Chapter 4

Coupled Channel Approximation

In this chapter, we give an introduction to the coupled channel method, used in this work to solve the two-centre Dirac equation numerically. Although this method has been widely used for many years, also for the solution of the two-centre Schrödinger equation, a brief account of this ansatz is necessary to explain its principal ideas and present notational conventions. Here, particular emphasis is given to the fundamental solution of the coupled channel equations and its properties. In this respect the following sections differ from standard presentations of the numerical method [BM92, EM95].

4.1 Coupled channel equations for the semiclassical approximation

The principal idea of the coupled channel ansatz is to construct an approximate solution $\tilde{\Psi}(t, \boldsymbol{x})$ of the Dirac equation (2.11) as a finite time-dependent linear combination of asymptotic configurations $\Phi_{\Gamma,i}(t, \boldsymbol{x})$:

$$\tilde{\Psi}(t, \boldsymbol{x}) = \sum_{\Gamma,i} c_{\Gamma,i}(t)\, \Phi_{\Gamma,i}(t, \boldsymbol{x}). \tag{4.1}$$

The states $\Phi_{\Gamma,i}$ included in this finite sum are usually referred to as the *basis functions* of the coupled channel expansion [BM92, EM95]. Note that generally an exact solution of the two-centre Dirac equation cannot be written as *finite* sum of asymptotic configurations. However, in the case of the two-centre Dirac equation an infinite series expansion is suitable to represent an arbitrary solution. The accuracy and usefulness of this ansatz depends on the physical situation under consideration and the corresponding choice of basis functions. More general expansions are possible in which the basis functions are equal to the asymptotic configurations $\Phi_{\Gamma,i}$ only asymptotically (i.e. for large times).

The determination of the complex expansion coefficients $c_{\Gamma,i}(t)$ is guided by the following reasoning. Assume that a solution $\Psi(t, \boldsymbol{x})$ of a Dirac equation with a time-dependent Hamilton operator $H(t)$,

$$[H(t) - \mathrm{i}\partial_t]\, \Psi(t, \boldsymbol{x}) = 0,$$

may be approximated by a wave function of the type given in equation (4.1), then $\tilde{\Psi}(t, \boldsymbol{x})$ approximately solves that Dirac equation:

$$[H(t) - \mathrm{i}\partial_t] \sum_{\Gamma,i} c_{\Gamma,i}(t)\, \Phi_{\Gamma,i}(t, \boldsymbol{x}) \approx 0. \tag{4.2}$$

Multiplying this equation from the left by the adjoint of some basis function $\Phi^\dagger_{\Delta,j}$ and integrating over x yields a set of *approximate* equations for the coefficients $c_{\Gamma,i}(t)$. By turning the approximate equality into an exact equality a *prescription* for the determination of the coefficients $c_{\Gamma,i}(t)$ is obtained. Therefore, given the time-dependent

Dirac-Hamiltonian $H(t)$, according to this prescription the expansion coefficients $c_{\Gamma,i}(t)$ have to be determined by solving the following set of differential equations:

$$\sum_{\Gamma,i} c_{\Gamma,i}(t)\Big(\Phi_{\Delta,j}(t), [H(t) - \mathrm{i}\partial_t]\,\Phi_{\Gamma,i}(t)\Big) - \mathrm{i}\sum_{\Gamma,i} \left(\partial_t\, c_{\Gamma,i}(t)\right)\Big(\Phi_{\Delta,j}(t), \Phi_{\Gamma,i}(t)\Big) = 0. \quad (4.3)$$

These equations will be referred to as the *coupled channel equations*. In the nonrelativistic impact parameter model, based, e.g., on the Schrödinger equation, the coupled channel equations may also be derived from a variational principle [BM92]. Note that in the literature on atomic physics the term coupled channel equations sometimes also refers to other (integro-differential) equations which are more or less related to the present set of equations (4.3) [BM92, Fri90].

The important, distinctive property of the coupled channel equations is that the norm $\|\tilde{\Psi}(t)\|$ of an approximate solution $\tilde{\Psi}(t, \boldsymbol{x})$ is independent of the time t. Following [BM92] it is verified as follows. As a consequence of equation (4.3) we have,

$$\int \tilde{\Psi}(t, \boldsymbol{x})^\dagger \Big([H(t) - \mathrm{i}\partial_t]\,\tilde{\Psi}(t, \boldsymbol{x})\Big)\,\mathrm{d}^3x = 0,$$

although $\tilde{\Psi}(t, \boldsymbol{x})$ is not an exact solution of the Dirac equation in general. Due to the hermitian property of the Hamiltonian $H(t)$ the time-independence of the norm $\|\tilde{\Psi}(t)\|$ is obtained by taking the time derivative of the norm squared:

$$\begin{aligned}\partial_t\|\tilde{\Psi}(t)\|^2 &= \Big(\partial_t\tilde{\Psi}(t), \tilde{\Psi}(t)\Big) + \Big(\tilde{\Psi}(t), \partial_t\tilde{\Psi}(t)\Big) \\ &= \Big(-\mathrm{i}H(t)\tilde{\Psi}(t), \tilde{\Psi}(t)\Big) + \Big(\tilde{\Psi}(t), -\mathrm{i}H(t)\tilde{\Psi}(t)\Big) = 0. \quad (4.4)\end{aligned}$$

