Appendix A

Numerical methods

This appendix describes several numerical techniques that were used throughout this thesis. The spline method gets special attention.

A.1 Interpolation

Let us first look at the problem of approximating a function f on a finite domain $[a, b]$ by an interpolating polynomial function. For this purpose we define a *grid* on the interval $[a, b]$, *i.e.*, we define a set of *knots* $\{k_0, \ldots, k_n\}$ dividing the interval into n *subintervals*:

$$a = k_0 < k_1 < \cdots < k_n = b\,, \tag{A.1}$$

and we require the approximating polynomial f_n to interpolate f in the knots:

$$f_n(k_i) \quad = \quad f(k_i)\,, \quad i = 0, \ldots, n\,. \tag{A.2}$$

For every set of $n+1$ distinct knots there exists exactly one interpolating polynomial of degree n. Such a polynomial is called a polynomial *interpolant*. To check our hope that polynomial interpolants can be reasonable approximations of the original function, we calculate the error

$$f(x) - f_n(x) \quad = \quad \frac{(x-k_0)\cdots(x-k_n)}{(n+1)!} f^{(n+1)}(\xi)\,, \tag{A.3}$$

where $\xi \in [a, b]$ depends on x, provided $f^{(n+1)}$ exists. For insufficiently smooth functions, the error function is not well defined, and hence convergence for $n \to \infty$ cannot be guaranteed. Unfortunately, it is even impossible to guarantee convergence for the class of infinitely many times differentiable functions. The most famous example, due to Runge, is

$$f(x) = \frac{1}{1+x^2}\,, \quad -5 \le x \le 5\,. \tag{A.4}$$

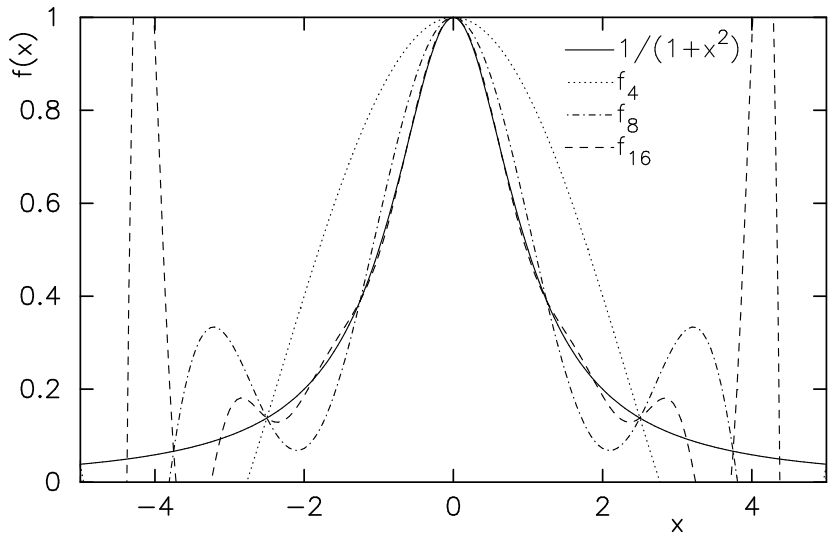


Figure A.1: Runge's example of nonconvergence of the polynomial interpolation.

The polynomial interpolant on a uniform grid, *i.e.*, using evenly spaced knots (*i.e.*, $k_{i+1} - k_i = (b-a)/n$, for all $i = 0, \ldots, n-1$) for this function does not converge to the original function. In fact, it can be shown [Isaacson and Keller, 1966] that

$$\sup_{n \geq k} \|f - f_n\| = \infty \,, \quad \text{for all } k \geq 0. \tag{A.5}$$

Figure A.1 illustrates this problem. For this particular function the problem may be fixed by using a nonuniform distribution of knots, but there is no general solution.

The failure of polynomials to accurately (*i.e.*, to any desired degree of accuracy) approximate even infinitely many times differentiable functions can be circumvented by enlarging the class of approximating functions. The simplest way to do this is to replace the polynomial function by a *piecewise* polynomial: the interpolant will be required to be polynomial only on every subinterval $[k_i, k_{i+1}]$. By using polynomials of a low degree, say m, the smoothness conditions on the function f can be relaxed to being $m+1$ times differentiable. The simplest continuous piecewise polynomial interpolant is the *piecewise linear* interpolant

$$f_n(x) \quad = \quad \frac{f(k_i)(k_{i+1} - x) + f(k_{i+1})(x - k_i)}{k_{i+1} - k_i} \,, \quad x \in [k_i, k_{i+1}] \,. \tag{A.6}$$

The interpolation error is given by

$$f(x) - f_n(x) \quad = \quad \frac{(x - k_i)(x - k_{i+1})}{2} f^{(2)}(\xi) \,, \tag{A.7}$$

for some ξ on $[k_i, k_{i+1}]$. The L_∞ norm of the error function satisfies the following

bound:

$$\|f(x) - f_n(x)\|_\infty \quad \leq \quad \frac{h^2}{8}\|f^{(2)}\|_\infty \,, \tag{A.8}$$

where h is the length of the longest subinterval:

$$h \quad = \quad \max_{i=0,\ldots,n-1} k_{i+1} - k_i \,. \tag{A.9}$$

This indicates that any function which is twice continuously differentiable on $[a, b]$ can be approximated to any desired degree of accuracy, simply by dividing the interval into sufficiently small subintervals. Clearly, the linear interpolant of Runge's counter example, Eq. (A.4), converges neatly when $n \to \infty$. (Actually, even when f is not twice differentiable on $[a, b]$, the approximation may still converge to the actual function. For example, the linear interpolant of the function $f(x) = \sqrt{x}$ (which is not differentiable in 0) on $[0, 1]$ will have an error of $\mathrm{O}(\sqrt{h})$. Therefore, the linear interpolant approaches $\sqrt{x}$ when $h \downarrow 0$.)

We can try to improve the approximation by using piecewise cubic functions. Since there are four degrees of freedom, four knots are needed to fix the parameters. For example, the points $k_{i-1}, \ldots, k_{i+2}$ might be used to determine the parameters for the cubic piece on the interval $[k_i, k_{i+1}]$. (Note that the first and last interval need a different treatment.) Such a cubic interpolant will have an error of $\mathrm{O}(h^4)$, provided f is four times differentiable.

Clearly, piecewise (or *local*) approximations have a much wider applicability than *global* approximations. However, piecewise approximations of the type described above (*i.e.*, *Lagrange*-type interpolants) have the disadvantage of not being continuously differentiable. This is major drawback, since in many applications derivatives of functions are required (such as in differential equations). For such applications, *Hermite* interpolation is good alternative. A Hermite interpolant is just a piecewise polynomial function interpolating not only the function itself, but also its first r derivatives:

$$f_n^{(d)}(k_i) \quad = \quad f^{(d)}(k_i) \,, \quad i = 0, \ldots, n \,, \quad \text{and} \quad d = 0, \ldots, r \,. \tag{A.10}$$

When the condition of interpolating the derivatives is dropped and replaced by continuity of the derivatives, one speaks of a *spline* approximant. Such an approximant is very useful when the derivative of the function is unavailable. The next section discusses spline interpolants.

A.2 Spline interpolation[1]

Let us start with the cubic spline interpolant. On a grid containing n intervals there are $4n$ degrees of freedom, and $2n$ interpolation and continuity restrictions.

[1] **spline** \'splīn\ *n* [origin unknown] (1756) **1:** a thin wood or metal strip used in building construction **...** [Webster's Ninth New Collegiate Dictionary, Merriam–Webster, Springfield, 1987.]

Requiring the first and second derivative to be continuous yields $2n-2$ additional conditions. The $4n-2$ conditions must be supplemented by two additional restrictions in order fix the $4n$ degrees of freedom. If the derivative of f is known at the end points a and b, we could require the first derivative to be interpolated at the end points. If, on the other hand, the derivative is not known at the end points, the "natural" choice is to put

$$f_n''(a) \quad = \quad f_n''(b) \quad = \quad 0\,. \tag{A.11}$$

The reason for calling this choice the natural one can be understood by looking at the following functional problem. Consider all twice continuously differentiable functions g interpolating a function f at the knots k_i $(i = 0, \ldots, n)$. The solution to the following minimalization problem

$$\min_g \int_a^b \mathrm{d}x\,[g''(x)]^2\,, \tag{A.12}$$

is just the cubic spline interpolant with the natural end-point choice given by Eq. (A.11). This functional minimalization can also be interpreted as the minimalization of the stress energy in a thin beam of flexible material (*i.e.*, a *spline*); g is the shape such a thin beam takes when it is fixed at a number of n points, since it will tend to minimize its stress energy [Ahlberg *et al.*, 1967; Seagrave, 1970].

A spline approximant can be written as a sum of basis functions with compact support. It can be shown that a nontrivial cubic spline function must have a support of at least four contiguous subintervals. Also, the spline function with a support of precisely four intervals is unique [Prenter, 1975]. It is the natural spline approximant of a function f satisfying (on a uniform grid):

$$f(k_0) \quad = \quad f(k_4) \quad = \quad 0\,, \tag{A.13a}$$

$$f(k_1) \quad = \quad f(k_3) \quad = \quad 1\,, \tag{A.13b}$$

$$f(k_2) \quad = \quad 4\,. \tag{A.13c}$$

The resulting approximant is known as a B spline. (Cf. Fig. A.2.)

The B splines are not well suited when solving differential equations by collocation (see Sec. A.3 for a description of collocation methods), due to the slow convergence. For example: if cubic splines are used to solve a second-order ordinary differential equation by requiring the equation to be satisfied at the knots only, the approximant has an error of $\mathrm{O}(h^2)$, which is h^{-2} times the *interpolation* error for a spline approximant of a given function [Prenter, 1975]. In the next section, a different set of basis functions will be defined, which does lead to optimal convergence if the collocation points are suitably carefully chosen.

A.3 Orthogonal collocation

An ordinary differential equation can be approximated by replacing the (unknown) function by a spline approximation, and requiring the equation to be satisfied in

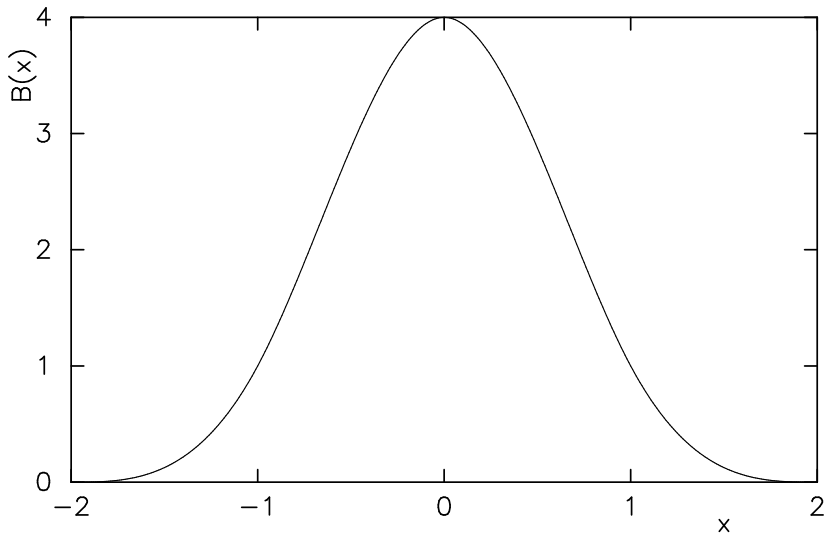


Figure A.2: A B spline.

a finite number of so-called *collocation* points only. Such a method is known as a *collocation method*, and it has the advantage of being very simple to implement, but usually also has the disadvantage of having a low rate of convergence. For example, using cubic splines and collocating at the knots leads to an error of $\mathrm{O}(h^2)$, which compares unfavorably with the error ($\mathrm{O}(h^4)$) of variational methods such as the Galerkin method [Prenter, 1975]. There is, however, no *a priori* reason for taking the knots as the collocation points. It turns out that by using a suitable choice of collocation points, collocation methods can be made to converge as fast as Galerkin methods.

A.3.1 Collocation points

Optimal convergence can be achieved by using the Gauss points of the subintervals, rather than the end points. This is known as *orthogonal* collocation. Orthogonal collocation is based on the same idea as Gauss quadrature, a method for approximating an integral by a finite sum:

$$\int_a^b \mathrm{d}x\, f(x) \quad \approx \quad \sum_{i=1}^{m} w_i f(x_i)\,, \tag{A.14}$$

where x_i are the quadrature points and w_i are the associated weights, with the property that polynomials of degree less than $2m$ are integrated exactly. It turns out that this is achieved when the quadrature points are taken to be the zeros of the mth Legendre polynomial P_m, and the weights are given by

$$w_i \quad = \quad \frac{1}{f'(x_i)} \int_a^b \mathrm{d}x\, \frac{P_m(x)}{x - x_i}\,. \tag{A.15}$$

The error will be $O(h^{2m+1})$, where $h = b - a$, provided that f is $2m$ times continuously differentiable. This is also the maximum degree of precision which can be achieved with an m-point quadrature rule [Isaacson and Keller, 1966].

Orthogonal collocation dates back at least to Lanczos [1938], and has been used extensively in engineering and chemistry to solve initial- and boundary-value problems arising in reactor dynamics and other systems. De Boor and Swartz [1973] first proved existence and uniqueness of the solution, and provided error estimates. They showed that an approximate solution to an mth order differential equation with m boundary conditions can be found by using piecewise polynomial approximants of degree less than $m + k$, possessing $m - 1$ continuous derivatives, and collocating in the k-point Gauss points of every subinterval. The global error of the approximate solution will be $O(h^{m+k})$ provided the solution has $m + 2k$ continuous derivatives, and the differential equation itself is sufficiently smooth. (The proof depends upon the existence of a sufficiently smooth Green's function.) At the end points of each subinterval, the approximation and its first $m - 1$ derivatives are $O(h^{2k})$ accurate.

A.3.2 Basis functions

The simplest orthogonal collocation method is based on cubic Hermite polynomials and two-point quadrature. It exhibits *fourth-order convergence*, *i.e.*, the error is $O(h^4)$. Collocation fixes $2n$ degrees of freedom, and continuity and differentiability at the knots fix $2n - 2$ degrees of freedom. The two remaining degrees of freedom are fixed by the two boundary conditions of the differential equation. The piecewise cubic function can be written as a sum of basis functions, each supported by two consecutive subintervals. The two basis functions with support $[k_{i-1}, k_{i+1}]$ will be denoted by ϕ_i and ξ_i. The basis functions must be continuously differentiable, and therefore satisfy

$$\phi_i(k_{i-1}) = \phi_i'(k_{i-1}) = 0\,, \tag{A.16a}$$
$$\phi_i(k_{i+1}) = \phi_i'(k_{i+1}) = 0\,, \tag{A.16b}$$
$$\xi_i(k_{i+1}) = \xi_i'(k_{i+1}) = 0\,, \tag{A.16c}$$
$$\xi_i(k_{i-1}) = \xi_i'(k_{i-1}) = 0\,. \tag{A.16d}$$

The two basis functions are completely fixed by specifying the value and derivative at the central knot k_i, which can be done conveniently as follows:

$$\phi_i(k_i) = 1\,, \tag{A.17a}$$
$$\phi_i'(k_i) = 0\,, \tag{A.17b}$$
$$\xi_i(k_i) = 0\,, \tag{A.17c}$$
$$\xi_i'(k_i) = 1\,. \tag{A.17d}$$

If we take -1, 0, and 1 to be the three relevant knots, the two piecewise cubic Hermite functions satisfying the conditions (A.16) and (A.17) are:

$$\phi(x) = \theta(1-|x|)(1-|x|)^2(1+2|x|)\,, \tag{A.18a}$$
$$\xi(x) = \theta(1-|x|)(1-|x|)^2 x\,, \tag{A.18b}$$

where θ is the Heavyside function ($\theta(x)$ is zero if $x<0$ and equal to one if $x>1$). These functions, often denoted by *local* basis functions, are plotted in Fig. A.3. The actual or *global* basis functions s_i are just

$$s_i(x) = \begin{cases} \phi_j(x)\,, & \text{if } i=2j\ , \\ \xi_j(x)\,, & \text{if } i=2j+1\ . \end{cases} \tag{A.19}$$

In Fig. A.4 all the global basis functions are plotted for a specific grid. The $2n+2$ basis functions must reduced to the desired number of $2n$, by requiring that all basis functions satisfy the (homogeneous) boundary conditions at the end points a and b:

$$\alpha_a f(a) + \beta_a f'(a) = 0\,, \tag{A.20a}$$
$$\alpha_b f(b) + \beta_b f'(b) = 0\,. \tag{A.20b}$$

The complete set of basis functions $\tilde{s}_i$ satisfying these conditions is defined by

$$\tilde{s}_j = s_j\,, \tag{A.21a}$$

for $2 \le j \le 2n-1$, and

$$\tilde{s}_1 = \beta_a s_0 - \alpha_a s_1\,, \tag{A.21b}$$
$$\tilde{s}_{2n} = \beta_b s_{2n} - \alpha_b s_{2n+1}\,. \tag{A.21c}$$

The two-point Gauss quadrature points on the interval $[0,1]$ are $\frac{1}{2}(1\pm 1/\sqrt{3})$, with weights $\frac{1}{2}$. The method of approximation by piecewise cubic Hermite functions and orthogonal collocation is commonly known as the *spline method*.

