Chapter 3

Multi-Channel Scattering Theory

The two-centre Dirac equation has been introduced as a model, for describing charge transfer, ionisation and pair creation in peripheral collisions of highly charged heavy-ions. Intuition suggests that the two-centre Dirac equation should have solutions which correspond to particles asymptotically bound to the electrostatic potential V_Γ of centre A or centre B, or move away from both centres, as time t tends to $+\infty$ or $-\infty$. This corresponds to three different scattering channels or three different types of scattering states: those, which are essentially subject to either one of the external fields $W_\mathrm{A}(t, \boldsymbol{x})$ or $W_\mathrm{B}(t, \boldsymbol{x})$, and those, which are not significantly influenced by any external field, as t tends to $\pm\infty$.

The scattering theory of the two-centre Dirac equation is presented here essentially for two reasons. First, it seems that a formal discussion of this scattering theory is not available; although several authors have discussed the scattering theory of the similar two-centre Schrödinger equation from a conceptional and mathematical point of view [Yaj80, Hag82, Wül88, Gra90]. Second, a precise definition of the transition amplitude is given. This is a necessary prerequisite in order to prove the relativistic invariance of the scattering theory. Boost invariance is not a trivial property in the present case, as it is for the scattering theory of the two-centre Schrödinger equation: Lorentz boosts transform the time axes, with respect to which the (necessarily) time-dependent scattering theory is formulated.

3.1 Scattering channels

First, let us introduce some notation. The three different scattering channels mentioned above correspond to three different Dirac equations, describing Dirac particles, which are bound to either of the external fields $W_\Gamma(t, \boldsymbol{x})$ or move freely. The Hamilton operators of these scattering-channel Dirac equations are:

$$\begin{aligned} H_\mathrm{A}(t) &= H_0 + W_\mathrm{A}(t, \boldsymbol{x}) \\ H_\mathrm{B}(t) &= H_0 + W_\mathrm{B}(t, \boldsymbol{x}) \\ H_\mathrm{C} &= H_0. \end{aligned} \tag{3.1}$$

As opposed to conventional quantum-mechanical multi-particle scattering theory [San72, San74, Thi94], these scattering channel Hamiltonians have an explicit time-dependence. The time-dependence of the Hamiltonian operators $H_\mathrm{A}(t)$ and $H_\mathrm{B}(t)$ cannot be removed simultaneously by a Poincaré transformation, if the centres are moving with different velocities. The unitary time-evolution operators of the scattering-channel Dirac equations are respectively denoted by,

$$U_\mathrm{A}(t, s), \quad U_\mathrm{B}(t, s) \quad \text{and} \quad U_\mathrm{C}(t, s) = \exp(-\mathrm{i}(t - s)H_0).$$

Solutions of the scattering-channel Dirac equations are denoted by the uppercase Greek letter Φ, with a lower index indicating the respective scattering channel, for example:

$$[H_0 + W_{\mathrm{A}}(t,\boldsymbol{x}) - \mathrm{i}\partial_t]\ \Phi_{\mathrm{A},k}(t,\boldsymbol{x}) = 0.$$

The second index k is used to differentiate between different solutions of the same Dirac equation symbolically. These wave functions $\Phi_{\Gamma,k}(t,\boldsymbol{x})$, where $\Gamma = \mathrm{A}, \mathrm{B}, \mathrm{C}$ will be referred to as *asymptotic configurations*, following [BH63, Tha92]. In other literature, they are also called in- and out-states [New82, Wei95].

3.1.1 Scattering states. A principal problem of scattering theory, as presenting itself in present context, is to find solutions $\Psi^+_{\Gamma,k}(t,\boldsymbol{x})$ and $\Psi^-_{\Gamma,k}(t,\boldsymbol{x})$ of the two-centre Dirac equation, which asymptotically approach the asymptotic configuration $\Phi_{\Gamma,k}(t,\boldsymbol{x})$:

$$\lim_{t\to-\infty} \|\Phi_{\Gamma,k}(t) - \Psi^+_{\Gamma,k}(t)\| = 0$$
$$\lim_{t\to+\infty} \|\Phi_{\Gamma,k}(t) - \Psi^-_{\Gamma,k}(t)\| = 0.$$

Here $\|.\|$ denotes the Hilbert-space norm of a wave function (cf. appendix C). The wave functions $\Psi^+_{\Gamma,k}(t,\boldsymbol{x})$ and $\Psi^-_{\Gamma,k}(t,\boldsymbol{x})$ are usually referred to as the *incoming* and the *outgoing scattering states* respectively. The seemingly paradoxical notation, in which Ψ^+ corresponds to the limit $t \to -\infty$ and vice versa, originates in the time-independent formulation of scattering theory. Although the latter cannot be applied in the present situation, this notation, common to many presentations of quantum scattering theory [BD66, San72, RS79, New82, Hag82, Gra90], is employed here as well. The question, whether scattering states $\Psi^+_{\Gamma,k}(t)$ and $\Psi^-_{\Gamma,k}(t)$ exist, for an arbitrary solution $\Phi_{\Gamma,k}(t,\boldsymbol{x})$ of the Dirac equation of the scattering channel Γ, is known as the problem of *asymptotic convergence*. For certain classes of electrostatic potentials $V_\Gamma(r)$ asymptotic convergence is proved in section 3.3 below.

In the case of the scattering channels A and B, only such asymptotic configurations that correspond to *bound states* of the respective potential are admitted. Wave functions corresponding to continuum eigenfunctions of the electrostatic potentials in their respective rest frames are moving away from their centres as time increases. Therefore, they are attributed to scattering channel C. Taking this convention into account, it will be shown that scattering states corresponding to different scattering channels are orthogonal to each other (see section 3.4 below):

$$\left(\Psi^+_{\Gamma,k}(t), \Psi^+_{\Delta,l}(t)\right) = \left(\Psi^-_{\Gamma,k}(t), \Psi^-_{\Delta,l}(t)\right) = 0, \qquad \text{if } \Gamma \neq \Delta.$$

This property is known as *asymptotic orthogonality.*

3.1.2 Wave operators. For the two-centre Dirac equation, asymptotic convergence is equivalent to the existence of the following strong operator limits:

$$\begin{aligned}
\Omega^\pm_{\mathrm{A}}(s) &= \operatorname*{s-lim}_{t\to\mp\infty}\ \Omega_{\mathrm{A}}(t,s) = \operatorname*{s-lim}_{t\to\mp\infty}\ U(t,s)^{-1}\, U_{\mathrm{A}}(t,s)\, P_{\mathrm{A}}(s). \\
\Omega^\pm_{\mathrm{B}}(s) &= \operatorname*{s-lim}_{t\to\mp\infty}\ \Omega_{\mathrm{B}}(t,s) = \operatorname*{s-lim}_{t\to\mp\infty}\ U(t,s)^{-1}\, U_{\mathrm{B}}(t,s)\, P_{\mathrm{B}}(s), \\
\Omega^\pm_{\mathrm{C}}(s) &= \operatorname*{s-lim}_{t\to\mp\infty}\ \Omega_{\mathrm{C}}(t,s) = \operatorname*{s-lim}_{t\to\mp\infty}\ U(t,s)^{-1}\, \exp(-\mathrm{i}(t-s)H_0).
\end{aligned} \tag{3.2}$$

The Møller operators $\Omega^\pm_\Gamma(s)$ are time-dependent in the present situation, which has its origin in the time-dependence of the scattering-channel Hamiltonians (3.1). In conventional multi-channel scattering theory the Møller wave operators are not time-dependent. But the same time-dependence occurs for the scattering theory of the two-centre Schrödinger equation (see e.g. [HAG82]).

In equations (3.2) the projection operators $P_{\rm A}(s)$ and $P_{\rm B}(s)$ have been introduced, in order to project onto the subspace of asymptotic configurations $\Phi_\Gamma(t,\boldsymbol{x})$ that correspond to bound states of the external fields $W_{\rm A}(t,\boldsymbol{x})$ and $W_{\rm B}(t,\boldsymbol{x})$ respectively. The projection operators are included into the definition of the wave operators $\Omega^\pm_{\rm A}(s)$ and $\Omega^\pm_{\rm B}(s)$, in order to obtain orthogonality of their ranges, which are then orthogonal proper subspaces of the state space $L^2(\mathbb{R}^3)^4$ of the classical Dirac equation.

