Stäckel Separation of the Helmholtz Equation

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last update: Feb 10, 2014
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1. Introduction and Summary

Nothing "new" is presented in this document. The Stäckel separation theory is treated in Morse & Feshbach (see References) and elsewhere. It is probably fair to say, however, that the treatments are far and few between, and the subject is not always presented in a systematic fashion. It is the purpose of this monograph to provide a simple, complete and systematic presentation without too much technical baggage. It is assumed only that the reader has some rudimentary knowledge of differential equations.

References to the original papers of Stäckel (1891,1893,1897), Robertson (1927) and Eisenhart (1934) and to a later work of Moon & Spencer (1952) are given at the end.

The subject at hand is separation of the Helmholtz equation (and its special case the Laplace equation) in various 3D curvilinear coordinate systems whose coordinates we shall call ξ_1,ξ_2,ξ_3. The term "separation" means that one starts with the 3D Helmholtz equation $(\nabla^2 + K_1{}^2)\ \psi = 0$, which is of course a *partial* differential equation (PDE), and tries to find solutions of the form

$$\psi(\xi_1,\xi_2,\xi_3) = X_1(\xi_1)X_2(\xi_2)X_3(\xi_3)/\ R(\xi_1,\xi_2,\xi_3)\ , \tag{1.1}$$

where an *ordinary* differential equation (ODE_n) can be produced for each of the functions $X_n(\xi_n)$. Thus, one can search for solutions "separately" for each X_n. If the X_n are any solutions of their respective ODE_n, then the ψ shown above is a solution of the Helmholtz equation.

First, this is useful way generically to *solve* the Helmholtz problem, and second, because boundary conditions are often specified separately for the three coordinates, this separation (usually) turns at least one of the ODE_n into its own little 1D boundary value problem. These ODE's always contain self-adjoint differential operators and are therefore (usually) amenable to normal 1D "Sturm-Liouville theory", a subject reviewed in Appendix A.

We say "usually" because in some cases the entanglement of the separation constants forces one to consider 2D or even 3D Sturm-Liouville situations, where the problem cannot be factored into 1D problems each of which causes quantization of its isolated separation constant. Hopefully this statement will become clearer below. A classic 3D case occurs in ellipsoidal coordinates as discussed in Section 12, while a 2D case occurs in conical coordinates. Both these systems involve the Lamé functions.

If the separation can be done as outlined above for a certain orthogonal curvilinear coordinate system where the function R is not a constant, then one says that the system is **R-separable**. If this can be done with R=constant, it is **simple-separable** and one can then take R = 1 without loss of generality.

It turns out that only the 11 "classical" 3D Euclidean orthogonal coordinate systems are simple separable for the Helmholtz equation (and therefore also for the Laplace equation). These systems are discussed in the first chapter (called Section I) of Moon & Spencer (1961). This separability is why they are the classical systems.

There are no coordinate systems in which the Helmholtz equation ($K_1{}^2 \neq 0$) is R-separable. Thus, apart from the 11 classical systems in which it is simple-separable, the Helmholtz equation is *non*-separable. For example, in toroidal coordinates (see graphic below) the Helmholtz equation is non-separable. We shall use toroidal coordinates as an ongoing example in the work below, and the reader should understand that this system is separable only for the Laplace equation (for which it is in fact R-separable).

When we speak in this document of the Helmholtz equation, we always mean the *scalar* Helmholtz equation. Moon and Spencer devote a whole Chapter (their Section V) to the *vector* Helmholtz equation. They refer to the vector Laplacian operator as ✡ to avoid confusion with the scalar ∇^2 operator. Beyond

Cartesian coordinates for which the components of the vector Helmholtz equation are each scalar Helmholtz equations, separability is obtained only for special forms of the vector function **F** in ✡ **F**.

Here then is a summary of the classification of the separability of 3D coordinate systems:

R-separable for Laplace *only* $\psi = X_1X_2X_3/R$ ($R \neq$ constant) M&S list the following 10 "rotational" systems in this category: • tangent-sphere • cardiod • bispherical • toroidal • inverse prolate spheroidal • inverse oblate spheroidal • bi-cyclide • flat-ring cyclide • disk cyclide • cap cyclide • 6-sphere (inverse Cartesian, not a rotational system) (no "cylindrical" systems in this category) Problem B	Simple-separable for (scalar) Helmholtz *and* Laplace $\psi = X_1X_2X_3$ (R = constant =1 without loss of generality) (the 11 classical systems) • Cartesian • spherical • circular-cylinder • elliptic-cylinder • parabolic-cylinder • parabolic • paraboloidal • ellipsoidal • prolate spheroidal • oblate spheroidal • conical Problem A
Vector Helmholtz • Cartesian (simple-separable) • some other systems for special cases only (see M&S Section V)	R-separable for Helmholtz ψ = no exist ($R \neq$ constant) (no systems known in this category) Problem C

Classification of Separable Coordinate Systems

The red references to Problems A,B,C will be explained in Section 4 below.

The Helmholtz equation is extremely significant because it arises very naturally in problems involving the heat conduction (diffusion) equation and the wave equation, where the time derivative term in the PDE is replaced by a constant parameter by applying a Laplace or Fourier time transform to the PDE. A huge swath of mathematical physics is dominated by these two PDE equation types. One always needs to solve the Helmholtz equation that results, and that then involves the notion of "separation". Section 11 provides as an example the Schrodinger Equation PDE of quantum mechanics, which is the heat conduction equation with scaled imaginary time.

Methods of generating equivalent Stackel matrices are given in Section 6, and Section 13 generalizes the whole theory to N dimensions.

A brief summary of the document is in order.

Section 2 sets up our "systematic" notation and conventions, and discusses the notion of a functional-form equation which differs in an operational sense from a normal equation.

Section 3 starts with the Helmholtz equation and grinds away on it, making one functional-form assumption (3.5) along the way. We define a support function Q, compute it for toroidal coordinates, and then digress to discuss the notion of separation constants as they appear in Cartesian coordinates.

Section 4 assumes a most-general self-adjoint form for the desired separated L_n which defines ODE_n and then inserts this form into the ground-down Helmholtz equation, thus grinding it down even more to equation (4.4). Finally one is in a position to introduce the Stäckel Matrix Φ and with it one can formulate two potentially solvable problems, called Problem A and Problem B, and one insolvable Problem C. Problem A (simple-separation) is seen to be a special case of Problem B (R-separation). The problem is to "find the Stäckel matrix Φ" and various supporting functions, and in so doing to "solve" Problem B, and thus also Problem A. Here "solve" means to achieve separation and thus to have at hand all the ODE_n which can then be solved subject to their boundary conditions. Basically Problems A and B are treated at the same time, something not done in the referenced books.

Section 5 takes Problem B and, using elementary linear algebra, recasts it into a new form which appears as certain conditions on the matrix Φ. The Robertson Condition appears here.

Section 6 digresses momentarily to derive a set of "equivalence rules" allowing one to obtain new valid Stäckel matrices from an existing valid Stäckel matrix. This matrix is thus not unique. We have not seen these simple rules stated anywhere, but they are doubtless out there somewhere.

Section 7 discusses the solution of Problem B as recast at the end of Section 5. Section 7 (a) specifies a set of Conditions which must be met for a solution to exist, and Section 7 (b) gives a sequence of Steps one can follow to find the solution. These Steps are then applied to two examples. The first is a Problem B problem: R-separation of toroidal coordinates. The second is a Problem A problem: simple-separation of circular cylindrical coordinates. The examples are just exercises in turning a crank. In each case the solution functions are stated, these being the toroidal and cylindrical harmonics.

Section 8 attempts to specialize the solution method to a class of *cylindrical* systems in which the non-trivial scale factors h_1 and h_2 are not multiples of each other. Such systems are uncommon with the exception of the circular cylindrical system considered in Section 7.

Section 9 first considers cylindrical systems for which $h_2 = \alpha h_1$, and then sets $\alpha = 1$ as a further special case. Most practical cylindrical systems have $h_1 = h_2$ since they come from conformal maps of the Cartesian system. The Stäckel matrix is computed for three cylindrical systems of this type and the 21 such systems considered by Moon and Spencer are mentioned.

Section 10 specializes the Section 7 Conditions and Steps to *rotational* systems, and again toroidal coordinates are considered as an example. The 11 such systems listed in Moon and Spencer are mentioned.

Section 11 considers how separation is affected when some function is rudely added to the constant in the Helmholtz equation. If this function has a certain simple form, the resulting equation can still be separated. A prototype of this situation is the Schrodinger Equation of quantum mechanics where that added function is the potential field imposed on a quantum particle. As an example we mention the notion of a central potential in spherical coordinates and take a passing glance at the solution of the hydrogen atom.

Section 12, as a solid exercise of our systematic machinery, carries out the separation of the Helmholtz equation in ellipsoidal coordinates, the most complicated of the classical systems. Two very different-looking Stäckel matrices are obtained, both of which appear in the literature, and it is shown they are equivalent by the rules of Section 6. Our notation matches Morse & Feshbach and a sign error in that book is noted.

Section 13 generalizes the Stäckel formalism from 3 to N dimensions, which is quite easy to do, though carrying out the computational Steps is more complicated for $N > 3$.

Section 14 examines the Stäckel theory for $N = 2$ dimensions, writes some general results, and then treats polar and elliptical coordinates as examples for $h_1 \neq h_2$ and $h_1 = h_2$. A certain polar coordinates Helmholtz Green's Function problem is considered to illustrate how the Sturm-Liouville analysis can be carried out in either coordinate.

Appendix A gives a concise review of the 1D Sturm-Liouville Problem and the transform associated with such a problem. The Kantorovich-Lebedev transform is presented as an example.

A short list of **References** is then provided.

2. Notation and Cast of Players

The entire analysis is a study of **functional forms** and this makes it a bit slippery. By functional form is meant the way a function of multiple variables depends on those variables in terms of possible factorization of the form. For example, some u(x,y,z) might be expressible as v(x)w(y,z) and this would then be the functional form of u. Another sense of functional form is simply what variables a function is a function of. One might write v(x) simply as v if an expressions get complicated, but one must remember than that its functional form is v(x).

The symbols ξ_1, ξ_2, ξ_3 (these are "xi", pronounced "zeye", different from ζ = zeta and χ = chi) are often used for ellipsoidal coordinates since those coordinates are so closely related to each other. Below ξ_1, ξ_2, ξ_3 shall represent an arbitrary triplet of orthogonal curvilinear coordinates. The notation ∂_n is used for a partial derivative,

$$\frac{\partial f}{\partial \xi_n} = \partial f/\partial \xi_n = \partial_n f \qquad\qquad n = 1,2,3$$

along with the following other symbols,

$\Sigma_n \equiv \Sigma_{n=1}^{3}$ LHS = left hand side of some equation RHS = right hand side
PDE = partial differential equation ODE = ordinary diff eq

There will be many function symbols used below, and each symbol has an implied functional form. At first one needs to show the forms in full detail, but eventually one learns to work without doing this. Here is a triplet of function symbols each having four different notations,

$$g_1(\xi_2, \xi_3) = g_1(23) = g_1(\neq 1) = g_1$$
$$g_2(\xi_3, \xi_1) = g_2(31) = g_2(\neq 2) = g_2$$
$$g_3(\xi_1, \xi_2) = g_3(12) = g_3(\neq 3) = g_3 \quad .$$

Each row is the forward cyclic permutation of the previous row. Only the notations of the last two columns are amenable to the generic notation

$$g_n(\neq n) = g_n \qquad n = 1,2,3 \quad .$$

Notice these facts:

$$\partial_1 g_1 = 0 \qquad\qquad \partial_1(g_1 F) = g_1(\partial_1 F)$$
$$\partial_n g_n = 0 \qquad\qquad \partial_n(g_n F) = g_n(\partial_n F) \quad .$$

These follow, for example, since g_1 is a function only of ξ_2 and ξ_3. "Facts" like these will be crucial in the analysis below. The functions g_n are "helper functions" which have no particular significance.

Only one other function symbol set will have this same functional form

$$M_n(\neq n) = M_n \qquad\qquad n = 1,2,3 \quad .$$

The letter M stands for "minor" as in the minor of a 3x3 matrix, but in fact M is really a cofactor. This confusion seems to go back to Morse and Feshbach who use the word "minor" to mean what is now usually called a "cofactor". In current terminology $\text{cofactor}_{pq} = (-1)^{p+q}\ \text{minor}_{pq}$ where p and q label the rows and columns of a matrix, as in A_{pq}. To be a little more specific, the M_n will be the cofactors of the elements of the first column of a certain 3x3 matrix called the Stäckel matrix Φ discussed soon below.

Certain function symbols imply a very simple functional form as follows

$f_n(\xi_n) = f_n(n) = f_n \qquad n = 1,2,3$

$X_n(\xi_n) = X_n(n) = X_n \qquad n = 1,2,3$.

The X_n are the factors of the ψ solution shown in the introduction. The f_n functions are just more helper functions that will be used in the analysis and which appear in the separated ODE equations.

There are several function symbols that are assumed to have in general no factored functional form, and here they are :

$R(\xi_1,\xi_2,\xi_3) = R(123) = R$ // the function appearing in (1) above ("modulation factor")

$Q(\xi_1,\xi_2,\xi_3) = Q(123) = Q$ // a helper function (called u by Morse & Feshbach)

$S(\xi_1,\xi_2,\xi_3) = S(123) = S$ // the determinant of Φ (coming soon)

$h_n(\xi_1,\xi_2,\xi_3) = h_n(123) = h_n$ // the curvilinear system scale factors $h_n^2 = g_{nn}$ (metric tensor)

$H(\xi_1,\xi_2,\xi_3) = H(123) = H \equiv h_1h_2h_3$.

The symbol H is "non standard" but it is convenient to use it as the product of the three curvilinear scale factors. One might say that all the quantities listed here have a generic (123) functional form. This does not mean they cannot also have some kind of factored form.

The symbol ψ, the Helmholtz equation solution function, has the special functional form noted in (1.1). That is, one *seeks* solutions ψ of this functional form,

$\psi(\xi_1,\xi_2,\xi_3) = X_1(\xi_1)X_2(\xi_2)X_3(\xi_3)/ R(\xi_1,\xi_2,\xi_3)$

$\psi(123) = X_1(1)X_2(2)X_3(3)/ R(123)$

$\psi = X_1X_2X_3/R$

Historically it seems that R was defined "in the denominator of ψ".

Certain constants shall appear below:

K_1^2 = the parameter appearing in the Helmholtz equation $(\nabla^2 + K_1^2)\psi = 0$

k_2^2, k_3^2 = two generic constants which will be called "separation constants"

Although K_1^2 and the k_n^2 are written "squared", they are really meant to be arbitrary real numbers, so if some $k_i^2 < 0$ then the corresponding k_i is imaginary. The squared notation arises from the way the Helmholtz equation looks when it derives from a transformed wave equation. It is probably an unfortunate notation, but we use it to be compatible with Morse and Feshbach.

For equations with three terms where the last two terms are cyclic permutations of the first term, we sometimes write first term " + cyclic" to save writing obvious extra terms. That is to say,

$$f(123) + f(231) + f(312) \; = \; f(123) + \text{cyclic} \; .$$

We now come finally to the Stäckel matrix which Morse and Feshbach (and Stäckel) call Φ

$$\Phi = \begin{pmatrix} \Phi_{11}(1) & \Phi_{12}(1) & \Phi_{13}(1) \\ \Phi_{21}(2) & \Phi_{22}(2) & \Phi_{23}(2) \\ \Phi_{31}(3) & \Phi_{32}(3) & \Phi_{33}(3) \end{pmatrix} \qquad \text{" the Stäckel Matrix"}$$

$$S = \det(\Phi) \qquad \text{" the Stäckel Determinant"}$$

A key fact to recognize is that the three functions of row n are functions only of ξ_n , as indicated by the notation

$$\Phi_{nm}(n) = \Phi_{nm}(\xi_n) \; ,$$

so the *first* index of Φ matches the argument. The cofactors of the elements of the first column of the Φ matrix are these,

$$M_n \equiv \text{cof}(\Phi_{n1}) = (-1)^{n+1} \, \text{minor}(\Phi_{n1}) \; .$$

For example,

$$M_2 = (-1)^{2+1} \, \text{minor}(\Phi_{n1}) = - \begin{vmatrix} \Phi_{12}(1) & \Phi_{13}(1) \\ \Phi_{32}(3) & \Phi_{33}(3) \end{vmatrix} = - [\Phi_{12}(\xi_1) \, \Phi_{33}(\xi_3) - \Phi_{13}(\xi_1) \, \Phi_{32}(\xi_3)] \; .$$

Notice that M_2 has the functional form $M_2(\neq 2) = M_2(\xi_1,\xi_3)$, and in general $M_n = M_n(\neq n)$, as it was presented earlier in this section. Sometimes the following notations are used

$$M_n(\Phi) \qquad S(\Phi)$$

to stress that these quantities are functions of the Stäckel matrix elements.