A.3.3 The collocation process

In this subsection I will describe the collocation process in some detail for two examples. The simplest example is that of fitting a function f. The approximant can be written as

$$f_n(x) = \sum_{j=1}^{2n} a_j s_j(x)\,, \tag{A.22}$$

where a_j are expansion coefficients. Collocation implies that

$$f_n(x_i) = f(x_i)\,, \tag{A.23}$$

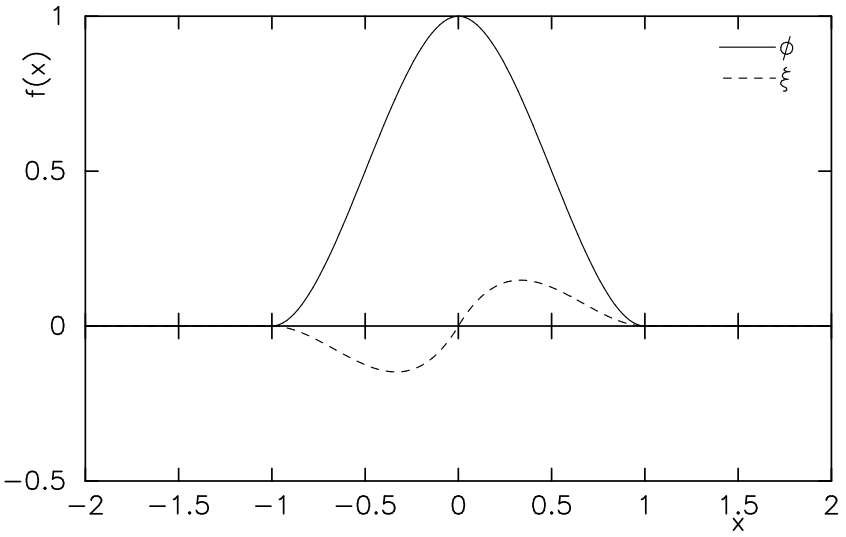


Figure A.3: Local piecewise cubic Hermite basis functions.

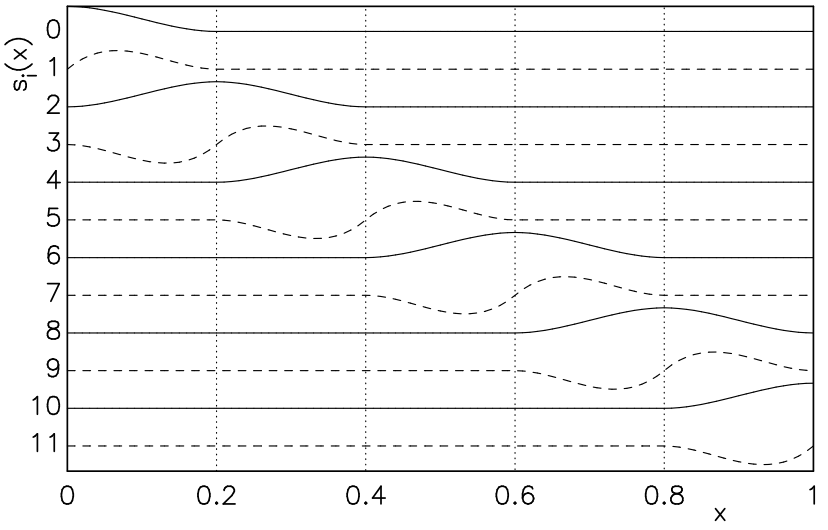


Figure A.4: Globally defined basis functions with compact support. (The odd-numbered basis functions are blown up by a factor 25.)

$$\begin{pmatrix}
\times & \times & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\times & \times & \times & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\
0 & \times & \times & \times & \times & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \times & \times & \times & \times & 0 & 0 & 0 \\
0 & 0 & 0 & \times & \times & \times & \times & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \times & \times & \times & \times & 0 \\
0 & 0 & 0 & 0 & 0 & \times & \times & \times & \times & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times
\end{pmatrix}$$

Figure A.5: General matrix structure.

must hold at every collocation point x_i ($i = 1, \ldots, 2n$). Substituting the expansion Eq. (A.22) gives the following set of conditions

$$\sum_{j=1}^{2n} a_j s_j(x_i) \quad = \quad f(x_i)\,, \tag{A.24}$$

which can be written as

$$S\boldsymbol{a} \quad = \quad \boldsymbol{f}\,, \tag{A.25}$$

where $\boldsymbol{a}$ is the vector of expansion coefficients a_i, $\boldsymbol{f}$ is the vector of function values $f(x_j)$, and S is a matrix whose elements are

$$S_{ij} \quad = \quad s_j(x_i)\,. \tag{A.26}$$

This matrix has a banded structure due to the limited support of the basis functions, as is shown in Fig. A.5. Equation (A.25) is a problem of linear algebra, which can be solved using standard techniques (*e.g.*, Gaussian elimination). This completes the first example.

The next step is to illustrate how to solve an ordinary differential equation using the spline method. Consider, for example, the following linear second-order differential equation:

$$a(x)f''(x) + b(x)f'(x) + c(x)f(x) \quad = \quad g(x)\,, \tag{A.27}$$

subject to given boundary conditions. Substituting the expansion (A.22) satisfying these boundary conditions, and collocating at the Gauss points, leads to

$$\sum_{j=1}^{2n} a_j[a(x_i)s_j''(x_i) + b(x_i)s_j'(x_i) + c(x_i)s_j(x_i)] \quad = \quad g(x_i)\,, \tag{A.28}$$

which can be put into matrix form:

$$M\boldsymbol{a} \quad = \quad \boldsymbol{g}\,, \tag{A.29}$$

where $\boldsymbol{a}$ is the vector of expansion coefficients, $\boldsymbol{g}$ the vector of function values of the inhomogeneous term, and M an $2n \times 2n$ matrix whose elements are

$$M_{ij} \quad = \quad a(x_i)s_j''(x_i) + b(x_i)s_j'(x_i) + c(x_i)s_j(x_i)\,. \tag{A.30}$$

This matrix again has the banded structure shown in Fig. A.5.

A.3.4 Quadrature

Due to the close relation between orthogonal collocation and Gauss quadrature, integral operators can be incorporated in the spline method in a very simple manner. Consider, for example, the operation

$$f(x) \quad = \quad \int_a^b \mathrm{d}x'\, K(x,x')g(x')\,. \tag{A.31}$$

This can be approximated using Gauss quadrature:

$$f(x) \quad = \quad \sum_{j=1}^{2n} w_j K(x,x_j)g(x_j) + \mathrm{O}(h^4)\,, \tag{A.32}$$

which, when taken at the collocation points, reduces to

$$f(x_i) \quad = \quad \sum_{j=1}^{2n} w_j K(x_i,x_j)g(x_j) + \mathrm{O}(h^4)\,, \tag{A.33}$$

or

$$\boldsymbol{f} \quad \approx \quad K\boldsymbol{g}\,, \tag{A.34}$$

where K is the $2n \times 2n$ matrix containing the kernel values $K(x_i,x_j)$ multiplied by the integration weights w_j. If we assume $g(x)$ to be a piecewise cubic Hermite function with expansion coefficients a_k, we may write

$$\boldsymbol{f} \quad = \quad KS\boldsymbol{a}\,. \tag{A.35}$$

The error made in the integration is $\mathrm{O}(h^4)$ (provided the kernel is sufficiently smooth), which is of the same order as the collocation error. Therefore, integrals can be performed without loss of accuracy in a very simple manner. The matrix KS is a product of the kernel matrix and the spline matrix, and will in general

not have a banded structure, unless the kernel itself has some locality. However, we will often be dealing with degenerate kernels, *i.e.*, kernels of the form

$$K(x,x') \quad = \quad k(x)k(x')\,, \tag{A.36}$$

in which case Eq. (A.35) can be rewritten into:

$$\boldsymbol{f} \quad = \quad \boldsymbol{k}\tilde{\boldsymbol{k}}^{\mathrm{T}}\boldsymbol{a}\,, \tag{A.37}$$

where $\boldsymbol{k}$ contains the values $k(x_i)$, and $\tilde{\boldsymbol{k}}$ is the product

$$\tilde{k}_j \quad = \quad \sum_{i=1}^{2n} w_i k_i S_{ij}\,. \tag{A.38}$$

The question of hermiticity and the orthogonality properties for such separable terms will discussed further on.

In most cases the above procedure is adequate. However, sometimes the integration limits do not coincide with knots, or more accurate integration is needed. The matrix elements of $P^{\alpha_i\beta_j}$ (cf. Eq. (5.53d)), are an example of the first case. Here one is forced to use a different integration rule (*i.e.*, using points and weights which are not the two-point Gauss points and weights for the interval). More accurate integration is often needed to distinguish between errors due to the spline approximation and quadrature errors. A relatively simple approach is to recalculate the spline expansion coefficients on a grid containing more intervals, and performing two-point Gauss quadrature on this new grid. The new spline expansion coefficients are simply:

$$\boldsymbol{b} \quad = \quad S^{-1}T\boldsymbol{a}\,, \tag{A.39}$$

where S is the spline matrix for the new grid, and T is a rectangular matrix defined by

$$T_{ij} \quad = \quad s_j(x_i)\,, \tag{A.40}$$

where s_j is a spline function defined on the *old grid*, and x_i is a collocation point on the *new grid*. Note that this recalculation introduces an additional error of $\mathrm{O}(h^4)$, where h is the length of the largest interval of the new grid. For the special case where the new grid "contains" the old grid, *i.e.*, if every knot of the old grid is also a knot of the new grid, the new spline approximant will be identical to the old one.

A.3.5 Spline matrices

It can be very fruitful to think of the matrices which result from applying the spline method to operators, as representing, or even being the operators themselves, since many of the properties of the original operator are (approximately) retained.

Locality

Locality of operators shows up as bandedness in the collocation matrix. The unit operator is replaced by the banded matrix S and local (differential) operators by matrices having the same banded structure as S, whereas nonlocal operators are replaced by general (*i.e.*, full) matrices.

Separability

A separable operator such as the degenerate kernel K of Eq. (A.36) is represented by an outer products of vectors $\boldsymbol{k}\tilde{\boldsymbol{k}}^{\mathrm{T}}$.

Hermiticity

The matrix representation of a Hermitian matrix is certainly not Hermitian. However, the generalized eigenvalue problem

$$H\boldsymbol{a} \quad = \quad \lambda S\boldsymbol{a}\,, \tag{A.41}$$

appears to have *real* eigenvalues. This can be shown exactly for the radial Hamiltonian on a finite domain. In that case, the matrix

$$S^{\mathrm{T}}WH\,, \tag{A.42}$$

where W is a diagonal matrix containing the Gauss weights on as the diagonal elements, is *symmetric*, as can be seen by explicitly constructing the matrix. Also, the matrix

$$S^{\mathrm{T}}WS\,, \tag{A.43}$$

is *symmetric* and *positive*, so that the generalized eigenvalue problem can be rewritten as

$$S^{\mathrm{T}}WH\boldsymbol{a} \quad = \quad \lambda S^{\mathrm{T}}WS\boldsymbol{a}\,, \tag{A.44}$$

which has only real eigenvalues, if both matrices are symmetric and at least one is positive.

For more complicated Hermitian operators such a simple argument does not hold. However, remembering the analogy between vectors of expansion coefficients and state vectors, and between matrices and operators, the following may be recognized:

$$\boldsymbol{a}S^{\mathrm{T}}WH\boldsymbol{b} \quad \approx \quad \langle a\,|\,Hb\rangle \quad = \quad \langle Ha\,|\,b\rangle \quad \approx \quad \boldsymbol{a}H^{\mathrm{T}}WS\boldsymbol{b}\,, \tag{A.45}$$

suggesting an *approximate* symmetry of the matrix $S^{\mathrm{T}}WH$. It should be noted, however, that the approximation will only be accurate for smooth states. This

allows one to show, for example, that the approximate ground-state eigenvalue will be real. (If an eigenvalue is well separated from the rest of the spectrum, a small perturbation can shift the eigenvalue, but it must still be real.)

Note that the disappearance of exact hermiticity can lead to problems when the orthogonality of eigenstates corresponding to different energies is required, such as for projection operators. Exact orthogonality only holds as the biorthogonality conditions for left and right eigenvectors:

$$\boldsymbol{a}_{iL}^{\mathrm{T}}\boldsymbol{a}_{jR} \quad = \quad \delta_{ij}\,, \tag{A.46}$$

where $\boldsymbol{a}_{iL}$ and $\boldsymbol{a}_{jR}$ are left and right eigenvectors corresponding to energy eigenvalues E_i and E_j, respectively:

$$H\boldsymbol{a}_{iR} \quad = \quad E_i S\boldsymbol{a}_{iR}\,, \tag{A.47}$$

$$\boldsymbol{a}_{iL}^{\mathrm{T}}H \quad = \quad E_i \boldsymbol{a}_{iL}^{\mathrm{T}}S\,. \tag{A.48}$$

A projection on a state $|\psi_i\rangle$ can now be written as:

$$\boldsymbol{a}_{jR}\boldsymbol{a}_{iL}^{\mathrm{T}}\,. \tag{A.49}$$

Note that this expression projects out the expansion coefficient representation of state $|\psi_i\rangle$. The corresponding operator working in the space of function values at collocation points is

$$S\boldsymbol{a}_{jR}\boldsymbol{a}_{iL}^{\mathrm{T}}S^{-1} \quad = \quad (S\boldsymbol{a}_{jR})(S^{-\mathrm{T}}\boldsymbol{a}_{iL})^{\mathrm{T}}\,. \tag{A.50}$$

A.4 The Lanczos method

The Lanczos method, which was originally only applicable to symmetric matrices, was modified to deal with nonsymmetric matrices by Saad [1982]. The modified Lanczos method is an *oblique projection method*, which means that it generates a basis which approximately spans an invariant subspace. (The basis consists of two sets of vectors, one for the left eigenvectors, and one for the right eigenvectors. The basis vectors satisfy an biorthogonality condition.) I will now describe the extension to complex matrices.

A complex Lanczos algorithm should at least retain biorthonormality with respect to the dot product on a complex vector space. For this to be the case, the following iterative steps must be used:

$$\hat{\boldsymbol{v}}_{i+1} \quad = \quad A\boldsymbol{v}_i - \alpha_i\boldsymbol{v}_i - \beta_i\boldsymbol{v}_{i-1}\,, \tag{A.51}$$

$$\hat{\boldsymbol{w}}_{i+1} \quad = \quad A^{\mathrm{H}}\boldsymbol{w}_i - \alpha_i^*\boldsymbol{w}_i - \delta_i^*\boldsymbol{w}_{i-1}\,. \tag{A.52}$$

It is easy to check that these steps do indeed generate a biorthogonal basis. Normalization is obtained using

$$\alpha_i \quad = \quad \boldsymbol{w}_i^{\mathrm{H}}A\boldsymbol{v}_i\,, \tag{A.53}$$

$$\beta_i \delta_i = \boldsymbol{w}_i^{\mathrm{H}} \boldsymbol{v}_i \,, \tag{A.54}$$

$$\delta_i = \sqrt{|\boldsymbol{w}_i^{\mathrm{H}} \boldsymbol{v}_i|} \,, \tag{A.55}$$

$$\boldsymbol{v}_i = \hat{\boldsymbol{v}}_i / \delta_i \,, \tag{A.56}$$

$$\boldsymbol{w}_i = \hat{\boldsymbol{w}}_i / \beta_i^* \,. \tag{A.57}$$

The next step is to extract the solution from the data generated by the iterative process. The vectors $\boldsymbol{v}_i$ and $\boldsymbol{w}_i$ can be gathered into two (rectangular) matrices V and W, which have the following property:

$$W^{\mathrm{H}} A V = T_m \,, \tag{A.58}$$

where T_m is the following tridiagonal matrix:

$$T_m = \begin{pmatrix} \alpha_1 & \beta_2 & & \\ \delta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_m \\ & & \delta_m & \alpha_m \end{pmatrix} . \tag{A.59}$$

Now an approximate inverse of the matrix A can be written as

$$A^{-1} \approx V T^{-1} W^{\mathrm{H}} \,. \tag{A.60}$$

(This equation has to be taken in a very specific sense, more on this later.) The solution to the problem

$$A\boldsymbol{x} = \boldsymbol{b} \,, \tag{A.61}$$

can now be written as

$$\boldsymbol{x} = A^{-1}\boldsymbol{b} \approx V T^{-1} W^{\mathrm{H}} \boldsymbol{b} \,. \tag{A.62}$$

If the iteration is started with

$$\boldsymbol{v}_1 = \boldsymbol{w}_1 = \frac{\boldsymbol{r}_0}{\|\boldsymbol{r}_0\|} \,, \tag{A.63}$$

where $\boldsymbol{r}_0$ is

$$\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0 \,, \tag{A.64}$$

and $\boldsymbol{x}_0$ is an initial guess at the solution, the following formula is obtained:

$$\boldsymbol{x} = \boldsymbol{x}_0 + A^{-1}\boldsymbol{r}_0 \approx \boldsymbol{x}_0 + V T^{-1} W^{\mathrm{H}} \boldsymbol{r}_0 = \boldsymbol{x}_0 + V T^{-1} \boldsymbol{e}_1 \|\boldsymbol{r}_0\| \,. \tag{A.65}$$

The error can easily be calculated from the above equation:

$$\|\boldsymbol{b} - A\boldsymbol{x}\| \quad = \quad \|\boldsymbol{r}_0\| \, \|\hat{\boldsymbol{v}}_{m+1}\| \, |T_m^{-1}| \, . \tag{A.66}$$

Note that Eq. (A.66) allows the error to be calculated very efficiently, without forming the entire approximate solution. This equation also expresses the specific sense in which $V_m T_M^{-1} W_m^{\mathrm{H}}$ is close to A^{-1}, and therefore how Eq. (A.60) should be interpreted.