For later reference, explicit representations of these time-dependent projection operators, $P_{\rm A}(s)$ and $P_{\rm B}(s)$, are given in the following. Let $(\Lambda_{\rm A}, a_{\rm A})$ denote the Poincaré transformation from the unprimed reference frame to a primed rest frame of centre A in which centre A is located at the spatial origin, i.e. $\boldsymbol{R}'_{\rm A}(t') = 0$. In the primed frame, the Hamiltonian $H'_{\rm A}$ of scattering channel A does not depend on the time t':

$$H'_{\rm A} = H'_0 - eV_{\rm A}(|\boldsymbol{x}'|).$$

Throughout this chapter, the potential $V_{\rm A}$ is assumed to be of such a form that $H'_{\rm A}$ has bound states. In the primed frame, choose a complete set of orthonormal bound state eigenfunctions, denoted by $\phi_{{\rm A},k}(\boldsymbol{x}')$, with eigenenergies $\epsilon_{{\rm A},k}$. Then the projector $P'_{\rm A}$ onto the subspace of the bound states of the potential $V_{\rm A}$ in the primed frame is time-independent and given by:

$$(P'_{\rm A}\phi)(\boldsymbol{x}') = \sum_k (\phi_{{\rm A},k}, \phi)'\, \phi_{{\rm A},k}(\boldsymbol{x}').$$

In the unprimed frame, the asymptotic configuration $\Phi_{{\rm A},k}(t,\boldsymbol{x})$, corresponding to the bound state $\phi_{{\rm A},k}(\boldsymbol{x}')$ in the primed frame, is obtained by a Poincaré transformation:

$$\Phi_{{\rm A},k}(t,\boldsymbol{x}) = S(\Lambda_{\rm A})^{-1} \exp(-{\rm i}t'\epsilon_{{\rm A},k})\phi_{{\rm A},k}(\boldsymbol{x}'), \tag{3.3}$$

Here $S(\Lambda_{\rm A})$ is the spinor-representation matrix of the Lorentz transformation $\Lambda_{\rm A}$ and the primed coordinates are given by $(t',\boldsymbol{x}') = \Lambda_{\rm A}(t,\boldsymbol{x}) + (a^0,\boldsymbol{a})$. The time-dependent projector $P_{\rm A}(s)$ in the unprimed reference frame, projecting onto the bound states of the external field $W_{\rm A}(t,\boldsymbol{x})$, is thus given by:

$$(P_{\rm A}(s)\psi) = \sum_k (\Phi_{{\rm A},k}(s), \psi)\, \Phi_{{\rm A},k}(s,\boldsymbol{x}). \tag{3.4}$$

An explicit representation of $P_{\rm B}(s)$ is given analogously.

3.2 Transition amplitudes

The two-centre Dirac equation is used by many authors as a model in order to describe atomic processes in collisions of heavy and highly charged ions, like excitation, ionisation, charge transfer and pair creation [EM95]. For example, an electron initially bound to either of the colliding nuclei is represented in this model by an incoming scattering state, $\Psi^+_{\rm A}(t,\boldsymbol{x})$ or $\Psi^+_{\rm B}(t,\boldsymbol{x})$. Electron states after the collision are represented by outgoing scattering states $\Psi^-_\Gamma(t,\boldsymbol{x})$.

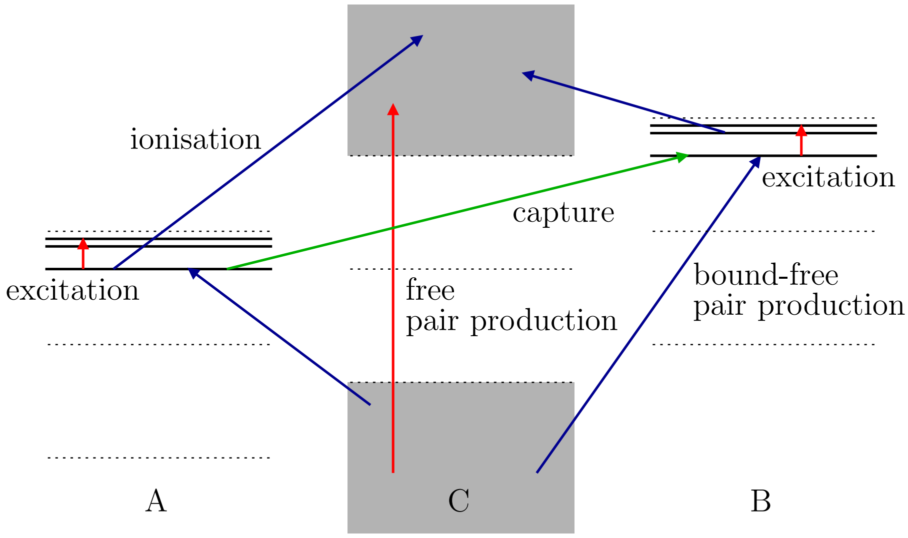

FIGURE 3.1. This figure illustrates the scattering theory of the two-centre Dirac equation. Transitions within the same scattering channel, i.e. excitation and free pair production, are depicted by red arrows. Blue arrows correspond to processes of ionisation and bound-free pair production. Finally, charge transfer is shown as a green arrow. The three different energy spectra represent the three scattering channels A, B and C.

The probability amplitude $a_{\Delta l,\Gamma k}$ for a state of incoming configuration $\Phi_{\Gamma,k}(s)$ to have the outgoing configuration $\Phi_{\Delta,l}(s)$ is given by,

$$a_{\Delta l,\Gamma k} = \Big(\Psi^-_{\Delta,l}(s), \Psi^+_{\Gamma,k}(s)\Big) . \tag{3.5}$$

Due to the unitarity of the time-evolution of the two-centre Dirac equation, the definition of the transition amplitude is independent of the time s. The various atomic processes are depicted in figure 3.1. There are other equivalent expressions for the transition amplitude, some of them listed below. In particular, the post and prior forms frequently appear in the literature.

$$\begin{aligned}
a_{\Delta l,\Gamma k} &= \Big(\Omega^-_\Delta(s)\Phi_{\Delta,l}(s), \Omega^+_\Gamma(s)\Phi_{\Gamma,k}(s)\Big)\\
&= \lim_{\substack{t_1\to-\infty\\ t_2\to\infty}} \Big(U(s,t_2)U_\Delta(t_2,s)\Phi_{\Delta,l}(s), U(s,t_1)U(t_1,s)\Phi_{\Gamma,k}(s)\Big)\\
&= \lim_{\substack{t_1\to-\infty\\ t_2\to\infty}} \Big(\Phi_{\Delta,l}(t_2), U(t_2,t_1)\Phi_{\Gamma,k}(t_1)\Big)\\
&= \lim_{t\to\infty} \Big(\Phi_{\Delta,l}(t), \Psi^+_{\Gamma,k}(t)\Big) \quad \text{(post form)}\\
&= \lim_{t\to-\infty} \Big(\Psi^-_{\Delta,l}(t), \Phi_{\Gamma,k}(t)\Big) \quad \text{(prior form)}.
\end{aligned}$$

For the discussion of asymptotic completeness we refer to section 3.6 below.

3.3 Asymptotic convergence

In this section, we will prove the existence of the operator-limits (3.2), defining the Møller wave operators $\Omega^\pm_\Gamma(s)$, under the assumption that the external fields $W_{\mathrm{A}}(t, \boldsymbol{x})$

and $W_{\mathrm{B}}(t,\boldsymbol{x})$ are short-ranged. Asymptotic convergence is essential for an unambiguous definition of the transition amplitude $a_{\Delta l,\Gamma k}$ in equation (3.5). The case of particular interest, in which moving point charges are the source of external fields, is not covered in this section. This principal model of the literature has long-range external fields (cf. sections 3.6 and 3.7 below).

The material presented in the following has not appeared in literature, but some aspects resemble a discussion of the nonrelativistic charge-transfer model in [Yaj80]. Furthermore, the first subsection recalls standard mathematical results. For detailed explanations of the notation the reader is referred to appendix C.

3.3.1 Cook's method. The proofs of convergence given below are based on a method which was introduced by Cook [Coo57]. Cook's method has become a standard tool for convergence proofs of wave operators, see e.g. [Kat80, Dol64, DV66, RS79, Yaj80, Wül88]. In this subsection Cook's reasoning, as applicable in the present context, will be reviewed shortly (see in particular [Kat80, subsec. X.3.3] and [RS79, sec. XI.3]).