This Φ matrix is named after German mathematician **Paul Stäckel** (shtay'kel), 1962-1919.

Our symbols match exactly those of Morse and Feshbach except for Q which they call u, and except for our added symbol H for $h_1h_2h_3$. Our symbols match Moon and Spencer except they use $U^n(u_n)$ in place of our $X_n(\xi_n)$.

Morse and Feshbach address this 3D separation subject in two places in their first volume: simple separation is treated pp 508-511, while R-separation is treated pp 518-519. They do not use the term "R-separation" and call the R function a "modulation factor".

Moon and Spencer discuss simple separation on pp 5-7, and R-separation on p 96. They provide more detail in some of their other books and papers.

One last notational item: when an already-numbered equation is later replicated for the reader's convenience, the equation number in the replicated line is put into italics to show that this is not the first occurrence of the equation.

3. Initial Processing of the Helmholtz Equation

We are going to treat R-separation and simple separation at the same time, and branch off later into the two cases. Remember that simple separation just means R = 1. In *orthogonal* curvilinear coordinates, using our notation as defined above, the Helmholtz equation can be written (see e.g. Morse and Feshbach p 115)

$$\mathcal{L}\psi \equiv (\nabla^2+K_1^2)\psi = 0 \qquad \mathcal{L} \equiv (\nabla^2+K_1^2) = \text{the Helmholtz operator}$$

$$\mathcal{L}\psi = H^{-1}\{ \partial_1[(H/h_1^2)(\partial_1\psi)] + \text{cyclic}\} + K_1^2\psi = 0 \qquad H \equiv h_1h_2h_3$$

$$\mathcal{L}\psi = H^{-1} \Sigma_n \partial_n[(H/h_n^2)(\partial_n\psi)] + K_1^2\psi = 0 \tag{3.1}$$

where sometimes the + cyclic notation is more useful for observing functional forms. We seek a solution of this functional form

$$\psi = X_1X_2X_3/R \tag{3.2}$$

where the four functions X_n and R are as yet unknown. Inserting this ψ form into (3.1) gives

$$\mathcal{L}\psi = H^{-1}\{ \partial_1[(H/h_1^2)(\partial_1\{ X_1X_2X_3/R \})] + \text{cyclic}\} + K_1^2\psi = 0$$

$$\mathcal{L}\psi = H^{-1}\{ X_2X_3\partial_1[(H/h_1^2)\, \partial_1\{ X_1/R \}] + \text{cyclic}\} + K_1^2\psi = 0 \ . \tag{3.3}$$

Here one sees how the implicit functional forms come into play, as the factors X_2X_3 quietly slip to the left through both ∂_1 operators. The following is then inserted into (3.3)

$$\partial_1(X_1/R) = \partial_1(R^{-1}X_1) = R^{-1}\partial_1X_1 - R^{-2}X_1\partial_1R = R^{-2}\{ (\partial_1X_1)R - X_1(\partial_1R) \}$$

to get

$$\mathcal{L}\psi = H^{-1}\{ X_2X_3\partial_1[(H/[R^2h_1^2])\{ (\partial_1X_1)R - X_1(\partial_1R) \}] + \text{cyclic}\} + K_1^2\psi = 0 \ . \tag{3.4}$$

In order to move toward a "separated form" wherein the terms above are less coordinate-entangled, we shall attempt to select function R so the following equation is satisfied in terms of functional form (comments below),

$$(H/[R^2h_n^2]) = f_n(n)g_n(\neq n) \qquad n = 1,2,3 \tag{3.5}$$

$$(H/[R^2h_1^2]) = f_1(1)g_1(23) \qquad \text{// for example}$$

because, if one inserts this into (3.4), one can pull $g_1(23)$ to the left through ∂_1 to get

$$H^{-1}\{ X_2X_3\partial_1[f_1(1)g_1(23) \{ (\partial_1X_1)R - X_1(\partial_1R) \}] + \text{cyclic}\}\psi + K_1^2\psi = 0$$

$$H^{-1}\{ X_2X_3\, g_1\partial_1[f_1 \{ (\partial_1X_1)R - X_1(\partial_1R) \}] + \text{cyclic}\}\psi + K_1^2\psi = 0$$

and, recalling that $\psi = X_1X_2X_3/R$ from (3.2), one can then divide by ψ to get

$$(\mathcal{L}\psi)/\psi = (R/H)\{(1/X_1)\, g_1\partial_1[f_1\, \{ (\partial_1X_1)R - X_1(\partial_1R) \}] + \text{cyclic}\} + K_1^2 = 0$$

$$(\mathcal{L}\psi)/\psi = (R/H)\, \Sigma_n[(g_n/X_n)\, \partial_n[f_n\, \{ R(\partial_nX_n) - X_n(\partial_nR) \}] + K_1^2 = 0 \quad .$$

Now using (3.5) to replace g_n in favor of f_n, our processed Helmholtz equation appears as

$$(\mathcal{L}\psi)/\psi = (1/R)\, \Sigma_n[\ (1/[h_n^2X_n])\, (1/f_n)\partial_n[f_n\, \{ R(\partial_nX_n) - X_n(\partial_nR) \}] + K_1^2 = 0 \qquad (3.6)$$

It is not obvious from the discussion above that having (3.5) be true is *the only* possible pathway to finding a separated solution, though probably that can be proven. It will be shown that this (3.5) pathway *does* in fact lead to separated solutions.

For a coordinate system which satisfies (3.5), where one has found the f_n , g_n and R, one can write ∇^2 in an alternate form. In (3.1) ∇^2 is given in terms of the scale factors h_n,

$$\nabla^2 = H^{-1}\ \Sigma_n\, \partial_n[(H/h_n^2)\, \partial_n\,] \quad .$$

From (3.5) one can replace $(H/h_n^2) = f_n(n)g_n(\neq n)R^2$ to get

$$\nabla^2 = H^{-1}\ \Sigma_n\, \partial_n[f_n(n)g_n(\neq n)R^2\partial_n\,] \ = H^{-1}\ \Sigma_n\, g_n(\neq n)\partial_n[f_n(n)\, R^2\partial_n\,]$$

$$= H^{-1}\ \Sigma_n\, (H/[h_n^2R^2])\, (1/f_n)\, \partial_n[f_n\, R^2\partial_n\,]$$

$$= \Sigma_n\, (1/[h_n^2R^2])\, (1/f_n)\, \partial_n[f_n\, R^2\partial_n\,] \quad . \qquad (3.7)$$

Then in the special case that R = 1, one has

$$\nabla^2 = \ \Sigma_n\, (1/h_n^2)\, (1/f_n)\, \partial_n[f_n\partial_n\,] \qquad (3.7a)$$

showing ∇^2 in terms of the f_n and the scale factors h_n. In either case $\mathcal{L} = \nabla^2 + K_1^2$.

Comments on (3.5) and example of toroidal coordinates

Conditions (3.5) above,

$$(H/[R^2h_n^2]) = f_n(n)g_n(\neq n) \qquad n = 1,2,3 \qquad \textit{(3.5)}$$

require that the LHS factor in a certain specific manner. One can certainly find an R(123) that works for the first equation with n=1: one could just select two arbitrary functions $f_1(1)$ and $g_1(23)$ and then define R by

$$[R(123)]^{-2} \equiv f_1(1)g_1(23)\,(H/h_1^2) \ .$$

But if this is done, it is unlikely that (3.5) will be viable for n=2 and 3! So one has to *assume* one can find a set of 7 functions (three f_n, three g_n and one R) which make (3.5) valid. Any curvilinear system for which one *cannot* find a happy set of 7 functions is therefore not separable. So one views (3.5) as a restriction or condition on the curvilinear coordinate system which must be met to obtain any separation. We do not address the question of whether there might be some other possible separation solution where (3.5) is not assumed.

Example. Since this is perhaps a confusing concept, consider the **toroidal** coordinate system as an example. The Moon and Spencer page 112 notation is used, where η labels toroids, θ labels bowls, ψ labels azimuthal half planes, a is the radius of the limiting toroid, and then $(\xi_1,\xi_2,\xi_3) = (\eta,\theta,\psi)$. In this system the basic parameters come out being

$$\mathcal{R}^{-2} \equiv [\mathrm{ch}(\xi_1)-\cos(\xi_2)]$$

$$h_1 = h_2 = a/[\mathrm{ch}(\xi_1)-\cos(\xi_2)] \qquad => \qquad h_1 = h_2 = a\mathcal{R}^2$$

$$h_3 = a\,\mathrm{sh}(\xi_1)/[\mathrm{ch}(\xi_1)-\cos(\xi_2)] \qquad => \qquad h_3 = a\,\mathrm{sh}(\xi_1)\mathcal{R}^2 \ .$$

As a candidate for R one tries R = $\mathcal{R}$ and finds then that

$$(H/h_1^2) = h_2h_3/h_1 = h_3 = a\,\mathrm{sh}(\xi_1)/[\mathrm{ch}(\xi_1)-\cos(\xi_2)]$$

$$(H/h_2^2) = h_3h_1/h_2 = h_3 = a\,\mathrm{sh}(\xi_1)/[\mathrm{ch}(\xi_1)-\cos(\xi_2)]$$

$$(H/h_3^2) = h_1h_2/h_3 = a^2/[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^2 * [\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,/a\,\mathrm{sh}(\xi_1) = a/\{[\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,\mathrm{sh}(\xi_1)\} \ .$$

Can a set of 6 functions f_n and g_n be found which satisfy (3.5) ?

$$f_n(1)g_n(23) = (1/R^2)\,(H/h_n^2) = [\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,(H/h_n^2) \qquad \text{for } n = 1,2,3$$

The answer is yes:

$$f_1(1)g_1(23) = [\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,a\,\mathrm{sh}(\xi_1)/[\mathrm{ch}(\xi_1)-\cos(\xi_2)] = a\,\mathrm{sh}(\xi_1) = [\mathrm{sh}(\xi_1)]\,[a]$$

$$f_2(2)g_2(31) = [\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,a\,\mathrm{sh}(\xi_1)/[\mathrm{ch}(\xi_1)-\cos(\xi_2)] = a\,\mathrm{sh}(\xi_1) = [1]\,[a\,\mathrm{sh}(\xi_1)]$$

$$f_3(3)g_3(12) = [\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,a/\{[\mathrm{ch}(\xi_1)-\cos(\xi_2)]\,\mathrm{sh}(\xi_1)\} = a/\mathrm{sh}(\xi_1) = [a]\,[1/\mathrm{sh}(\xi_1)] \ .$$

Thus, with this candidate R, a solution set for the 6 functions has been found:

$$f_1(1) = \mathrm{sh}(\xi_1) \qquad g_1(23) = a \qquad R = \mathcal{R} = [\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{-1/2}$$

$$f_2(2) = 1 \qquad g_2(31) = a\,\mathrm{sh}(\xi_1)$$

$$f_3(3) = a \qquad g_3(12) = 1/\mathrm{sh}(\xi_1) \ .$$

Therefore, the toroidal system at least has a chance of being R-separable. It is in fact R-separable (for Laplace), but we don't know that yet since there might be other restrictions that will need checking.

Had one tried R = 1 in the above toroidal discussion, the problem would have been to find 6 functions f_n and g_n which satisfy (3.5). The n=1 condition would read,

$$f_1(1)g_1(23) = (H/h_1^2) = a\, sh(\xi_1)/[ch(\xi_1)-cos(\xi_2)] .$$

The only chance is to select $f_1(1) = a\, sh(\xi_1)$ but then one is stuck with $g_1(23) = 1/[ch(\xi_1)-cos(\xi_2)]$ which involves coordinate ξ_1 which violates the functional form $g_1(23)$! Therefore the toroidal system is not simple-separable!

The Definition of Q

Processing of the Helmholtz equation now resumes where it left off, which was here

$$(\mathcal{L}\psi)/\psi = (1/R)\, \Sigma_n[\ (1/[h_n^2 X_n])\, (1/f_n)\partial_n[f_n \{ R(\partial_n X_n) - X_n(\partial_n R) \}] + K_1^2 = 0 \qquad (3.6)$$

where (3.5) has been assumed. Note that there is serious variable entanglement in each term of the sum, since R = R(123) and $h_n = h_n(123)$.

To further process (3.6), compute the ∂_n derivatives,

$$\partial_n[R\, f_n(\partial_n X_n)] = \partial_n[R\{f_n(\partial_n X_n)\}] = R\partial_n\{f_n(\partial_n X_n)\} + (\partial_n R)\, \{f_n(\partial_n X_n)\}$$
$$\partial_n[f_n X_n(\partial_n R)] = \partial_n[X_n\{f_n(\partial_n R)\}] = X_n\partial_n\{f_n(\partial_n R)\} + (\partial_n X_n)\, \{f_n(\partial_n R)\} \quad .$$

Therefore, for the quantity appearing in (3.6),

$$\partial_n[f_n \{ R(\partial_n X_n) - X_n(\partial_n R) \})] = R\partial_n\{f_n(\partial_n X_n)\} - X_n\partial_n\{f_n(\partial_n R)\}$$

since the two second terms cancel. Then (3.6) for $(\mathcal{L}\psi)/\psi$ becomes

$$(1/R)\, \Sigma_n\, (1/[h_n^2 X_n f_n])\, [R\partial_n\{f_n(\partial_n X_n)\} - X_n\partial_n\{f_n(\partial_n R)\}] + K_1^2 = 0$$

$$(1/R)\, \Sigma_n[\ (1/[h_n^2 X_n f_n])\, [R\partial_n\{f_n(\partial_n X_n)\}] - (1/R)\, \Sigma_n[\ (1/[h_n^2 X_n f_n])\ [X_n\partial_n\{f_n(\partial_n R)\}] + K_1^2 = 0$$

or

$$(\mathcal{L}\psi)/\psi = \Sigma_n[\ (1/[h_n^2 X_n f_n])\, [\partial_n\{f_n(\partial_n X_n)\}] - \Sigma_n[\ (1/[h_n^2 R f_n])\, [\partial_n\{f_n(\partial_n R)\}] + K_1^2 = 0 . \qquad (3.8)$$

Notice that the X_n part is segregated from the R part. Since a viable set of functions f_n and R has already been determined from (3.5), the second term sum shown in (3.8) can be computed. It is going to be some general function of 123 which we now write in a fairly strange manner,

$$\Sigma_n\, (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} \equiv - k_1^2/Q(123) \ . \qquad (3.9)$$

Here, it is the RHS which is fully determined by the LHS and we choose to partition the RHS into two factors, a constant $-k_1^2$ (Moon and Spencer call this constant $-\alpha_1$) and 1/Q(123) (Morse and Feshbach call this 1/u). Remember that the Helmholtz parameter is K_1^2 and has nothing to do with this new constant

$k_1{}^2$ just introduced. In theory, $k_1{}^2$ can be any constant, but one usually chooses it to make the resulting Q(123) have some simple form. The reason for calling this constant $k_1{}^2$ will be seen later.

For the simple separation case with R = 1, we will choose Q(123) = 1 and $k_1{}^2 = 0$ in (3.9), which of course makes it still valid since $(\partial_n R) = 0$.