I will not discuss convergence of the Lanczos process, breakdown of the process by generating two basis vectors which are orthogonal to one another, or the difficulties which arise by imperfect biorthogonality of the basis. It is my experience that provided the problem is not too ill conditioned, these problems hardly ever become important. (An attempt at dealing with the breakdown is described in Parlett *et al.* [1985].)

A.5 Special functions

The accurate numerical evaluation of special functions is a highly nontrivial matter. In this thesis I have used two classes of functions. The first is that of orthogonal polynomials and Legendre functions. The second is that of hypergeometric functions, Coulomb functions, and Bessel functions. The first class can usually be calculated with sufficient accuracy by simple recursion relations, although care must be taken, since not all recursion relations are inherently stable.

The second class is a set of functions which are related to the hypergeometric function ${}_2F_1(a, b; c; z)$, and the confluent hypergeometric functions ${}_1F_1(a; c; z)$ and $U(a, c, z)$. These functions were calculated using combinations of series expansions and Chebyshev expansions, as described in the excellent book of Luke [1975].

Appendix B

Example systems

This appendix contains a description of a number of example few-body systems, which are useful in one way or another. Some are useful because they are exactly solvable, others are useful because of their widespread use.

B.1 Exactly solvable systems

In this section potentials are defined for which exact solutions can be found, some of which can be used to check the numerical methods used in this thesis. The potentials will be defined with a "normalized" strength parameter V_0: the potential has negative-energy states if, and only if, $V_0 > 1$. (Such a normalization may not be possible if the potential is not well-behaved, or long ranged.)

B.1.1 Harmonic oscillator

The problem of N identical bodies interacting via harmonic-oscillator pair potentials can be solved exactly. The harmonic oscillator has an infinite number of bound states, and it can therefore not be normalized. The potential is defined by

$$V(r) \quad = \quad \tfrac{1}{4}a^2 r^2 \,, \tag{B.1}$$

where a^2 is a measure of the strength of the potential, or, equivalently, a^{-1} is a measure of the width of the well. In one dimension, the solutions are

$$\psi_n(r) \quad = \quad \left(2a^{-1}\pi^{\frac{1}{2}}n!\right)^{-\frac{1}{2}} \mathrm{e}^{-ar^2/4}\,\mathrm{He}_n(a^{\frac{1}{2}}r)\,, \tag{B.2}$$

where He_n is a Hermite polynomial (cf. Appendix D), for $n = 0, 1, 2, \ldots$. The corresponding energies are

$$E_n \quad = \quad a(n + \tfrac{1}{2})\,. \tag{B.3}$$

The N-body Hamiltonian can be written as

$$-\sum_{i=1}^{N-1} \nabla^2_{\boldsymbol{r}^{f_i}_{g_i}} + \sum_{i,j>i} \tfrac{1}{4}a^2(2\mu^i_j)^{-1}(\boldsymbol{r}^i_j)^2\,, \tag{B.4}$$

where I have used the notational conventions for the Jacobi coordinates of Chapter 4. The interaction can be simplified by using the following identity:

$$\sum_{i,j>i} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \quad = \quad \tfrac{1}{2} N \sum_i (\boldsymbol{r}_{g_i}^{f_i})^2 \,. \tag{B.5}$$

This leads to

$$\sum_{i=1}^{N-1} -\nabla^2_{\boldsymbol{r}_{g_i}^{f_i}} + \tfrac{1}{8} N a^2 (\boldsymbol{r}_{g_i}^{f_i})^2 \,, \tag{B.6}$$

which is just the $3(N-1)$-dimensional harmonic oscillator. The following fully symmetric N-body states are easily found:

$$\psi(\boldsymbol{r}_{g_1}^{f_1}, \ldots, \boldsymbol{r}_{g_{N-1}}^{f_{N-1}}) \quad = \quad \left(2c^{-1}\pi^{\frac{1}{2}} n!\right)^{-\frac{3}{2}(N-1)} \prod_{i=1}^{N-1} \mathrm{e}^{-\frac{c}{4}(r_{g_i}^{f_i})^2} \, \mathrm{He}_n(c^{\frac{1}{2}} r_{g_i}^{f_i}) \,, \tag{B.7}$$

with bound-state energy

$$E_n \quad = \quad 3c(N-1)(n+\tfrac{1}{2}) \,, \tag{B.8}$$

for n even, and with $c = a\sqrt{N/2}$. In the test cases used in Chapters 2, 5, and 7, a was taken to be two, leading to the following bound-state energies:

$$E_n \quad = \quad 3\sqrt{2N}\,(N-1)(n+\tfrac{1}{2}) \,. \tag{B.9}$$

To avoid the problems associated with the potential going to infinity for large distances, a cutoff and a shift are introduced:

$$\tilde{V}(r) \quad = \quad \begin{cases} a^2 r^2 - b^2 \,, & \text{if } \; ar < b, \\ 0 \,, & \text{if } \; ar \geq b. \end{cases} \tag{B.10}$$

This modified potential has the advantage of being exponentially bounded, at the expense of having a discontinuity in its first derivative at $ar = b$, and not being exactly equal to the harmonic oscillator. However, for sufficiently large b, the lowest lying states will be extremely close to the exact harmonic oscillator states, and the discontinuity can be expected to have a negligible effect on the convergence of the spline method, since the wave function is extremely small for $ar > b$ if b is sufficiently large. If b is not taken sufficiently large, a substantial shift in the energy and a noticeable effect on the convergence of the spline method. In Chapter 2, the cutoff value was $b = 2$, which leads to a ground-state energy of approximately 2.908... (instead of 3, for the pure harmonic oscillator), and in Chapters 5 and 7 the cutoff value was $b = 5$, which is sufficiently large to have negligible effect on the ground-state energy. The three-body harmonic oscillator ground state has been studied analytically and graphically by Friar *et al.* [1980].

B.1.2 Hulthén

The Hulthén potential is another interesting test case, since its two-body s-wave bound-state and scattering wave functions can be expressed in closed form using hypergeometric functions [Newton, 1982]. The potential can be seen as a model for a screened Coulomb potential. It has $1/r$ behavior near the origin and is exponentially bounded:

$$V_a(r) \quad = \quad \frac{-a^{-2}V_0}{\mathrm{e}^{r/a}-1}\,, \tag{B.11}$$

where $a > 0$ is a range parameter and the strength V_0 is real. The radial equation with the Hulthén potential can be transformed into the hypergeometric equation by substituting $\mathscr{f}^{+}_{0,k}(r) = \mathrm{e}^{\mathrm{i}kr}g(k,r)$ and $x = \mathrm{e}^{-r/a}$. The s-wave Jost solutions are given by

$$\mathscr{f}^{+}_{0,k}(r) \quad = \quad \mathrm{e}^{\mathrm{i}kr}\,{}_2F_1(A,B;C;\mathrm{e}^{-r/a})\,, \tag{B.12}$$

with

$$A \quad = \quad -\mathrm{i}ak + \mathrm{i}(a^2k^2 - V_0)^{\frac{1}{2}}\,, \tag{B.13}$$

$$B \quad = \quad -\mathrm{i}ak - \mathrm{i}(a^2k^2 - V_0)^{\frac{1}{2}}\,, \tag{B.14}$$

$$C \quad = \quad 1 - 2\mathrm{i}ak\,. \tag{B.15}$$

The Jost function is therefore

$$\mathscr{f}_0(k) \quad = \quad {}_2F_1(A,B;C;1) \quad = \quad \frac{\Gamma(1-2\mathrm{i}ak)}{\Gamma(1+B)\Gamma(1+A)}\,, \tag{B.16}$$

which has poles in the lower half of the k plane (*i.e.*, virtual states) at

$$k \quad = \quad -\frac{\mathrm{i}n}{2a}\,, \quad \text{for } n = 1,2,\ldots\,. \tag{B.17}$$

Bound states are found if $V_0 > 1$:

$$k_n \quad = \quad \frac{\mathrm{i}(V_0 - n^2)}{2an}\,, \quad \text{for } n = 1,2,\ldots < V_0^{1/2}. \tag{B.18}$$

The Lippmann–Schwinger kernel G_0V has eigenvalues

$$\alpha_n \quad = \quad \frac{-V_0}{n(2\mathrm{i}ak - n)}\,, \quad \text{for } n = 1,2,\ldots\,, \tag{B.19}$$

which are all inside the unit circle if

$$|V_0| \quad < \quad (1 + 4a^2k^2)^{1/2}\,, \tag{B.20}$$

(for real k), *i.e.*, the necessary and sufficient condition for the Born series to converge for all energies (for this case), is clearly that the attractive version of the potential has no bound states.

B.1.3 Coulomb

The long-ranged behavior of the Coulomb potential has two important consequences: (*i*) it supports an infinite number of bound states, and (*ii*) its scattering states cannot be considered free at large separation distances. Systems which have a short-ranged plus Coulomb interaction suffer from this same problem, and its asymptotic states must be expressed in the Coulomb asymptotic states. In this subsection the Coulomb scattering states are given, as well as the bound states, which are useful as tests for numerical accuracy. (The Coulomb potential is apart from the harmonic oscillator and the r^{-2} potential one of the few for which an analytic solution can be given for $\ell \neq 0$.)

Since the Coulomb potential has an infinite number of bound states, a normalized strength parameter cannot be defined. Instead, we will fix the ground-state energy at -1 for strength s equal to one:

$$V(r) \quad = \quad -\frac{2s}{r} \quad = \quad \frac{2k\gamma}{r}\,, \tag{B.21}$$

where Sommerfeld's parameter $\gamma = -s/k$ has been introduced. The radial equation with the Coulomb interaction reads

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2k\gamma}{r} + k^2\right)\psi_\ell(r) \quad = \quad 0\,. \tag{B.22}$$

The substitution $\psi_\ell(r) \equiv w(-2\mathrm{i}kr)r^{\ell+1}\mathrm{e}^{\mathrm{i}kr}$ transforms this equation into Kummer's equation (D.23), with $a = \ell + 1 + \mathrm{i}\gamma$ and $c = 2\ell + 2$. The regular solution is proportional to

$$\psi_\ell(r) \quad = \quad r^{\ell+1}\mathrm{e}^{\mathrm{i}kr}\,{}_1F_1(\ell + 1 + \mathrm{i}\gamma; 2\ell + 2; -2\mathrm{i}kr)\,, \tag{B.23}$$

where ${}_1F_1$ is a confluent hypergeometric function (cf. Appendix D). In order to obtain a bound state $\psi_\ell(r)$ must be imposed to go to 0 when r goes to ∞. This condition can only be met when the series terminates, *i.e.*, when $-\mathrm{i}\gamma \in \{\ell + 1, \ell + 2, \ldots\}$. The bound states are therefore found at energies $E = -\kappa_n^2$ with

$$\kappa_n \quad = \quad \frac{s}{\ell + n}\,, \tag{B.24}$$

($k = \mathrm{i}\kappa$) for all $n \in \{1, 2, \ldots\}$. The corresponding (unnormalized) wave functions are

$$\psi_\ell(r) \quad = \quad r^{\ell+1}\mathrm{e}^{-\kappa_n r}\sum_{p=0}^{n-1}\frac{(1-n)_p}{(2\ell+2)_p}\frac{(2\kappa_n r)^p}{p^n}\,. \tag{B.25}$$

The Coulomb scattering wave functions which are the analogues of the free scattering wave functions $\hat{\jmath}_\ell$ and $\hat{h}_\ell^+$, are F_ℓ and u_ℓ^+, respectively. These are defined in Appendix D.

B.1.4 Square well

The square well is of interest because of its discontinuity:

$$V(r) \quad = \quad \begin{cases} -\left(\frac{\pi}{2a}\right)^2 V_0\,, & \text{if } \ 0 \le r < a\,, \\ 0\,, & \text{if } \ a < r\,. \end{cases} \tag{B.26}$$

The (unnormalized) s-wave bound-state solutions are given by

$$\psi(r) \quad = \quad \begin{cases} \sin(\frac{\pi q}{2}\frac{r}{a})\,, & \text{if } \ 0 \le r < a\,, \\ \sin(\frac{\pi}{2}q)\mathrm{e}^{-\kappa(r-a)}\,, & \text{if } \ a < r\,, \end{cases} \tag{B.27}$$

with $\kappa = +\sqrt{-E}$ and $q^2 = E + \pi^2 V_0/(4a^2)$, where E is the bound-state energy. Matching the first derivative at $r = a$ gives

$$\tfrac{2a}{\pi}\kappa \quad = \quad -\,q\cot\tfrac{\pi}{2}q\,. \tag{B.28}$$

This is a transcendental equation in q since $\kappa^2 = q^2 - \pi^2 V_0/(4a^2)$ for which we can construct solutions in closed form by taking special cases. For example, for $V_0 = 9/2$ (and $a = 1$), the ground-state solution is

$$\psi(r) \quad = \quad \begin{cases} \sin\tfrac{3}{4}\pi r\,, & \text{if } \ 0 \le r < 1\,; \\ \tfrac{1}{2}\sqrt{2}\mathrm{e}^{-\frac{3}{4}\pi(r-1)}\,, & \text{if } \ 1 \le r\,, \end{cases} \tag{B.29}$$

which corresponds to a bound-state energy of $-\frac{9}{16}\pi^2$. This is the test case used in Chapter 2. In Chapter 5 the critical strength, $V_0 = 1$, was used instead.

B.1.5 Zero-range interaction

The zero-range interaction is peculiar, since it is both local and separable. Its potential is in one dimension

$$V(x) \quad = \quad -\,2s\delta(x)\,, \tag{B.30}$$

where s is a real strength parameter. It has a single bound state at $E = -s^2$, for all $s > 0$. The corresponding wave function is

$$\psi(x) \quad = \quad \left(\frac{s}{2}\right)^{\frac{1}{2}}\mathrm{e}^{-s|x|}\,. \tag{B.31}$$

The Green's operator for the Hamiltonian

$$H \quad = \quad -\,\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2s\delta(x)\,, \tag{B.32}$$

can be written as

$$G(k^2;x,x') = \frac{1}{2\mathrm{i}k}\left(\mathrm{e}^{\mathrm{i}k|x-x'|} - \frac{s}{\mathrm{i}k+s}\mathrm{e}^{\mathrm{i}k(|x|+|x'|)}\right). \tag{B.33}$$

A scattering state may be constructed using

$$\begin{aligned}\psi_\epsilon &= \mathrm{i}\varepsilon\int \mathrm{d}x'\, G((k+\mathrm{i}\varepsilon)^2;x,x')\mathrm{e}^{\mathrm{i}kx'} \\ &= \frac{\varepsilon}{2k}\left(\frac{1}{\varepsilon} - \frac{1}{2\mathrm{i}k-\varepsilon}\right)\left(\mathrm{e}^{\mathrm{i}kx} - \frac{s\mathrm{e}^{-\varepsilon|x|}}{\mathrm{i}k+s}\mathrm{e}^{\mathrm{i}k|x|}\right),\end{aligned} \tag{B.34}$$

and taking the limit $\varepsilon \downarrow 0$:

$$\psi = \frac{1}{2k}\left(\mathrm{e}^{\mathrm{i}kx} - \frac{s}{\mathrm{i}k+s}\mathrm{e}^{\mathrm{i}k|x|}\right). \tag{B.35}$$

This procedure shows the effect of the small positive imaginary part $+\mathrm{i}\varepsilon$ on the scattering wave function: it suppresses the scattered part of the wave function (*i.e.*, the part proportional to $\exp(\mathrm{i}k|x|)$) for very large radii.