The convergence of the limit,

$$\Omega_\Gamma^-(s) = \operatorname*{s-lim}_{t\to\infty} \Omega_\Gamma(t,s)$$

with respect to the strong operator topology (cf. [RS80]) is equivalent to,

$$\|(\Omega_\Gamma(t_1,s) - \Omega_\Gamma(t_0,s))\,\phi\| \to 0,$$

as $t_0, t_1 \to \infty$ for all $\phi(\boldsymbol{x})$, elements of the Hilbert space $L^2(\mathbb{R}^3)^4$. This equivalence holds due to the completeness of $L^2(\mathbb{R}^3)^4$ (Cauchy criterion). The convergence on a dense subspace already implies convergence on the complete state space in the present situation (see e.g. [Kat80, p. 151]). The estimate,

$$\|\Omega_\Gamma(t_1,s)\phi - \Omega_\Gamma(t_0,s)\phi\| = \left\|\int_{t_0}^{t_1} \left[\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega_\Gamma(t,s)\phi\right] \mathrm{d}t\right\| \le \int_{t_0}^{t_1} \left\|\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega_\Gamma(t,s)\phi\right\| \mathrm{d}t,$$

leads to the following conclusion: A sufficient condition for the existence of the wave operator $\Omega_\Gamma^-(s)$ is the finiteness of the following time-integral,

$$\int_{t_0}^{\infty} \left\|\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega_\Gamma(t,s)\phi\right\| \mathrm{d}t \,<\, \infty, \tag{3.6}$$

for some (arbitrary but finite) time t_0 and all $\phi(\boldsymbol{x})$ of a subspace of wave functions that is dense in the state space $L^2(\mathbb{R}^3)^4$.

Obviously, a sufficient condition for the convergence as $t\to-\infty$, i.e. the existence of the wave operator $\Omega_\Gamma^+(s)$, is established in a similar manner.

3.3.2 Asymptotically bound particles. In this subsection, we prove the existence of the strong operator limit $\Omega_{\mathrm{A}}^-(s)$. The other three wave operators $\Omega_{\mathrm{A}}^+(s)$ and $\Omega_{\mathrm{B}}^\pm(s)$ are treated analogously. The Cook integral (3.6) for $\Omega_{\mathrm{A}}^-(s)$ reads:

$$\int_{t_0}^{\infty} \left\|\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega_{\mathrm{A}}(t,s)\phi\right\| \mathrm{d}t \;=\; \int_{t_0}^{\infty} \|W_{\mathrm{B}}(t)U_{\mathrm{A}}(t,s)P_{\mathrm{A}}(s)\phi\|\,\mathrm{d}t. \tag{3.7}$$

Recalling the definition (2.14) of $W_{\mathrm{B}}(t, \boldsymbol{x})$, the integrand on the right hand side of equation (3.7) is estimated as follows:

$$\begin{aligned}
&\|W_{\mathrm{B}}(t)U_{\mathrm{A}}(t,s)P_{\mathrm{A}}(s)\phi\| \\
&= \left\| W_{\mathrm{B}}(t)\sum_k c_k \Phi_{\mathrm{A},k}(t)\right\| \\
&\le \sum_k |c_k(s)|\,\|W_{\mathrm{B}}(t)\Phi_{\mathrm{A},k}(t)\| \\
&= \sum_k |c_k(s)|\,\|\gamma_{\mathrm{B}}(1-\boldsymbol{v}_{\mathrm{B}}\cdot\boldsymbol{\alpha})\,V_{\mathrm{B}}(r_{\mathrm{B}}(t,\boldsymbol{x}))\,\Phi_{\mathrm{A},k}(t,\boldsymbol{x})\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)^4} \\
&\le \sum_k \gamma_{\mathrm{B}}|c_k(s)|\,\|(1-\boldsymbol{v}_{\mathrm{B}}\cdot\boldsymbol{\alpha})\|_2\,\|V_{\mathrm{B}}(r_{\mathrm{B}}(t,\boldsymbol{x}))\Phi_{\mathrm{A},k}(t,\boldsymbol{x})\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)^4}\,,
\end{aligned} \tag{3.8}$$

with $c_k(s) = (\Phi_{\mathrm{A},k}(s), \phi)$ and $\|.\|_2$ denotes the matrix norm with respect to the scalar product in $\mathbb{C}^4$ (see appendix C or [GV96]). The following inequality may be proved for the straight line trajectories $\boldsymbol{R}_{\mathrm{A}}(t)$ and $\boldsymbol{R}_{\mathrm{B}}(t)$, as in equation (2.1), and arbitrary $\boldsymbol{x} \in \mathbb{R}^3$ and $t \in \mathbb{R}$:

$$\frac{1}{1+|\boldsymbol{x}-\boldsymbol{R}_{\mathrm{A}}(t)|^2}\,\frac{1}{1+|\boldsymbol{x}-\boldsymbol{R}_{\mathrm{B}}(t)|^2} \le \frac{2}{1+|\boldsymbol{R}_{\mathrm{A}}(t)-\boldsymbol{R}_{\mathrm{B}}(t)|^2}.$$

In conjunction with inequality (2.5) and the Hölder inequality [For84, RS80] the estimate of the integrand of the Cook integral (3.7) may be continued as follows:

$$\begin{aligned}
&\|W_{\mathrm{B}}(t)\Phi_{\mathrm{A},k}(t)\| \\
&\le \frac{2\gamma_{\mathrm{B}}\,\|(1-\boldsymbol{v}_{\mathrm{B}}\cdot\boldsymbol{\alpha})\|_2}{1+|\boldsymbol{R}_{\mathrm{A}}(t)-\boldsymbol{R}_{\mathrm{B}}(t)|^2}\times \\
&\qquad \left\|\left(1+r_{\mathrm{B}}(t,\boldsymbol{x})^2\right)V_{\mathrm{B}}(r_{\mathrm{B}}(t,\boldsymbol{x}))\left(1+r_{\mathrm{A}}(t,\boldsymbol{x})^2\right)\Phi_{\mathrm{A},k}(t,\boldsymbol{x})\right\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)^4} \\
&\le \frac{2\gamma_{\mathrm{B}}\,\|(1-\boldsymbol{v}_{\mathrm{B}}\cdot\boldsymbol{\alpha})\|_2}{1+|\boldsymbol{R}_{\mathrm{A}}(t)-\boldsymbol{R}_{\mathrm{B}}(t)|^2}\left\|\left(1+r_{\mathrm{B}}(t,\boldsymbol{x})^2\right)V_{\mathrm{B}}(r_{\mathrm{B}}(t,\boldsymbol{x}))\right\|_{L^p(\mathbb{R}^3,\mathrm{d}^3x)}\times \\
&\qquad \sum_{i=1}^{4}\left\|\left(1+r_{\mathrm{A}}(t,\boldsymbol{x})^2\right)\,\Phi_{\mathrm{A},k;i}(t,\boldsymbol{x})\right\|_{L^q(\mathbb{R}^3,\mathrm{d}^3x)}
\end{aligned}$$

Here, the positive real numbers p and q have to be chosen such that $\frac{1}{p}+\frac{1}{q}=\frac{1}{2}$. The index i denotes the spinor index of the Dirac four-spinor $\Phi_{\mathrm{A},k}(t,\boldsymbol{x})$.

It remains to show that the norms,

$$\begin{aligned}
&\left\|\left(1+r_{\mathrm{A}}(t,\boldsymbol{x})^2\right)\,\Phi_{\mathrm{A},k;i}(t,\boldsymbol{x})\right\|_{L^p(\mathbb{R}^3,\mathrm{d}^3x)} \quad \text{and} \\
&\left\|\left(1+r_{\mathrm{B}}(t,\boldsymbol{x})^2\right)V_{\mathrm{B}}(r_{\mathrm{B}}(t,\boldsymbol{x}))\right\|_{L^q(\mathbb{R}^3,\mathrm{d}^3x)}\,,
\end{aligned}$$

are finite and moreover time-independent. This is true for arbitrary p and q, if the radial electrostatic potentials V_Γ are of the form (2.10) with $\mu_\Gamma > 0$ and $\rho_\Gamma > 0$. Furthermore, it can be verified that suitable p and q can be determined also in the case the Yukawa potentials, $\varrho_\Gamma = 0$, if $e^2 Z_{\mathrm{B}} < \frac{\sqrt{3}}{2}$ holds. The sum in equation (3.8) is finite if $\mu_\Gamma > 0$. In the cases mentioned, the estimate,

$$\int_{t_0}^{\infty}\left\|\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega_{\mathrm{A}}(t,s)\phi\right\|\mathrm{d}t \le \int_{t_0}^{\infty}\frac{\text{const.}}{1+|(\boldsymbol{b}_{\mathrm{A}}-\boldsymbol{b}_{\mathrm{B}})+t(\boldsymbol{v}_{\mathrm{A}}-\boldsymbol{v}_{\mathrm{B}})|^2}\,\mathrm{d}t<\infty,$$

holds and, thereby, shows that the Cook integral (3.6) for $\Omega_{\mathrm{A}}^-(s)$ is finite.