Equations (3.8,9) appears as (5.1.46,47) in Morse and Feshbach p 519, with Q→ u.

Example: Compute Q for the toroidal system using (3.9)

Start with the numerators in (3.9). First,

$$(\partial_1 R) = \partial_1[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{-1/2} = (-1/2)\mathrm{sh}(\xi_1)\,[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{-3/2} = (-1/2)\mathrm{sh}(\xi_1)\,R^3$$
$$(\partial_2 R) = \partial_2[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{-1/2} = (-1/2)\sin(\xi_2)\,[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{-3/2} = (-1/2)\sin(\xi_2)\,R^3$$
$(\partial_3 R) = 0$ => entire third term in the sum is 0, so ignore it from now on

The following tedious algebra must then be done:

$$\begin{aligned}
[\partial_1\{f_1(\partial_1 R)\}] &= [\partial_1\{\ \mathrm{sh}(\xi_1) * (-1/2)\mathrm{sh}(\xi_1)\,R^3\}] = (-1/2)\,\partial_1[\mathrm{sh}^2(\xi_1)R^3] \\
&= (-1/2)\,[\,2\mathrm{sh}(\xi_1)\mathrm{ch}(\xi_1)\,R^3 + \mathrm{sh}^2(\xi_1)3R^2(\partial_1 R)\,] \\
&= (-1/2)\,[\,2\mathrm{sh}(\xi_1)\mathrm{ch}(\xi_1)\,R^3 + \mathrm{sh}^2(\xi_1)3R^2(-1/2)\mathrm{sh}(\xi_1)\,R^3\,] \\
&= (-1/2)\,[\,2\mathrm{sh}(\xi_1)\mathrm{ch}(\xi_1)\,R^3 - \mathrm{sh}^3(\xi_1)(3/2)R^5\,] \\
&= (-1/4)\mathrm{sh}(\xi_1)R^5\,[\,4\mathrm{ch}(\xi_1)\,R^{-2} - 3\mathrm{sh}^2(\xi_1)\,] \\
&= (-1/4)\mathrm{sh}(\xi_1)R^5\,[\,4\mathrm{ch}(\xi_1)\,[\mathrm{ch}(\xi_1)-\cos(\xi_2)] - 3\mathrm{sh}^2(\xi_1)\,] \\
&= (-1/4)\mathrm{sh}(\xi_1)R^5\,[\,4\mathrm{ch}^2(\xi_1) - 4\,\mathrm{ch}(\xi_1)\cos(\xi_2)] - 3\mathrm{sh}^2(\xi_1)\,] \\
&= (-1/4)\mathrm{sh}(\xi_1)R^5\,[\,3 + \mathrm{ch}^2(\xi_1) - 4\,\mathrm{ch}(\xi_1)\cos(\xi_2)]
\end{aligned}$$

$$\begin{aligned}
[\partial_2\{f_2(\partial_2 R)\}] &= [\partial_2\{1 *(\partial_2 R)\}] = \partial_2[(-1/2)\sin(\xi_2)\,R^3 \\
&= (-1/2)[\,\cos(\xi_2)R^3 + \sin(\xi_2)3R^2\,(\partial_2 R)\,] \\
&= (-1/2)[\,\cos(\xi_2)R^3 + \sin(\xi_2)3R^2\,(-1/2)\sin(\xi_2)\,R^3\,] \\
&= (-1/2)[\,\cos(\xi_2)R^3 - \sin^2(\xi_2)(3/2)R^5\,] \\
&= (-1/2)\,R^5\,[\,\cos(\xi_2)R^{-2} - \sin^2(\xi_2)(3/2)] \\
&= (-1/4)\,R^5\,[\,2\cos(\xi_2)\,[\mathrm{ch}(\xi_1)-\cos(\xi_2)] - 3\sin^2(\xi_2)] \\
&= (-1/4)\,R^5\,[\,2\cos(\xi_2)\,\mathrm{ch}(\xi_1)-2\cos^2(\xi_2) - 3\sin^2(\xi_2)] \\
&= (-1/4)\,R^5\,[\,2\cos(\xi_2)\,\mathrm{ch}(\xi_1) - 2 - \sin^2(\xi_2)]
\end{aligned}$$

which can be summarized as

$$[\partial_1\{f_1(\partial_1 R)\}] = (-1/4)\,R^5\,[\,3 + \mathrm{ch}^2(\xi_1) - 4\,\mathrm{ch}(\xi_1)\cos(\xi_2)]\,\mathrm{sh}(\xi_1)$$
$$[\partial_2\{f_2(\partial_2 R)\}] = (-1/4)\,R^5\,[\,2\cos(\xi_2)\,\mathrm{ch}(\xi_1) - 2 - \sin^2(\xi_2)]\ .$$

The denominator factors of the Q expression are these,

$$h_1{}^2 f_1 R = a^2 R^4\,\mathrm{sh}(\xi_1)\,R = a^2\,\mathrm{sh}(\xi_1)\,R^5$$
$$h_2{}^2 f_2 R = a^2 R^4\,1\,R = a^2\,R^5\ .$$

Now the LHS of (3.9) can be evaluated:

$\Sigma_n (1/[h_n^2 f_n R]) [\partial_n\{f_n(\partial_n R)\}] =$

$[a^2 \,sh(\xi_1)\, R^5]^{-1} * \;\; (-1/4)sh(\xi_1)R^5 \,[\, 3 + ch^2(\xi_1) - 4\, ch(\xi_1)\, cos(\xi_2)]$
$+ \;\; [a^2\, R^5]^{-1} * \;\; (-1/4)\, R^5 \,[\, 2cos(\xi_2)\, ch(\xi_1) - 2 - sin^2(\xi_2)]$

$= (-1/4a^2)\, [\, 3 + ch^2(\xi_1) - 4\, ch(\xi_1)\, cos(\xi_2)] \;\; + \;\; (-1/4a^2)\;\; [\, 2cos(\xi_2)\, ch(\xi_1) - 2 - sin^2(\xi_2)]$
$= (-1/4a^2)\, [3 + ch^2(\xi_1) - 4\, ch(\xi_1)\, cos(\xi_2) + 2cos(\xi_2)\, ch(\xi_1) - 2 - sin^2(\xi_2)\,]$
$= (-1/4a^2)\, [1 + ch^2(\xi_1) - 4\, ch(\xi_1)\, cos(\xi_2) + 2cos(\xi_2)\, ch(\xi_1) - sin^2(\xi_2)\,]$
$= (-1/4a^2)\, [cos^2(\xi_2) + ch^2(\xi_1) - 2\, ch(\xi_1)\, cos(\xi_2)]$
$= (-1/4a^2)\, [ch(\xi_1)-cos(\xi_2)]^2 = (-1/4a^2)\, R^{-4}$.

Therefore (3.9) says

$-k_1^2/Q(123) = \Sigma_n (1/[h_n^2 f_n R]) [\partial_n\{f_n(\partial_n R)\}] = \;(-1/4a^2)\, R^{-4} = (-1/4) \,/\, \{a^2 R^4\}$

so one can make this simple partitioning

$k_1^2 = \;\alpha_1 = (1/4)$ $\qquad\qquad$ $Q = a^2R^4 = a^2[ch(\xi_1)-cos(\xi_2)]^2$

which agrees with Moon and Spencer page 97.

So after this brute force sum computation, Q comes out being a very simple function. The toroidal information found so far can now be summarized :

$h_1 = h_2 = a/[ch(\xi_1)-cos(\xi_2)]$ $\quad$ => $\quad$ $h_1 = h_2 = aR^2$ $\qquad$ $H = sh(\xi_1)a^3R^6$
$h_3 = a\, sh(\xi_1)/[ch(\xi_1)-cos(\xi_2)]$ $\quad$ => $\quad$ $h_3 = a\, sh(\xi_1)R^2$

$f_1(1) = \; sh(\xi_1)$	$g_1(23) = a$	$R = [ch(\xi_1)-cos(\xi_2)]^{-1/2}$
$f_2(2) = 1$	$g_2(31) = a\, sh(\xi_1)$	$Q = a^2[ch(\xi_1)-cos(\xi_2)]^2 = a^2R^4$
$f_3(3) = a$	$g_3(12) = 1/\, sh(\xi_1)$	$k_1^2 = (1/4)$

Finish Processing

So here is where things stood prior to the above example :

$(\mathcal{L}\psi)/\psi \;= \Sigma_n[\;\; (1/[h_n^2 X_n f_n])\, [\partial_n\{f_n(\partial_n X_n)\}] \;-\Sigma_n[\;\; (1/[h_n^2 R f_n])\, [\partial_n\{f_n(\partial_n R)\}] \;+ K_1^2 \;= 0$ $\qquad$ *(3.8)*

$\Sigma_n (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} \;\; = - k_1^2/Q$. $\qquad$ *(3.9)*

Therefore,

$(\mathcal{L}\psi)/\psi \;= \;\Sigma_n(1/[h_n^2 X_n])\, (1/f_n)\partial_n[f_n(\partial_n X_n)] \;+ k_1^2/Q \;+ K_1^2 \;= 0$. $\qquad$ (3.10)

For later reference, notice in (3.10) the position of the two copies of function f_n. Equation (3.10) is not separated because $h_n = h_n(123)$ and $Q = Q(123)$. At least in the simple separation case the Q term goes away, since as noted above $k_1^2 = 0$ and $Q = 1$.

This concludes the "initial processing of the Helmholtz equation". The PDE (3.10) essentially *is* the Helmholtz equation $\mathcal{L}\psi = (\nabla^2+K_1^2)\psi = 0$ where various assumptions have been made: the form $\psi = X_1X_2X_3/R$, equation (3.5), and the definition of Q and k_1^2 from (3.9). At this point, then, for a given curvilinear coordinate system, we *know* all these items in full detail:

$$K_1^2 \quad h_n(123) \quad H(123) \quad R(123) \quad f_n(n) \quad g_n(\neq n) \quad Q(123) \quad k_1^2 \ .$$

Comment on separation in Cartesian coordinates

Cartesian coordinates have $h_n = 1$ and so $f_n = 1$, R=1, Q=1, $k_1^2 = 0$ and (3.10) reads

$$\Sigma_n (1/X_n) (\partial_n^2 X_n) + K_1^2 = 0 \qquad (3.11)$$

or

$$(1/X_1) (\partial_1^2 X_1) + (1/X_2) (\partial_2^2 X_2) + (1/X_3) (\partial_3^2 X_3) + K_1^2 = 0 \ . \qquad (3.11a)$$

If one were to fix ξ_2 and ξ_3 and vary just ξ_1, one would conclude that $(1/X_1) (\partial_1^2 X_1)$ is a constant, since the other three terms in (3.11a) are then constant. By this argument, one is led to claim that

$$(1/X_1) (\partial_1^2 X_1) = c_1$$
$$(1/X_2) (\partial_2^2 X_2) = c_2$$
$$(1/X_3) (\partial_3^2 X_3) = c_3 \qquad (3.12)$$

and then (3.11a) says $\qquad c_1 + c_2 + c_3 = -K_1^2 \ . \qquad (3.13)$

One can then regard any *two* of the c_i as *free parameters*, say c_1 and c_2, then the third is not free and is constrained to be $c_3 = K_1^2 - c_1 - c_2$. The two free parameters are called **separation constants**.

This is the simple way separation works in Cartesian coordinates, and it works this way because each term in the sum (3.11) is completely "detangled" from the other two terms in the sense that the first term does not involve variables ξ_2 and ξ_3 whatsoever. In general curvilinear coordinates, there will still be two separation constants, which will be called k_2^2 and k_3^2, but the simple arrangement shown in (3.12) does not obtain, and both the free parameters will (in the general case) appear *in each* of the three separated equations! As shown below, in curvilinear coordinates the separated equations end up having this form

$$(1/f_nX_n)\partial_n[f_n(\partial_nX_n)] + [\ K_1^2\Phi_{n1}(\xi_n) + k_2^2\Phi_{n2}(\xi_n) + k_3^2\Phi_{n3}(\xi_n)] = 0 \qquad n = 1,2,3$$

where the $\Phi_{ni}(\xi_n)$ are a set of nine functions which can in principle all be different (and they *are* all different in ellipsoidal coordinates, for example, see Section 12). Here the two separation constants k_2^2 and k_3^2 appear in each of the three separated equations as advertised, and they cannot be simply extracted as in (3.12). Nevertheless, they are free parameters and are still called separation constants. That is to say, all three equations above will be valid *for any values* of k_2^2 and k_3^2.

4. Starting from the other end: The Stäckel Matrix Φ and a Formulation of the Problem

The goal is to find differential operators L_n in terms of which (3.10) can be separated. The most general second-order linear L_n can be written this way, where p_n, r_n and q_n are real functions,

$$L_n X_n = (1/p_n)\partial_n[p_n(\partial_n X_n)] + r_n(\partial_n X_n) + q_n X_n = 0 \quad . \qquad (4.1)$$

For several reasons, one wants L_n to be formally self-adjoint, L=L*. If (f,g) is the scalar product for the space of functions upon which L_n acts, L=L* means that (u,Lv) = (Lu,v), where one ignores the contributions of the "parts" terms as L is swung from one side to the other in the integration which this scalar product represents. Since $L = r_n\partial_n X_n \Rightarrow L^* = - r_n\partial_n X_n$, one must have $r_n = 0$ so then

$$L_n X_n = (1/p_n)\partial_n[p_n(\partial_n X_n)] + q_n X_n = 0 \quad . \qquad (4.1A)$$

If one takes $r_n \neq 0$, the process given below leads to an intractable set of equations which it is not hard to show is insolvable. Secondly, L_n being self-adjoint is essential to the application of Sturm-Liouville theory to the separated equations.

Looking now at (3.10),

$$(\mathcal{L}\psi)/\psi = \Sigma_n(1/[h_n^2 X_n])\,(1/f_n)\partial_n[f_n(\partial_n X_n)] + k_1^2/Q + K_1^2 = 0, \qquad \textit{(3.10)}$$

one is highly motivated to set $p_n = f_n$ in (4.1A) and then the candidate form for L_n is

$$L_n X_n = (1/f_n)\partial_n[f_n(\partial_n X_n)] + q_n X_n = 0 \qquad (4.2)$$

which says

$$(1/X_n)(1/f_n)\partial_n[f_n(\partial_n X_n)] = - q_n \quad . \qquad (4.3)$$

Inserting (4.3) into (3.10),

$$(\mathcal{L}\psi)/\psi = - \Sigma_n(1/h_n^2)q_n + k_1^2/Q + K_1^2 = 0 \quad . \qquad (4.4)$$

This then is the final form of the processed Helmholtz equation, assuming that X_n satisfies the equation (4.2) .

Introduction of the Stäckel Matrix

Now comes a fairly inspired and unexpected step in the development. Suppose one chooses to write the $q_n(n)$ function of (4.2) in this manner, which is to say, the unknown function $q_n(n)$ is simply written as a linear combination of three other unknown functions,

$$q_n(n) = [\, \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] \qquad n = 1,2,3 \qquad (4.5)$$

where κ_1^2, k_2^2 and k_3^2 are at the moment three arbitrary real constants, and the $\Phi_{nm}(n)$ are the 9 functions of what is called the Stäckel matrix mentioned in Section 2 above,

$$\Phi = \begin{pmatrix} \Phi_{11}(1) & \Phi_{12}(1) & \Phi_{13}(1) \\ \Phi_{21}(2) & \Phi_{22}(2) & \Phi_{23}(2) \\ \Phi_{31}(3) & \Phi_{32}(3) & \Phi_{33}(3) \end{pmatrix} \qquad S(\Phi) \equiv \det(\Phi) \tag{4.6}$$

$$M_n(\Phi) \equiv \mathrm{cof}(\Phi_{n1}) = (-1)^{n+1}\,\mathrm{minor}(\Phi_{n1}) \quad . \tag{4.7}$$

With (4.5) used in (4.2), the assumed form for L_n becomes

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\ \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \tag{4.8}$$

and the processed Helmholtz equation (4.4) becomes

$$Q(\mathcal{L}\psi)/\psi = -\,\Sigma_n(Q/h_n^2)\,[\ \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] + k_1^2 + QK_1^2 = 0 \quad . \tag{4.9}$$

This then is the form the processed Helmholtz equation takes if one expands the q_n of (4.4) as shown in (4.5). The goal is to find a set of functions Φ_{nm} which makes (4.9) be true. It is not obvious that such a set of Φ_{nm} exists. The sum is still entangled due to $h_n(123)$ and $Q(123)$.