In the same way it is proved that the scalar product between two arbitrary approximate solutions $\tilde{\Psi}^{(1)}(t)$ and $\tilde{\Psi}^{(2)}(t)$, which are different linear combination of the same basis functions, is conserved:

$$\partial_t \Big(\tilde{\Psi}^{(1)}(t), \tilde{\Psi}^{(2)}(t)\Big) = 0 \quad (4.5)$$

This property, which will be used below, is in fact equivalent to (4.4) due to the polarisation identity of the scalar product [RS80, Kat80].

To conclude this section, we note that the coupled channel ansatz (4.1) can be formulated in various relativistic frames of reference. Then the coupled channel equations (4.3) stated in two different reference frames differ if the Lorentz frames are moving with respect to each other. This constitutes a peculiarity of the relativistic theory of coupled channel equations. Nonrelativistic inertial frames all have the same time axis and the coupled equations are the same in all nonrelativistic inertial frames. By contrast, in the relativistic theory the time axis is transformed by a Lorentz boost. The influence of the choice of the relativistic frame of reference on transition amplitudes computed by means of the coupled channel method is investigated systematically in this thesis, numerical results are presented in chapter 6.

4.2 Fundamental solution and asymptotic unitarity

In this section, the general mathematical properties of solutions $c_{\Gamma,i}(t)$ of the coupled channel equations (4.3) are discussed. In order to simplify the notation in the subsequent presentation, the double indices (Γ, i) of the basis functions are mapped one

to one and onto the integers from 1 to n, where n is the number of basis functions occurring in the expansion (4.1). Given such a mapping for some particular set of basis functions $\Phi_{\Gamma,i}$, the basis functions may be labelled more simply by a single integer i. Defining the overlap matrix $N(t)$ of the basis functions $\Phi_i(t, \boldsymbol{x})$ as,

$$N_{ij}(t) = (\Phi_i(t), \Phi_j(t)) \,, \tag{4.6}$$

and the interaction matrix $V(t)$ as,

$$V_{ij}(t) = (\Phi_i(t), [H(t) - \mathrm{i}\partial_t] \, \Phi_j(t)) \,, \tag{4.7}$$

the coupled channel equations (4.3) may be rewritten in the equivalent matrix form [BM92, EM95]:

$$\partial_t \, c(t) = -\mathrm{i} N(t)^{-1} V(t) c(t). \tag{4.8}$$

Here, $c(t)$ denotes a vector of expansion coefficients, $c(t) = (c_1(t), \ldots, c_n(t))$. Equation (4.8) is a homogeneous linear ordinary differential equation. It is assumed in the following that every initial value problem of equation (4.8) has a unique solution defined for all times t. It is known from the theory of ordinary differential equations that, under this assumption, a system of n linear independent solutions exists such that every solution of (4.8) is a linear combination of these linear independent solutions [CL55, Wal93].

We introduce the fundamental solution of equation (4.8) and discuss its properties: Let $F(t, t_\mathrm{i})$ denote the matrix of column-vectors $c^{(i)}(t, t_\mathrm{i})$ which are solutions of (4.8) and meet the initial condition $c^{(i)}_j(t_\mathrm{i}, t_\mathrm{i}) = \delta_{ij}$ at time t_i:

$$F(t_\mathrm{i}, t_\mathrm{i}) = \left(c^{(1)}(t_\mathrm{i}, t_\mathrm{i}), c^{(2)}(t_\mathrm{i}, t_\mathrm{i}), \ldots, c^{(n)}(t_\mathrm{i}, t_\mathrm{i}) \right) = 1. \tag{4.9}$$

Throughout this work, multiples of the unit matrix are represented simply by complex numbers, therefore, the numeral 1 in the previous equation stands for the unit matrix. Such a system of solutions is commonly known as a fundamental system of solutions [Wal93]. It exists for any initial time t_i (see above). The two-parameter matrix-valued function $F(t, t_\mathrm{i})$ will be referred to as *the* fundamental solution of the coupled channel equations for the initial time t_i. The properties of this fundamental solution have not yet been explicitly discussed in the literature on coupled channel calculations.