3.3.3 Asymptotically free particles. In order to show the existence of of $\Omega_{\mathrm{C}}^{-}(s)$ we consider the Cook integral (3.6) for scattering channel C:

$$\begin{aligned}\int_{t_0}^{\infty} \left\| \tfrac{\mathrm{d}}{\mathrm{d}t}\, \Omega_{\mathrm{C}}(t,s)\phi \right\| \mathrm{d}t &= \int_{t_0}^{\infty} \left\| [W_{\mathrm{A}}(t) + W_{\mathrm{B}}(t)]\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi \right\| \mathrm{d}t \\ &\leq \sum_{\Gamma=\mathrm{A},\mathrm{B}} \int_{t_0}^{\infty} \left\| W_{\Gamma}(t)\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi \right\| \mathrm{d}t.\end{aligned}$$

Here $\phi(\boldsymbol{x})$ shall be a regular free Dirac wave packet,

$$\phi(\boldsymbol{x}) = (2\pi)^{-3/2} \int \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p}}\, \hat{\phi}(\boldsymbol{p})\ \mathrm{d}^3 p,$$

with $\hat{\phi}(\boldsymbol{p}) \in C_0^{\infty}(\mathbb{R}^3)^4$ (cf. section B.1). It is sufficient to consider regular wave packets because they are dense in the state space $L^2(\mathbb{R}^3)^4$. The estimate is continued as follows:

$$\begin{aligned}&\left\| W_{\Gamma}(t)\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi \right\| \\ &= \left\| \gamma_{\Gamma}(1 - \boldsymbol{v}_{\Gamma}\cdot\boldsymbol{\alpha}) V_{\Gamma}(r_{\Gamma}(t,\boldsymbol{x}))\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi(\boldsymbol{x}) \right\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)^4} \\ &\leq \gamma_{\Gamma} \left\| 1 - \boldsymbol{v}_{\Gamma}\cdot\boldsymbol{\alpha} \right\|_2 \left\| V_{\Gamma}(r_{\Gamma}(t,\boldsymbol{x}))\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi(\boldsymbol{x}) \right\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)^4} \\ &\leq 2\gamma_{\Gamma} \left\| 1 - \boldsymbol{v}_{\Gamma}\cdot\boldsymbol{\alpha} \right\|_2 \sup_{\boldsymbol{x}\in\mathbb{R}^3} \left\| \mathrm{e}^{-\mathrm{i}(t-s)H_0}\, \phi(\boldsymbol{x}) \right\|_2 \left\| V_{\Gamma}(r_{\Gamma}(t,\boldsymbol{x})) \right\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x)} \\ &\leq \frac{\text{const.}}{(1+|t-s|^{3/2})} \int_0^{\infty} |r\, V_{\Gamma}(r)|^2\, \mathrm{d}r\end{aligned}$$

For the last step, a propagation estimate for regular free wave packets has been used, which is reviewed in section B.1. Provided that the integral over $rV_{\Gamma}(r)$ is finite, the Cook integral for a regular wave packet ϕ is finite as well:

$$\int_{t_0}^{\infty} \left\| \tfrac{\mathrm{d}}{\mathrm{d}t}\, \Omega_{\mathrm{C}}(t,s)\phi \right\| \mathrm{d}t \leq \int_{t_0}^{\infty} \frac{\text{const.}'}{(1+|t-s|)^{3/2}}\, \mathrm{d}t < \infty.$$

The integrability of $rV_{\Gamma}(r)$ holds in particular for potentials $V_{\Gamma}(r)$ as in equation (2.10), if $\mu_{\Gamma} > 0$.

3.4 Asymptotic orthogonality

In this section, we demonstrate the asymptotic orthogonality of the wave operators. The calculations are simple and given here for the sake of completeness. Asymptotic orthogonality means that the ranges of the wave operators are mutually orthogonal subspaces of the state space, i.e. $\operatorname{Ran}\Omega_{\Gamma}^{\pm}(s) \perp \operatorname{Ran}\Omega_{\Delta}^{\pm}(s)$ if $\Gamma \neq \Delta$. By definition this relation means that for any pair of states ϕ_1 and ϕ_2 the following scalar product vanishes,

$$\left(\Omega_{\Delta}^{\pm}(s)\phi_2, \Omega_{\Gamma}^{\pm}(s)\phi_1\right) = 0, \qquad \text{if } \Gamma \neq \Delta,$$

which is equivalent to,

$$\lim_{t\to\mp\infty} \left(U_{\Delta}(t,s) P_{\Delta}(s)\phi_2, U_{\Gamma}(t,s) P_{\Gamma}(s)\phi_1\right) = 0.$$

Here the projector $P_{\mathrm{C}}(s)$ is trivially defined as the unit operator. It is sufficient to consider the following two cases:

$$\operatorname{Ran}\Omega_{\mathrm{A}}^{-}(s) \perp \operatorname{Ran}\Omega_{\mathrm{B}}^{-}(s), \tag{3.9}$$

$$\operatorname{Ran}\Omega_{\mathrm{A}}^{-}(s) \perp \operatorname{Ran}\Omega_{\mathrm{C}}^{-}(s). \tag{3.10}$$

3.4.1 Orthogonality of channels A and B. Recalling the form (3.4) of the projection operators $P_{\mathrm{A}}(s)$ and $P_{\mathrm{B}}(s)$, it must be shown for any pair of asymptotic configurations $\Phi_{\mathrm{A},k}(t,\boldsymbol{x})$ and $\Phi_{\mathrm{B},l}(t,\boldsymbol{x})$ of the form (3.3) that

$$\lim_{t\to\infty}\Big(\Phi_{\mathrm{A},k}(t),\Phi_{\mathrm{B},l}(t)\Big) = 0, \tag{3.11}$$

in order to verify relation (3.9). We estimate the scalar product (3.11) as follows:

$$\begin{aligned}
&\Big|\Big(\Phi_{\mathrm{A},k}(t),\Phi_{\mathrm{B},l}(t)\Big)\Big| \\
&\quad\le \int \Big|\phi_{\mathrm{A},k}(\boldsymbol{x}')^\dagger S(\Lambda_{\mathrm{A}})^{\dagger^{-1}} S(\Lambda_{\mathrm{B}})^{-1}\phi_{\mathrm{B},l}(\boldsymbol{x}'')\Big|\,\mathrm{d}^3x \\
&\quad\le \|S(\Lambda_{\mathrm{A}})^{\dagger^{-1}} S(\Lambda_{\mathrm{B}})^{-1}\|_2 \int \|\phi_{\mathrm{A},k}(\boldsymbol{x}')\|_2\,\|\phi_{\mathrm{B},l}(\boldsymbol{x}'')\|_2\,\mathrm{d}^3x \\
&\quad\le \frac{2\,\|S(\Lambda_{\mathrm{A}})^{\dagger^{-1}} S(\Lambda_{\mathrm{B}})^{-1}\|_2}{1+|(\boldsymbol{b}_{\mathrm{B}}-\boldsymbol{b}_{\mathrm{A}})+t(\boldsymbol{v}_{\mathrm{B}}-\boldsymbol{v}_{\mathrm{A}})|^2}\,\times \\
&\qquad\times\int \Big\|(1+r_{\mathrm{A}}(t,\boldsymbol{x})^2)\,\phi_{\mathrm{A},k}(\boldsymbol{x}')\Big\|_2\,\Big\|(1+r_{\mathrm{B}}(t,\boldsymbol{x})^2)\,\phi_{\mathrm{B},l}(\boldsymbol{x}'')\Big\|_2\,\mathrm{d}^3x \\
&\quad\le \frac{\text{const.}}{1+|(\boldsymbol{b}_{\mathrm{B}}-\boldsymbol{b}_{\mathrm{A}})+t(\boldsymbol{v}_{\mathrm{B}}-\boldsymbol{v}_{\mathrm{A}})|^2}\,\times \\
&\qquad\times\Big\{\int(1+\boldsymbol{x}'^2)\,\|\phi_{\mathrm{A},k}(\boldsymbol{x}')\|_2^2\,\mathrm{d}^3x'\Big\}^{\frac12}\Big\{\int(1+\boldsymbol{x}''^2)\,\|\phi_{\mathrm{B},l}(\boldsymbol{x}'')\|_2^2\,\mathrm{d}^3x''\Big\}^{\frac12}
\end{aligned}$$

Here, the Cauchy–Schwarz and Hölder inequalities have been used. Doubly primed coordinates $\boldsymbol{x}''$ refer to the rest frame coordinates of centre B. The two integrals of the last expression are independent of the time t and finite, provided the eigenfunctions $\phi_{\mathrm{A},k}(\boldsymbol{x}')$ and $\phi_{\mathrm{B},l}(\boldsymbol{x}'')$ are decreasing sufficiently fast towards spatial infinity. In particular, if the potentials V_{A} and V_{B} are of the form (2.10) the eigenfunctions have the necessary fall-off property and equation (3.11) directly follows from the estimate above.