Formulation of separation Problems A, B and C

Problem A: (simple separation of the Helmholtz equation).

In this case R = 1, so Q = 1 and $k_1^2 = 0$ in (4.9), and set $\kappa_1^2 = K_1^2$ in both (4.8) and (4.9) to get

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\ K_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \tag{4.8A}$$

$$(\mathcal{L}\psi)/\psi = -\,\Sigma_n(1/h_n^2)\,[\ K_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] + K_1^2 = 0 \ . \tag{4.9A}$$

Problem B: (R-separation of the *Laplace* Equation).

In this case $K_1^2 = 0$ in (4.9), and set $\kappa_1^2 = k_1^2$ in both (4.8) and (4.9) to get

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\ k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \tag{4.8B}$$

$$Q(\mathcal{L}_0\psi)/\psi = -\,\Sigma_n(Q/h_n^2)\,[k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] + k_1^2 = 0 \tag{4.9B}$$

where $\mathcal{L}_0 = \nabla^2$ is the Laplace operator.

Comparing the A and B equations, one sees that Problem A is a special case of Problem B having Q = 1 and $k_1^2 = K_1^2$. Below in the systematic solution of Problem B, we may apply any intermediate equation of that solution to Problem A by making these two substitutions (and R=1). This explains why we (and Morse and Feshbach) gave the constant in (3.9) the strange name k_1^2.

One now treats Problem B as an abstract mathematical problem. That mathematical problem is to find a set of 9 functions Φ_{nm} and 3 functions f_n that makes (4.8B) and (4.9B) be consistent.

The method used for solving this problem is straightforward, the details appear in the next section. One requires that the coefficient of each k_i^2 in (4.9B) vanish, since the equation should be true for all real values of the three k_i^2 parameters. One then writes (4.9B) as a vector equation $\Phi^T \mathbf{V} = \mathbf{W}$ where $V_n = (Q/h_n)^2$ and $W_n = \delta_{n,1}$. This equation is inverted to obtain a simple expression for the cofactors M_n of the elements of the first column of Φ. From these cofactors one can (hopefully) deduce the 6 components of the rightmost two columns of Φ. We postulate a second condition as an ansatz (the Robertson Condition), and this condition then leads (potentially) to an evaluation of the elements of the first column of Φ. One then has all of Φ! The functions f_n are determined from (3.5). If this program can be completed successfully, the separated L_n are obtained, and the Robertson ansatz is justified. The solution will be summarized as a sequence of Steps that one must execute one at a time. A list of Conditions is first stated which, if met, ensure that the Steps can be carried out.

Problem C: (R-separation of the *Helmholtz* Equation with $K_1^2 \neq 0$).

Here one has the full bore (4.9) to contend with

$$- \Sigma_n(Q/h_n^2)\,[\,\kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] + k_1^2 + QK_1^2 = 0\,. \qquad (4.9C)$$

Remember that Q = Q(123) is (in general) a function of all three coordinates. It is not clear how to decouple that last two terms in this equation. What should κ_1^2 be set to? The method just outlined above for solving Problem B *does not work* for Problem C. Moon and Spencer state (p 96, 1961) that no curvilinear system has ever been found in which the Helmholtz equation with $K_1^2 \neq 0$ separates via R-separation (by which they mean with $R \neq$ constant). So having at least stated it, we shall give up on Problem C and continue now to solve Problem B.

5. Recasting Problem B into a new form

Equations (4.9B) and (4.8B) are replicated here with new equations numbers,

$$- \Sigma_n(Q/h_n^2)\ [k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]\ + k_1^2\ = 0 \tag{5.1}$$

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\ k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \quad . \tag{5.2}$$

If one can find the 3 functions f_n appearing in (5.2) and the 9 functions Φ_{nm} of the Stäckel matrix that solve (5.1), then (5.2) gives the separated ODE for functions X_n. The plan is to find a solution of (5.1) which is valid for all three k_n^2 constants having arbitrary (complex in fact) values. Such a solution requires that the coefficients of each k_n^2 be set to 0 so that

$$\Sigma_n\ (Q/h_n^2)\ \Phi_{n1}(n)\ = 1$$
$$\Sigma_n\ (Q/h_n^2)\ \Phi_{n2}(n)\ = 0$$
$$\Sigma_n(Q/h_n^2)\ \Phi_{n3}(n)\ \ = 0\ \ .$$

To put this into a standard vector equation form, use $[\Phi^T]_{mn}(n) \equiv \Phi_{nm}\ (n)$ so that

$$\Sigma_n\ \Phi^T{}_{1n}(n)\ (Q/h_n^2)\ = 1$$
$$\Sigma_n\ \Phi^T{}_{2n}(n)\ (Q/h_n^2)\ = 0$$
$$\Sigma_n\ \Phi^T{}_{3n}(n)\ (Q/h_n^2)\ = 0$$

and the vector equation is then

$$\Phi^T\ \mathbf{V} = \mathbf{W} \qquad\qquad \text{where} \tag{5.3}$$

$$\mathbf{V} = \begin{pmatrix} Q/h_1^2 \\ Q/h_2^2 \\ Q/h_3^2 \end{pmatrix} \qquad \mathbf{W} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \Phi\ = \begin{pmatrix} \Phi_{11}(1) & \Phi_{12}(1) & \Phi_{13}(1) \\ \Phi_{21}(2) & \Phi_{22}(2) & \Phi_{23}(2) \\ \Phi_{31}(3) & \Phi_{32}(3) & \Phi_{33}(3) \end{pmatrix} \qquad S \equiv \det(\Phi)\ \ .$$

This equation can easily be solved for **V** using the rule that $A^{-1} = \text{cof}(A^T)/\det(A)$:

$$\mathbf{V} = \{\ \text{cof}(\Phi^{T,T})/\det(\Phi^T)\}\ \mathbf{W}\ =\ \text{cof}(\Phi)\ \mathbf{W}\ /\det(\Phi)\ = (1/\ S(\Phi))\ \ \text{cof}(\Phi)\ \mathbf{W}\ .$$

In components

$$V_n\ = (1/\ S(\Phi))\ \ [\text{cof}(\Phi)]_{nm}\ W_m\ = (1/S(\Phi))\ \ [\text{cof}(\Phi_{nm})]\ \delta_{m,1} =\ \ (1/S(\Phi))\ \ [\text{cof}(\Phi_{n1})] \quad . \tag{5.4}$$

Following tradition, define M_n according to

$$M_n \equiv \text{cof}(\Phi_{n1})\ \ = \text{the cofactor of the first element in the } n^{th} \text{ row of } \Phi \tag{5.5}$$

and insert this on the right of (5.4) and $V_n = (Q\ /h_n^2)$ on the left, giving the **Cofactor Conditions**,

$$M_n/S = (Q / h_n^2) \;. \qquad (5.6)$$

Alternatively, write (5.6) as

$$M_n(\Phi)/S(\Phi) = (Q/h_n^2) \qquad n=1,2,3 \qquad \text{" Cofactor conditions"} \qquad (5.6a)$$

and this emphasizes that there are 3 conditions that the Φ matrix must satisfy for a given coordinate system with scale factors h_n. Notice that these conditions arise from the assumed form for L_n in (5.2), they are not "imposed". The reason that *cofactors* appear in (5.6) is because one had to invert the matrix Φ^T and matrix inversion always gives rise to cofactors. Since **W** was the unit vector $\mathbf{e_1}$, only the cofactors of the first column of Φ play a role.

If the three cofactor conditions are satisfied by some matrix Φ, then equation (5.1) is satisfied. But equation (5.1) is the "ground down" Helmholtz equation, so this provides a solution to the initial problem. Moreover, equation (5.2) then gives the L_n operators such that $L_nX_n = 0$ from which the X_n may be determined.

[Repeated Warning: Morse and Feshbach use cofactor M_n exactly as described above, but unfortunately they refer to M_n as a "minor", and they never use the word "cofactor". In modern parlance, cofactors are minors with signs added, which make a lot of difference.]

The next step is to impose an extra condition on the Φ matrix known as the **Robertson Condition**. This is done just as an *ansatz* to see if it helps find a solution. The requirement is that S = det(Φ) take this form,

$$S(\Phi) = H / (f_1f_2f_3QR^2) \;. \qquad \text{"Robertson condition"} \qquad (5.7)$$

It is not obvious that, for a given coordinate system, one can even *find* a matrix Φ which satisfies the Cofactor and Robertson conditions, but we shall try to construct a solution Φ. Combining (5.6) and (5.7) gives

$$M_n = (SQ/h_n^2) = (H/h_n^2) /(f_1f_2f_3R^2) \;. \qquad (5.8)$$

The Robertson condition causes the solution M_n to be expressed directly in terms of known quantities. If a full solution matrix Φ can be found, then this Robertson condition is retroactively justified. Using (3.5) which says $(H/h_n^2) = f_ng_n R^2$, (5.8) can be written in an alternate form

$$M_n = g_nf_n/(f_1f_2f_3) \qquad (5.8a)$$

or

$$M_1 = g_1 /(f_2f_3)$$
$$M_2 = g_2 /(f_3f_1)$$
$$M_3 = g_3 /(f_1f_2) \;. \qquad (5.8b)$$

These are the three *cofactors* of the elements of the first column of Φ. Notice there are no factors of R or Q in (5.8b). This was the motivation for installing the Q and R factors in the Robertson condition as done above in (5.7).

It remains to find the *elements* of the first column of Φ. They appear in this standard expansion of the determinant of Φ,

$$S = \Phi_{11}(1)\, M_1 + \Phi_{21}(2)\, M_2 + \Phi_{31}(3)\, M_3 \ . \qquad (5.9)$$

Install now S from (5.7) and the M_n from (5.8) to get

$$[\, H / (f_1 f_2 f_3 Q R^2)] = \Phi_{11}(1)\, (H/h_1^2) /(f_1 f_2 f_3 R^2) + \Phi_{21}(2)\, (H/h_2^2) /(f_1 f_2 f_3 R^2) + \Phi_{31}(3)\, (H/h_3^2) /(f_1 f_2 f_3 R^2)$$

or

$$1/Q = \Phi_{11}(1)\, (1/h_1^2) + \Phi_{21}(2)\, (1/h_2^2) + \Phi_{31}(3)\, (1/h_3^2) \ . \qquad (5.10)$$

This is a non-trivial functional-form equation that may or may not have solutions for the $\Phi_{n1}(n)$.

One is now left with this problem: Given

$$S(\Phi) = H / (f_1 f_2 f_3 Q R^2) \qquad // \text{ Robertson}$$
$$M_n(\Phi) = S(\Phi)\, (Q/h_n^2) \qquad // \text{ Cofactor} \qquad (5.11)$$

how *exactly* does one find the 9 elements of Φ ? This is Problem B restated in a simple form. If one can solve for the elements of matrix Φ, then the Robertson condition is justified because it led to a solution of equation (5.1).

Having thus reformulated the problem of finding a separable solution to the Helmholtz equation as a problem of finding the matrix Φ solving (5.11), we put our development in temporary stasis to discuss the non-uniqueness of the Stäckel matrix Φ. The development then resumes in Section 7.

6. The non-uniqueness of Stäckel matrix Φ: Equivalence Operations

Suppose one has successfully found a solution for Φ satisfying (5.11). Write it as

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi) \ .$$

The cofactors of the elements of the first column are given by

$$\begin{aligned} M_1(23) &= e(2)i(3)-f(2)h(3) \\ -M_2(31) &= b(1)i(3)-c(1)h(3) \\ M_3(12) &= b(1)f(2)-c(1)e(2) \ . \end{aligned}$$

(1) Look what happens if one scales up the elements of column 2 by constant factor α, and scales down those of column 3 by the same factor. The above three equations become

$$\begin{aligned} M'_1(23) &= \alpha e(2)\,(1/\alpha)i(3)-(1/\alpha)f(2)\alpha h(3) = e(2)i(3)-f(2)h(3) = M_1(23) \\ -M'_2(31) &= \alpha b(1)\,(1/\alpha)i(3)-(1/\alpha)c(1)\alpha h(3) = b(1)i(3)-c(1)h(3) = -M_2(31) \\ M'_3(12) &= \alpha b(1)\,(1/\alpha)f(2)-(1/\alpha)c(1)\alpha e(2) = b(1)f(2)-c(1)e(2) = M_3(12) \end{aligned}$$

Since $S = a(1)\,M_1 + d(2)\,M_2 + g(3)\,M_3$ and the M's stayed the same, S also stays the same, and (5.11) is still satisfied. Therefore, this up/down scaling of the last two columns is an "equivalence" operation for Φ -- it creates a new Stäckel matrix that is just as good as the original Φ. In the special case α = -1, one sees that negating the last two columns of a Stäckel matrix is an equivalence operation.

(2) Next, suppose one swaps columns 2 and 3 and then negates either of the swapped columns. For example, swapping columns 2 and 3 and then negating column 2 gives,

$$\Phi' = \begin{pmatrix} a(1) & -c(1) & b(1) \\ d(2) & -f(2) & e(2) \\ g(3) & -i(3) & h(3) \end{pmatrix} \qquad S = \det(\Phi) \ . \qquad // \ \Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix}$$

A quick inspection shows that $M'_n = M_n$. Also, swapping two columns negates the determinant, and then negating a column restores it. Negating the third column instead of the second is the same as taking Φ' as shown above and negating both columns 2 and 3. But from (1) that is an equivalence operation.

(3) Adding a multiple of one of the last two columns to the other is also an equivalence operation as is now shown. Linear algebra says that such an operation does not change S. Suppose one adds a multiple α of column 2 to column 3:

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi)$$

$$c'(1) = c(1) + \alpha\, b(1)$$
$$f'(2) = f(2) + \alpha\, e(2)$$
$$i'(3) = i(3) + \alpha\, h(3)$$

Then :

$$M_1'(23) = e(2)i'(3)-f'(2)h(3) = e(2)[\, i(3) + \alpha\, h(3)]-[\, f(2) + \alpha\, e(2)]h(3)$$

$$= e(2)i(3)-f(2)h(3) + \alpha\, [e(2)\, h(3) - e(2)\, h(3)] = e(2)i(3)-f(2)h(3) = M_1(23)$$

and similarly for the other two M_n. Of course one could add a multiple of one of the last two columns to the *first* column, and that would also be an equivalence operation since the M_n and S are both unaltered.

Summary of Stäckel Matrix Equivalence Operations

(1) multiply one of the last two columns by any (nonzero) constant α and the other by $1/\alpha$. (6.1)
(2) swap the last two columns of Φ and then negate either of these columns. (6.2)
(3) add any multiple of one of the last two columns to a different column. (6.3)

These rules are useful if one computes a Stäckel matrix and it does not agree with a Stäckel matrix appearing in the literature. Some examples will be shown in Section 12.