As a consequence of the unique solvability of the initial value problem, the fundamental solution F has the following additional properties:

$$F(t_2, t_1) F(t_1, t_0) = F(t_2, t_0), \tag{4.10}$$

$$F(t_1, t_0)^{-1} = F(t_0, t_1), \tag{4.11}$$

satisfied for arbitrary times t_0, t_1 and t_2.

Note that F is generally not a unitary matrix (i.e. a unitary time evolution), because the matrix $-\mathrm{i} N(t)^{-1} V(t)$ of the coefficients of the linear differential equation (4.8) is not anti-hermitian. However, this coefficient matrix may be anti-hermitian in particular cases, e.g. in single-centre coupled channel equations. In such cases $F(t, t_\mathrm{i})$ is unitary for all arguments t and t_i [CL55, Wal93]. However, the matrix $F(t_2, t_1)$ is *asymptotically* unitary, if the overlap matrix $N(t)$ converges to the unit

matrix as $t \to \pm\infty$, i.e. if the basis functions are asymptotically orthogonal. Asymptotic unitarity is useful later in this work in order to check and assess the accuracy of a numerically evaluated fundamental solution $F(t_\mathrm{f}, t_\mathrm{i})$.

It can be verified that the time-independence of the scalar product (4.5) is equivalent to the following relation between the fundamental solution F and the overlap matrix $N(t)$:

$$F(t_1, t_0)^\dagger N(t_1) F(t_1, t_0) = N(t_0). \tag{4.12}$$

Given the asymptotic orthonormality of the basis functions, the asymptotic unitarity of the fundamental solution F is obtained by taking the limits $t_1 \to \infty$ and $t_0 \to -\infty$:

$$\lim_{t_1 \to \infty} \lim_{t_0 \to -\infty} F(t_1, t_0)^\dagger F(t_1, t_0) = 1. \tag{4.13}$$

This means in particular that the norms at $t = \pm\infty$ of some arbitrary solution $c(t)$ of the coupled channel equations are equal,

$$\lim_{t \to -\infty} \|c(t)\|_2 = \lim_{t \to \infty} \|c(t)\|_2, \tag{4.14}$$

if $N(t) \to 1$ as t approaches $\pm\infty$.

Note that the existence of the limits $\lim_{t \to \pm\infty} c(t)$ themselves is not implied by (4.14). Their existence can be deduced from the asymptotic convergence of the fundamental solution,

$$\lim_{t_1 \to \infty} \lim_{t_0 \to -\infty} F(t_1, t_0) = F(\infty, -\infty), \tag{4.15}$$

which is likewise not implied by (4.13) and, in principle, requires a separate mathematical discussion. The limit $F(\infty, -\infty)$ takes the role of the 'coupled channel scattering matrix' (see section 4.3 below) and satisfies:

$$F(\infty, -\infty)^\dagger = F(\infty, -\infty)^{-1} = F(-\infty, \infty). \tag{4.16}$$

4.2.1 Unitarity criterion. In this subsection a numerically useful method is developed in order to assess the deviation of the fundamental solution $F(t, t_\mathrm{i})$ from unitarity. The unitarity of a fundamental solution $F(t, t_\mathrm{i})$ is equivalent to the property,

$$\|F(t, t_\mathrm{i})u\|_2 = 1, \tag{4.17}$$

for all times t and unit vectors u. The unit vector u describes an initial condition at some initial time t_i of a solution $c(t) = F(t, t_\mathrm{i})u$ of the coupled channel equations. It has been mentioned in the previous section that the fundamental solution is generally not unitary, which means that,

$$\|F(t, t_\mathrm{i})u\|_2 \neq 1.$$

As a measure of the deviation of F from unitarity, one may compute the range of the vector norm $\|F(t, t_\mathrm{i})u\|_2$ substituting all unit vectors u. It turns out that the upper limit,

$$\max_{\|u\|_2 = 1} \|F(t, t_\mathrm{i})u\|_2,$$

and the lower limit,

$$\min_{\|u\|_2 = 1} \|F(t, t_\mathrm{i})u\|_2,$$

of this range, may be computed easily, because they are related to the so-called singular values of the the matrix $F(t, t_\mathrm{i})$. The singular values of a matrix F are defined as the positive square roots of the eigenvalues of the matrix $F^\dagger F$ [Wil65, Kat80, RS80, DH93]. Due to the positivity of $F^\dagger F$, the singular values of F are positive numbers and they will be denoted, in descending order, by $\sigma_1, \ldots, \sigma_n$. We may then compute:

$$\min_{\|u\|_2=1} \|Fa_\mathrm{i}\|_2 = \left(\min_{v\in\mathbb{C}^n} \frac{\|Fv\|_2^2}{\|v\|_2^2} \right)^{\frac{1}{2}} = \left(\min_{v\in\mathbb{C}^n} \frac{v^\dagger F^\dagger F v}{v^\dagger v} \right)^{\frac{1}{2}} = \sigma_n. \tag{4.18}$$