3.4.2 Orthogonality of the channels A and C. Equation (3.10), which expresses the asymptotic orthogonality of the outgoing channels A and C, is equivalent to,

$$\lim_{t\to\infty}\Big(U_{\mathrm{A}}(t,s)P_{\mathrm{A}}(s)\phi_2,\mathrm{e}^{-\mathrm{i}(t-s)H_0}\,\phi_1\Big) = 0,$$

for any pair of states $\phi_1(\boldsymbol{x})$ and $\phi_2(\boldsymbol{x})$. However, it is again sufficient to assume that $\phi_1(\boldsymbol{x})$ is a regular wave packet (cf. section B.1). Therefore, it remains to show that,

$$\lim_{t\to\infty}\Big(\Phi_{\mathrm{A},k}(t),\mathrm{e}^{-\mathrm{i}(t-s)H_0}\,\phi\Big) = 0,$$

for any regular wave packet $\phi(\boldsymbol{x})$ and asymptotic configuration $\Phi_{\mathrm{A},k}(t)$ of scattering channel A as in equation (3.3). The following sequence of estimates,

$$\begin{aligned}
&\left|\left(\Phi_{\mathrm{A},k}(t), \mathrm{e}^{-\mathrm{i}(t-s)H_0}\,\phi\right)\right| \\
&\quad\leq \int \left|\Phi_{\mathrm{A},k}(t,\boldsymbol{x})^\dagger \left(\mathrm{e}^{-\mathrm{i}(t-s)H_0}\,\phi\right)(\boldsymbol{x})\right| \mathrm{d}^3x \\
&\quad\leq \|S(\Lambda_{\mathrm{A}})^{-1}\|_2 \int \|\phi_{\mathrm{A},k}(\boldsymbol{x}')\|_2 \left\|\left(\mathrm{e}^{-\mathrm{i}(t-s)H_0}\,\phi\right)(\boldsymbol{x})\right\|_2 \mathrm{d}^3x \\
&\quad\leq \|S(\Lambda_{\mathrm{A}})^{-1}\|_2 \,\frac{\text{const.}}{(1+|t-s|)^{3/2}} \int \|\phi_{\mathrm{A},k}(\boldsymbol{x}')\|_2 \,\mathrm{d}^3x',
\end{aligned}$$

yields the desired convergence to zero as $t \to \infty$, if the remaining spatial integral is finite. Note that this remaining spatial integral does not depend on time t. It is finite if the bound state eigenfunctions $\phi_{\mathrm{A},k}$ are L^1-integrable, which is true in particular for the class of electrostatic potentials $V_\Gamma(r)$ as in equation (2.10). The estimate again makes use of estimate (B.2) for regular wave packets, described in the appendix B.

3.5 Relativistic invariance

The existence proofs in section 3.3 refer to some particular, although arbitrarily chosen, Lorentz frame. In different, relatively moving Lorentz frames, the limits appearing in the definition of wave operators and scattering states have to be taken with respect to different time axes. It is, therefore, necessary to prove that the transition amplitudes are nevertheless Lorentz invariant quantities.

Consider an arbitrary asymptotic configuration $\Phi_{\Gamma,k}(t,\boldsymbol{x})$ and the corresponding outgoing scattering state $\Psi^-_{\Gamma,k}(t,\boldsymbol{x})$ of the two-centre Dirac equation. Given a Poincaré transformation, $(t',\boldsymbol{x}') = \Lambda(t,\boldsymbol{x}) + (a^0,\boldsymbol{a})$, to an arbitrary primed coordinate system, the transformed wave functions in the primed coordinates are:

$$\begin{aligned}
\Phi'_{\Gamma,k}(t',\boldsymbol{x}') &= S(\Lambda)\,\Phi_{\Gamma,k}(\Lambda^{-1}(t'-a^0,\boldsymbol{x}'-\boldsymbol{a})), \\
{\Psi^-_{\Gamma,k}}'(t',\boldsymbol{x}') &= S(\Lambda)\,\Psi^-_{\Gamma,k}(\Lambda^{-1}(t'-a^0,\boldsymbol{x}'-\boldsymbol{a})).
\end{aligned}$$

The question arises whether the transformed wave function ${\Psi^-_{\Gamma,k}}'(t',\boldsymbol{x}')$ is identical to the (unique) outgoing scattering state that corresponds to the asymptotic configuration $\Phi'_{\Gamma,k}(t',\boldsymbol{x}')$ in the primed frame of reference. In other words, it has to be checked whether the following holds:

$$\lim_{t'\to\infty} \|{\Psi^-_{\Gamma,k}}'(t',\boldsymbol{x}') - \Phi'_{\Gamma,k}(t',\boldsymbol{x}')\|_{L^2(\mathbb{R}^3,\mathrm{d}^3x')^4} = 0. \tag{3.12}$$

Of course, the analogous convergence as $t' \to -\infty$ is similarly conjectured for the Poincaré-transformed incoming scattering state ${\Psi^+_{\Gamma,k}}'(t',\boldsymbol{x}')$.

If these conjectures can be verified, then, in the primed frame, the transition amplitude $a'_{\Delta l,\Gamma k}$ is given in terms of the Poincaré-transformed scattering states of the unprimed frame, according to:

$$a'_{\Delta l,\Gamma k} = \left({\Psi^-_{\Delta,l}}'(t'), {\Psi^+_{\Gamma,k}}'(t')\right).$$

The relativistic invariance of the transition amplitude is then simply a consequence of the Poincaré invariance of the scalar product between two wave functions that solve the same Dirac equation (cf. section B.2):

$$a'_{\Delta l,\Gamma k} = \Big(\Psi^{-\,\prime}_{\Delta,l}(t'), \Psi^{+\,\prime}_{\Gamma,k}(t')\Big)' = \Big(\Psi^{-}_{\Delta,l}(t), \Psi^{+}_{\Gamma,k}(t)\Big) = a_{\Delta l,\Gamma k}.$$

Note that in this equation the two scalar products refer to different spatial integrations or hypersurfaces in Minkowski space.

Equation (3.12) is most easily verified, if the Poincaré transformation is only a product of spatial rotations and space-time translations, which do not mix time and spatial coordinates. For a verification of equation (3.12) only Lorentz boosts need to be considered.

3.5.1 Boost invariance of the excitation and capture amplitudes. In this subsection, it is demonstrated that (3.12) holds for $\Gamma = \mathrm{A}$. The case $\Gamma = \mathrm{B}$ and the limits $t \to -\infty$ are treated similarly. In the course of the following calculations, several assumptions about the radially symmetric potentials V_A and V_B are necessary. These assumptions hold in particular, if both electrostatic potentials $V_\Gamma(r)$ are of the form (2.10) with $\varrho_\Gamma > 0$ and $\mu_\Gamma > 0$.

Without loss of generality, it may be assumed that the unprimed Lorentz frame is a rest frame of centre A, where centre A is located at the origin. This is sufficient because the Poincaré transformation between two arbitrary Lorentz frames can be decomposed into a product of a boost into a rest frame of centre A, spatial rotations, space-time translations, and the inverse of another boost into a rest frame of centre A. Hence, the primed coordinates, for which the convergence (3.12) must be proved, are connected to the unprimed coordinates by a pure boost. In this section the velocity of this boost is denoted by $\boldsymbol{v}$. Again, without loss of generality, the parameter $\boldsymbol{b}_\mathrm{B}$ of the trajectory $\boldsymbol{R}_\mathrm{B}(t) = \boldsymbol{b}_\mathrm{B} + t\boldsymbol{v}_\mathrm{B}$ of centre B in the unprimed coordinates can be taken to be perpendicular to the boost velocity $\boldsymbol{v}$. Hence, $\boldsymbol{b}_\mathrm{B} = \boldsymbol{b}'_\mathrm{B}$ holds. Assuming this case, the following estimates hold for the Lorentz scalars $r_\Gamma(t,\boldsymbol{x})$ and $r'_\Gamma(t',\boldsymbol{x}')$ in the primed and unprimed frames respectively:

$$\begin{aligned} \frac{1}{1+r_\mathrm{A}(t,\boldsymbol{x})^2}\,\frac{1}{1+r_\mathrm{B}(t,\boldsymbol{x})^2} &\le \frac{2}{1+|\boldsymbol{b}_\mathrm{B}+t\boldsymbol{v}_\mathrm{B}|^2}, \\ \frac{1}{1+r'_\mathrm{A}(t',\boldsymbol{x}')^2}\,\frac{1}{1+r'_\mathrm{B}(t',\boldsymbol{x}')^2} &\le \frac{2}{1+|\boldsymbol{b}_\mathrm{B}+t'(\boldsymbol{v}+\boldsymbol{v}'_\mathrm{B})|^2}, \end{aligned} \tag{3.13}$$

where $\boldsymbol{v}'_\mathrm{B}$ is the velocity of centre B in the primed coordinates.