7. Solving Problem B

To save writing lots of subscripts, write the to-be-determined Φ matrix as shown above,

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi) \ . \tag{7.1}$$

The cofactors of interest appear in these equations

$$\begin{aligned} M_1(23) &= e(2)i(3)-f(2)h(3) \\ -M_2(31) &= b(1)i(3)-c(1)h(3) \\ M_3(12) &= b(1)f(2)-c(1)e(2) \end{aligned} \tag{7.2}$$

and now insert the M_n expressions from (5.8b) to get

$$\begin{aligned} g_1/(f_2f_3) &= e(2)i(3)-f(2)h(3) \\ -g_2/(f_3f_1) &= b(1)i(3)-c(1)h(3) \\ g_3/(f_1f_2) &= b(1)f(2)-c(1)e(2) \ . \end{aligned} \tag{7.3}$$

Now define rescaled upper-case functions of the form

$$E(2) = e(2)\, f_2(2) \tag{7.4}$$

and similarly for the other five functions appearing above, so (7.3) becomes,

$$\begin{aligned} g_1(23) &= E(2)I(3)-F(2)H(3) \\ -g_2(31) &= B(1)I(3)-C(1)H(3) \\ g_3(12) &= B(1)F(2)-C(1)E(2) \end{aligned} \tag{7.5}$$

where the g_n are those helper functions appearing in (3.5). Recall that it was assumed at the start that the curvilinear coordinate system and its scale factors h_n were *compatible* with the three equations of (3.5) and that one could find a set of 7 functions f_n, g_n and R, all unique apart from constant allocation. In particular, the analysis of (3.5) yields the three g_n which appear on the LHS of equations (7.5). The question is now whether these g_n have the functional form shown in (7.5) ! For example, does the $g_1(23)$ obtained from (3.5) have a form which is at most two terms each showing simple factorization? One has to regard (7.5) as three *functional-form conditions* for the chosen coordinate system! If the g_n don't have the functional form shown in (7.5), then given the three cofactors M_n , one cannot successfully obtain the elements of the rightmost two columns of Φ and the entire plan collapses.

Suppose the g_n *do* in fact have the functional form shown in (7.5). Even in this case, it is not clear that (7.5) can be solved for the capital letter functions. The reason is that there is correlation in the three equations in that each function shows up in two equations. So even if the functional form requirements are met, one still has to actually be able to solve 7.5 for the 6 capital letter functions. If this can be done, then one uses (7.4) to find the lower case functions which are the actual Φ matrix elements for the rightmost two columns.

In many examples studied below, each of equations (7.5) will have only a single term on the RHS. In this case, at least two of the capital letter functions will vanish. (But this does not happen in Section 12.)

We now turn to the S equation which is this from (5.10)

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \qquad (7.6)$$

Of course the $(1/h_n^2)$ and Q(123) objects are completely determined by the choice of coordinate system, so once again one has a functional-form question concerning the solvability of (7.6). To see if it is solvable, we have to examine a specific curvilinear system, or perhaps a family of such systems. When (7.6) has a solution, one often finds that two of the three matrix elements a(1), d(2), g(3) can be set to 0.

In the next two subsections, we summarize first the Conditions needed for a successful separation, then the sequence of Steps needed to actually do the separation.

(a) Conditions required for Separability

If the following conditions are all met, then Problem B (and therefore Problem A) has a solution, and the corresponding curvilinear coordinate system is separable.

<u>Condition (1)</u> Equations (3.5) must be solvable for the 7 functions f_n, g_n and R. If some f_n is a constant, that constant is set to 1. (If one is doing Problem A, R=1.)

$$(H/h_1^2) = f_1(1)g_1(23)\,R^2 \qquad H = h_1h_2h_3$$
$$(H/h_2^2) = f_2(2)g_2(31)\,R^2$$
$$(H/h_3^2) = f_3(3)g_3(12)\,R^2\ . \qquad (3.5)$$

Assuming one can solve equations (3.5), one computes the M_n as follows,

$$M_1 = g_1\,/(f_2f_3) \qquad // = g_1f_1\,/\,(f_2f_2f_3)$$
$$M_2 = g_2\,/(f_3f_1)$$
$$M_3 = g_3\,/(f_1f_2)\ . \qquad (5.8b)$$

<u>Condition (2)</u> Equations (7.2) must have a solution. This is a triplet of functional-form conditions, where the M_n are as given above,

$$M_1(23) = e(2)i(3)-f(2)h(3)$$
$$-M_2(31) = b(1)i(3)-c(1)h(3)$$
$$M_3(12) = b(1)f(2)-c(1)e(2)\ . \qquad (7.2)$$

<u>Condition (3)</u> If conditions (1) and (2) are met, one then does the work of computing Q and k_1^2 from (3.9),

$$\Sigma_n\,(1/[h_n^2f_nR])\,\partial_n\{f_n(\partial_nR)\} \;= -\,k_1^2/Q(123)\ . \qquad (3.9)$$

For Problem A, Q = 1 and $k_1^2 = 0$ and no work is needed.

Then with this Q expression, equation (7.6) must have a solution for a, d and g,

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \qquad (7.6)$$

and this is another functional-form condition.

(b) Steps for finding Φ and related quantities

Here it is assumed that the Conditions of 7(a) are all met, so we proceed with our Stäckel solution. Some of the Steps listed here were already carried out to check the Conditions, but they are listed here anyway. If one knows ahead of time that separation is going to work, one can ignore the Conditions and then just carry out the Steps listed here.

Step 0: Write down the h_n for the curvilinear system of interest and compute $H = h_1h_2h_3$. Perhaps write down other useful facts concerning the system of interest.

Step (1) As noted above, the first task is to solve (3.5) for the 7 functions f_n, g_n and R

$$(H/h_1^2) = f_1(1)g_1(23)\, R^2$$
$$(H/h_2^2) = f_2(2)g_2(31)\, R^2$$
$$(H/h_3^2) = f_3(3)g_3(12)\, R^2\ . \qquad (3.5)$$

This task is pretty much just one of "inspection" when the LHS's of (3.5) are inserted.

Step (2) One can then immediately write down the three first-column cofactors from (5.8b)

$$M_1 = g_1/(f_2f_3)$$
$$M_2 = g_2/(f_3f_1)$$
$$M_3 = g_3/(f_1f_2)\ . \qquad (5.8b)$$

Step (3) If Problem A, then Q = 1. Otherwise compute Q and k_1^2 from (3.9),

$$\Sigma_n\, (1/[h_n^2f_nR])\, \partial_n\{f_n(\partial_nR)\} = -\,k_1^2/Q(123)\ . \qquad (3.9)$$

Step (4) Knowing Q, compute S from the Robertson condition,

$$S(\Phi) = H / (f_1f_2f_3QR^2)\ . \qquad \text{"Robertson condition"} \qquad (5.7)$$

Step (5) One must next find the *rightmost* two columns of the Stäckel matrix,

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi) \ . \qquad (7.1)$$

This can be done by solving the following equation set, using the M_n found in Step (2)

$$\begin{aligned} M_1 &= e(2)i(3)-f(2)h(3) \\ -M_2 &= b(1)i(3)-c(1)h(3) \\ M_3 &= b(1)f(2)-c(1)e(2) \ . \end{aligned} \qquad (7.2)$$

Step (6) One must next find the *first* column of the Stäckel matrix by solving (7.6) or (5.9)

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \qquad (7.6)$$

$$S = a(1)\, M_1 + d(2)\, M_2 + g(3)\, M_3 \qquad (5.9)$$

Step (7) At this point, one may want to apply some of the Section 6 equivalence operations to obtain a Stäckel matrix Φ that is of the simplest possible form, or of a form that matches the literature.

(c) Problem B Example (R-separation of Laplace): Toroidal Coordinates

The Φ matrix

Section 3 (see (3.8) above) states our accumulated facts about toroidal coordinates and their separation, and those facts are copied here :

$$h_1 = h_2 = a/[ch(\xi_1)-\cos(\xi_2)] \quad => \quad h_1 = h_2 = aR^2 \qquad H = sh(\xi_1)a^3R^6$$
$$h_3 = a\, sh(\xi_1)/[ch(\xi_1)-\cos(\xi_2)] \quad => \quad h_3 = a\, sh(\xi_1)R^2$$

$$f_1(1) = sh(\xi_1) \qquad g_1(23) = a \qquad R = [ch(\xi_1)-\cos(\xi_2)]^{-1/2}$$
$$f_2(2) = 1 \qquad g_2(31) = a\, sh(\xi_1) \qquad Q = a^2[ch(\xi_1)-\cos(\xi_2)]^2 = a^2R^4$$
$$f_3(3) = a \qquad g_3(12) = 1/ sh(\xi_1) \qquad k_1^2 = (1/4)$$

Steps (0),(1) and (3) of Section 7 (b) have already been carried out.

For Step (2) compute the cofactors,

$$\begin{aligned} M_1 &= g_1 /(f_2f_3) = a/a = 1 \\ M_2 &= g_2 /(f_3f_1) = a\, sh(\xi_1)/ a\, sh(\xi_1) = 1 \\ M_3 &= g_3 /(f_1f_2) = (1/sh(\xi_1))/(sh(\xi_1) = 1/sh^2(\xi_1) \end{aligned} \qquad (5.8b)$$

For Step (4) one has

$$S(\Phi) = H / ([f_1 f_2 f_3] Q R^2) \quad = sh(\xi_1) a^3 R^6 / ([a\, sh(\xi_1)]\, a^2 R^4\, R^2) = 1$$

For Step (5) :

$$\begin{aligned} M_1(23) &= 1 && = e(2)i(3)-f(2)h(3) \\ -M_2(31) &= -1 && = b(1)i(3)-c(1)h(3) \\ M_3(12) &= 1/sh^2(\xi_1) && = b(1)f(2)-c(1)e(2) \end{aligned} \qquad (7.2)$$

We try h(3) = 0 and f(2) = 0 (trial and error!)

$$\begin{aligned} 1 &= e(2)i(3) \\ -1 &= b(1)i(3) \\ 1/sh^2(\xi_1) &= -c(1)e(2) \end{aligned}$$

The first two lines say e(2) = 1, i(3) = 1 and b(1) = -1. The third line is then

$$1/sh^2(\xi_1) = -c(1)$$

The Stäckel matrix at this point is then

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \Phi = \begin{pmatrix} a(1) & -1 & -1/sh^2(\xi_1) \\ d(2) & 1 & 0 \\ g(3) & 0 & 1 \end{pmatrix}$$

For Step (6) write

$$1/Q = a(1)\,[1/h_1^2] + d(2)\,[1/h_2^2] + g(3)\,[1/h_3^2] \qquad (7.6)$$

$$1/(a^2R^4) = a(1)\,[1/(a^2R^4)] + d(2)\,[1/(a^2R^4)] + g(3)\,[1/(a^2R^4\, sh^2(\xi_1))]$$

$$1 = a(1) + d(2) + g(3)\,[1/(sh^2(\xi_1))]$$

A solution here is a(1) = 1 and d(2) = g(3) = 0. So here is the filled-in Φ matrix along with our results found above:

$$\Phi = \begin{pmatrix} a(1) & -1 & -1/sh^2(\xi_1) \\ d(2) & 1 & 0 \\ g(3) & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -1 & -1/sh^2(\xi_1) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (7.7)$$

$f_1(1) = sh(\xi_1)$	$g_1(23) = a$	$R = [ch(\xi_1)-cos(\xi_2)]^{-1/2}$
$f_2(2) = 1$	$g_2(31) = a\, sh(\xi_1)$	$Q = a^2[ch(\xi_1)-cos(\xi_2)]^2 = a^2R^4$
$f_3(3) = a$	$g_3(12) = 1/ sh(\xi_1)$	$k_1^2 = (1/4)$

$M_1 = 1$ $\qquad\qquad$ $S = 1$
$M_2 = 1$
$M_3 = 1/sh^2(\xi_1)$

These results are in agreement with Moon and Spencer p 112, so Step (7) is not needed.

The separated equations and their solutions: toroidal harmonics

Here then are the separated equations from (5.2)

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\ k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \qquad (5.2)$$

We now install the Φ matrix elements from (7.7) above showing enough lines for the reader to quickly verify each step:

$$L_1X_1 = (1/f_1)\partial_1[f_1(\partial_1X_1)] + [\ k_1^2\Phi_{11}(1) + k_2^2\Phi_{12}(1) + k_3^2\Phi_{13}(1)]X_1 = 0$$
$$L_1X_1 = (1/f_1)\partial_1[f_1(\partial_1X_1)] + [\ k_1^2\ 1 + k_2^2(-1) + k_3^2(-1/sh^2(\xi_1)]X_1 = 0$$
$$L_1X_1 = (1/sh(\xi_1))\partial_1[sh(\xi_1)\ (\partial_1X_1)] + [\ k_1^2 - k_2^2 + k_3^2(-1/sh^2(\xi_1)]X_1 = 0$$
$$L_1X_1 = (1/sh(\xi_1))\{\ sh(\xi_1)\ \partial_1^2X_1 + ch(\xi_1)\ \partial_1X_1\} + [\ k_1^2 - k_2^2 - k_3^2/sh^2(\xi_1)]X_1 = 0$$
$$L_1X_1 = \partial_1^2X_1 + coth(\xi_1)\ \partial_1X_1 + [(1/4) - k_2^2 - k_3^2/sh^2(\xi_1)]X_1 = 0$$

$$L_2X_2 = (1/f_2)\partial_2[f_2(\partial_2X_2)] + [\ k_1^2\Phi_{21}(2) + k_2^2\Phi_{22}(2) + k_3^2\Phi_{23}(2)]X_2 = 0$$
$$L_2X_2 = (1/1)\partial_2[f_1(\partial_2X_2)] + [\ k_1^20 + k_2^21 + k_3^20]X_2 = 0$$
$$L_2X_2 = \partial_2^2X_2 + k_2^2X_2 = 0$$

$$L_3X_3 = (1/f_3)\partial_3[f_3(\partial_3X_3)] + [\ k_1^2\Phi_{31}(3) + k_2^2\Phi_{32}(3) + k_3^2\Phi_{33}(3)]X_3 = 0$$
$$L_3X_3 = (1/a)\partial_3[a(\partial_3X_3)] + [\ k_1^20 + k_2^20 + k_3^21]X_3 = 0$$
$$L_3X_3 = \partial_3^2X_3 + k_3^2X_3 = 0 \quad .$$

So here are the separated equations :

$$L_1X_1 = \partial_1^2X_1 + coth(\xi_1)\ \partial_1X_1\} + [(1/4) - k_2^2 - k_3^2/sh^2(\xi_1)]X_1 = 0$$
$$L_2X_2 = \partial_2^2X_2 + k_2^2X_2 = 0$$
$$L_3X_3 = \partial_3^2X_3 + k_3^2X_3 = 0 \quad .$$

in agreement with Moon and Spencer page 114. For this system, the appearance of the separation constants in the last two separated equations looks just like our c_2 and c_3 equations shown in (3.12) for Cartesian coordinates. However, the first equation involves both separation constants in a tangled manner. For ellipsoidal coordinates in Section 12, one finds full entanglement in all three separation equations.

Moon and Spencer use $k_2^2 = \alpha_2 = p^2$ and $k_3^2 = \alpha_3 = q^2$. Whereas the X_2 and X_3 are simple trig functions, the X_1 (it turns out) are Legendre functions of the type $P^q{}_{p-1/2}(ch\xi_1)$. Thus, in a most-general toroidal problem, the **"toroidal harmonics"** would be (we have added 1/R on the right to get $\psi = X_1X_2X_3/R$)

$[P^q{}_{p-1/2}(\mathrm{ch}\xi_1), Q^q{}_{p-1/2}(\mathrm{ch}\xi_1)$ [$\sin(p\xi_2), \cos(p\xi_2)$] [$\sin(q\xi_3), \cos(q\xi_3)$] * $[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{1/2}$.

This notation means that each bracket $[f_1, f_2]$ can be an arbitrary linear combination Af_1+Bf_2 and the constants can be different for each bracket. The functions are called "harmonics" because they are functions which solve the Laplace equation. Elsewhere we refer to the above combinations as "atoms" or "atomic forms" with the idea that one can assemble a problem solution by linearly combining the atoms.

Since ξ_3 is an azimuthal coordinate, in a problem with a full 2π azimuthal range one would find that $k_3 = q$ was an integer, and in an problem with azimuthal symmetry one finds q = 0. Legendre functions of this kind are called toroidal or ring functions. If $k_2^2 = p^2 < 0$, one writes $p = i\tau$ to get

$[P^q{}_{i\tau-1/2}(\mathrm{ch}\xi_1), Q^q{}_{i\tau-1/2}(\mathrm{ch}\xi_1)$ [$\mathrm{sh}(\tau\xi_2), \mathrm{ch}(\tau\xi_2)$] [$\sin(q\xi_3), \cos(q\xi_3)$] * $[\mathrm{ch}(\xi_1)-\cos(\xi_2)]^{1/2}$

and Legendre functions of this type are called Mehler functions.

