here $i = 1, 2, 3$ and K denotes the operator of complex conjugation. Consequently, the eigenvalues of both $\mathcal{P}_i$ and $\mathcal{T}_i$ are ± 1. Note, however, that $\mathcal{P}_1\mathcal{P}_2\mathcal{P}_3 = \mathrm{i}\mathcal{P}$. The following commutation and anti-commutation properties of the operators $\mathcal{P}_i$ and $\mathcal{T}_i$ are easily verified:[2]

$$[\mathcal{P}_i, \mathcal{T}_j] = 0. \{\mathcal{T}_i, \mathcal{T}_j\} = \{\mathcal{P}_i, \mathcal{P}_j\} = 2\delta_{ij}, \tag{2.20}$$

$$\tag{2.21}$$

2.4.1 Commutation properties. Next, it must be demonstrated that both of the commuting operators $\mathcal{P}_2$ and $\mathcal{T}_3$ implement a symmetry of the two-centre Dirac equation (2.11). Due to the particular choice of the Lorentz frame in this section, the scalars $r_\mathrm{A}(t, \boldsymbol{x})$ and $r_\mathrm{B}(t, \boldsymbol{x})$ satisfy the following identities:

$$r_\Gamma(t, \boldsymbol{x}) = r_\Gamma(t, \boldsymbol{x} - 2x^2\boldsymbol{e}_2) = r_\Gamma(-t, \boldsymbol{x} - 2x^3\boldsymbol{e}_3),$$

with $\Gamma = \mathrm{A}, \mathrm{B}$. Using this, we are able to verify that the external field operators W_A and W_B commute with both $\mathcal{P}_2$ and $\mathcal{T}_3$:

$$[\mathcal{P}_2, W_\Gamma] = [\mathcal{T}_3, W_\Gamma] = 0. \tag{2.22}$$

[2]For the standard Dirac-Pauli representation a valid choice for C is the real matrix $\mathrm{i}\gamma^2\gamma^0$ (see section C.2 and [BD66, ch. 5]). Hence, the spinor transformation matrices of $\mathcal{P}_2$ and $\mathcal{T}_3$ take the form:

$$\gamma^2\gamma^5 = \mathrm{i}\gamma^2\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix}\sigma_2 & 0\\ 0 & -\sigma_2\end{pmatrix},$$

$$\gamma^3 C = \mathrm{i}\gamma^3\gamma^2\gamma^0 = \begin{pmatrix}\sigma_1 & 0\\ 0 & -\sigma_1\end{pmatrix}.$$

First, it will be checked that the commutator of W_Γ and $\mathcal{P}_2$ vanishes:

$$\begin{aligned}(\mathcal{P}_2 W_\Gamma \mathcal{P}_2 \Psi)(t,\boldsymbol{x}) &= \gamma^2\gamma^5\ (W_\Gamma \mathcal{P}_2\Psi)(t,\boldsymbol{x}-2x^2\boldsymbol{e}_2)\\ &= \gamma^2\gamma^5\ W_\Gamma(t,\boldsymbol{x}-2x^2\boldsymbol{e}_2)\ (\mathcal{P}_2\Psi)(t,\boldsymbol{x}-2x^2\boldsymbol{e}_2)\\ &= -\gamma_\Gamma e\, V_\Gamma(r_\Gamma(t,\boldsymbol{x}-2x^2\boldsymbol{e}_2))\ \gamma^2\gamma^5\,(1-v_\Gamma\gamma^0\gamma^3)\,\gamma^2\gamma^5\,\Psi(t,\boldsymbol{x})\\ &= W_\Gamma(t,\boldsymbol{x})\ \Psi(t,\boldsymbol{x}) \ = \ (W_\Gamma\Psi)(t,\boldsymbol{x}).\end{aligned}$$

Repeatedly using relation (C.9) of the appendix, the calculation for $\mathcal{T}_3$ is carried out similarly:

$$\begin{aligned}(\mathcal{T}_3 W_\Gamma \mathcal{T}_3 \Psi)(t,\boldsymbol{x}) &= \gamma^3 C\ (W_\Gamma \mathcal{T}_3\Psi)^*(-t,\boldsymbol{x}-2x^3\boldsymbol{e}_3)\\ &= \gamma^3 C\ W_\Gamma^*(-t,\boldsymbol{x}-2x^3\boldsymbol{e}_3)\ (\mathcal{T}_3\Psi)^*(-t,\boldsymbol{x}-2x^3\boldsymbol{e}_3)\\ &= \gamma^3 C\ W_\Gamma^*(-t,\boldsymbol{x}-2x^3\boldsymbol{e}_3)\ \gamma^{3^*}C^*\ \Psi(t,\boldsymbol{x})\\ &= -\gamma_\Gamma e\, V_\Gamma^*(r_\Gamma(-t,\boldsymbol{x}-2x^3\boldsymbol{e}_3))\,\gamma^3 C(1-v_\Gamma\gamma^{0^*}\gamma^{3^*})C^*\gamma^3\,\Psi(t,\boldsymbol{x})\\ &= -\gamma_\Gamma e\, V_\Gamma(r_\Gamma(t,\boldsymbol{x}))\,\gamma^3 CC^*(1-v_\Gamma\gamma^0\gamma^3)\gamma^3\,\Psi(t,\boldsymbol{x})\\ &= W_\Gamma(t,\boldsymbol{x})\ \Psi(t,\boldsymbol{x}) \ = \ (W_\Gamma\Psi)(t,\boldsymbol{x}).\end{aligned}$$