The asymptotic condition $\Phi_\mathrm{A}(t,\boldsymbol{x})$ (for the sake of simplicity omitting the second index in this subsection) may be chosen as,

$$\Phi_\mathrm{A}(t,\boldsymbol{x}) = \exp(-\mathrm{i}t\epsilon_\mathrm{A})\phi_\mathrm{A}(\boldsymbol{x}),$$

where $\phi_\mathrm{A}(\boldsymbol{x})$ is a normalised bound state eigenfunction of the electrostatic potential V_A. The statement, that $\Psi^-_\mathrm{A}(t,\boldsymbol{x})$ is the outgoing scattering state which corresponds to the asymptotic condition $\Phi_\mathrm{A}(t,\boldsymbol{x})$, is equivalent to the following convergence property:

$$\lim_{t\to\infty} \Big(\Psi^-_\mathrm{A}(t), \Phi_\mathrm{A}(t)\Big) = 1. \tag{3.14}$$

Similarly, the asymptotic convergence of the two transformed Dirac wave functions ${\Psi_{\mathrm{A}}^{-}}'(t',\boldsymbol{x}')$ and $\Phi'_{\mathrm{A}}(t',\boldsymbol{x}')$ in the primed frame is equivalent to:

$$\lim_{t'\to\infty}\left({\Psi_{\mathrm{A}}^{-}}'(t'),\Phi'_{\mathrm{A}}(t')\right)' = 1. \tag{3.15}$$

In order to prove that (3.15) follows from (3.14), the difference of both scalar products is considered for some finite times $t=\zeta$ and $t'=\gamma\zeta$. Here γ denotes the Lorentz factor corresponding to the boost velocity $\boldsymbol{v}$. The limit of this difference of scalar products is shown to vanish as ζ tends to $+\infty$. Using the Gaussian integral theorem in Minkowski space, the difference of the scalar products is transformed into a four-dimensional integral:

$$\begin{aligned}\left(\Psi_{\mathrm{A}}^{-}(\zeta),\Phi_{\mathrm{A}}(\zeta)\right)-\left({\Psi_{\mathrm{A}}^{-}}'(\gamma\zeta),\Phi'_{\mathrm{A}}(\gamma\zeta)\right)' &= \int_{D(\zeta)}\partial_\mu\left(\overline{\Psi_{\mathrm{A}}^{-}}(y)\,\gamma^\mu\,\Phi_{\mathrm{A}}(y)\right)\,\mathrm{d}^4y\\ &= \int_{D(\zeta)}\Psi_{\mathrm{A}}^{-}(y)^\dagger\,W_{\mathrm{B}}(y)\,\Phi_{\mathrm{A}}(y)\,\mathrm{d}^4y.\end{aligned}\tag{3.16}$$

For the second step, we have used that $\Psi_{\mathrm{A}}^{-}(t,\boldsymbol{x})$ solves the two-centre Dirac equation, whereas $\Phi_{\mathrm{A}}(t,\boldsymbol{x})$ solves the Dirac equation of scattering channel A. The four-volume of integration $D(\zeta)$ is given by:

$$D(\zeta)=\left\{y\in\mathbb{R}^4 : 0\le y^0-\zeta\le\boldsymbol{v}\cdot\boldsymbol{y}\quad\text{or}\quad 0\ge y^0-\zeta\ge\boldsymbol{v}\cdot\boldsymbol{y}\right\}.$$

It is the volume of space-time bounded by the two spacelike hypersurfaces, which are determined by $t=\zeta$ and $t'=\gamma\zeta$. (See section B.2 for a similar calculation.)

According to the inequalities (3.13), the following estimate holds for sufficiently large parameter ζ:

$$\sup_{y\in D(\zeta)}\frac{1}{1+r_{\mathrm{A}}(y)^2}\,\frac{1}{1+r_{\mathrm{B}}(y)^2}\le\frac{1}{C_1\zeta^2} \tag{3.17}$$

Here the constant $C_1>0$ depends on $\boldsymbol{b}_{\mathrm{B}}$, $\boldsymbol{v}_{\mathrm{B}}$ and $\boldsymbol{v}$ only.

Since the time-dependence of the scattering state $\Psi_{\mathrm{A}}^{-}(t,\boldsymbol{x})$ is not known explicitly, the integral (3.16) must be estimated in order to demonstrate that it converges to zero as $\zeta\to\infty$. The following estimate is based on the assumption that the solution $\Psi_{\mathrm{A}}^{-}(t,\boldsymbol{x})$ of the two-centre Dirac equation is bounded in space-time by some constant C_2:

$$\Big\|\,\|\Psi_{\mathrm{A}}^{-}(y)\|_2\Big\|_{L^\infty(\mathbb{R}^4)}\le C_2 \tag{3.18}$$

This cannot be expected to be true in general. In fact, it is false if the external fields $W_\Gamma(t,\boldsymbol{x})$ correspond to linearly moving Yukawa potentials. But a suitable assumption on the electrostatic fields $V_\Gamma(r)$ should be sufficient in order to obtain this property. Although a proof is not given here, (3.18) is expected to hold in particular if the radial potentials $V_\Gamma(r)$ are of the form (2.10), with $\varrho_\Gamma>0$ and $\mu_\Gamma>0$. The latter condition provides that the potentials $V_\Gamma(r)$, their eigenfunctions, and the multiplication operators $W_\Gamma(t,\boldsymbol{x})$ are bounded.

The estimate of the integral (3.16) is done as follows:

$$
\begin{aligned}
&\left| \int_{D(\zeta)} \Psi_{\mathrm{A}}^{-}(y)^{\dagger}\, W_{\mathrm{B}}(y)\, \Phi_{\mathrm{A}}(y)\, \mathrm{d}^4 y \right| \\
&\quad\leq \int_{D(\zeta)} \|\Psi_{\mathrm{A}}^{-}(y)\|_2\, \gamma_{\mathrm{B}}\, \|1 - \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{\alpha}\|_2\, |V_{\mathrm{B}}(r_{\mathrm{B}}(y))|\, \|\Phi_{\mathrm{A}}(y)\|_2\, \mathrm{d}^4 y \\
&\quad\leq \frac{\gamma_{\mathrm{B}} \|1 - \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{\alpha}\|_2}{C_1 \zeta^2} \\
&\qquad\qquad \int_{D(\zeta)} \|\Psi_{\mathrm{A}}^{-}(y)\|_2\, (1 + r_{\mathrm{B}}(y)^2)\, |V_{\mathrm{B}}(r_{\mathrm{B}}(y))|\, (1 + r_{\mathrm{A}}(y)^2)\, \|\Phi_{\mathrm{A}}(y)\|_2\, \mathrm{d}^4 y \\
&\quad\leq \frac{C_2 C_3 \gamma_{\mathrm{B}} \|1 - \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{\alpha}\|_2}{C_1 \zeta^2} \int_{D(\zeta)} (1 + \boldsymbol{y}^2)\, \|\phi_{\mathrm{A}}(\boldsymbol{y})\|_2\, \mathrm{d}^4 y \\
&\quad\leq \frac{C_2 C_3 \gamma_{\mathrm{B}} \|1 - \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{\alpha}\|_2\, |\boldsymbol{v}|}{C_1 \zeta^2} \int_{\mathbb{R}^3} |\boldsymbol{y}| (1 + \boldsymbol{y}^2) \|\phi_{\mathrm{A}}(\boldsymbol{y})\|_2\, \mathrm{d}^3 y.
\end{aligned}
$$

The remaining integral is finite, in particular, if the bound state eigenfunction $\phi_{\mathrm{A}}(\boldsymbol{x})$ is exponentially decreasing towards spatial infinity. Furthermore, it has been used that the term $|(1 + r^2)\, V_{\mathrm{B}}(r)|$ is bounded by a constant C_3. Both requirements are satisfied for the class of potentials $V_\Gamma(r)$ of equation (2.10) with $\mu_\Gamma > 0$ and $\varrho_\Gamma > 0$. Therefore, the integral (3.16) vanishes as ζ approaches infinity.