The problem of three particles with zero-range interactions in one dimension can also be solved exactly. (In three dimensions, the three-body system collapses [Thomas, 1935].) The general scattering wave function is of the form

$$\psi_i(x,y) = \sum_{\alpha\sigma\tau} a_{\alpha i}^{\sigma\tau}\phi_\alpha^{\sigma\tau}(x,y), \tag{B.36}$$

where i denotes any of the six regions defined in Fig. B.1, σ and τ are ± 1, and α can be thought of as denoting a particle number, which are numbered -1, 0, and 1 for convenience. The coordinates x and y can be any of the pair of Jacobi coordinates (x_γ, y_γ), representing a point in region i. The basis functions are

$$\phi_\alpha^{\sigma\tau}(x,y) = \exp\left[(\sigma q, \mathrm{i}\tau k)\, R_\alpha \begin{pmatrix} x \\ y \end{pmatrix}\right], \tag{B.37}$$

where

$$R_\alpha = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}. \tag{B.38}$$

The basis functions have the following transformation property

$$\phi_{\alpha+\beta}^{\sigma\tau} = \phi_\alpha^{\sigma\tau} R_\beta, \tag{B.39}$$

(where $\alpha+\beta$ is wrapped around so that $-1 \le \alpha+\beta \le 1$) and the derivative

$$\frac{\partial\phi_\alpha^{\sigma\tau}(x,y)}{\partial x_\beta} = \left[(\sigma q, \mathrm{i}\tau k) R_{\alpha-\beta}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right]\phi_\alpha^{\sigma\tau}(x,y), \tag{B.40}$$

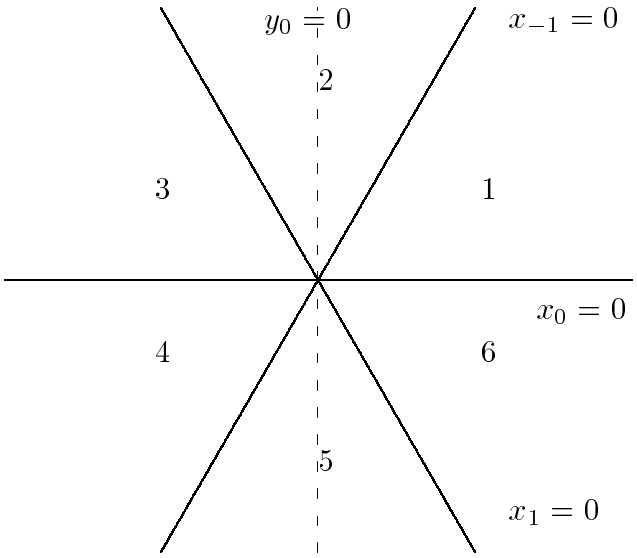


Figure B.1: Regions in configuration space for a three-body system in one dimension with zero-range interaction.

where x_β is defined by

$$\begin{pmatrix} x_\beta \\ y_\beta \end{pmatrix} \quad = \quad R_\beta \begin{pmatrix} x \\ y \end{pmatrix} . \tag{B.41}$$

This leads to the following matching matrix:

$$(M_{\beta\lambda})^{\sigma\tau,\sigma'\tau'}_{\alpha,\alpha'} \quad = \quad \delta^{\tau'}_{\tau}\delta^{\alpha'\sigma'-\beta\sigma'}_{\alpha\sigma-\beta\sigma}[(1-\lambda c^{\tau\sigma}_{\alpha-\beta})\delta^{\sigma'}_{\sigma} + \lambda c^{\tau\sigma}_{\alpha-\beta}\delta^{\sigma'}_{-\sigma}] , \tag{B.42}$$

where c is defined as

$$c^{\tau\sigma}_{\alpha} \quad = \quad \frac{2q}{(\sigma q, \mathrm{i}\tau k)R_\alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} - (-\sigma q, \mathrm{i}\tau k)R_{-\alpha} \begin{pmatrix} 1 \\ 0 \end{pmatrix}} . \tag{B.43}$$

The sign λ is positive if the line $x_\beta = 0$ is crossed from the positive to the negative side, and negative if otherwise. The matrix M matches the wave functions on both sides of the line $x_\beta = 0$ as follows:

$$\boldsymbol{a}_i \quad = \quad M_{\beta\lambda}\boldsymbol{a}_{i+1} , \tag{B.44}$$

where $\boldsymbol{a}_i$ is the vector of expansion coefficients $a^{\sigma\tau}_{\alpha i}$ in region i. The matrix mapping the coefficients for region i to itself (constructed as a product of six matrices M) turns out to be the unit matrix. Scattering solutions are therefore all bounded

Table B.1: Expansion coefficients for a specific solution of a system of three identical particles interacting via a zero-range potential in one dimension. The constants a and b are $-2q(q+\mathrm{i}\sqrt{3}k)/(3k^2+q^2)$ and $2q(q-\mathrm{i}\sqrt{3}k)/(3k^2+q^2)$, respectively. The sign τ is taken positive here.

σ	α	1	2	3	4	5	6
$-$	-1	0	0	b	a	0	0
$+$	-1	0	0	0	0	a	0
$-$	0	0	0	0	$1-a-b$	$1-a$	1
$+$	0	1	$1-a$	$1-a-b$	0	0	0
$-$	1	0	a	0	0	0	0
$+$	1	0	0	a	b	0	0

solutions. As it turns out, if the solution is bounded on one region, it is automatically bounded on all other regions. Obviously, the problem separates in fully "incoming" ($\tau<0$) and fully "outgoing" ($\tau>0$) parts.

The expansion coefficients $c_{\alpha i}^{\sigma\tau}$ are tabulated in Table B.1, for a specific case. Other cases can be easily derived. There are two remarkable conclusions to be drawn here. First, there appear to be no breakup solutions. (They are of course ruled out by assuming the basis functions in the specific manner shown here, but there is no breakup if all possible basis functions are used.) Second, from the matching conditions, it follows that τ is a good quantum number of the system. The three-body bound state is located at $E=-4s^2$:

$$\Psi(x_{-1},x_0,x_1) \quad = \quad \mathrm{e}^{-s(|x_{-1}|+|x_0|+|x_1|)}\,. \tag{B.45}$$

The problem of three-particles on a line with δ interactions has been investigated using various techniques (see, for example, McGuire [1964], Yang [1967, 1968], and Dodd [1970]). Gerjuoy [1987] used it as a test ground for exploring the mathematical problems with three-body scattering.

B.2 Common examples

Over the years, many models for the nuclear interaction have been used, varying from simple Gaussian or Yukawa-type potentials to accurate phenomenological potentials and potentials based on a meson-exchange model. These potentials are constructed to fit to low-energy scattering data and the deuteron binding energy. In this section I give the exact definition for some of the simpler potentials, since some of these come in many versions.

Table B.2: Parameters for the S3 potential. Potential strengths V_{si} are in MeV, range parameters β_{si} are in fm^{-2}.

s	V_{s1}	β_{s1}	V_{s2}	β_{s2}	V_{s3}	β_{s3}
0	1000.0	3.00	−326.7	1.05	−43.0	0.60
1	1000.0	3.00	−166.0	0.80	−23.0	0.40

B.2.1 Afnan–Tang

Afnan and Tang [1968] defined a set of four simple nucleon–nucleon potentials (denoted by S1 through S4) which can be written as a sum of three Gaussians, to investigate the properties of three- and four-nucleon bound systems:

$$V_s(r) \quad = \quad \sum_{i=1}^{3} V_{si} \mathrm{e}^{-\beta_{si} r^2} \,, \tag{B.46}$$

where s is the two-particle spin. In this thesis, the S3 potential, whose parameters are listed in Table B.2, was used. A spin-averaged potential is defined as well:

$$V_{\mathrm{avg}}(r) \quad = \quad \tfrac{1}{2}(V_0(r) + V_1(r)) \,. \tag{B.47}$$

B.2.2 Malfliet–Tjon

Malfliet and Tjon [1969] introduced potentials of the following form, as simple test cases for three-body bound-state calculations:

$$V(r) \quad = \quad V_1 \frac{\mathrm{e}^{-\mu_1 r}}{r} - V_2 \frac{\mathrm{e}^{-\mu_2 r}}{r} \,, \tag{B.48}$$

with $\mu_1 = 2\mu_2$. There are two spin dependent potentials, one with a repulsive core (denoted by MT-I/III), and one purely attractive (denoted by MT-II/IV). For both potentials the first potential (*i.e.*, MT-I and MT-II, respectively) is used for the singlet interaction, and the second for the triplet interaction. The averages of MT-I and MT-III is denoted by MT-V and the average of MT-II/IV is denoted by MT-VI.

Unfortunately the authors do not specify their units, and take $\mu_1 \neq \mu_2$, which has caused a lot of confusion in the literature. The parameters denoted by MT in Table B.3 were obtained using the conversion constant $\hbar c = 197.3\,\mathrm{MeV\,fm}$. However, the MT-III potential does not reproduce the experimental deuteron binding energy of 2.224 MeV. This is why Payne *et al.* [1980] scaled the MT-I/III pair and its average, MT-V, such that the correct deuteron binding energy is reproduced.

Table B.3: Parameters and two-body bound-state energies E_2 for Malfliet–Tjon potentials. The nucleon mass is defined by $\hbar^2/M = 41.47\,\mathrm{MeV\,fm^2}$. References are explained in the text.

Potential no.	V_1 (MeV fm)	μ_1 (fm^{-1})	V_2 (MeV fm)	μ_2 (fm^{-1})	E_2 (MeV)	Ref.
I	1458.047	3.110	520.872	1.550		MT
Ia	1438.720	3.110	513.968	1.550		PF
Ic	1458.047	3.110	520.872	1.555		NS
III	1458.047	3.110	635.306	1.550	−2.409	MT
IIIa	1438.720	3.110	626.885	1.550	−2.231	PF
IIIc	1458.047	3.110	635.306	1.555	−2.242	NS
V	1458.047	3.110	578.089	1.550	−0.414	MT
Va	1438.4812	3.110	570.316	1.550	−0.350	PF
Vb	1438.4812	3.110	570.3316	1.550	−0.350	PA
Vc	1458.047	3.110	578.089	1.555	−0.351	NS
II			52.4818	0.809		MT
IV			65.1090	0.633	−2.209	MT
VI			58.7954	0.723	−0.343	MT

Note that Table 1 of Payne *et al.* [1980] contains two mistakes. (The inverse range of the MT-IV potential is incorrectly listed as $0.663\,\mathrm{fm}^{-1}$ and V_2 of the MT-V potential should be 570.3316 MeV fm, as correctly listed by Payne [1987], instead of 570.316 MeV fm.) The parameters from Payne *et al.* [1980] are denoted by PF, and the correct parameters for MT-V from Payne [1987] are denoted by PA. Several other versions of the Malfliet–Tjon potentials can be found in the literature, due to differences in the conversion constant used, or differences in the nucleon mass. However, these closely resemble either the original MT potentials or the revised PF potentials. Finally, I would like to point out that if the relation $\mu_1 = \mu_2$ is restored by taking $\mu_2 = 1.555\,\mathrm{fm}^{-1}$ instead of $1.55\,\mathrm{fm}^{-1}$ (these parameters are denoted by NS), the two-body binding energy is very reasonable. The three-body binding energy is approximately 8.54 MeV for both MT-I/IIIa and MT-I/IIIc.

Appendix C

Angular momentum

This appendix summarizes the formulas related to angular momentum in few-body systems. These formulas supplement expressions which can be found mainly in Chapters 2, 4, and 5, and are needed to implement the few-body problem in a computer code.

First, I will concentrate on the angular-momentum operator and its eigenfunctions for both a single particle and a composite system. Next, I will look at the coupling and recoupling of angular momenta.

C.1 Angular momentum of a single particle

The angular momentum of a particle is defined by $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{k}$. If the particle moves in a spherically symmetric potential, its equation of motion can be separated into a radial and an angular part. This section briefly discusses the angular motion of a single particle or, equivalently, the angular motion of two particles interacting only with each other, in the center-of-mass frame.

The problem is most conveniently expressed in *polar coordinates*:

$$\boldsymbol{r} \;=\; r \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} . \tag{C.1}$$

The components of the angular-momentum operator expressed in polar coordinates are

$$L_x \;=\; \mathrm{i}\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right), \tag{C.2}$$

$$L_y \;=\; \mathrm{i}\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right), \tag{C.3}$$

$$L_z \;=\; -\,\mathrm{i}\frac{\partial}{\partial\phi}\,. \tag{C.4}$$

The square of $\boldsymbol{L}$ can be written as

$$\boldsymbol{L}^2 \quad = \quad -\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \csc^2\theta\frac{\partial^2}{\partial\phi^2}\right), \tag{C.5}$$

and the useful raising and lowering operators, L_+ and L_- are

$$L_\pm \quad = \quad L_x \pm \mathrm{i}L_y \quad = \quad \mathrm{e}^{\pm\mathrm{i}\phi}\left(\pm\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}\right), \tag{C.6}$$

The simultaneous eigenfunctions of $\boldsymbol{L}^2$ and L_z are the *spherical harmonics*:

$$\boldsymbol{L}^2 Y_{\ell m} \quad = \quad \ell(\ell+1)Y_{\ell m}\,, \quad \ell = 0, 1, 2, \ldots\,, \tag{C.7}$$

$$L_z Y_{\ell m} \quad = \quad mY_{\ell m}\,, \quad m = -\ell, -\ell+1, \ldots, \ell-1, \ell\,. \tag{C.8}$$

The spherical harmonics can be given in terms of the associated Legendre functions P_ℓ^m:

$$Y_{\ell m}(\theta,\phi) \quad = \quad (-1)^m\left[\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}\right]^{\frac{1}{2}} P_\ell^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}\,. \tag{C.9}$$

The spherical harmonics form a complete basis for functions on a unit sphere. They satisfy the following orthogonality relation:

$$\int_0^{2\pi}\mathrm{d}\phi\int_{-1}^{1}\mathrm{d}\cos\theta\, Y^*_{\ell m}(\theta,\phi)Y_{\ell' m'}(\theta,\phi) \quad = \quad \delta_{\ell\ell'}\delta_{mm'}\,. \tag{C.10}$$

The spherical harmonics for negative values of m can be calculated as follows:

$$Y_{\ell -m}(\theta,\phi) \quad = \quad (-1)^m Y^*_{\ell m}(\theta,\phi)\,. \tag{C.11}$$

A final useful relation is:

$$(2\ell+1)P_\ell(\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{y}}) \quad = \quad \sum_m Y_{\ell m}(\hat{\boldsymbol{x}})Y^*_{\ell m}(\hat{\boldsymbol{y}})\,, \tag{C.12}$$

where P_ℓ is a Legendre polynomial.

C.2 Angular momentum of composite systems

The angular-momentum operator for a system of N particles reads:

$$\boldsymbol{L} \quad = \quad \sum_{i=1}^{N}\boldsymbol{r}_i\times\boldsymbol{k}_i\,. \tag{C.13}$$

If the particles interact only with each other, the motion of the system may be separated in the collective angular motion and the internal motion of the particles with respect to each other. The orientation of a system of three or more particles cannot be described by two angles, as is the case for two particles. Different orientations are related by general rotations in three-body space, requiring three angles. It is convenient to use the Euler parameterization for these rotations. Such a rotation will be denoted by $D(\alpha,\beta,\gamma)$, which, when viewed as coordinate transformation, is defined by

$$\begin{aligned} & D(\alpha,\beta,\gamma) \\ = & \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} . \end{aligned} \tag{C.14}$$

Instead of $D(\alpha,\beta,\gamma)$, a short-hand notation, $D(\omega)$, can be used. The operator for functions in coordinate space will also be denoted by D, and is defined as follows:

$$D(\omega) f[D(\omega)\boldsymbol{r}] \quad = \quad f(\boldsymbol{r}) \,, \tag{C.15}$$

for any scalar field f. Using this definition, the following form for the rotation operator can be obtained:

$$D(\alpha,\beta,\gamma) \quad = \quad \mathrm{e}^{\mathrm{i}\gamma L_z} \mathrm{e}^{\mathrm{i}\beta L_y} \mathrm{e}^{\mathrm{i}\alpha L_z} \,, \tag{C.16}$$

where the L_y and L_z are the y and z components of the total-angular-momentum operator $\boldsymbol{L}$, respectively. The components of the angular momentum operator can be expressed in the Euler angles as follows:

$$L_x \quad = \quad -\,\mathrm{i} \left(-\cos\alpha \cot\beta \frac{\partial}{\partial\alpha} - \sin\alpha \frac{\partial}{\partial\beta} + \cos\alpha \csc\beta \frac{\partial}{\partial\gamma} \right) , \tag{C.17}$$

$$L_y \quad = \quad -\,\mathrm{i} \left(-\sin\alpha \cot\beta \frac{\partial}{\partial\alpha} + \cos\alpha \frac{\partial}{\partial\beta} + \sin\alpha \csc\beta \frac{\partial}{\partial\gamma} \right) , \tag{C.18}$$

$$L_z \quad = \quad -\,\mathrm{i} \frac{\partial}{\partial\alpha} \,. \tag{C.19}$$

Often, it is convenient to work with the raising and lowering operators L_+ and L_-, defined by

$$L_\pm \quad = \quad L_x \pm \mathrm{i} L_y \quad = \quad \mathrm{e}^{\pm\mathrm{i}\alpha} \left(\mathrm{i} \cot\beta \frac{\partial}{\partial\alpha} \pm \frac{\partial}{\partial\beta} - \mathrm{i} \csc\beta \frac{\partial}{\partial\gamma} \right) . \tag{C.20}$$

Finally, the square of the angular momentum operator can be written as

$$\boldsymbol{L}^2 \quad = \quad -\frac{\partial^2}{\partial\beta^2} - \cot\beta \frac{\partial}{\partial\beta} - \csc^2\beta \left(\frac{\partial^2}{\partial\alpha^2} - 2\cos\beta \frac{\partial}{\partial\alpha} \frac{\partial}{\partial\gamma} + \frac{\partial^2}{\partial\gamma^2} \right) . \tag{C.21}$$

It is convenient to introduce the following notation for the matrix elements of the rotation operators:

$$\langle \ell\, m' \,|\, D(\alpha,\beta,\gamma) \,|\, \ell\, m \rangle \quad = \quad \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,. \tag{C.22}$$