It remains to establish the commutation properties of $\mathcal{P}_2$ and $\mathcal{T}_3$ with H_0 and $\mathrm{i}D_0$. Up to a complex phase, the operators $\mathcal{P}_i$ and $\mathcal{T}_i$ are products of space-inversions, time-reversals and spatial rotations. Hence, the commutation relations can be deduced from well-known properties of the free Dirac equation. More precisely the following relations hold for $i = 1, 2, 3$ (for the notation cf. appendix C):

$$[\mathcal{P}_i, H_0] = [\mathcal{T}_i, H_0] = 0, \tag{2.23}$$

$$[\mathcal{P}_i, \mathrm{i}D_0] = [\mathcal{T}_i, \mathrm{i}D_0] = 0 \tag{2.24}$$

As an example the second part of (2.23) will be verified:

$$\begin{aligned}(\mathcal{T}_k H_0 \mathcal{T}_k \Psi)(t,\boldsymbol{x}) &= \gamma^k C\left(\gamma^0\left(-i\gamma^i D_i + 1\right)\mathcal{T}_k\Psi\right)^*(-t,\boldsymbol{x}-2x^k\boldsymbol{e}_k)\\ &= \gamma^k C\gamma^{0^*}\left(\mathrm{i}\gamma^{i^*}\partial_i - 2\mathrm{i}\gamma^{k^*}\partial_k + 1\right)\ (\mathcal{T}_k\Psi)^*(-t,\boldsymbol{x}-2x^k\boldsymbol{e}_k)\\ &= \gamma^k C\gamma^{0^*}\left(\mathrm{i}\gamma^{i^*}\partial_i - 2\mathrm{i}\gamma^{k^*}\partial_k + 1\right)\ \gamma^{k^*}C^*\Psi(t,\boldsymbol{x}-2x^k\boldsymbol{e}_k)\\ &= -\gamma^k CC^*\gamma^0\left(\mathrm{i}\gamma^{i^*}\partial_i - 2\mathrm{i}\gamma^{k^*}\partial_k - 1\right)\gamma^k\Psi(t,\boldsymbol{x})\\ &= \gamma^0\left(\mathrm{i}\gamma^{i^*}\partial_i + 1\right)\Psi(t,\boldsymbol{x}) \ = \ (H_0\Psi)(t,\boldsymbol{x}).\end{aligned}$$

Note that in the previous calculation there shall not be a summation over the repeated index $k = 1, 2, 3$.

2.4.2 Unitary time-evolution. Since $\mathcal{P}_2$ commutes with the time-dependent Hamiltonian of the two-centre Dirac equation and with the time-derivative, it is verified that $\mathcal{P}_2 U(t,s)\mathcal{P}_2$ is also a unitary time-evolution of the two-centre Dirac equation and, therefore, identical with $U(t,s)$. Hence, the operators $\mathcal{P}_2$ and $U(t,s)$ commute:

$$U(t,s)\,\mathcal{P}_2 = \mathcal{P}_2\,U(t,s).$$

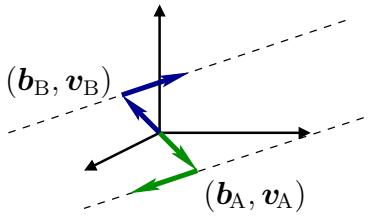
We conclude that solutions $\Psi(t,\boldsymbol{x})$ of the two-centre Dirac equation may be constructed such that they are eigenfunctions of both $\mathcal{P}_2$ and $\mathcal{T}_3$. In other words $\mathcal{P}_2$ and $\mathcal{T}_3$ represent conserved quantities of the time-dependent two-centre Dirac equation in any frame of reference where the trajectories are given by (2.17). In other

coordinate systems the symmetry operators corresponding to these conserved quantities may be obtained by a Poincaré-transformation of $\mathcal{P}_2$ and $\mathcal{T}_3$ respectively. It can be shown that $\mathcal{P}_2$ and $\mathcal{T}_3$ commute with Lorentz boosts in $\boldsymbol{e}_3$-direction and also with spatial translations in $\boldsymbol{e}_1$-direction. Hence, the definitions (2.18) and (2.19) are unambiguous.

The physical importance of these symmetries is that they lead to corresponding symmetries of the transition amplitudes, which are defined in the next chapter.

2.5 Homonuclear collisions

In the following a two-centre Dirac equation (2.11) is considered for which the radial electrostatic potentials V_A and V_B are equal. This situation corresponds to a homonuclear collision system. In order to discuss the additional symmetry, parity, present only in those homonuclear collisions, it is useful to chose a coordinate system, in which both centres move with equal but opposite velocities and have the same dis-



tance to the origin at time $t = 0$. Hence, the trajectories shall be given by equations (2.1) with,

$$\boldsymbol{v}_\mathrm{B} = -\boldsymbol{v}_\mathrm{A},$$
$$\boldsymbol{b}_\mathrm{B} = -\boldsymbol{b}_\mathrm{A}.$$

Then the following relation holds:

$$r_\mathrm{B}(t, \boldsymbol{x}) = r_\mathrm{A}(t, -\boldsymbol{x}). \tag{2.25}$$

It can be shown similarly to the previous section that the parity operator $\mathcal{P}$ (cf. equation (C.5) of appendix C) transforms the external field operators W_A and W_B into each other:

$$\mathcal{P} W_\mathrm{A} \mathcal{P} = W_\mathrm{B},$$
$$\mathcal{P} W_\mathrm{B} \mathcal{P} = W_\mathrm{A}.$$

Therefore, in the reference frame considered here, the parity operator $\mathcal{P}$ commutes with the time-dependent Hamiltonian $H(t) = H_0 + W_\mathrm{A}(t) + W_\mathrm{B}(t)$ of the two-centre Dirac equation. Parity is a constant of motion.