3.6 Remarks

3.6.1 Two-centre Dirac equation with moving point charges. In section 3.3, asymptotic convergence has *not* been shown for the two-centre Dirac equation with moving unscreened point charges. The proofs cannot be extended to include Coulomb potentials, because the inverse screening lengths μ_{A} and μ_{B} must not vanish. This means that the radial potentials $V_\Gamma(r)$ have to be short-ranged.

Furthermore, it seems hardly possible that asymptotic convergence can be proved for long-range electrostatic potentials $V_\Gamma(r)$, like the Coulomb potential, without a modification of the dynamics of the scattering channels. The reason for this conviction is as follows: For the nonrelativistic and relativistic quantum mechanical scattering by a *single* Coulomb potential, the corresponding fact has been demonstrated by Dollard in [Dol64, DV66] (reviewed in [Tha92]). Also, the scattering theory of the *two-centre* Schrödinger equation with long-range potentials has been investigated by Wüller in [Wül88]. There, it was found that modified dynamics for the scattering channels of the two-centre Schrödinger equation are necessary, in order to prove the existence and asymptotic completeness of the Møller wave operators if long-range forces are present. The modified dynamics of each of the three different scattering channels closely resembles the distorted free-time-evolution that was given by Dollard for the nonrelativistic case.

Wüller, in his analysis [Wül88], made use of geometrical methods of scattering theory, which have been developed by Enß and have also been applied to the discussion of the Dirac equation [Tha92]. Therefore, a proper discussion of the scattering theory for the Dirac equation with moving point charges may be feasible by using similar methods as in [Wül88]. Such a mathematical investigation does not exist in the literature, but it is required, in particular, for a proof of relativistic invariance in the long-range case. See, however, the next section for the discussion of Coulomb boundary conditions.

3.6.2 Asymptotic completeness. Note that *asymptotic completeness* of the scattering theory of the two-centre Dirac equation is neither proved in this thesis nor has it been considered in the literature. It is conjectured that it can be shown similarly to the complicated, corresponding proofs that have been published for the nonrelativistic charge-transfer model [YAJ80, HAG82, WÜL88, GRA90].

Asymptotic completeness is defined as the existence of complete sets of orthonormal incoming scattering states $\Psi^+_{\Gamma,k}(t,\boldsymbol{x})$ and outgoing scattering states $\Psi^-_{\Gamma,k}(t,\boldsymbol{x})$. It means that *any* solution $\Psi(t,\boldsymbol{x})$ of the two-centre Dirac equation can be written rigorously as linear combination of either incoming or outgoing scattering states:

$$\Psi(t,\boldsymbol{x}) = \sum_{\Gamma,k} a^+_{\Gamma,k}\,\Psi^+_{\Gamma,k}(t,\boldsymbol{x}) = \sum_{\Gamma,k} a^-_{\Gamma,k}\,\Psi^-_{\Gamma,k}(t,\boldsymbol{x}).$$

As the scattering states $\Psi^\pm_{\Gamma,k}(t,\boldsymbol{x})$ are asymptotically equal to asymptotic configurations $\Phi_{\Gamma,k}(t,\boldsymbol{x})$ as $t\to\mp\infty$, formally the linear expansions above turn into linear combinations of asymptotic configurations $\Phi_{\Gamma,k}(t,\boldsymbol{x})$ in the limit $t\to\mp\infty$ (cf. chapter 4).

If the solution $\Psi(t,\boldsymbol{x})$ is itself a scattering state, the coefficients of linear expansion are identical to the transition amplitudes $a_{\Delta l,\Gamma k}$ defined in section 3.2:

$$\Psi^+_{\Gamma,k}(t,\boldsymbol{x}) = \sum_{\Delta,l} a_{\Delta l,\Gamma k}\,\Psi^-_{\Delta,l}(t,\boldsymbol{x}),$$
$$\Psi^-_{\Gamma,k}(t,\boldsymbol{x}) = \sum_{\Delta,l} a^*_{\Gamma k,\Delta l}\,\Psi^+_{\Delta,l}(t,\boldsymbol{x}).$$

Therefore, the 'conservation of probability',

$$\|\Psi^\pm_{\Gamma,k}(t)\| = \sum_{\Delta,l} |a_{\Delta l,\Gamma k}|^2 = 1, \tag{3.19}$$

is a consequence of asymptotic completeness. Suppose that an initial configuration (Γ,k) is a bound state of either centre A or centre B. In general, the sum over transition probabilities $|a_{\Delta l,\Gamma k}|^2$ to final configurations (Δ,l) which are not asymptotic configurations of channel C with negative energy is strictly less then one. This means that the naive interpretation of the initial configuration as a one-particle state is not entirely correct, since the total probability of finding an initial bound state (Γ,k) in a final configuration of positive energy is not one, as it must be for a single-particle theory. This reflects that the Dirac theory can only be interpreted as a multi-particle theory.

3.6.3 Problem of second quantisation. A multi-particle theory requires a multi-particle state space, namely the Fock space of quantum field theory. The Fock space formalism of pair creation in external fields makes use of the fact that the *time-dependent* external fields vanish everywhere in space as time t tends to $\pm\infty$. This property is necessary, it allows for the construction of the Fock space (the 'second quantisation') based on a spectral decomposition of the state space of the classical Dirac field with respect to the time-independent Hamiltonian at $t=\pm\infty$ [THA92, Sch95].[1] This time-independent Hamiltonian is identical to the Hamiltonian the interaction picture of quantum field theory refers to (see e.g. [RS75, FGS91, Sch95]). In common presentations of quantum field theory this is frequently the free Hamiltonian $H_0 = -\mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta$ (e.g. [FGS91, Sch95, Wei95]) or the free Hamiltonian plus a stationary Coulomb field, referred to as the Furry picture of quantum field theory [MPS98].

Clearly, for the two-centre Dirac equation there is no such limit of the time-dependent Dirac Hamiltonian as $t \to \pm\infty$. Therefore, the usual Fock space construction is not possible, although, as we have seen above, a multi-particle interpretation of the transition amplitudes is inevitable. The problem of second quantisation of the scattering theory presented in this chapter remains unsolved. For the present work we take the pragmatic point of view that transition amplitudes between an asymptotic configuration of negative energy and an asymptotic configuration of positive energy have to be interpreted as probability amplitudes of single pair production or annihilation processes, as depicted in figure 3.1. Furthermore, in numerical calculations of this work these amplitudes are so small that the 'one-particle' interpretations of other transition amplitudes, namely those between asymptotic configurations of positive energy as depicted in 3.1, are reasonable, because numerical uncertainties are much larger than the 'error due to a loss of probability' as a consequence of transitions to negative energy configurations of scattering channel C.

Finally, we take a look at the role of quantum field theory in other approaches to pair creation in peripheral heavy-ion collisions. Note, that the scattering channels A and B of the two-centre Dirac equation can be removed by an adiabatic switching formalism, namely by replacing the external fields $W_\Gamma(t,\boldsymbol{x})$, for example, by fields $\mathrm{e}^{-\varepsilon^2 t^2}\, W_\Gamma(t,\boldsymbol{x})$ that vanish as time t tends to infinity. For a Dirac field with such an external potential all particles are asymptotically free. The scattering channels A and B are removed by the exponential damping factor and the scattering theory can be formulated with respect to the free particle Fock space (Feynman–Dyson QED). Although not mentioned explicitly, this point of view is taken implicitly, e.g., in [BS89, WBS90]. A second possibility, allowing for an asymmetrical description of bound-free pair production, is given by exponentially damping only the external field of one of the centres, say $W_{\mathrm{B}}(t,\boldsymbol{x})$. Then, in a rest frame of centre A, the total two-centre Hamiltonian also becomes stationary as time t tends to $\pm\infty$. This allows for a proper Fock space theory as well and corresponds to the single-centre approaches to pair creation making use of the Furry picture. It is clearly asymmetrical, since one of the nuclei only acts as a perturbation.

It is well-known that in quantum field theories, subject to asymptotically vanishing time-dependent external field, transition amplitudes of the multi-particle theory are directly related to transition amplitudes of the scattering theory of the classical Dirac field (e.g. [FGS91, Sch95]) and it is, therefore, sufficient to consider the latter. In conclusion, we have argued in this subsection that the scattering theory of the

[1] Strictly speaking even stronger assumptions on the time-dependent external fields are necessary for a second quantised field theory: The scattering matrix of the classical Dirac field must be implementable in Fock space. A sufficient condition for the implementability is known as the Shale–Stinesping criterion. (See e.g. [Rui77a, Rui77b, Rui77c, Tha92, Sch95].)

two-centre Dirac equation, which allows for bound states of both centres, represents a more complicated case, for which a proper multi-particle theory is not known.