These *Wigner* $\mathscr{D}$ functions have the following properties:

$$\boldsymbol{L}^2\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma) \quad = \quad \ell(\ell+1)\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,, \tag{C.23}$$

$$L_z\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma) \quad = \quad m'\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,, \tag{C.24}$$

$$-\mathrm{i}\frac{\partial}{\partial\gamma}\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma) \quad = \quad m\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,, \quad \text{and} \tag{C.25}$$

$$L_\pm\, \mathscr{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma) \quad = \quad \sqrt{(\ell\mp m)(\ell\pm m+1)}\, \mathscr{D}^{(\ell)}_{m'm\pm1}(\alpha,\beta,\gamma)\,, \tag{C.26}$$

implying that they are the eigenfunctions of $\boldsymbol{L}^2$ and L_z, and also of $-\mathrm{i}\partial/\partial\gamma$, the analogue of L_z in the "moving" coordinate system, which commutes with both $\boldsymbol{L}^2$ and L_z. The Wigner $\mathscr{D}$ functions can be written as

$$\mathscr{D}^{(j)}_{m'm}(\alpha,\beta,\gamma) \quad = \quad \mathrm{e}^{\mathrm{i}m'\gamma} d^{(j)}_{m'm}(\beta) \mathrm{e}^{\mathrm{i}m\alpha}\,, \tag{C.27}$$

where $d^{(j)}_{m'm}$ is related to the Jacobi polynomials as follows:

$$\begin{aligned} d^{(j)}_{m'm}(\beta) \quad = \quad & \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}\right]^{1/2} \\ & \times \left(\cos\frac{\beta}{2}\right)^{m'+m} \left(\sin\frac{\beta}{2}\right)^{m'-m} P^{(m'-m,m'+m)}_{j-m'}(\cos\beta)\,. \end{aligned} \tag{C.28}$$

The value of $d^{(j)}_{m'm}(\beta)$ can be determined by using the following recursion relation:

$$\begin{aligned} d^{(j)}_{m'm}(\beta) \quad = \quad & \left(\frac{j-m'}{j-m}\right)^{1/2} \left(\cos\frac{\beta}{2}\right) d^{(j-\frac{1}{2})}_{m'+\frac{1}{2}\, m+\frac{1}{2}}(\beta) \\ & - \left(\frac{j+m'}{j-m}\right)^{1/2} \left(\sin\frac{\beta}{2}\right) d^{(j-\frac{1}{2})}_{m'-\frac{1}{2}\, m+\frac{1}{2}}(\beta)\,, \end{aligned} \tag{C.29}$$

for $m \neq j$, and

$$\begin{aligned} d^{(j)}_{m'j}(\beta) \quad = \quad & (-1)^{j-m'} \left[\frac{(2j)!}{(j+m')!(j-m')!}\right]^{1/2} \\ & \times \left(\cos\frac{\beta}{2}\right)^{j+m'} \left(\sin\frac{\beta}{2}\right)^{j-m'}\,. \end{aligned} \tag{C.30}$$

The Wigner $\mathscr{D}$ functions are the generalization of the spherical harmonics. They form a complete basis on the space of orientations of a composite system.

C.3 Coupling of angular momenta

The eigenstates of the total angular momentum $\boldsymbol{J} = \boldsymbol{J}_1 + \boldsymbol{J}_2$ can be constructed from eigenstates of the two angular momenta $\boldsymbol{J}_1$ and $\boldsymbol{J}_2$ as follows:

$$|j_1\, j_2\, j\, m\rangle \quad = \quad \sum_{m_1 m_2} \langle j_1\, m_1\, j_2\, m_2 | J\, M\rangle |j_1\, m_1\rangle |j_2\, m_2\rangle\,, \tag{C.31}$$

where $\langle j_1\, m_1\, j_2\, m_2 | J\, M\rangle$ are the *vector-coupling* or *Clebsch–Gordan* (CG) coefficients. There are many different notations for the CG coefficients. I use a short-hand form of the notation used in Edmonds [1960]:

$$\langle j_1\, m_1\, j_2\, m_2 | j\, m\rangle \quad = \quad \langle j_1\, m_1\, j_2\, m_2\, |\, j_1\, j_2\, j\, m\rangle\,, \tag{C.32}$$

since usually there is no need to write the quantum numbers j_1 and j_2 in the ket part of the matrix element. (This definition implies the Condon–Shortley convention for the phases of the CG coefficients.) The CG coefficients satisfy the following unitarity relations:

$$\sum_{jm} \langle j_1\, m_1\, j_2\, m_2 | j\, m\rangle \langle j_1\, m_1'\, j_2\, m_2' | j\, m\rangle \quad = \quad \delta_{m_1 m_1'} \delta_{m_2 m_2'}\,, \tag{C.33}$$

$$\sum_{m_1 m_2} \langle j_1\, m_1\, j_2\, m_2 | j\, m\rangle \langle j_1\, m_1\, j_2\, m_2 | j'\, m'\rangle \quad = \quad \delta_{jj'} \delta_{mm'}\,. \tag{C.34}$$

The CG coefficients can be given in closed form, using the following formula, due to Racah:

$$\begin{aligned}
&\langle j_1\, m_1\, j_2\, m_2 | j\, m\rangle \\
= \quad & \delta_{m_1+m_2,m} \left[\frac{(2j+1)(j_1+j_2-j)!(j_1-j_2+j)!(-j_1+j_2+j)!}{(j_1+j_2+j+1)!}\right]^{\frac{1}{2}} \\
& \times [(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!]^{\frac{1}{2}} \\
& \times \sum_z \frac{(-1)^z}{z!(j_1+j_2-j-z)!(j_1-m_1-z)!} \\
& \qquad \times \frac{1}{(j_2+m_2-z)!(j-j_2+m_1+z)!(j-j_1-m_2+z)!}\,.
\end{aligned} \tag{C.35}$$

The Clebsch–Gordan coefficients are not very symmetrical, as opposed to the Wigner 3-j symbol:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad = \quad (-1)^{j_1-j_2-m_3} (2j_3+1)^{-\frac{1}{2}} \langle j_1\, m_1\, j_2\, m_2 | j_3\; -m_3\rangle\,. \tag{C.36}$$

The Wigner 3-j symbol has many simple symmetries. It is invariant under even permutations of the columns, and changes sign under odd permutations if $j_1 +$

$j_2 + j_3$ is odd. Finally, we have:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} . \tag{C.37}$$

C.4 Recoupling

Matrix elements of noncentral operators have traditionally been calculated using six-, nine-, twelve-, ... j symbols. These objects can be seen to be contained in these formulas, by reducing the explicit sums over magnetic quantum numbers of products of CG coefficients to products of recoupling coefficients (*i.e.*, $3N$-j symbols), using (for example) diagram techniques [Baz and Castel, 1972]. The reason for doing this is that the explicit evaluation of the sums over the magnetic quantum numbers of products of CG coefficients can be a huge task, when done manually. A reduction to products of $3N$-j symbols leads to a simplification, since these objects can (and have been) tabulated. However, the reduction procedure is a task that requires insight and experience, and therefore very hard to code into a computer program. (I have used these techniques to calculate the quadrupole moment of the ^{6}Li nucleus. The (tedious) calculation can be found in Appendix E.) Therefore, and also because computers have no trouble calculating and adding up huge numbers of CG coefficients, this method can now be regarded as outdated. It is possible, of course, that the reduction process leads to a smaller numerical task than the brute-force approach of blindly performing the summations, but the advantage of being able to write a code that calculates recoupling coefficients and noncentral operators in a very general fashion usually overrules this possible disadvantage.

For this reason, I do not give any formulas of recoupling coefficients in this section. The only formulas regarding recoupling are given in Sec. 5.1.4, and are intended just as an illustration, since I do not use six- or nine-j symbols in my computer code, but instead I use a code that can recouple any coupling scheme into any other (for any number of particles). This has the practical advantage that, provided this code is correct, the possibility of errors introduced by the manual reduction process, or by convention problems, has been ruled out. I will describe this aspect in Appendix F.

Appendix D

Special functions

This appendix contains definitions and properties of the special functions used throughout this thesis. Note that there exist several different definitions for some of these special functions. My precise choice as well as the most common differences in the literature are pointed out. My main sources of reference were Erdélyi [1953], and Magnus *et al.* [1966]. Other sources were Abramowitz and Stegun [1965] and Gradshteyn and Ryzhik [1980]. An excellent reference for functions related to the Coulomb potential is van Haeringen [1985]. These references will be denoted by EH, MOS, AS, GR, and HA, respectively.

D.1 The Gamma function

The Gamma function can be defined by

$$\Gamma(z) \quad = \quad z^{-1} \prod_{n=1}^{\infty} \left(1+\frac{1}{n}\right)^{z} \left(1+\frac{z}{n}\right)^{-1} . \tag{D.1}$$

It can be regarded as the generalization of the factorial function:

$$\Gamma(1+z) \quad = \quad z\Gamma(z)\,, \tag{D.2}$$

and behaves asymptotically as

$$\Gamma(z) \quad = \quad z^{-\frac{1}{2}} \mathrm{e}^{z(\log z - 1)} \sqrt{2\pi} (1 + \mathrm{O}(z^{-1}))\,, \tag{D.3}$$

for $|z| \to \infty$ and $|\arg z| < \pi$. This equation can be used to calculate the Coulomb phase shift for low energies. Using

$$\begin{aligned} & \Gamma(\ell + 1 + \mathrm{i}\gamma) \\ = \quad & \sqrt{2\pi} |\gamma|^{\ell+\frac{1}{2}} \mathrm{e}^{-\pi|\gamma|/2} \\ & \times \exp\left[\mathrm{i}\,\mathrm{sgn}(\gamma)\left(\tfrac{\pi}{4}(2\ell+1) + |\gamma|(-1+\log|\gamma|)\right)\right] (1 + \mathrm{O}(\gamma^{-1}))\,, \end{aligned} \tag{D.4}$$

the following expression is found:

$$\sigma_\ell(\gamma) \quad = \quad \mathrm{sgn}(\gamma)\left(\tfrac{\pi}{4}(2\ell+1) + |\gamma|(-1+\log|\gamma|)\right)(1+\mathrm{O}(\gamma^{-1}))\,. \tag{D.5}$$

The digamma function, $\psi(z)$, is defined as the logarithmic derivative of the Gamma function:

$$\psi(z) \quad = \quad \frac{\Gamma'(z)}{\Gamma(z)}\,. \tag{D.6}$$

It can be written as

$$\begin{aligned}\psi(z) \quad &= \quad -\gamma + \sum_{n=0}^{\infty}\Big(\frac{1}{n+1} - \frac{1}{z+n}\Big) \\ &= \quad \lim_{n\to\infty}\left(\log n - \sum_{i=0}^{n}\frac{1}{z+i}\right).\end{aligned} \tag{D.7}$$

In this equation, γ is Euler's constant:

$$\gamma \quad = \quad \lim_{n\to\infty}\left(-\log n + \sum_{i=1}^{n}\frac{1}{i}\right) \quad = \quad 0.577215\ldots\,. \tag{D.8}$$

D.2 The hypergeometric function

The hypergeometric function ${}_2F_1$ is a special case of a class of functions ${}_pF_q$, defined by the *generalized hypergeometric series*:

$${}_pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;z) \quad = \quad \sum_{n=0}^{\infty}\frac{(a_1)_n\cdots(a_p)_n}{(b_1)_n\cdots(b_q)_n}\frac{z^n}{n!}\,, \tag{D.9}$$

where $(a)_n$ is the Pochhammer symbol, defined by

$$(a)_n \quad = \quad a(a+1)\cdots(a+n-1) \quad = \quad \frac{\Gamma(a+n)}{\Gamma(a)}\,. \tag{D.10}$$

For $p=2$ and $q=1$ we have

$${}_2F_1(a,b;c;z) \quad = \quad \sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!}\,. \tag{D.11}$$

The series converges for $|z|<1$ and diverges for $|z|>1$. The behavior on the unit circle depends on the parameters a, b, and c. If either a or b is a negative

integer, the hypergeometric function reduces to a polynomial. The hypergeometric function is one solution (for $|z| < 1$) of the hypergeometric differential equation

$$z(1-z)\frac{\mathrm{d}^2 w}{\mathrm{d}z^2} + [c - (a+b+1)z]\frac{\mathrm{d}w}{\mathrm{d}z} - abw \quad = \quad 0\,, \tag{D.12}$$

unless $c = 1 - n$ for $n = 1, 2, \ldots$. The second solution can usually be expressed through hypergeometric functions as well. (However, in some cases, such as $c = 1-n$, the second solution is logarithmic.) The hypergeometric differential equation has three regular-singular points ($z = 0$, $z = 1$, and $z = \infty$), which can be mapped onto each other using simple transformations. This allows one to extend the solution to the entire z plane. (Note, however, that since the case $c = 1 - n$ poses a problem close to the origin, similar problems occur near the other singular points.)

The hypergeometric function contains a large class of special functions. For example, the classical orthogonal polynomials are special cases of the hypergeometric function. The Legendre functions can also be expressed using hypergeometric functions. Finally, the confluent hypergeometric function, or Kummer's function, is a limit of the hypergeometric function.

D.3 Coulomb functions

The Coulomb functions are defined by

$$F_\ell(\gamma; kr) \quad = \quad C_\ell \mathrm{e}^{\mathrm{i}kr}(kr)^{\ell+1}\,{}_1F_1(\ell+1+\mathrm{i}\gamma; 2\ell+2; -2\mathrm{i}kr)\,, \tag{D.13}$$

$$u_\ell^+(\gamma; kr) \quad = \quad \mathrm{i}(-2kr)^{\ell+1}\mathrm{e}^{\mathrm{i}kr+\pi\gamma/2}U(\ell+1+\mathrm{i}\gamma, 2\ell+2, -2\mathrm{i}kr)\,, \tag{D.14}$$

(notation from HA) with

$$C_\ell \quad = \quad \frac{C_0}{(2\ell+1)!!}\prod_{n=1}^{\ell}\left(1+\frac{\gamma^2}{n^2}\right)^{\frac{1}{2}}\,, \tag{D.15}$$

$$C_0 \quad = \quad \left(\frac{2\pi\gamma}{\mathrm{e}^{2\pi\gamma}-1}\right)^{\frac{1}{2}}\,. \tag{D.16}$$

(For $\gamma = 0$, we define $C_0 = 1$.) For real γ this can also be written as

$$C_\ell \quad = \quad 2^\ell \mathrm{e}^{-\pi\gamma/2}\frac{|\Gamma(\ell+1+\mathrm{i}\gamma)|}{(2\ell+1)!}\,. \tag{D.17}$$

These functions have the following long-range behavior:

$$F_\ell(\gamma; kr) \quad \sim \quad \sin(kr - \gamma\log 2kr - \tfrac{1}{2}\ell\pi + \sigma_\ell)\,, \tag{D.18}$$

$$u_\ell^\pm(\gamma; kr) \quad \sim \quad \exp[\pm\mathrm{i}(kr - \gamma\log 2kr - \tfrac{1}{2}\ell\pi)]\,, \tag{D.19}$$

for $r \to \infty$.

The functions ${}_1F_1$ and U (notation from MOS and HA) are the confluent hypergeometric functions of the first and second kind, respectively:

$$ {}_1F_1(a;c;z) \quad = \quad \sum_{n=0}^{\infty} \frac{(a)_n}{(c)_n} \frac{z^n}{n!} \quad = \quad \frac{\Gamma(c)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(c+n)} \frac{z^n}{n!} \,, \tag{D.20} $$

(for $c \neq 0, -1, -2, \ldots$), and

$$ \begin{aligned} & U(a,c,z) \\ = \quad & \frac{\pi}{\sin(\pi c)} \left[\frac{{}_1F_1(a;c;z)}{\Gamma(c)\Gamma(1+a-c)} - z^{1-c} \frac{{}_1F_1(a+1-c;2-c;z)}{\Gamma(a)\Gamma(2-c)} \right] , \end{aligned} \tag{D.21} $$

(this is a multivalued function; its principal branch is given by $-\pi < \arg z \leq \pi$). (Note that, although ${}_1F_1(a;-m;z)$ does not exist, the limit of ${}_1F_1(a;c;z)/\Gamma(c)$ for $c \to -m$ does exist.) In the limit that c goes to a positive integer, U can be expressed as

$$ \begin{aligned} & U(a,n+1,z) \\ = \quad & \frac{(n-1)!}{\Gamma(a)} \sum_{r=0}^{n-1} \frac{(a-n)_r}{(1-n)_r} \frac{z^{r-n}}{r!} \\ & + \frac{(-1)^{n+1}}{\Gamma(a-n)\Gamma(n+1)} \left[{}_1F_1(a;n+1;z) \log z \right. \\ & \qquad \left. + \sum_{r=0}^{\infty} \frac{(a)_r}{(n+1)_r} \frac{z^r}{r!} \left\{ \psi(a+r) - \psi(1+r) - \psi(n+1+r) \right\} \right] . \end{aligned} \tag{D.22} $$

The confluent hypergeometric functions are solutions to Kummer's differential equation

$$ z \frac{\mathrm{d}^2 w}{\mathrm{d}z^2} + (c-z) \frac{\mathrm{d}w}{\mathrm{d}z} - aw \quad = \quad 0 \,, \tag{D.23} $$

which has a regular singularity at $z = 0$ and an irregular singularity at $z = \infty$. The irregular singularity is the result of the confluence of the singularity at $z = 1$ and $z = \infty$ of the hypergeometric equation, which occurs when z is replaced by z/b, and the limit $b \to \infty$ is taken. Therefore,

$$ {}_1F_1(a;c;z) \quad = \quad \lim_{b \to \infty} {}_2F_1(a,b;c;z/b) \,. \tag{D.24} $$

Different notations are in use for the confluent hypergeometric functions. For the confluent hypergeometric function of the first kind the following names are in use:

${}_1F_1(a;c;z)$ (MOS), $\Phi(a,c;z)$ (EH and GR), $M(a,c,z)$ (AS), and $F(a|c|z)$ [Messiah, 1961]. The confluent hypergeometric function of the second kind, $U(a,c,z)$ (MOS and AS), is often denoted by $\Psi(a,c;z)$ (EH and GR), and by $W_1(a|c|z)$ [Messiah, 1961].