The last step is obtained by writing the vector $v \in \mathbb{C}^n$ as a linear combination of orthonormal eigenvectors of the hermitian matrix $F^\dagger F$. In the same way the relation,

$$\max_{\|u\|_2=1} \|Fu\|_2 = \sigma_1, \tag{4.19}$$

is obtained. We conclude that,

$$\sigma_n(t, t_\mathrm{i}) \leq \|F(t, t_\mathrm{i})u\|_2 \leq \sigma_1(t, t_\mathrm{i}), \tag{4.20}$$

for any unit vector u. In particular, a fundamental solution matrix $F(t, t_\mathrm{i})$ is unitary if and only if $\sigma_1(t, t_\mathrm{i}) = \sigma_n(t, t_\mathrm{i}) = 1$. Therefore, the determination of the singular values is an appropriate method to assess the unitarity of $F(t, t_\mathrm{i})$ in numerical calculations. It is also an efficient method because stable iterative methods for the evaluation of singular values of square matrices exist (see [GV96, DH93, ABB+99]).

4.3 Approximate transition amplitudes

The coupled channel method is used to compute approximate transition amplitudes numerically. In order to deduce the relation between the analytically defined transition amplitude and the fundamental solution matrix, recall the post form of the transition amplitude, presented in section 3.2:

$$a_{\Delta l, \Gamma k} = \lim_{t\to\infty} \Big(\Phi_{\Delta,l}(t), \Psi^+_{\Gamma,k}(t) \Big). \tag{4.21}$$

Consider an approximate solution $\tilde{\Psi}^+_{\Gamma,k}(t, \boldsymbol{x})$ of the two-centre Dirac equation, which is obtained by means of the coupled channel method and approaches the asymptotic configuration $\Phi_{\Gamma,k}(t, \boldsymbol{x})$ as $t \to -\infty$,

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

The approximate transition amplitude $\tilde{a}_{\Delta l, \Gamma k}$ is defined similarly to equation (4.21) by,

$$\tilde{a}_{\Delta l, \Gamma k} = \lim_{t\to\infty} \left(\Phi_{\Delta,l}(t), \tilde{\Psi}^+_{\Gamma,k}(t) \right). \tag{4.22}$$

Assuming asymptotic orthogonality of the basis functions $\Phi_{\Gamma,k}(t,\boldsymbol{x})$ of the coupled channel expansion, the short calculation,

$$\begin{aligned}\tilde{a}_{\Delta l,\Gamma k} &= \lim_{t\to\infty}\Big(\Phi_{\Delta,l}(t),\sum_{\Theta,m} c_{\Theta,m}(t)\,\Phi_{\Theta,m}(t)\Big) \qquad (\text{where } \lim_{t\to-\infty} c_{\Theta,m}(t)=\delta_{\Theta m,\Gamma k})\\ &= \sum_{\Theta,m}\lim_{t\to\infty} c_{\Theta,m}(t)\,\lim_{t\to\infty}(\Phi_{\Delta,l}(t),\Phi_{\Theta,m}(t))\\ &= \lim_{t\to\infty} c_{\Delta,l}(t),\end{aligned}$$

shows that the approximate transition amplitudes are identical to the elements of the matrix $F(\infty,-\infty)$ defined in equation (4.15),

$$F(\infty,-\infty)_{\Delta l,\Gamma k}=\tilde{a}_{\Delta l,\Gamma k}.$$

As a consequence of the unitarity of $F(\infty,-\infty)$ the finite sum over all approximate transition probabilities is one, for any initial configuration (Γ,k), i.e.

$$\sum_{\Delta,l}|\tilde{a}_{\Delta l,\Gamma k}|^2=1.$$

This property is not a consequence of the conservation of probability (3.19), which was discussed in the context of the exact scattering theory of the two-centre Dirac equation. But it is a feature of the coupled channel equations. In general the corresponding finite sum over the *exact* transition probabilities $|a_{\Delta l,\Gamma k}|^2$ will be smaller than one.

As demonstrated by numerical calculations presented in chapter 6, the approximate transition amplitude $\tilde{a}_{\Delta l,\Gamma k}$ is not invariant under Lorentz boosts. This fact also reflects the breaking of the Lorentz invariance due to the coupled channel approximation.

Certainly, the matrix of transition amplitudes $F(\infty,-\infty)$ must be approximated in numerical calculations by a fundamental solution matrix $F(t_{\mathrm{f}},t_{\mathrm{i}})$ with finite initial and final times t_{i} and t_{f}.