3.7 Coulomb boundary conditions

In this section, the case of long-range forces is considered. This means that the electrostatic potential of a charge distribution ρ_Γ in its rest frame is Coulomb-like at large distances from the corresponding centre. It has been argued in the previous section 3.6 that scattering theory as described in section 3.1 is not applicable in this case, because the potential is not decreasing sufficiently fast towards spatial infinity to obtain asymptotic convergence. A workaround for that is the modification of the wave equations for the scattering channels.

Modified Dirac equations for the scattering channels A and B have been proposed in [Eic87], and reviewed in [TE90] and [EM95, ch. 5], where they have been termed asymptotic equations. In these wave equations the residual interaction of centre B with bound states of centre A is added to the corresponding channel Hamiltonian of centre A, and vice versa, leading to *modified scattering-channel Hamiltonians.*

A relativistically moving point charge not only induces a long-range electric-field, but also a long-range magnetic field. The magnetic field only vanishes in the rest frame of the point source. Therefore, the asymptotic influence of centre B on bound states of centre A is best considered in the rest frame of centre B. A state bound to centre A means here that it is localised in the vicinity of centre A for *all* times. Such a bound state is subject to the long-range Coulomb potential of centre B also at arbitrarily large times. This is expressed by the fact that asymptotic convergence is not achieved, if this large-time influence of centre B is neglected. It has, therefore, been proposed by Eichler [Eic87, TE90, EM95] to include the following residual interaction into the Hamiltonian of scattering channel A:

$$W_{\mathrm{B}}^{\infty\prime\prime}(t'', \boldsymbol{x}'') = \frac{-e^2 \tilde{Z}_{\mathrm{B}}}{d''_{\mathrm{B}}(t'', \boldsymbol{x}'')}. \tag{3.20}$$

Here, doubly primed coordinates denote rest frame coordinates of centre B and the distance between the centres A and B as determined in the rest frame of centre B is given by the Lorentz scalar $d''_{\mathrm{B}}(t'', \boldsymbol{x}'')$ (cf. section 2.1). The charge number $\tilde{Z}_{\mathrm{B}}$ has been introduced to indicate the strength of the Coulomb-like tail of the electrostatic potential of centre B. It is distinguished from the charge number Z_{B}, since the latter has been used as well for the Yukawa potential, in order to indicate its field strength near the origin. Clearly, $Z_{\mathrm{B}} = \tilde{Z}_{\mathrm{B}}$ for the Coulomb potential.

In fact, in the doubly primed frame the external field $W_{\mathrm{B}}^{\infty\prime\prime}(t'', \boldsymbol{x}'')$ does not depend on spatial coordinates $\boldsymbol{x}''$. In the rest frame of centre B, it corresponds to the Coulomb potential at the position of the moving centre A, of a point charge $e\tilde{Z}_{\mathrm{B}}$ located at the origin. A Poincaré transformation from the doubly primed coordinates back to an unprimed coordinate system yields the residual external field of centre B on bound states of centre A,

$$W_{\mathrm{B}}^{\infty}(t, \boldsymbol{x}) = \frac{-e^2 \tilde{Z}_{\mathrm{B}}}{d_{\mathrm{B}}(t, \boldsymbol{x})}\, \gamma_{\mathrm{B}}(1 - \boldsymbol{v}_{\mathrm{B}} \cdot \boldsymbol{\alpha}), \tag{3.21}$$

where $\boldsymbol{v}_{\mathrm{B}}$ is the velocity of centre B in the unprimed frame. Similarly, the residual external field of centre A on bound states of centre B is given in terms of the parameter $\tilde{Z}_{\mathrm{A}}$ and the Lorentz scalar $d_{\mathrm{A}}(t,\boldsymbol{x})$. These residual fields have non-vanishing magnetic-field components, to which bound states are exposed at arbitrarily large times.

The modified Hamiltonians of the scattering channels A and B are therefore:

$$\begin{aligned} H_{\mathrm{A}}^{\infty}(t) &= H_0 + W_{\mathrm{A}}(t,\boldsymbol{x}) + W_{\mathrm{B}}^{\infty}(t,\boldsymbol{x}), \\ H_{\mathrm{B}}^{\infty}(t) &= H_0 + W_{\mathrm{B}}(t,\boldsymbol{x}) + W_{\mathrm{A}}^{\infty}(t,\boldsymbol{x}). \end{aligned} \tag{3.22}$$

These Hamilton operators are time-dependent in any Lorentz frame. For the rest frames of centre A and B they have been described in the works of Eichler and co-workers. It was recognised first in [Eic87] that the corresponding scattering-channel Dirac equations have *bound-state* solutions, because the residual fields $W_{\Gamma}^{\infty}(t,\boldsymbol{x})$ can be removed by a gauge transformation.

A gauge function suitable to remove the external field $W_{\mathrm{B}}^{\infty}(t,\boldsymbol{x})$ is given by:

$$g_{\mathrm{B}}(t,\boldsymbol{x}) = \frac{e^2\tilde{Z}_{\mathrm{B}}}{v}\log\left[d_{\mathrm{B}}(t,\boldsymbol{x}) - \frac{\gamma_{\mathrm{A}}\boldsymbol{v}_{\mathrm{A}}\cdot\boldsymbol{d}}{\gamma v} + \frac{\gamma_{\mathrm{B}}\boldsymbol{v}_{\mathrm{B}}\cdot\boldsymbol{d}}{\gamma^2 v} + v\gamma_{\mathrm{B}}\Big(t - \boldsymbol{v}_{\mathrm{B}}\cdot(\boldsymbol{x}-\boldsymbol{b}_{\mathrm{B}})\Big)\right]. \tag{3.23}$$

The abbreviations v,γ and $\boldsymbol{d}$ have been introduced in section 2.1, where $d_{\mathrm{B}}(t,\boldsymbol{x})$ has been defined as well. Similarly a gauge function $g_{\mathrm{A}}(t,\boldsymbol{x})$ removing $W_{\mathrm{A}}^{\infty}(t,\boldsymbol{x})$ is obtained, by interchanging in equation (3.23) the indices A and B and reversing the sign of $\boldsymbol{d}$, which was defined as $\boldsymbol{d} = \boldsymbol{b}_{\mathrm{B}} - \boldsymbol{b}_{\mathrm{A}}$. These gauge functions satisfy:

$$\{\partial_t + \boldsymbol{\alpha}\cdot\nabla\}\, g_{\Gamma}(t,\boldsymbol{x}) = -W_{\Gamma}^{\infty}(t,\boldsymbol{x}).$$

The gauge functions $g_{\Gamma}(t,\boldsymbol{x})$ are determined only up to constant and, therefore, other, equivalent gauge functions exist. Given a solution $\Phi_{\mathrm{A}}(t,\boldsymbol{x})$ of the unperturbed scattering channel Dirac equation,

$$[H_0 + W_{\mathrm{A}}(t,\boldsymbol{x}) - \mathrm{i}\partial_t]\,\Phi_{\mathrm{A}}(t,\boldsymbol{x}) = 0,$$

the gauge transformed wave function $\Phi_{\mathrm{A}}^{\infty}(t,\boldsymbol{x})$, given by,

$$\Phi_{\mathrm{A}}^{\infty}(t,\boldsymbol{x}) = \exp(\mathrm{i}g_{\mathrm{B}}(t,\boldsymbol{x}))\,\Phi_{\mathrm{A}}(t,\boldsymbol{x}),$$

then solves the Coulomb-distorted channel Dirac equation,

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

By virtue of this connection, Dirac equations of the scattering channels A and B, with Hamilton operators according to equation (3.22), have solutions which *permanently* remain localised in the vicinity of their respective centre. Therefore, they are appropriate for the description of bound states, if Coulomb forces are present. Following Eichler and Dewangan the wave function $\Phi_{\mathrm{A}}^{\infty}(t,\boldsymbol{x})$ is said to satisfy *Coulomb boundary conditions* [EM95].

Recently, it has been asserted in [WSE99] that the asymptotic equations, as presented in this section, are 'not formally correct' (see in particular appendix A of [WSE99]). Another residual interaction has been proposed by Segev in the article quoted. The present author does not agree with Segev for the following reason: The Hamilton operator of the asymptotic equation, as proposed by Segev, is time-dependent in a nontrivial way in *any* Lorentz frame. This means that there are no solutions of Segev's asymptotic equations, which remain localised at a single centre for all times. Clearly, the asymptotic equations of Segev are not suitable to describe bound states. Contrary to the argument in [WSE99], the earlier proposal of Eichler [Eic87] seems to be the only appropriate choice for the Coulomb-modified Dirac equations of the scattering channels A and B, corresponding to asymptotically bound particles of the two-centre Dirac equation with unscreened nuclear charges.