(d) Problem A Example (simple-separation of Helmholtz): Circular Cylindrical Coordinates

The Φ matrix

Here are the Steps of Section 7 (b) :

Step (0)

$1,2,3 = \rho,\varphi,z$

$h_1 = 1$ $\quad h_2 = \xi_1$ $\quad h_3 = 1$ $\quad H = \xi_1$ $\quad R = 1$

Step (1) Examine equation (3.5) with R=1

$(H/h_n^2) = f_n(n)g_n(\neq n)$ $\qquad n = 1,2,3$

$\xi_1 = f_1(1)g_1(23) = [\ \xi_1\ ][\ 1\ ]$ => $f_1 = \xi_1$ $\quad g_1 = 1$
$1/\xi_1 = f_2(2)g_3(31) = [\ 1\ ][\ 1/\xi_1]$ => $f_2 = 1$ $\quad g_2 = 1/\xi_1$
$\xi_1 = f_3(3)g_3(12) = [1][\ \xi_1]$ => $f_3 = 1$ $\quad g_3 = \xi_1$

Step (2)

$M_1 = g_1/(f_2f_3) = 1/1 = 1$
$M_2 = g_2/(f_3f_1) = (1/\xi_1)/\xi_1 = 1/\xi_1^2$
$M_3 = g_3/(f_1f_2) = \xi_1/\alpha_1 = 1$ *(5.8b)*

Step (3) $\quad Q = 1 \quad k_1^2 = 0$

Step (4) $\quad S(\Phi) = H / ([f_1f_2f_3]QR^2) = \xi_1/(\xi_1) = 1$

Step (5)

$$M_1(23) = 1 \quad = e(2)i(3)-f(2)h(3)$$
$$-M_2(31) = -1/\xi_1^2 = b(1)i(3)-c(1)h(3)$$
$$M_3(12) = 1 \quad = b(1)f(2)-c(1)e(2) \qquad (7.2)$$

Try h(3) = 0 and f(2) = 0

$$1 = e(2)i(3) \quad \Rightarrow \quad e(2) = 1 \text{ and } i(3) = 1$$
$$1/\xi_1^2 = -b(1)i(3)$$
$$1 = -c(1)e(2) \quad \Rightarrow \quad c(1) = -1$$

The second line then says $-1/\xi_1^2 = b(1)$. The Stäckel matrix at this point is then

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \begin{pmatrix} a(1) & -1/\xi_1^2 & -1 \\ d(2) & 1 & 0 \\ g(3) & 0 & 1 \end{pmatrix}$$

Step (6)

$$1/Q = a(1)\,[1/h_1^2] + d(2)\,[1/h_2^2] + g(3)\,[1/h_3^2] \qquad (7.6)$$
$$1 = a(1)\,1 + d(2)\,[1/\xi_1^2] + g(3)\,1$$

One can then take g(3) = 1 and a(1) = d(2) = 0. So here is the filled-in Φ matrix along with the results found above:

$$\Phi = \begin{pmatrix} a(1) & -1/\xi_1^2 & -1 \\ d(2) & 1 & 0 \\ g(3) & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1/\xi_1^2 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$f_1(1) = \xi_1 \qquad g_1(23) = 1 \qquad R = 1$$
$$f_2(2) = 1 \qquad g_2(31) = 1/\xi_1 \qquad Q = 1 \qquad (7.8)$$
$$f_3(3) = 1 \qquad g_3(12) = \xi_1 \qquad k_1^2 = 0$$

$$M_1 = 1 \qquad S = 1$$
$$M_2 = 1/\xi_1^2$$
$$M_3 = 1$$

These results are in agreement with Moon and Spencer p 12, so we don't need Step (7).

The separated equations and their solutions: cylindrical harmonics

Here then are the separated equations from (5.2)

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\, k_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \quad . \qquad (5.2)$$

We now install the Φ matrix elements from (7.8),

$$L_1X_1 = (1/f_1)\partial_1[f_1(\partial_1X_1)] + [\, K_1^2\Phi_{11}(1) + k_2^2\Phi_{12}(1) + k_3^2\Phi_{13}(1)]X_1 = 0$$
$$L_1X_1 = (1/\xi_1)\partial_1[\xi_1(\partial_1X_1)] + [\, -k_2^2/\xi_1^2 - k_3^2]X_1 = 0$$
$$L_1X_1 = \partial_1^2X_1 + (1/\xi_1)(\partial_1X_1) - [\, k_2^2/\xi_1^2 + k_3^2]X_1 = 0$$

$$L_2X_2 = (1/f_2)\partial_2[f_2(\partial_2X_2)] + [\, K_1^2\Phi_{21}(2) + k_2^2\Phi_{22}(2) + k_3^2\Phi_{23}(2)]X_2 = 0$$
$$L_2X_2 = (1/1)\partial_2[1(\partial_2X_2)] + [\, K_1^2 0 + k_2^2 1 + k_3^2 0]X_2 = 0$$
$$L_2X_2 = \partial_2^2X_2 + k_2^2X_2 = 0$$

$$L_3X_3 = (1/f_3)\partial_3[f_3(\partial_3X_3)] + [\, K_1^2\Phi_{31}(3) + k_2^2\Phi_{32}(3) + k_3^2\Phi_{33}(3)]X_3 = 0$$
$$L_3X_3 = (1/1)\partial_3[1(\partial_3X_3)] + [\, K_1^2 1 + k_2^2 0 + k_3^2 1)]X_3 = 0$$
$$L_3X_3 = \partial_3^2X_3 + (K_1^2 + k_3^2)]X_3 = 0 \quad .$$

So here are the separated equations :

$$L_1X_1 = \partial_1^2X_1 + (1/\xi_1)(\partial_1X_1) - [\, k_2^2/\xi_1^2 + k_3^2]X_1 = 0$$
$$L_2X_2 = \partial_2^2X_2 + k_2^2X_2 = 0$$
$$L_3X_3 = \partial_3^2X_3 + (K_1^2 + k_3^2)]X_3 = 0 \quad .$$

in agreement with Moon and Spencer page 15 (they use $K_1^2 = \kappa^2$, $k_2^2 = \alpha_2 = p^2$, and $k_3^2= \alpha_3 = q^2$). The solutions of the X_1 equation have the form $J_p(iq\xi_1)$. The X_2 is trig of the form $\sin(k_2\xi_2)$, and X_3 is also trig of the form $\sin(\sqrt{K_1^2 + k_3^2}\ \xi_3)$. The **"cylindrical harmonics"** can then be written (R=1 so $\psi = X_1X_2X_3$)

$$[J_p(ik_3\xi_1), Y_p(i\, k_3\xi_1)]\ [\sin(k_2\xi_2), \cos(k_2\xi_2)]\ [\sin(\sqrt{K_1^2 + k_3^2}\ \xi_3), \cos(\sqrt{K_1^2 + k_3^2}\ \xi_3)]$$

or (ignoring constants) one can put in the usual modified Bessel functions,

$$[I_p(k_3\xi_1), K_p(k_3\xi_1)]\ [\sin(k_2\xi_2), \cos(k_2\xi_2)]\ [\sin(\sqrt{K_1^2 + k_3^2}\ \xi_3), \cos(\sqrt{K_1^2 + k_3^2}\ \xi_3)]$$

all of which agrees with Moon and Spencer page 15. Notice that if we had selected a(1) = 1 back in Step (6), the constants get shuffled around in the three factors in a trivial manner. The point here is that k_2 and k_3 are arbitrary separation constants and one can "shuffle" them however one wants. If $k_3^2 < 0$, then $k_3 = -i\sigma_3$ to get these harmonics instead.

$$[J_p(\sigma_3\xi_1), Y_p(\sigma_3\xi_1)]\ [\sin(k_2\xi_2), \cos(k_2\xi_2)]\ [\sin(\sqrt{K_1^2 - \sigma_3^2}\ \xi_3), \cos(\sqrt{K_1^2 - s_3^2}\ \xi_3)] \quad .$$

8. Separability in Cylindrical Systems when $h_1 \neq \alpha\, h_2$

For the moment, assume some *general* h_1 and h_2 where one h is not just a multiple of the other. They define a 2D orthogonal system of some sort. Then just extrude in the "z direction" (ξ_3) to get a 3D cylindrical coordinate system. This gives

$$h_1 = h_1(12) \qquad (8.1)$$
$$h_2 = h_2(12)$$
$$h_3 = 1 \qquad H = h_1 h_2 \qquad H/h_1^2 = h_2/h_1 \quad H/h_2^2 = h_1/h_2 \quad H/h_3^2 = h_1 h_2 \ .$$

Here then is an examination of the Conditions stated in Section 7 (a) applied to this situation, with a summary at the end:

Condition (1) From (3.5)

$$(H/h_1^2) = f_1(1) g_1(23)\, R^2$$
$$(H/h_2^2) = f_2(2) g_2(31)\, R^2$$
$$(H/h_3^2) = f_3(3) g_3(12)\, R^2 \ . \qquad \textit{(3.5)}$$

One can define some new functions $G_1(2)$ and $G_2(1)$ that might simplify things in terms of functional form, since the h_1 and h_2 scale factors don't depend on coordinate 3:

$$(h_2/h_1) = f_1(1)\, g_1(23) R^2 \quad \Rightarrow \quad g_1(23) \equiv G_1(2)$$
$$(h_1/h_2) = f_2(2)\, g_2(13) R^2 \quad \Rightarrow \quad g_2(13) \equiv G_2(1)$$
$$(h_1 h_2) = f_3(3)\, g_3(12) R^2 \quad \Rightarrow \quad f_3(3) = 1 \qquad (8.2)$$

or

$$(h_2/h_1) = f_1(1)\, G_1(2) R^2$$
$$(h_1/h_2) = f_2(2)\, G_2(1) R^2$$
$$(h_1 h_2) = g_3(12) R^2 \ . \qquad (8.3)$$

One is still faced with the problem of solving (8.3) for the 6 functions f_1, f_2, G_1, G_2, g_3 and R. It is not clear that a solution set exists for some very strange h_1 and h_2.

For example, suppose $h_1 = 1$ and $h_2 = \sqrt{\xi_1^2 - \xi_2^2}$. The first equation of (8.3) forces $f_1 = G_1 = 1$ and then $R^2 = \sqrt{\xi_1^2 - \xi_2^2}$. Then the second equation says $1/\sqrt{\xi_1^2 - \xi_2^2} = f_2(2)\, G_2(1) \sqrt{\xi_1^2 - \xi_2^2}$ and one ends up with $f_2(2)\, G_2(1) = 1/(\xi_1^2 - \xi_2^2)$ and there is no solution for f_2 and G_2 that works.

So the duty to find the solutions to (3.5) remains for cylindrical systems. If there is a solution, one can multiply the first two equations of (8.3) to find that R must have this form

$$1/R^4 = [f_1(1)\, G_2(1)]\, [G_1(2)\, f_2(2)] \qquad (8.4)$$

so R is seen to factorize into $R = r_1(1)\, r_2(2)$. One can also compute the three cofactors

$$M_1 = g_1 /(f_2 f_3) = G_1(2)/f_2(2)$$
$$M_2 = g_2 /(f_3 f_1) = G_2(1)/f_1(1)$$
$$M_3 = g_3 /(f_1 f_2) = g_3(12) /[f_1(1)f_2(2)] \quad . \qquad \textit{(5.8b)}$$

<u>Condition (2)</u> requires the solution of

$$M_1(23) = e(2)i(3)-f(2)h(3)$$
$$-M_2(31) = b(1)i(3)-c(1)h(3)$$
$$M_3(12) = b(1)f(2)-c(1)e(2) \qquad \textit{(7.2)}$$

and in the current situation this says

$$G_1(2)/f_2(2) = e(2)i(3)-f(2)h(3)$$
$$- G_2(1)/f_1(1) = b(1)i(3)-c(1)h(3)$$
$$g_3(12) /[f_1(1)f_2(2)] = b(1)f(2)-c(1)e(2) \quad .$$

From the first line we must choose either i(3) = 0 or h(3) = 0 and we choose the latter. The reader can show that selecting i(3) = 0 introduces nothing new. Then the above becomes

$$G_1(2)/f_2(2) = e(2)i(3)$$
$$- G_2(1)/f_1(1) = b(1)i(3)$$
$$g_3(12) /[f_1(1)f_2(2)] = b(1)f(2)-c(1)e(2) \quad .$$

From the first two lines select

$$e(2) = G_1(2)/f_2(2) \qquad i(3) = 1$$
$$b(1) = - G_2(1)/f_1(1) \qquad i(3) = 1 \quad .$$

The third line then says

$$g_3(12) /[f_1(1)f_2(2)] = [- G_2(1)/f_1(1)]f(2) - c(1)[G_1(2)/f_2(2)]$$
$$g_3(12) = [- G_2(1) f_2(2)]f(2) - c(1)f_1(1)G_1(2)$$

or

$$- g_3(12) = c(1)f_1(1)G_1(2) + f(2) f_2(2) G_2(1) \quad . \qquad (8.5)$$

This is a very strict requirement on the form $g_3(12)$ must have in order to allow the Stäckel separation process to succeed. One is free to select c(1) and f(2), but $G_1(2)$, $G_2(1)$ and f_1,f_2 are already determined and none of these factors vanishes. Installation of (8.5) and then (8.4) into the last line of (8.3) gives

$$-(h_1h_2) = -g_3(12)R^2 = [c(1)\, f_1(1)G_1(2) + f(2)\, f_2(2)\, G_2(1)]\, R^2$$

$$= [c(1)\, f_1(1)G_1(2) + f(2)\, f_2(2)\, G_2(1)] / \{ [f_1(1)\, G_2(1)]^{1/2} [f_2(2)G_1(2)]^{1/2}\}$$

$$= c(1)\, f_1(1)G_1(2) / \{ [f_1(1)\, G_2(1)]^{1/2} [f_2(2)G_1(2)]^{1/2}\}$$
$$+ f(2)\, f_2(2)\, G_2(1)] / \{ [f_1(1)\, G_2(1)]^{1/2} [f_2(2)G_1(2)]^{1/2}\}$$

$$= c(1)\, [f_1(1)\, G_2(1)]^{1/2} / [f_2(2)G_1(2)]^{1/2}$$
$$+ f(2)\, [f_2(2)G_1(2)]^{1/2} / [f_1(1)\, G_2(1)]^{1/2} .$$

Absorbing $[f_1(1)\, G_2(1)]^{1/2}$ into c(1) and similarly for f(2),

$$c(1)\, [f_1(1)\, G_2(1)]^{1/2} \equiv c'(1) \qquad [f_2(2)G_1(2)]^{1/2} f(2) \equiv f'(2) ,$$

produces this functional form requirement

$$-(h_1h_2) = c'(1) / [f_2(2)G_1(2)]^{1/2} + f'(2) / [f_1(1)G_2(1)]^{1/2} , \tag{8.6}$$

so one must find c'(1) and f'(2) to satisfy this equation. So condition (8.5) is replaced with a condition directly on the product of the scale factors, and it still looks very strict for some completely arbitrary pair of functions $h_1(12)$ and $h_2(12)$. Equation (8.6) can be regarded as Condition 2.