The confluent hypergeometric functions are related to the Bessel functions. They are found by switching off the Coulomb potential, *i.e.*, by putting $\gamma = 0$:

$$ {}_1F_1(\nu+\tfrac{1}{2};2\nu+1;2\mathrm{i}z) = \Gamma(1+\nu)\mathrm{e}^{\mathrm{i}z}\left(\frac{z}{2}\right)^{-\nu} J_\nu(z)\,, \tag{D.25} $$

$$ U(\nu+\tfrac{1}{2},2\nu+1,\mp 2\mathrm{i}z) = \pm\tfrac{1}{2}\mathrm{i}\pi^{\frac{1}{2}}\mathrm{e}^{\pm\mathrm{i}(\pi\nu-z)}(2z)^{-\nu}H_\nu^{(1,2)}(z)\,. \tag{D.26} $$

More specifically, we find

$$ F_\ell(0;kr) = \hat{\jmath}_\ell(kr)\,, \tag{D.27} $$

$$ u_\ell^+(0;kr) = \hat{h}_\ell^+(kr)\,, \tag{D.28} $$

where $\hat{\jmath}$ and $\hat{h}$ are the Riccati–Bessel functions.

The zero-energy limit, *i.e.*, the limit $\gamma \to \pm\infty$ (k positive) of the Coulomb functions is:

$$ \lim_{k\downarrow 0}\left(\frac{-2\pi\gamma}{C_0}\right)F_\ell(\gamma;kr) = (\operatorname{sgn} s)^\ell \pi\sqrt{2sr}J_{2\ell+1}(\sqrt{8sr})\,, \tag{D.29} $$

$$ \lim_{k\downarrow 0} C_0\mathrm{e}^{\mathrm{i}\sigma_\ell}u_\ell^+(\gamma;kr) = \mathrm{i}(\operatorname{sgn} s)^\ell \pi\sqrt{2sr}H^{(1)}_{2\ell+1}(\sqrt{8sr})\,. \tag{D.30} $$

D.4 Bessel functions

The Bessel functions are solutions of

$$ z^2\frac{\mathrm{d}^2w}{\mathrm{d}z^2} + z\frac{\mathrm{d}w}{\mathrm{d}z} + (z^2-\nu^2)w = 0\,, \tag{D.31} $$

where ν and z can be arbitrarily complex. The Bessel functions (of the first kind) are defined by

$$ J_\nu(z) = \sum_{m=0}^{\infty}\frac{(-1)^m\left(\frac{z}{2}\right)^{\nu+2m}}{m!\Gamma(\nu+m+1)} = \frac{\left(\frac{z}{2}\right)^\nu}{\Gamma(\nu+1)}{}_0F_1(\nu+1;-\tfrac{1}{4}z^2)\,, \tag{D.32} $$

from which the Neumann (Bessel functions of the second kind, denoted by Y_ν, or by N_ν in GR) and Hankel functions (Bessel functions of the third kind, $H_\nu^{(1,2)}$) can be derived:

$$ Y_\nu(z) = (\sin\pi\nu)^{-1}\left[J_\nu(z)\cos\pi\nu - J_{-\nu}(z)\right]\,, \tag{D.33} $$

$$ H_\nu^{(1,2)}(z) = J_\nu(z) \pm \mathrm{i}Y_\nu(z)\,, \tag{D.34} $$

Note that for integer ν the above definitions are indefinite. The correct procedure is then to take the limit for $\nu \to n$. The Bessel functions have a cut along the negative real z axis.

The *modified* Bessel and Hankel functions can be defined by replacing the argument z of the Bessel and Hankel functions by iz:

$$I_\nu(z) = \mathrm{e}^{-\mathrm{i}\nu\pi/2} J_v\left(z\mathrm{e}^{\mathrm{i}\pi/2}\right), \tag{D.35}$$

$$K_\nu(z) = \tfrac{1}{2}\mathrm{i}\pi\mathrm{e}^{\mathrm{i}\nu\pi/2} H_\nu^{(1)}\left(z\mathrm{e}^{\mathrm{i}\pi/2}\right). \tag{D.36}$$

For integer order ($\nu = n$ for $n = 0, 1, 2, \ldots$), the irregular Bessel functions can be written in such a way that the singularity structure becomes explicit:

$$\begin{aligned} Y_n(z) &= \tfrac{2}{\pi}[\gamma + \log\tfrac{z}{2}]J_n(z) - \frac{1}{\pi}\sum_{m=0}^{n-1}\frac{(\frac{z}{2})^{2m-n}(n-m-1)!}{m!} \\ &\quad - \frac{1}{\pi}\sum_{m=0}^{\infty}(-1)^m\frac{(\frac{z}{2})^{n+2m}}{m!(n+m)!}(h_{m+n}+h_m), \end{aligned} \tag{D.37}$$

$$\begin{aligned} K_n(z) &= (-1)^{n+1}[\gamma + \log\tfrac{z}{2}]I_n(z) + \tfrac{1}{2}\sum_{m=0}^{n-1}(-1)^m\frac{(n-m-1)!}{m!}(\tfrac{z}{2})^{2m-n} \\ &\quad + \tfrac{1}{2}(-1)^n\sum_{m=0}^{\infty}\frac{(\frac{z}{2})^{n+2m}}{m!(n+m)!}(h_{m+n}+h_m). \end{aligned} \tag{D.38}$$

(for $n = 0$ the finite sum drops out) where h_m is defined by

$$h_m = \sum_{k=1}^{m} k^{-1}, \tag{D.39}$$

h_0 is zero, and γ is Euler's constant.

The Bessel functions of half-odd integer order are elementary functions. One form is:

$$J_{n+\frac{1}{2}}(z) = (-1)^n\left(\tfrac{1}{2}\pi z\right)^{-\frac{1}{2}} z^{n+1}\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^n\frac{\sin z}{z}, \tag{D.40}$$

$$Y_{n+\frac{1}{2}}(z) = -(-1)^n\left(\tfrac{1}{2}\pi z\right)^{-\frac{1}{2}} z^{n+1}\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^n\frac{\cos z}{z}, \tag{D.41}$$

$$H_{n+\frac{1}{2}}^{(1,2)}(z) = \mp\mathrm{i}(-1)^n\left(\tfrac{1}{2}\pi z\right)^{-\frac{1}{2}} z^{n+1}\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^n\frac{\mathrm{e}^{\pm\mathrm{i}z}}{z}, \tag{D.42}$$

$$I_{n+\frac{1}{2}}(z) = \left(\tfrac{1}{2}\pi z\right)^{-\frac{1}{2}} z^{n+1}\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^n\frac{\sinh z}{z}, \tag{D.43}$$

$$K_{n+\frac{1}{2}}(z) = (-1)^n\left(\frac{\pi}{2z}\right)^{\frac{1}{2}} z^{n+1}\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^n\frac{\mathrm{e}^{-z}}{z}. \tag{D.44}$$

The spherical Bessel functions j and h (often denoted by ψ_m and ζ_m, respectively) are defined by

$$j_\ell(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} J_{\ell+\frac{1}{2}}(z)\,, \tag{D.45}$$

$$n_\ell(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} Y_{\ell+\frac{1}{2}}(z)\,, \tag{D.46}$$

$$h_\ell^{(1,2)}(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} H_{\ell+\frac{1}{2}}^{(1,2)}(z)\,, \tag{D.47}$$

$$h_\ell^{\pm}(z) = \pm\,\mathrm{i} h_\ell^{(1,2)}(z)\,. \tag{D.48}$$

Taylor [1972] and Messiah [1961] define a function n_ℓ which differs from the one given here by an overall minus sign. The Riccati–Bessel functions are related to the spherical Bessel functions by

$$\hat{\jmath}_\ell(z) = z j_\ell(z)\,, \tag{D.49}$$

$$\hat{n}_\ell(z) = z n_\ell(z)\,, \tag{D.50}$$

$$\hat{h}_\ell^{\pm}(z) = z h_\ell^{\pm}(z)\,. \tag{D.51}$$

The Riccati–Bessel functions satisfy the following Wronskian property:

$$W(\hat{\jmath}_\ell, \hat{n}_\ell) = \hat{\jmath}_\ell(z)\hat{n}_\ell'(z) - \hat{n}_\ell(z)\hat{\jmath}_\ell'(z) = 1\,. \tag{D.52}$$

The zero-energy limit ($k \downarrow 0$) of the Riccati–Bessel functions is

$$\lim_{k\downarrow 0} k^{-\ell-1}\hat{\jmath}_\ell(kr) = \frac{r^{\ell+1}}{(2\ell+1)!!}\,, \tag{D.53}$$

$$\lim_{k\downarrow 0} k^{\ell}\hat{h}_\ell^{+}(kr) = (2\ell-1)!!\, r^{-\ell}\,. \tag{D.54}$$

D.5 Orthogonal polynomials

A set of polynomials p_n satisfying the orthonormality relation

$$\int_a^b \mathrm{d}x\, w(x) p_m^*(x) p_n(x) = \delta_{mn}\,, \tag{D.55}$$

($w(x)$ is a nonnegative real weight factor) is considered *orthonormal*. (If the normalization condition is dropped, the polynomials are considered *orthogonal*.) If the index n is equal to the degree of the polynomial p_n, this requirement uniquely specifies the polynomials, apart from phase factors. Let me summarize a few properties of orthogonal polynomials:

1. Any polynomial of degree $m < n$ is orthogonal to p_n.

2. The polynomial p_n has n different zeros on the open interval (a, b).

3. If p_n has zeros $\{x_i\}_1^n$, p_m $(m > n)$ has at least one zero in every interval $(x_i, x_i + 1)$, and exactly one zero if $m = n + 1$. (Note that we define $a = x_0$, and $b = x_{n+1}$.)

4. There is a recursion relation relating three consecutive orthonormal polynomials:

$$p_{n+1}(x) \quad = \quad (A_n x + B_n)p_n(x) - C_n p_{n-1}(x)\,, \tag{D.56}$$

   where A_n, B_n, and C_n depend on n only.

The best-known orthogonal polynomials are the Chebyshev, Gegenbauer, Hermite, Jacobi, Laguerre, and Legendre polynomials. These *classical* orthogonal polynomials have a few additional properties:

1. $\{p_n'(x)\}$ is a system of orthogonal polynomials.

2. The classical orthogonal polynomials satisfy the following differential equation:

$$A(x)\frac{\mathrm{d}^2 p_n}{\mathrm{d}x^2} + B(x)\frac{\mathrm{d}p_n}{\mathrm{d}x} + \lambda_n p_n \quad = \quad 0\,, \tag{D.57}$$

   for some functions $A(x)$, $B(x)$ independent of n, and some constant λ_n, depending only on n.

3. The polynomials can be expressed using a Rodrigues formula:

$$p_n(x) \quad = \quad \frac{1}{K_n w(x)}\frac{\mathrm{d}^n}{\mathrm{d}x^n}[w(x)(X(x))^n]\,, \tag{D.58}$$

   for some polynomial X independent of n, and some constant K_n depending only on n.

These properties are equivalent, and any system of orthogonal polynomials satisfying any of these conditions can be reduced to a system of classical polynomials.

D.5.1 Legendre polynomials

The Legendre polynomials P_n are orthogonal polynomials on $(-1, 1)$ with weight $w(x) = 1$. They satisfy the differential equation

$$\left[(1 - x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}}{\mathrm{d}x} + n(n + 1)\right] P_n(x) \quad = \quad 0\,, \tag{D.59}$$

with the boundary condition that $P_n(x)$ is finite at ± 1. They are normalized such that

$$P_n(1) \quad = \quad 1\,. \tag{D.60}$$

The corresponding orthonormal system is

$$(n+\tfrac{1}{2})^{\frac{1}{2}} P_n(x)\,. \tag{D.61}$$

The recursion relation is

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) \quad = \quad 0\,, \tag{D.62}$$

and the Rodrigues formula reads

$$P_n(x) \quad = \quad \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}((x^2-1)^n)\,. \tag{D.63}$$

The derivative can be expressed as follows:

$$(1-x^2)P_n'(x) \quad = \quad n[P_{n-1}(x) - xP_n(x)]\,. \tag{D.64}$$

D.5.2 Hermite polynomials

The Hermite polynomials H_n are orthogonal polynomials on $(-\infty,\infty)$ with weight $w(x) = \exp(-\frac{1}{2}x^2)$. They satisfy the differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}}{\mathrm{d}x} + 2n\right] H_n(x) \quad = \quad 0\,, \tag{D.65}$$

with the boundary condition that $H_n(x)$ behaves as a finite power of x at $\pm\infty$. The orthonormal system is

$$(\pi)^{-1/4}(2^n n!)^{-\frac{1}{2}} H_n(x)\,. \tag{D.66}$$

The recursion relation is

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) \quad = \quad 0\,, \tag{D.67}$$

and the Rodrigues formula reads

$$H_n(x) \quad = \quad (-1)^n \mathrm{e}^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(\mathrm{e}^{-x^2})\,. \tag{D.68}$$

The derivative can be expressed as follows:

$$H_n'(x) \quad = \quad 2nH_{n-1}(x) \quad = \quad 2xH_n(x) - H_{n+1}(x)\,. \tag{D.69}$$

The orthogonal polynomials associated with the weight $\exp(-x^2/2)$ are denoted by He_n. They are related to H_n as follows:

$$\mathrm{He}_n(x) \quad = \quad 2^{-\frac{n}{2}} H_n(2^{-\frac{1}{2}}x)\,. \tag{D.70}$$

D.5.3 Jacobi polynomials

The Jacobi polynomials $P_n^{(\alpha,\beta)}$ are orthogonal polynomials on $(-1,1)$ with weights $w(x) = (1-x)^\alpha(1+x)^\beta$. They satisfy the differential equation

$$\begin{aligned} & \left[(1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + [\beta-\alpha-(\alpha+\beta+2)x]\frac{\mathrm{d}}{\mathrm{d}x} + n(n+\alpha+\beta+1)\right] P_n^{(\alpha,\beta)}(x) \\ = \quad & 0\,, \end{aligned} \tag{D.71}$$

with the boundary condition that $P_n^{(\alpha,\beta)}(x)$ is finite at $x = \pm 1$. The Jacobi polynomials are normalized as follows:

$$P_n^{(\alpha,\beta)}(1) \quad = \quad \frac{(\alpha+1)_n}{n!}\,. \tag{D.72}$$

The orthonormal system is

$$\left[\frac{n!\Gamma(\alpha+\beta+n+1)(\alpha+\beta+2n+1)}{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}\right]^{\frac{1}{2}} P_n^{(\alpha,\beta)}(x)\,. \tag{D.73}$$

The recursion relation is

$$\begin{aligned} & 2(n+1)(\alpha+\beta+n+1)(\alpha+\beta+2n)P_{n+1}^{(\alpha,\beta)}(x) \\ -[(\alpha+\beta+2n)_3 x + (\alpha^2-\beta^2)(\alpha+\beta+2n+1)]P_n^{(\alpha,\beta)}(x) & \\ +2(\alpha+n)(\beta+n)(\alpha+\beta+2n+2)P_{n-1}^{(\alpha,\beta)}(x) \quad &= \quad 0\,, \end{aligned} \tag{D.74}$$

and the Rodrigues formula reads

$$P_n^{(\alpha,\beta)}(x) \quad = \quad \frac{(-1)^n}{n!2^n}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{\mathrm{d}^n}{\mathrm{d}x^n}[(1-x)^{\alpha+n}(1+x)^{\beta+n}]\,. \tag{D.75}$$

The derivative can be expressed as follows:

$$\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(x) \quad = \quad \frac{\alpha+\beta+n+1}{2}P_{n-1}^{(\alpha+1,\beta+1)}(x)\,, \tag{D.76}$$

or:

$$\begin{aligned} & (1-x^2)(\alpha+\beta+2n)\frac{\mathrm{d}}{\mathrm{d}x}P_n^{(\alpha,\beta)}(x) \\ = \quad & n[\alpha-\beta-(\alpha+\beta+2n)x]P_n^{(\alpha,\beta)}(x) + 2(\alpha+n)(\beta+n)P_{n-1}^{(\alpha,\beta)}(x)\,. \end{aligned} \tag{D.77}$$

D.6 Legendre functions

The Legendre functions are solutions of

$$(1-z^2)\frac{\mathrm{d}^2 w}{\mathrm{d}z^2} - 2z\frac{\mathrm{d}w}{\mathrm{d}z} + [\nu(\nu+1) - \mu^2(1-z^2)^{-1}]w \quad = \quad 0\,. \tag{D.78}$$

This equation has three regular-singular points at $z = -1$, $z = +1$, and $z = \infty$. Note that ν and μ may by any complex number, and that two cases must be distinguished: (i) z is real and between -1 and $+1$, and (ii) z is any other complex number, with the exclusion of the interval $(-\infty, +1]$. (The z plane is cut along the real axis from $-\infty$ to $+1$.) In the first case the fundamental system of solutions is denoted by $P^\mu_\nu(x)$ and $Q^\mu_\nu(x)$ (Legendre functions of the first kind), and in the second case they are denoted by $\mathcal{B}^\mu_\nu(z)$ and $\mathcal{D}^\mu_\nu(z)$ (Legendre functions of the second kind). The Legendre functions are special cases of the hypergeometric function ${}_2F_1(a, b; c; z)$:

$$\begin{aligned} & \Gamma(1-\mu)P^\mu_\nu(x) \\ = \quad & (1+x)^{\frac{1}{2}\mu}(1-x)^{-\frac{1}{2}\mu}\,{}_2F_1(-\nu, 1+\nu; 1-\mu; \tfrac{1}{2}-\tfrac{1}{2}x)\,, \end{aligned} \tag{D.79}$$

for $-1 < x < 1$. This expression is undefined when μ is a positive integer.