Assuming Conditions (1) and (2) are met as just outlined, one can construct the Stäckel matrix Φ

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \begin{pmatrix} a(1) & -G_2(1)/f_1(1) & c(1) \\ d(2) & G_1(2)/f_2(2) & f(2) \\ g(3) & 0 & 1 \end{pmatrix} .$$

<u>Condition (3)</u> One is supposed to compute Q using (3.9) which says

$$\Sigma_n (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} = -k_1^2/Q(123) . \tag{3.9}$$

Since $\partial_3 R = 0$, there will be only two terms in the sum

$$-k_1^2/Q(123) = (1/[h_1^2 f_1 R])\, [\partial_1\{f_1(\partial_1 R)\}] + (1/[h_2^2 f_2 R])\, [\partial_2\{f_2(\partial_2 R)\}]$$

$$= (1/[h_1^2 f_1 R])\, [\partial_1\{f_1(\partial_1 R)\}] + (1/[h_2^2 f_2 R])\, [\partial_2\{f_2(\partial_2 R)\}] = T1 + T2$$

Putting these terms into Maple as T1 and T2 with $R^{-4} = f_1g_1f_2g_2$ from (8.4), Maple does the derivatives:

```
T1 := 1/(h1(x1,x2)^2*f1(x1)*R(x1,x2))*diff(f1(x1)*diff(R(x1,x2),x1),x1):simplify(%);
```

$$\frac{\left(\frac{\partial}{\partial x1}\mathrm{f1}(x1)\right)\left(\frac{\partial}{\partial x1}\mathrm{R}(x1,x2)\right)+\mathrm{f1}(x1)\left(\frac{\partial^2}{\partial x1^2}\mathrm{R}(x1,x2)\right)}{\mathrm{h1}(x1,x2)^2\,\mathrm{f1}(x1)\,\mathrm{R}(x1,x2)}$$

```
T2 := 1/(h2(x1,x2)^2*f2(x2)*R(x1,x2))*diff(f2(x2)*diff(R(x1,x2),x2),x2):simplify(%);
```

$$\frac{\left(\frac{\partial}{\partial x2}\mathrm{f2}(x2)\right)\left(\frac{\partial}{\partial x2}\mathrm{R}(x1,x2)\right)+\mathrm{f2}(x2)\left(\frac{\partial^2}{\partial x2^2}\mathrm{R}(x1,x2)\right)}{\mathrm{h2}(x1,x2)^2\,\mathrm{f2}(x2)\,\mathrm{R}(x1,x2)}$$

```
R := (x1,x2) -> (f1(x1)*G2(x1)*G1(x2)*f2(x2))^(-1/4);
```

$$R := (x1,x2) \to \frac{1}{(\mathrm{f1}(x1)\,\mathrm{G2}(x1)\,\mathrm{G1}(x2)\,\mathrm{f2}(x2))^{\left(\frac{1}{4}\right)}}$$

```
T1: simplify(%);
```

$$-\frac{1}{16}\frac{-\left(\frac{\partial}{\partial x1}\mathrm{f1}(x1)\right)^2\mathrm{G2}(x1)^2+2\left(\frac{\partial}{\partial x1}\mathrm{f1}(x1)\right)\mathrm{G2}(x1)\,\mathrm{f1}(x1)\left(\frac{\partial}{\partial x1}\mathrm{G2}(x1)\right)-5\,\mathrm{f1}(x1)^2\left(\frac{\partial}{\partial x1}\mathrm{G2}(x1)\right)^2+4\,\mathrm{f1}(x1)\,\mathrm{G2}(x1)^2\left(\frac{\partial^2}{\partial x1^2}\mathrm{f1}(x1)\right)+4\,\mathrm{f1}(x1)^2\,\mathrm{G2}(x1)\left(\frac{\partial^2}{\partial x1^2}\mathrm{G2}(x1)\right)}{\mathrm{f1}(x1)^2\,\mathrm{G2}(x1)^2\,\mathrm{h1}(x1,x2)^2}$$

```
T2: simplify(%);
```

$$\frac{1}{16}\frac{-2\left(\frac{\partial}{\partial x2}\mathrm{G1}(x2)\right)\mathrm{f2}(x2)\,\mathrm{G1}(x2)\left(\frac{\partial}{\partial x2}\mathrm{f2}(x2)\right)+\mathrm{G1}(x2)^2\left(\frac{\partial}{\partial x2}\mathrm{f2}(x2)\right)^2+5\left(\frac{\partial}{\partial x2}\mathrm{G1}(x2)\right)^2\mathrm{f2}(x2)^2-4\,\mathrm{G1}(x2)\,\mathrm{f2}(x2)^2\left(\frac{\partial^2}{\partial x2^2}\mathrm{G1}(x2)\right)-4\,\mathrm{f2}(x2)\,\mathrm{G1}(x2)^2\left(\frac{\partial^2}{\partial x2^2}\mathrm{f2}(x2)\right)}{\mathrm{f2}(x2)^2\,\mathrm{G1}(x2)^2\,\mathrm{h2}(x1,x2)^2}$$

The details are less important than the general form of the result, visible from the last lines above,

$$T1 = t_1(1) / h_1^2$$
$$T2 = t_2(2) / h_2^2$$

$$\Rightarrow\ - k_1^2/Q(12) = t_1(1) / h_1^2 + t_2(2) / h_2^2 \quad . \tag{8.7}$$

Now having to some extent computed Q, one must examine condition (7.6),

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \tag{8.8}$$
$$1/Q(12) = a(1)\,(1/h_1(12)^2) + d(2)\,(1/h_2(12)^2) + g(3)\ 1\ .$$

Since Q = Q(12), g(3) must be a constant. As an ansatz set g(3)=0 to see if a solution results. Then,

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) \quad .$$

Comparing this to (8.7) one can make these choices

$a(1) = - t_1(1)/k_1^2$ $d(2) = - t_2(2)/k_1^2$ and of course $g(3) = 0$

so the Φ matrix now has this form

$$\Phi = \begin{pmatrix} a(1) & - G_2(1)/f_1(1) & c(1) \\ d(2) & G_1(2)/f_2(2) & f(2) \\ g(3) & 0 & 1 \end{pmatrix} = \begin{pmatrix} - t_1(1)/k_1^2 & - G_2(1)/f_1(1) & c(1) \\ - t_2(2)/k_1^2 & G_1(2)/f_2(2) & f(2) \\ 0 & 0 & 1 \end{pmatrix}$$

Summary of the three conditions:

(1) One must be able to find f_1, f_2, G_1, G_2, g_3 and R which satisfy these functional-form equations,

$$(h_2/h_1) = f_1(1)\, G_1(2)R^2$$
$$(h_1/h_2) = f_2(2)\, G_2(1)R^2$$
$$(h_1h_2) = g_3(12)R^2 \qquad (8.3)$$

(2) One must be able to find c'(1) and f'(2) which satisfy this functional form equation,

$$-(h_1h_2) = c'(1) / [f_2(2)G_1(2)]^{1/2} + f'(2) / [f_1(1)\, G_2(1)]^{1/2} \qquad (8.6)$$

(3) One *can* meet condition (3) for sure, and the first column of Φ is as shown above. If Q = 1, choose g(3) = 1 and the two elements above it 0.

Example: Circular cylindrical coordinates revisited

Cylindrical systems with $h_1 \neq \alpha\, h_2$ are uncommon for the reason discussed at the end of the next section, but there is one notable exception: circular cylinder coordinates, which we shall call ρ,φ,z. If one defines the ξ_n according to ρ,φ,z = exp(ξ_1),ξ_2,ξ_3, then this system fits into the conformal-mapping-of-Cartesians framework and one finds $h_1 = h_2 = \exp(2\xi_1)$, as in Moon and Spencer p 13. But normally one takes ρ,φ,z = ξ_1,ξ_2,ξ_3 so that $h_1 = 1$ and $h_2 = \xi_1$, so one can consider this system as an example of a cylindrical system with $h_1 \neq \alpha h_2$. This system was fully analyzed in Section 7 (d), so we just examine the first two conditions summarized above to see how they work out:

Condition (1): $h_1 = 1$ $h_2 = \xi_1$ and we know the R = 1

$$(h_2/h_1) = f_1(1)\, G_1(2)R^2$$
$$(h_1/h_2) = f_2(2)\, G_2(1))R^2$$
$$(h_1h_2) = g_3(12)R^2 \qquad (8.3)$$

$$\xi_1 = f_1(1)\, G_1(2)$$
$$1/\xi_1 = f_2(2)\, G_2(1)$$
$$\xi_1 = g_3(12)$$

Inspection shows a simple solution to equation (3.5),

$f_1(1) = \xi_1$	$G_1(2) = 1$	R=1	=>	Q=1 and $k_1^2 = 0$
$f_2(2) = 1$	$G_2(1)= 1/\xi_1$			
$f_3(3) = 1$	$g_3(12) = \xi_1$			

Condition (2):

$$-(h_1 h_2) = c'(1) / [f_2(2) G_1(2)]^{1/2} + f'(2) / [f_1(1) G_2(1)]^{1/2} \tag{8.6}$$

$$-\xi_1 = c'(1) / [1 * 1]^{1/2} + f'(2) / [\xi_1 * \xi_1^{-1}]^{1/2}$$

$$-\xi_1 = c'(1) + f'(2)$$

So this condition, noted in the general case to be "strict", has in this system the simple solution,

$$c'(1) = -\xi_1 \qquad f'(2) = 0 \qquad \Rightarrow \qquad c(1) = -1 \qquad f(2) = 0$$

Since Q=1, one can take g(3)=1 and a(1) = d(2) = 0 for the first column, so Φ comes out exactly as found in Section (7d),

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \begin{pmatrix} a(1) & -G_2(1)/f_1(1) & c(1) \\ d(2) & G_1(2)/f_2(2) & f(2) \\ g(3) & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1/\xi_1^2 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

9. Separability in Cylindrical Systems when $h_2 = \alpha h_1$

We review the three Conditions summarized just above (end of Section 8), but now instead of general h_1 and h_2, it is assumed that $h_2 = \alpha h_1$, α = a fixed constant.

The Conditions

(1) It must be possible to solve equations (8.3) for the 6 functions f_1, f_2, G_1, G_2, g_3 and R

$$(h_2/h_1) = f_1(1)\, G_1(2) R^2$$
$$(h_1/h_2) = f_2(2)\, G_2(1) R^2$$
$$(h_1 h_2) = g_3(12) R^2 \quad . \qquad \textit{(8.3)}$$

In this case,

$$\alpha = f_1(1)\, G_1(2) R^2$$
$$\alpha^{-1} = f_2(2)\, G_2(1) R^2$$
$$\alpha h_1^2 = g_3(12) R^2 \quad . \qquad (9.1)$$

Try R = 1 and search for a solution to

$$\alpha = f_1(1)\, G_1(2)$$
$$1/\alpha = f_2(2)\, G_2(1)$$
$$\alpha h_1^2 = g_3(12) \; .$$

The solution is pretty clear (recall $f_3 = 1$ for any cylindrical system),

$$f_1 = f_2 = f_3 = 1 \qquad G_1(2) = \alpha \quad G_2(1) = 1/\alpha \qquad g_3 = \alpha\, h_1^2 \qquad R=Q=1 \; . \qquad (9.2)$$

Since a solution was found, the R=1 assumption is justified.

(2) This condition was

$$-(h_1 h_2) = c'(1) / [f_2(2) G_1(2)]^{1/2} + f'(2) / [f_1(1)\, G_2(1)]^{1/2} \; . \qquad \textit{(8.8)}$$

It looked fairly strict in general, but in the current situation it says

$$- \alpha h_1^2 = c'(1) /\sqrt{\alpha} + f'(2) \sqrt{\alpha} \; . \qquad (9.3)$$

Tracing back we had

$$c(1)\, [f_1(1)\, G_2(1)]^{1/2} \equiv c'(1) \qquad f(2)\, [f_2(2) G_1(2)]^{1/2} \equiv f'(2)$$

or

$$c(1)\, [1/\alpha]^{1/2} \equiv c'(1) \qquad f(2)\, [\alpha]^{1/2} \equiv f'(2)$$

so that Condition 2 above becomes

$$- \alpha h_1^2 = c(1)/\alpha + f(2)\,\alpha$$

or

$$- h_1^2 = c(1)/\alpha^2 + f(2) . \tag{9.4}$$

(3) We shall redo this condition from scratch. The general condition is

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \tag{8.6}$$

but since Q = 1 and $h_3 = 1$ this becomes

$$1 = a(1)\,(1/h_1^2) + d(2)\,(1/\alpha^2 h_1^2) + g(3) . \tag{9.5}$$

The obvious solution here is a(1) = 0 , d(2) = 0 and g(3) = 1. The Stäckel matrix from Section 8 now takes this form

$$\Phi = \begin{pmatrix} a(1) & -G_2(1)/f_1(1) & c(1) \\ d(2) & G_1(2)/f_2(2) & f(2) \\ g(3) & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1/\alpha & c(1) \\ 0 & \alpha & f(2) \\ 1 & 0 & 1 \end{pmatrix} \tag{9.6}$$

This agrees in its general form with Moon and Spencer on page 7 equation (1.28).

Summary of Conditions: The only real condition for separation of this kind of coordinate system is the Condition 2 requirement found above,

$$- h_1^2 = c(1)/\alpha^2 + f(2) \tag{9.4}$$

and this, assuming it can be satisfied, fills in the two missing elements in the Φ matrix above.

Condition (9.4) of course rules out something like $\alpha = 1$ and $h_1^2 = (\xi_1^2 + \xi_2)^{-2}$ as occurs in "tangent cylinder coordinates" (Moon and Spencer p 79). That is to say, the general Laplace equation cannot be separated in such coordinates.

The Steps

From Section 7 (b) we track our 7 steps for the case $h_2 = \alpha h_1$:

Step (1) : Already done above where it was found that

$$f_1=f_2=f_3=1 \qquad G_1(2) = \alpha \quad G_2(1) = 1/\alpha \qquad g_3 = \alpha h_1^2 \qquad R=Q=1 \tag{9.2}$$

Step (2):

$M_1 = g_1 /(f_2f_3) = \alpha/1 = \alpha$
$M_2 = g_2 /(f_3f_1) = (1/\alpha)/1 = 1/\alpha$
$M_3 = g_3 /(f_1f_2) = \alpha h_1^2$ *(5.8b)*

Step (3): $R = 1$ so $Q = 1$

Step (4): $S = [H / (f_1f_2f_3QR^2)] = H = h_1h_2h_3 = \alpha h_1^2$

Step (5) and Step (6): Already done above where it was found that

$$\Phi = \begin{pmatrix} 0 & -1/\alpha & c(1) \\ 0 & \alpha & f(2) \\ 1 & 0 & 1 \end{pmatrix} \qquad \text{where } -h_1^2 = c(1)/\alpha^2 + f(2)$$

Moon and Spencer page 7 equation (1.28) gives a general form for the Stäckel matrix associated with a cylindrical system

$$\Phi = \begin{pmatrix} 0 & * & * \\ 0 & * & * \\ 1 & 0 & 1 \end{pmatrix}$$

and this is seen to agree with our result above.

Special Case $h_1 = h_2$

Practical curvilinear cylindrical coordinate systems have $h_1 = h_2$ so $\alpha = 1$, and for such systems the results above can be summarized :

$f_1=f_2=f_3=1$ $G_1(2) = 1$ $G_2(1) = 1$ $g_3 = h_1^2$ $R=Q=1$ *(9.2)*

$M_1 = 1$
$M_2 = 1$
$M_3 = h_1^2$ $S = h_1^2$ *(5.8b)*

$$\Phi = \begin{pmatrix} 0 & -1 & c(1) \\ 0 & 1 & f(2) \\ 1 & 0 & 1 \end{pmatrix} \qquad \text{where } -h_1^2 = c(1) + f(2)$$

This says $g_3 = M_3 = S = h_1^2$ so we won't repeat those results in the following examples. The critical functional-form condition is that $- h_1^2 = c(1) + f(2)$.