Since we are interested in the Legendre functions for integer values of μ and ν, other expressions are needed. Note that if ν is a nonnegative integer and μ is an integer satisfying $-\nu \le \mu \le \nu$, P^μ_ν is a polynomial of degree $\nu - |\mu|$ multiplied by an elementary function. More specifically, the following relation holds:

$$P^m_\nu(x) = (-1)^m(1-x^2)^{\frac{1}{2}m}\frac{\mathrm{d}^m}{\mathrm{d}x^m}P_\nu(x)\,, \tag{D.80}$$

$$P^{-m}_\nu(x) = (-1)^m(1-x^2)^{-\frac{1}{2}m}\int_1^x \mathrm{d}x_1 \cdots \int_1^{x_{m-1}} \mathrm{d}x_m\, P_\nu(x_m)\,, \tag{D.81}$$

where ν is any complex number, m is a positive integer, and P_ν is the Legendre function for $\mu = 0$, which for integer values of ν is just a Legendre polynomial.

For practical calculations, the following relations are sufficient:

$$P^0_0(x) = 1\,, \tag{D.82}$$

$$P^0_1(x) = x\,, \tag{D.83}$$

$$xP^\mu_\nu(x) - P^\mu_{\nu+1}(x) = (\nu+\mu)(1-x^2)^{\frac{1}{2}}P^{\mu-1}_\nu(x)\,, \tag{D.84}$$

$$(2\nu+1)xP^\mu_\nu(x) = (\nu-\mu+1)P^\mu_{\nu+1}(x) + (\nu+\mu)P^\mu_{\nu+1}(x)\,, \tag{D.85}$$

where it must be remembered that P^m_ℓ vanishes for $m > |\ell|$. Note that the same relations hold for Q^μ_ν. The first of the two recursion relations can be used to calculate P^ℓ_ℓ, for all nonnegative integer values of ℓ. The second recursion relation can then be used to calculate all other cases with $m \ge 0$. Negative values of m are not needed, since Eq. (C.11) can be used instead.

Appendix E

Formulas

This appendix contains a collection of formulas which I have found during my work on the three-body problem. Only a few of these formulas have been actually used in the various calculations. Of these some have become obsolete since alternative techniques were developed.

E.1 Three-body formulas

The geometry of the three-body problem as formulated in Chapter 6 provides a number of useful and elegant formulas. They are based on the definitions of the mass-weighted Jacobi coordinates and the polar coordinates. A number of interesting formulas are listed here. All formulas are valid for any permutation $\{ijk\}$ of $\{123\}$.

I will start with a number of formulas for the quantities μ_k^{ij} and mass ratios. Note that the masses are expressed as fractions of the total mass. (This is an unusual choice; the most natural choice for the unit mass would be the mass of the lightest particle.)

$$\mu_k^{ij} + \mu_i^{jk} + \mu_j^{ki} = \epsilon_{ijk}\pi\,, \tag{E.1}$$

$$-4\cos\mu_k^{ij}\cos\mu_i^{jk}\cos\mu_j^{ki} = 1 + \cos 2\mu_k^{ij} + \cos 2\mu_j^{ki} + \cos 2\mu_i^{jk}\,, \tag{E.2}$$

$$m_i = \frac{\cos\mu_k^{ij}\cos\mu_j^{ki}}{\sin\mu_k^{ij}\sin\mu_j^{ki}}\,, \tag{E.3}$$

$$m_j + m_k = \frac{\cos\mu_i^{jk}}{\sin\mu_k^{ij}\sin\mu_j^{ki}}\,, \tag{E.4}$$

$$\frac{m_i}{m_j + m_k} = \frac{\cos\mu_k^{ij}\cos\mu_j^{ki}}{\cos\mu_i^{jk}}\,, \tag{E.5}$$

$$\frac{m_j}{m_j+m_k} = \frac{\cos\mu_k^{ij}\sin\mu_j^{ki}}{\sin\mu_i^{jk}}\,, \tag{E.6}$$

$$\frac{m_i m_j}{m_i+m_j} = \frac{\cos\mu_k^{ij}\cos\mu_i^{jk}\cos\mu_j^{ki}}{\sin^2\mu_k^{ij}}\,, \tag{E.7}$$

$$\frac{m_i(m_j+m_k)}{m_i+m_j+m_k} = \frac{\cos\mu_k^{ij}\cos\mu_i^{jk}\cos\mu_j^{ki}}{\sin^2\mu_k^{ij}\sin^2\mu_j^{ki}}\,. \tag{E.8}$$

The following expression relates the polar angles:

$$\sin 2\mu_k^{ij}\cos 2\theta_k + \sin 2\mu_i^{jk}\cos 2\theta_i + \sin 2\mu_j^{ki}\cos 2\theta_j = 0\,. \tag{E.9}$$

For three particles with identical mass, the following (trivial) identities are obtained:

$$\mu_k^{ij} = \epsilon_{ijk}\tfrac{\pi}{3}\,, \tag{E.10}$$

$$\cos 2\theta_i + \cos 2\theta_j + \cos 2\theta_k = 0\,. \tag{E.11}$$

From Eq. (E.9) the following can be derived:

$$\theta_i^{\pm}(\theta_k) = \theta_j^{\mp}(\theta_k)\,, \tag{E.12}$$

In other words, the lower (upper) edge of the domain of valid angles Ω_{ik} corresponds to the upper (lower) edge of Ω_{jk}. The direction of curves of constant θ_j in Ω_{ik} can be determined from:

$$\frac{\partial\theta_k(\theta_i,\theta_j)}{\partial\theta_i} = -\frac{\sin 2\mu_i^{jk}}{\sin 2\mu_k^{ij}}\frac{\sin 2\theta_i}{\sin 2\theta_k(\theta_i,\theta_j)}\,. \tag{E.13}$$

$$\left.\frac{\partial\theta_k(\theta_i,\theta_j)}{\partial\theta_i}\right|_{\theta_i^{\pm}(\theta_j)} = -\frac{\sin 2\mu_i^{jk}}{\sin 2\mu_k^{ij}}\frac{\sin 2\theta_i^{\pm}(\theta_j)}{\sin 2\theta_k^{\mp}(\theta_j)}\,. \tag{E.14}$$

Finally: the distance of a particle to the center of mass is

$$r_i = \sqrt{\frac{m_{jk}}{2m_i m_{ijk}}}\,y_i = \frac{1}{\sqrt{m_{ijk}}}\sqrt{\frac{\cos\mu_i^{jk}}{2\cos\mu_k^{ij}\cos\mu_j^{ki}}}\,y_i\,, \tag{E.15}$$

Equations (E.9) and (E.15) can be used to find the following expression for $\langle r^2\rangle$ for a system of three identical particles:

$$\langle r^2\rangle = \tfrac{1}{6m}\langle\rho^2\rangle\,, \tag{E.16}$$

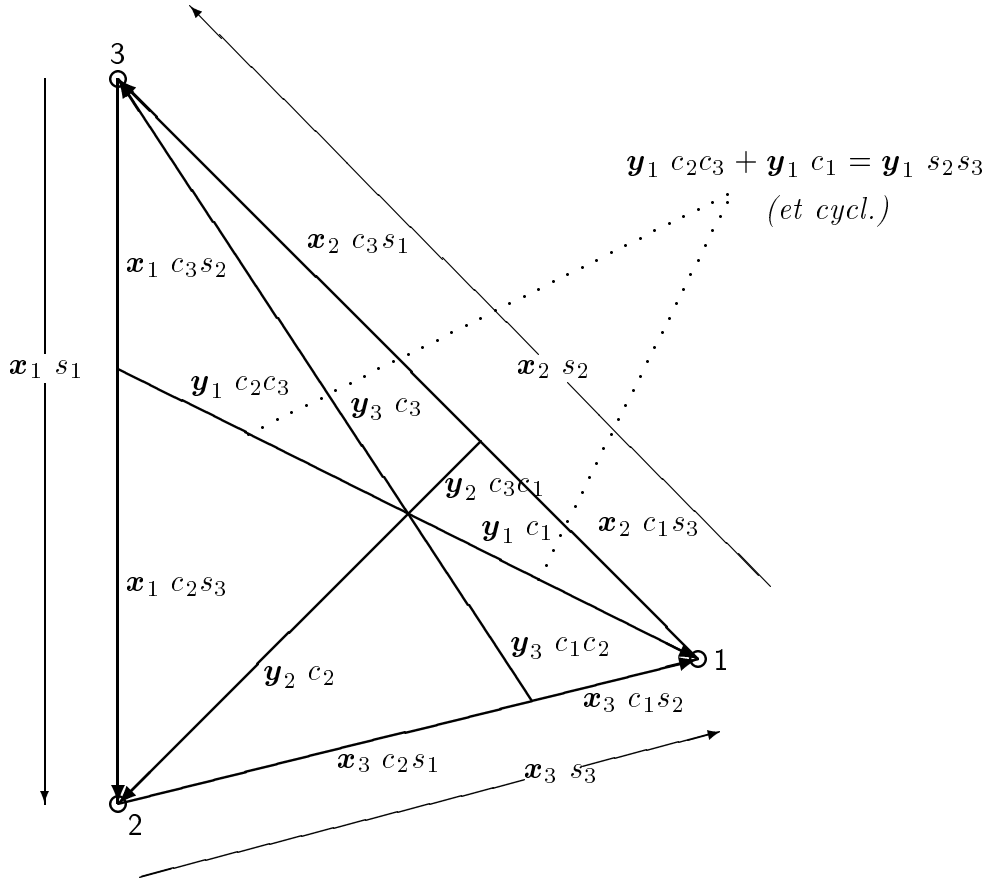


Figure E.1: The three-body triangle. See text for details.

where m is the particle mass expressed in the unit mass which was introduced in Chapter 4. (This unit mass is in the case of identical particles of course most conveniently chosen to be the particle mass, leading to $m = 1$.) A useful overview of the various lengths in the three-body system is given by Fig. E.1. The actual triangle can be retrieved by scaling this picture with a factor $(2Mc_1c_2c_3)^{-1/2}$. Note that in this figure, the notation $c_1 = \cos\mu_1^{23}$, $s_1 = \sin\mu_1^{23}$, *et cycl.* was used.

E.2 Angular momenta

Matrix elements of operators which have some angular dependence are very common. Examples can be found in the nuclear interaction, but also in the theory of (electromagnetic) reactions. For the two-body case these matrix elements can usually be calculated after some (often tedious) algebra. For the three-body case the situation is much more difficult, since the angular-momentum structure of such

a system is much more difficult than that of a two-body system. In this section I will show one nontrivial example of such a calculation, that of the quadrupole moment, Q. The quadrupole moment is defined as follows:

$$Q \quad = \quad \sqrt{\tfrac{16\pi}{5}} \sum_i Z_i \langle r_i^2 Y_{20}(\hat{\boldsymbol{r}}_i) \rangle \,, \tag{E.17}$$

where $\boldsymbol{r}_i$ is the distance of particle i to the center of mass and Z_i is the charge of particle i. It is related to the low-momentum limit of the quadrupole form factor. The multipole form factors are defined by Donnelly and Walecka [1975]:

$$F_{Cl}(q) \quad = \quad \frac{\sqrt{4\pi}}{Z} \sum_i \frac{Z_i}{\langle J\, J\, l\, 0 | J\, J \rangle} \langle \Psi \,|\, Y_{l0}(\hat{\boldsymbol{r}}_i) j_l(q r_i) \,|\, \Psi \rangle \,, \tag{E.18}$$

where Z is the total charge of the system, J is the total angular momentum, and where the wave function Ψ must have a specific total magnetic quantum number: $M = J$. The low-energy limit of the quadrupole moment, F_{C2}, is

$$\begin{aligned} &\frac{\sqrt{4\pi}}{Z} \sum_i \frac{Z_i}{\langle 1\, 1\, 2\, 0 | 1\, 1 \rangle} \langle \Psi \,|\, Y_{20}(\hat{\boldsymbol{r}}_i) j_2(q r_i) \,|\, \Psi \rangle \quad \longrightarrow \\ &\frac{\sqrt{4\pi}}{Z} \sum_i \frac{Z_i \sqrt{10}}{(2 \cdot 2 + 1)!!} \langle \Psi \,|\, Y_{20}(\hat{\boldsymbol{r}}_i) (qr)^2 \,|\, \Psi \rangle \quad = \quad \frac{1}{3Z\sqrt{2}} Q q^2 \,, \end{aligned} \tag{E.19}$$

which follows immediately from Eq. (D.53).

The key ingredient in all these expressions is the matrix element of $r_i^2 Y_{lm}(\hat{\boldsymbol{r}}_i)$. I will now calculate this matrix element. The matrix element can be factorized in a radial and an angular part. I will only look at the angular part here. In that case it suffices to calculate matrix elements $\langle \alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}_i \,|\, \beta \rangle$, where α and β are angular-momentum eigenstates. I will use a bipolar basis in L–S coupling:

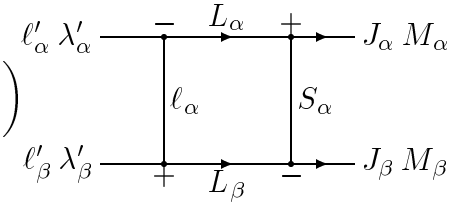
$$\begin{aligned} &\langle ((\ell_\alpha\, \ell'_\alpha) L_\alpha\, S_\alpha) J_\alpha\, M_\alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}) \,|\, ((\ell_\beta\, \ell'_\beta) L_\beta\, S_\beta) J_\beta\, M_\beta \rangle \\ = &\sum_{\substack{\lambda_\alpha \lambda'_\alpha \Lambda_\alpha \Sigma_\alpha \\ \lambda_\beta \lambda'_\beta \Lambda_\beta \Sigma_\beta}} \langle \ell_\alpha\, \lambda_\alpha\, \ell'_\alpha\, \lambda'_\alpha | L_\alpha\, \Lambda_\alpha \rangle \langle \ell_\beta\, \lambda_\beta\, \ell'_\beta\, \lambda'_\beta | L_\beta\, \Lambda_\beta \rangle \langle L_\alpha\, \Lambda_\alpha\, S_\alpha\, \Sigma_\alpha | J_\alpha\, M_\alpha \rangle \\ &\times \langle L_\beta\, \Lambda_\beta\, S_\beta\, \Sigma_\beta | J_\beta\, M_\beta \rangle \langle \ell_\alpha\, \lambda_\alpha\, \ell'_\alpha\, \lambda'_\alpha\, S_\alpha\, \Sigma_\alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}) \,|\, \ell_\beta\, \lambda_\beta\, \ell'_\beta\, \lambda'_\beta\, S_\beta\, \Sigma_\beta \rangle \\ = &\sum_{\substack{\lambda_\alpha \lambda'_\alpha \Lambda_\alpha \Sigma \\ \lambda'_\beta \Lambda_\beta}} \langle \ell_\alpha\, \lambda_\alpha\, \ell'_\alpha\, \lambda'_\alpha | L_\alpha\, \Lambda_\alpha \rangle \langle \ell_\alpha\, \lambda_\alpha\, \ell'_\beta\, \lambda'_\beta | L_\beta\, \Lambda_\beta \rangle \langle L_\alpha\, \Lambda_\alpha\, S_\alpha\, \Sigma | J_\alpha\, M_\alpha \rangle \\ &\times \langle L_\beta\, \Lambda_\beta\, S_\alpha\, \Sigma | J_\beta\, M_\beta \rangle \delta_{\ell_\alpha \ell_\beta} \delta_{S_\alpha S_\beta} \langle \ell'_\alpha\, \lambda'_\alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}) \,|\, \ell'_\beta\, \lambda'_\beta \rangle \,. \end{aligned} \tag{E.20}$$

The matrix element $\langle \ell'_\alpha\, \lambda'_\alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}) \,|\, \ell'_\beta\, \lambda'_\beta \rangle$ can be easily evaluated:

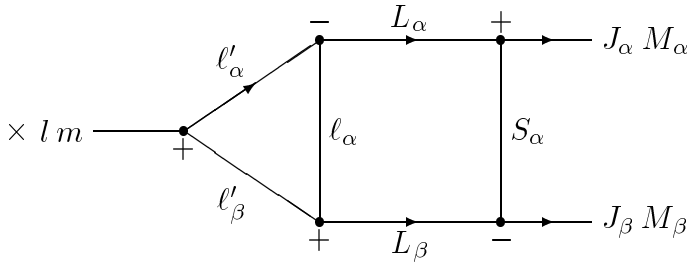
$$\langle \ell'_\alpha\, \lambda'_\alpha \,|\, Y_{lm}(\hat{\boldsymbol{y}}) \,|\, \ell'_\beta\, \lambda'_\beta \rangle \quad = \quad (-1)^{\lambda'_\alpha} \frac{\hat{\ell}'_\alpha \hat{l} \hat{\ell}'_\beta}{\sqrt{4\pi}} \begin{pmatrix} \ell'_\alpha & l & \ell'_\beta \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell'_\alpha & l & \ell'_\beta \\ -\lambda'_\alpha & m & \lambda'_\beta \end{pmatrix} . \tag{E.21}$$

The next step is to replace the sums over products of Clebsch–Gordan coefficients by a diagram following the rules of Baz and Castel [1972], and then applying simplification techniques, by cutting the diagram into smaller pieces:

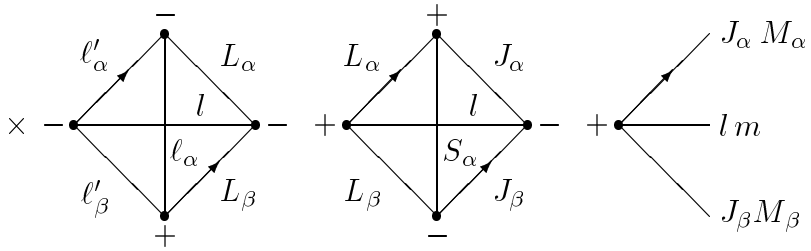
$$\begin{aligned}
&\langle((\ell_\alpha\,\ell'_\alpha)L_\alpha\,S_\alpha)J_\alpha\,M_\alpha\,|\,Y_{lm}(\hat{\boldsymbol{y}})\,|\,((\ell_\beta\,\ell'_\beta)L_\beta\,S_\beta)J_\beta\,M_\beta\rangle \\
&= \delta_{\ell_\alpha\ell_\beta}\delta_{S_\alpha S_\beta}\hat{L_\alpha}\hat{L_\beta}\hat{J_\alpha}\hat{J_\beta}(-1)^{2\ell_\alpha-\ell'_\alpha-\ell'_\beta-2S_\alpha-J_\alpha-J_\beta}\frac{\hat{\ell}'_\alpha\hat{l}\hat{\ell}'_\beta}{\sqrt{4\pi}}\begin{pmatrix}\ell'_\alpha & l & \ell'_\beta\\ 0 & 0 & 0\end{pmatrix} \\
&\quad\times\sum_{\lambda'_\alpha\lambda'_\beta}(-1)^{-\lambda'_\alpha}\begin{pmatrix}\ell'_\alpha & l & \ell'_\beta\\ -\lambda'_\alpha & m & \lambda'_\beta\end{pmatrix}
\end{aligned}$$



$$\begin{aligned}
&= \delta_{\ell_\alpha\ell_\beta}\delta_{S_\alpha S_\beta}(-1)^{2\ell_\alpha-\ell'_\beta-2S_\alpha-J_\alpha-J_\beta}\hat{L_\alpha}\hat{L_\beta}\hat{J_\alpha}\hat{J_\beta}\frac{\hat{\ell}'_\alpha\hat{l}\hat{\ell}'_\beta}{\sqrt{4\pi}}\begin{pmatrix}\ell'_\alpha & l & \ell'_\beta\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$



$$\begin{aligned}
&= \delta_{\ell_\alpha\ell_\beta}\delta_{S_\alpha S_\beta}(-1)^{2\ell_\alpha-\ell'_\beta-2S_\alpha-J_\alpha-J_\beta}\hat{L_\alpha}\hat{L_\beta}\hat{J_\alpha}\hat{J_\beta}\frac{\hat{\ell}'_\alpha\hat{l}\hat{\ell}'_\beta}{\sqrt{4\pi}}\begin{pmatrix}\ell'_\alpha & l & \ell'_\beta\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}$$



$$\begin{aligned}
&= \delta_{\ell_\alpha\ell_\beta}\delta_{S_\alpha S_\beta}(-1)^{J_\alpha-M_\alpha+J_\beta+S_\alpha+\ell_\alpha+l}\hat{L_\alpha}\hat{L_\beta}\hat{J_\alpha}\hat{J_\beta}\frac{\hat{\ell}'_\alpha\hat{l}\hat{\ell}'_\beta}{\sqrt{4\pi}}\begin{pmatrix}\ell'_\alpha & l & \ell'_\beta\\ 0 & 0 & 0\end{pmatrix} \\
&\quad\times\begin{Bmatrix}L_\beta & l & L_\alpha\\ \ell'_\alpha & \ell_\alpha & \ell'_\beta\end{Bmatrix}\begin{Bmatrix}J_\beta & l & J_\alpha\\ L_\alpha & S_\alpha & L_\beta\end{Bmatrix}\begin{pmatrix}J_\alpha & l & J_\beta\\ -M_\alpha & m & M_\beta\end{pmatrix}. \qquad \text{(E.22)}
\end{aligned}$$

In the final step, I replaced the final diagrams by the well-known three- and six-j symbols, again using rules from Baz and Castel [1972].

Clearly, this is an awkward procedure to follow. For more difficult operators (*e.g.*, magnetic moments), this procedure becomes even more complicated. Therefore, I have followed the "brute force" approach of simply summing up all the products of Clebsch–Gordan coefficients, without trying to reduce expressions to products of known recoupling coefficients. The only part that has to be done by hand is then the evaluation of the one-body matrix elements (cf. Eq. (E.21)).

Appendix F

Software design

The three- and four-body problems lead to complicated mathematical equations. The implementation of the corresponding numerical equations in a computer code is a nontrivial matter. This appendix addresses some of the problems that I have encountered, and their solutions. First, some general remarks on structured programming will be given, after which the global structure which was identified and implemented is described. Next, the problem of administrating permutations (*i.e.*, coordinate transformations between different Jacobi coordinate systems) is addressed in some detail. Finally, matters of portability and efficiency are discussed, and an outlook is given.

F.1 Structure

Computer programs exceeding a certain size tend to become unmanageable, due to many interconnections between the different parts. This situation can be improved by structuring the computer program in a collection of well-defined and semi-isolated parts, each dealing with a small part of the full problem. Structuring exists in both the procedures (subroutines) and the data on which the procedures operate (data structures). Recently, these two have become more and more intertwined, and the structuring into concepts or objects (known as object-oriented programming) has become the focus of attention. With the growth of computer programs, programming languages have evolved. Originally, FORTRAN was the language that was considered most suitable for doing numerical calculations. Later on, structured programming languages such as C appeared. Presently, object-oriented programming languages such as C++ are being used more and more. However, even today, FORTRAN is used extensively in scientific calculations. The reason for using this outdated language is sometimes its supposed efficiency and standardization, but more often, tradition: both standardization and efficiency of C has come to a level at least equal to that of FORTRAN, but there is still a large amount of (old) FORTRAN software, that is being used regularly, and many numerical libraries are written in FORTRAN.

Complex numerical problems lead to large computer codes. Clearly, structured programming is essential for the successful and efficient solution of these problems. However, structured programming becomes useful already on a much smaller scale. I will illustrate this by looking implementation of the spline method for the two-, three-, and four-body problem.

F.2 Discretization

The numerical few-body problem has a number of different aspects. First, there is the principal problem of representing the equations in a discretized form. As we have seen throughout this thesis, there is a simple systematic manner for representing the different operators by spline matrices. The spline matrices found in the two-, three-, and four-body problems have much in common. The spline matrices can be constructed in a systematic manner, once the spline basis is known. A spline basis consists of a grid, augmented by the basis functions. It is therefore useful, to design the computer code in this hierarchical fashion.

In the different computer codes (two-, three-, and four-body codes are separate programs), there is a large common section, dealing with the definition and construction of grids, spline bases, and spline matrices. Many standard operators are identical for these four problems, and can also be shared. An important example is the potential. Since I have allowed very general interactions, this is quite a complex piece of computer code, which can, however be shared between the programs. (Also, the general potential routine itself is thoroughly structured and organized to allow for the most general possible interaction, and still keep the computer code manageable: structuring occurs at all levels.) The differences between the programs occur at the higher level of combining these matrices into the full matrix problem.

F.3 Angular momentum

The two-, three-, and four-body problems involve increasingly difficult angular-momentum analysis. However, here also, a common factor can be recognized. All coupling schemes for the general N-body problem can be seen as a tree structure, very similar to the trees associated with partition chains or Jacobi coordinates. Therefore, it is possible design a data structure which describes an angular-momentum coupling scheme in a systematic fashion, and also structures to describe angular-momentum states. A general set of procedures can be defined to generate coupling structures, angular momentum states, and indeed, full angular-momentum bases.

Once a systematic description of angular-momentum states is given, it is possible to calculate matrix elements of operators in a systematic fashion, as well. This requires only a knowledge of the matrix elements at the lowest level required

(*e.g.*, the two-body level for the two-body interaction, or the one-body level for one-body operators). The remaining part of the matrix element can simply be expressed as sums of products Clebsch–Gordan coefficients. These products can be determined easily from the coupling structure, and the quantum numbers of the particular states.

Of course, this approach may lead to very inefficient code, since multiple sums must be evaluated. Therefore, care must be taken to keep the numerical effort at a reasonable level. I have implemented several optimizations and tricks to achieve this. For example, I have written a subroutine that calculates a general recoupling coefficient (*i.e.*, from any coupling scheme to any other, for any number of particles), exploiting the coupling order, disconnected trees, symmetries, as much as possible. It turns out to be sufficiently efficient for all the calculations that I have done so far.

F.4 Permutation

This section discusses the administration of partition chains and coordinate transformations, or permutations. It contains an attempt at a general scheme for dealing with the indistinguishability of particles in the N-body problem. The presence of indistinguishable particles has consequences for the number of independent partition chains, and hence Yakubovsky amplitudes. Another effect is, that some of the coordinate transformations coincide with permutation operators. The following subsections address the administration of independent amplitudes and the coordinate transformations.

Administration

First, the interdependence of the partition chains must be determined. Suppose that there are N_f partition channels if all particles are distinguishable. If some of the particles are identical, this number reduces to a new number N'_f, because the partitions chains can be grouped into sets of *dependent partitions chains*, or P-sets. Partition chains are labeled by i (or by i' for P-sets), where i ranges from 1 to N_p. The number of elements in P-set i' is denoted by $N_p^{i'}$.

I will assume that with every partition chain i an angular-momentum basis containing N_c^i basis functions is associated. I will call the combination of a partition chain and an angular-momentum basis function a *channel*. The channels are labeled by α, and are numbered consecutively. (The channels for partition chain 1 are numbered 1 through N_c^1, the channels for partition chain 2 are N_c^1+1 through $N_c^1+N_c^2$, and so on.) A similar counting is done for the combination of P-sets and angular-momentum basis functions. The channels belonging to different P-sets can be distinguished through a new "quantum number" $i(\alpha)$, describing to which P-set a particular channel belongs. It is sometimes useful to denote channels by two labels, such as $|i\alpha\rangle$, or $|i'\alpha'\rangle$.

Permutation

I will now show that it is possible to define Faddeev (or Yakubovsky) amplitudes $\phi_{i'\alpha'}$ corresponding to the P-set i', such that the Faddeev amplitudes $\phi_{i\alpha}$ (for all partitions i that are in set i') are related to $\phi_{i'\alpha'}$ in a very simple manner:

$$\phi_{i\alpha'} = \sum_{i'} \sigma_{ii'\alpha'}\phi_{i'\alpha'} , \tag{F.1}$$

where σ is the following object:

$$\sigma_{ii'\alpha'} = p(\alpha', i \leftrightarrow i^-)\delta_{i\in i'} . \tag{F.2}$$

Here $p(\alpha', i \leftrightarrow j)$ was written to denote the parity of $|i\alpha\rangle$ under the permutation that changes partition i into j (or its inverse). Note that this has only meaning if i and j are members of the same P-set. The symbol i^- denotes the lowest number which represents a partition in the set i'. Finally, $\delta_{i\in i'}$ is equal to one if $i \in i'$, and zero otherwise. The above description may be used to construct the complete wave function, or to calculate the effect of permutation operators.

The effect of the permutation operators can be constructed as follows:

$$(P\boldsymbol{\phi})_{i'\alpha'} = \sum_{jj'\beta'} P_{i'j\alpha'\beta'}\sigma_{jj'\beta'}\phi_{j'\beta'} , \tag{F.3}$$

where $P_{i'j\alpha'\beta'}$ is a matrix representing a coordinate transformation from the natural coordinate system corresponding to partition chain i' to the coordinate system corresponding to partition chain j. I will now show that the permutation operators can be reduced to operate on P-sets only. The decomposition is as follows:

$$P_{i'j\alpha'\beta'} = \sum_{j'} P_{i^-j^+\alpha'\beta'}\pi_{j'j\beta'}\bar{\delta}_{i^-j^+} , \tag{F.4}$$

where π is an object which is very similar to σ:

$$\pi_{j'j\beta'} = p(\beta', j \leftrightarrow j^+)\delta_{j\in j'} . \tag{F.5}$$

Note that it is necessary to use j^+ in order to be able to sensibly define permutations *inside* an P-set (*i.e.*, the diagonal elements $P_{i'i'\alpha'\beta'}$). The factor $\bar{\delta}_{i^-j^+}$ makes sure that we only consider permutations which differ from the unit operator, and the factor $p(\beta', j \leftrightarrow j^+)$ is present to give the correct sign if j is different from j^+.

Now the construction of the total permutation operator can be completed:

$$\begin{aligned}(P\boldsymbol{\phi})_{i'\alpha'} &= \sum_{k'jj'\beta'} \bar{\delta}_{i^-k^+}P_{i^-k^+\alpha'\beta'}p(\beta', j \leftrightarrow k^+)\delta_{j\in k'}p(\beta', j \leftrightarrow j^-)\delta_{j\in j'}\phi_{j'\beta'} \\ &= \sum_{j'\beta'} \bar{\delta}_{i^-j^+}N_p^{j'}P_{i^-j^+\alpha'\beta'}p(\beta', j^- \leftrightarrow j^+)\phi_{j'\beta'} .\end{aligned} \tag{F.6}$$

Note that $P_{i^-j^+\alpha'\beta'}$ may be separated into orbital, spin, and isospin parts, as described for the three-body problem in Eq. (5.19).

F.5 Flexibility, efficiency, and portability

It is convenient to have a single program that can deal with all possible three-body problems (two- and four-body problems may share a substantial part of the code, but can be considered too different from the three-body problem to be treated within the same program), since that reduces the maintenance effort considerably. Since it is very inconvenient to have to change parameters in the program determining the grid size and the number of channels, the size of temporary storage, and so on, the program should be designed such that no assumptions are made on the grid size and number of channels. This implies that the storage requirements are unknown at compile time, and therefore, that dynamic storage allocation must be used. Since FORTRAN does not support dynamic storage allocation, a different programming language must be chosen.

I have used the language C to write my programs. This language supports dynamic storage allocation and allows easy structuring of both procedures and data. There are other languages which have the same facilities, but none are in as widespread use as C. Since C has been designed to write the operating system UNIX, it is a good compromise between structure and efficiency. Also, it is very well suited for large computer programs. Its widespread use has led to an excellent standardization (ANSI C), significantly simplifying writing portable programs.

By exploiting the possibilities of C, it is possible to formulate a program for solving the few-body problem in a systematic, and well-maintainable manner. Also, through the use of dynamic memory, the memory requirements can be kept to the exact minimum that is required for a particular problem. Letting the program performing different tasks in one run is also a simple matter. The program was designed such that it determines all the necessary sizes and limits. Its input consists of a few simple text files, which the user must supply.

To optimize the speed of solving the numerical problem, it is necessary to have some knowledge of the computer hardware. For example, there is large difference between scalar and vector machines: the former are more efficient in long loops, whereas the latter are most efficient in short loops, which can be reduced to vector instructions. A substantial amount of system dependence can be removed by using standard libraries to perform the most expensive operations. I have used LINPACK and EISPACK for the linear algebra and eigenvalue problems. The rest of the code was written in a form that allows automatic vectorization, but has sufficiently long loops so that the performance is good on scalar machines perform as well.

F.6 Outlook

In principle, it is possible to summarize the two-, three-, and four-body codes into one program. This has the advantage that only a single program has to be maintained. The disadvantage is that the code becomes substantially more complicated. On the other hand, the two-, three-, and four-body programs contain a

lot of common code, and the code that is specific for any of them can be generalized into a new common general scheme. This would require a way of automatizing generating partition chains and the coordinate transformations between them. This is a feasible, but complicated task.

For such a project, one may wonder if C is a sufficiently structured language. Already in the three-body code that I have written now, many aspects of object-oriented programming can be found. Therefore, the step to C++ seems a logical one. Unfortunately, this language is not yet fully developed. Standardization is not yet complete, and libraries must still be developed. Also, reliable and efficient compilers are hard to find.