Example 1: elliptic cylinder coordinates

For this system,

$$h_1^2 = (\xi_1^2 + \xi_2^2) = -c(1) - f(2) \quad => \quad c(1) = -\xi_1^2 \qquad f(2) = -\xi_2^2$$

$$\Phi = \begin{pmatrix} 0 & -1 & c(1) \\ 0 & 1 & f(2) \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & -a^2 ch^2(\xi_1) \\ 0 & 1 & a^2\cos^2(\xi_2) \\ 1 & 0 & 1 \end{pmatrix}$$ // agrees with Moon and Spencer p 17 η,ψ,z

Example 2: parabolic cylinder coordinates

For this system,

$$h_1^2 = a^2 ch^2(\xi_1) - a^2\cos^2(\xi_2) = -c(1) - f(2) \quad => \quad c(1) = -a^2 ch^2(\xi_1) \qquad f(2) = a^2\cos^2(\xi_2)$$

$$\Phi = \begin{pmatrix} 0 & -1 & c(1) \\ 0 & 1 & f(2) \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & -\xi_1^2 \\ 0 & 1 & -\xi_2^2 \\ 1 & 0 & 1 \end{pmatrix}$$ // agrees with Moon and Spencer p 21 μ,ν,z

Example 3: circular cylinder coordinates

This case was treated in Section 7 (d) above, where $h_1 = 1$ and $h_2 = \xi_1 = r$. One can do an alternate analysis defining ξ_1 by $r = \exp(\xi_1)$, and in this case it turns out that $h_1 = h_2 = \exp(\xi_1)$ so,

$$h_1^2 = \exp(2\xi_1) = -c(1) - f(2) \quad => \quad c(1) = -\exp(2\xi_1) \qquad f(2) = 0$$

$$\Phi = \begin{pmatrix} 0 & -1 & c(1) \\ 0 & 1 & f(2) \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & -\exp(2\xi_1) \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$ // see Moon and Spencer p 13 ξ,ψ,z

Moon and Spencer have a rare typo in this matrix. They show its upper right element as $-\exp(-2\xi)$ which then disagrees with their $M_1 = \exp(2\xi)$ and $S = \exp(2\xi)$.

The 21 cylindrical systems of Moon and Spencer

In their third chapter (called Section III) Moon and Spencer consider 21 cylindrical curvilinear coordinate systems which presumably have proven useful in some applications. Each of these systems is obtained by doing some conformal mapping $w = f(z)$ of the Cartesian coordinates $z = x+iy$ to get $w = \xi_1+i\xi_2$. Such mappings preserve scaling, which is why $h_1 = h_2$, and also preserve angles, so the orthogonality of the Cartesian system maps into the orthogonality of the (ξ_1,ξ_2) system. Of these 21 systems, 18 do NOT meet our Condition 2 which says $-h_1^2 = c(1) + f(2)$, and are therefore not separable! Only 3 of the 21 systems are separable, and they are the three cylindrical examples presented above, all simple-separable for Helmholtz. These 3 systems are among the 11 classical systems Moon and Spencer discuss in their first chapter. In addition to Cartesian, the remaining 7 classical systems are: ellipsoidal and its two subcases prolate and oblate spheroidal and their special case spherical; parabolic-cylinder, parabolic (paraboloidal) and conical. Moon and Spencer give excellent data sets for all 11 systems including good drawings, which seem clearer than the interesting but hard to focus stereoscopic images of Morse and Feshbach. For the 21 cylindrical systems Moon and Spencer also have collected data including detailed 2D drawings of the level curves.

On page 78 Moon and Spencer state bluntly that "no cylindrical system allows R-separability". What they mean by this is that no $h_1 = h_2$ cylindrical system is separable with $R \neq$ constant. Certainly our three cylindrical systems noted above are R-separable with $R = 1$, and the more general case might be R separable for an obscure contrived system.

10. Separability in Rotational Systems

First of all, 2D orthogonal curvilinear systems often have one or two symmetry axes. If the 2D system is created by a conformal mapping of the Cartesian system, so w= f(z) or $\xi_1 + i\xi_2 = f(x +iy)$, then the 2D level curve drawing will be symmetric in x if it happens that f(x +iy) = f(-x +iy), and it will be symmetric in y if f(x +iy) = f(x -iy).

A 3D rotational system is formed by rotating such a 2D system about one of its symmetry axes. Such a system of course then has an azimuthal variable ξ_3. One could for example rotate any of the 21 2D systems that Moon and Spencer use to generate cylindrical systems, and some of those can be rotated about two different symmetry axes. All these systems have $h_1= h_2$ since the starting 2D systems are derived from conformal maps of the Cartesian 2D system.

An example is the rotation of a 2D bipolar system about one of its symmetry axes to form toroidal coordinates. Rotation about the other symmetry axis gives bispherical coordinates. A simpler example is the rotation of 2D polar coordinates to create 3D spherical coordinates.

Since $h_3 = 1$ is no longer true, one doesn't get much specialization of the general case treated back in Section 7. Since ξ_3 is an azimuth angle, the defining equations must have this general form,

$$x = A(\xi_1,\xi_2)\cos\xi_3$$
$$y = A(\xi_1,\xi_2)\sin\xi_3$$
$$z = B(\xi_1,\xi_2) \ .$$

The scale factors are given by (see derivation a few lines below)

$$h_n^2 = (\partial_n x)^2 + (\partial_n y)^2 + (\partial_n z)^2 \qquad\qquad \partial_n \equiv \partial/\partial\xi_n \ .$$

Therefore (see also Moon and Spencer p 50)

$$h_1^2 = [\partial_1 A(\xi_1,\xi_2)]^2\cos^2\xi_3 + [\partial_1 A(\xi_1,\xi_2)]^2\sin^2\xi_3 + [\partial_1 B(\xi_1,\xi_2)]^2$$
$$= [\partial_1 A(\xi_1,\xi_2)]^2 + [\partial_1 B(\xi_1,\xi_2)]^2$$

$$h_2^2 = [\partial_2 A(\xi_1,\xi_2)]^2\cos^2\xi_3 + [\partial_2 A(\xi_1,\xi_2)]^2\sin^2\xi_3 + [\partial_2 B(\xi_1,\xi_2)]^2$$
$$= [\partial_2 A(\xi_1,\xi_2)]^2 + [\partial_2 B(\xi_1,\xi_2)]^2$$

$$h_3^2 = [A(\xi_1,\xi_2)\ (-\sin\xi_3)]^2 + [A(\xi_1,\xi_2)\ (\cos\xi_3)]^2 = [A(\xi_1,\xi_2)]^2 \ .$$

If $h_1 = h_2$ one has an obvious condition on the various derivatives,

$$[\partial_1 A(\xi_1,\xi_2)]^2 - [\partial_2 A(\xi_1,\xi_2)]^2 = [\partial_2 B(\xi_1,\xi_2)]^2 - [\partial_1 B(\xi_1,\xi_2)]^2$$

but the main point is that the scale factors are functions only of ξ_1 and ξ_2 so one has $h_n(12)$. This is the same form arising in all cylindrical systems except there $h_3 = 1$.

Derivation of the above h_n^2 sum. The curvilinear covariant metric tensor g_{ij} can be related to $S_{in} \equiv \frac{\partial x_i}{\partial\xi_n}$ by the matrix equation $g = S^T S$. Since $h_n^2 = g_{nn}$ one finds that,

$$h_n^2 = g_{nn} = \Sigma_i (S^T)_{ni} S_{in} = \Sigma_i (S_{in})^2 = \Sigma_i \left(\frac{\partial x_i}{\partial \xi_n}\right)^2 = (\partial_n x_1)^2 + (\partial_n x_2)^2 + (\partial_n x_3)^2 .$$

This is true for any curvilinear coordinates, orthogonal or not. Morse and Feshbach derive it for a 3D orthogonal system on page 24, equation (1.3.4).

We shall now restrict our interest to rotational systems of the type considered in Moon and Spencer which are derived from conformal map 2D systems, so from now on $h_1 = h_2$.

A look at the Conditions of Section 7 (a):

Condition (1) Equations (3.5) must be solvable for the 7 functions f_n, g_n and R. If some f_n is a constant, that constant is set to 1. (If one is doing Problem A, R=1.)

$$(H/h_1^2) = f_1(1)g_1(23)\, R^2 \qquad\qquad H = h_1h_2h_3$$
$$(H/h_2^2) = f_2(2)g_2(31)\, R^2$$
$$(H/h_3^2) = f_3(3)g_3(12)\, R^2 \qquad\qquad (3.5)$$

which becomes, assuming $h_1 = h_2$,

$$h_3(12) = f_1(1)g_1(23)\, R^2$$
$$h_3(12) = f_2(2)g_2(31)\, R^2$$
$$h_1^2(12)/h_3(12) = f_3(3)g_3(12)\, R^2 .$$

As with the cylindrical case, define $G_1(2)$ in the obvious way and set $f_3 = 1$ to get

$$h_3(12) = f_1(1)G_1(2)\, R^2$$
$$h_3(12) = f_2(2)G_2(1)\, R^2$$
$$h_1^2(12)/h_3(12) = g_3(12)\, R^2 .$$

Divide the first two equations by R^2

$$f_1(1)G_1(2) = f_2(2)G_2(1)$$

which has this viable solution

$$G_2(1) = f_1(1)$$
$$G_1(2) = f_2(2)$$

allowing the three equations to be written as

$h_3(12) = f_1(1)\, f_2(2)\, R^2$
$h_3(12) = f_2(2)\, f_1(1)\, R^2$
$h_1^2(12)/h_3(12) = g_3(12)\, R^2$.

Since the first two are the same, Condition 1 requires the solution of the following *pair* of equations for the 4 quantities f_1, f_2, g_3 and R

$h_3(12) = f_1(1)\, f_2(2)\, R(12)^2$
$h_1^2(12)/h_3(12) = g_3(12)\, R(12)^2$

Assuming this problem has a solution, one then has

$R^2 = h_3/f_1f_2$

$$M_1 = g_1 /(f_2f_3) = G_1(2) /f_2(2) = f_2(2) /f_2(2) = 1$$
$$M_2 = g_2 /(f_3f_1) = G_2(1) /f_1(1) = f_1(1) /f_1(1) = 1$$
$$M_3 = g_3 /(f_1f_2) = g_3(12) /(f_1(1)f_2(2)) \quad . \qquad \textit{(5.8b)}$$

Condition (2) Equations (7.2) must have a solution:

$$M_1(23) = 1 = e(2)i(3)-f(2)h(3)$$
$$-M_2(31) = -1 = b(1)i(3)-c(1)h(3)$$
$$M_3(12) = g_3(12) /(f_1(1)f_2(2)) = b(1)f(2)-c(1)e(2) \quad . \qquad \textit{(7.2)}$$

Select h(3) = 0 based on the first two lines (nothing new if i(3)=0 instead) to get

$$1 = e(2)i(3)$$
$$-1 = b(1)i(3)$$
$$g_3(12) /(f_1(1)f_2(2))= b(1)f(2)-c(1)e(2) \quad .$$

From the first pair select i(3) = 1, e(2) = 1 and b(1) = -1. The last line is then

$$g_3(12) /(f_1(1)f_2(2))= - f(2)-c(1)$$

or

$$- g_3(12) = c(1)[f_1(1)f_2(2)] + f(2)[f_1(1)f_2(2)]$$

and this then is Condition 2. The Stäckel matrix now has this form

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \begin{pmatrix} a(1) & -1 & c(1) \\ d(2) & 1 & f(2) \\ g(3) & 0 & 1 \end{pmatrix} \quad .$$

Condition (3) If conditions (1) and (2) are met, we then do the work of computing Q and k_1^2 from (3.9),

$$\Sigma_n (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} \quad = - k_1^2/Q(123) \ . \qquad (3.9)$$

If R = 1, we then set Q = 1 and $k_1^2 = 0$ since in this case $\partial_n R = 0$. Then with this Q expression, equation (7.6) must have a solution for a, d and g,

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \qquad (7.6)$$

$$1/Q(12) = (1/h_1^2)\,[\ a(1) + d(2)\ ] + g(3)\,(1/h_3^2)$$

and this is another functional-form condition. Since nothing other than g(3) is a function of ξ_3, one must set g(3) = α, a constant. Then

$$1/Q(12) = (1/h_1^2)\,[\ a(1) + d(2)\ ] + \alpha\,(1/h_3^2)$$

so Condition 3 requires solution of the above equatino for α, a(1) and d(2). The Stäckel matrix is now

$$\Phi \ = \begin{pmatrix} a(1) & -1 & c(1) \\ d(2) & 1 & f(2) \\ \alpha & 0 & 1 \end{pmatrix} .$$

Adding -α times the third column to the first column , Equivalence Rule (6.3) gives us this new equivalent matrix

$$\Phi \ \approx \begin{pmatrix} a(1)-\alpha c(1) & -1 & c(1) \\ d(2)-\alpha f(2) & 1 & f(2) \\ 0 & 0 & 1 \end{pmatrix} .$$

Moon and Spencer page 7 equation (1.29) gives a general form for the Stäckel matrix associated with a rotational system

$$\Phi \ = \begin{pmatrix} * & * & * \\ * & * & * \\ 0 & 0 & 1 \end{pmatrix}$$

and this is seen to agree with our last result above.

A look at the Steps of Section 7 (b):

Step (1) As noted above in Condition 1, the first step is to solve the following 2 equations for the quantities f_1, f_2, g_3 and R

$$h_3(12) = f_1(1)\, f_2(2)\, R(12)^2$$
$$h_1^2(12)/h_3(12) = g_3(12)\, R(12)^2$$

Step (2) These items are taken from Condition 2 above

$R^2 = h_3/f_1f_2$

$M_1 = 1$
$M_2 = 1$
$M_3 = g_3(12) /(f_1(1)f_2(2))$

Step (3) If R=1 works in step (1), then Q = 1. Otherwise compute Q from (3.9),

$$\Sigma_n (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} = - k_1^2/Q(123) \qquad (3.9)$$

Step (4) Having Q, compute S from the Robertson condition

$$S(\Phi) = H / (f_1f_2f_3QR^2) \qquad \text{"Robertson condition"} \qquad (5.7)$$

But $f_3 = 1$ and $R^2f_1f_2 = h_3$ so this really says

$$S = [\, H / (Qh_3)] = h_1^2/Q$$

Step (5) Find the rightmost two columns of the Stäckel matrix,

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi) \qquad (7.1)$$

But in Condition 2 above (with a little Condition 3) we already know that

$$\Phi = \begin{pmatrix} a(1) & -1 & c(1) \\ d(2) & 1 & f(2) \\ \alpha & 0 & 1 \end{pmatrix}$$

and entries c(1) and f(2) are then determined by

$$- g_3(12) = c(1)[f_1(1)f_2(2)] + f(2)[f_1(1)f_2(2)]$$

Step (6) In Condition 3 above this was the same as solving

$$1/Q(12) = (1/h_1^2)\, [\, a(1) + d(2)\,] + \alpha\, (1/h_3^2)$$

Example 1: toroidal coordinates revisited

This case has already been fully solved, but we shall do it again using the systematic steps outlined above for rotational systems. From earlier work the following facts were obtained for the toroidal system,

$h_1 = h_2 = a/[ch(\xi_1)-cos(\xi_2)]$ => $h_1 = h_2 = a\mathcal{R}^2$ $H = sh(\xi_1)a^3\mathcal{R}^6$
$h_3 = a\, sh(\xi_1)/[ch(\xi_1)-cos(\xi_2)]$ => $h_3 = a\, sh(\xi_1)\, \mathcal{R}^2$

$f_1(1) = ash(\xi_1)$ $g_1(23) = 1$ $\mathcal{R} \equiv [ch(\xi_1)-cos(\xi_2)]^{-1/2}$
$f_2(2) = 1$ $g_2(31) = a\, sh(\xi_1)$ $Q = a^2[ch(\xi_1)-cos(\xi_2)]^2 = a^2\mathcal{R}^4$
$f_3(3) = 1$ $g_3(12) = a/sh(\xi_1)$ $k_1^2 = (1/4)$

We shall here pretend not to know the "blue facts" (6 lower left equations), but the earlier calculation of Q and k_1^2 will be utilized. Notice first that h_1 and h_3 are functions only of 12 and not 3, as expected. We use here the symbol $\mathcal{R} \equiv [ch(\xi_1)-cos(\xi_2)]^{-1/2}$ to distinguish it from the separation R below. And (in the blue) the constant a has been moved from f_3 over to g_3, and also from g_1 over to f_1 -- the allocation of constants is immaterial.

Here then are all our Stäckel calculation steps for rotational systems given above:

Step (1) As noted above in Condition 1, the first step is to solve the following 2 equations for the quantities f_1, f_2, g_3 and R

$h_3 = f_1\, f_2\, R^2$
$h_1^2/h_3 = g_3R^2$

and these now say

$a\, sh(\xi_1)\mathcal{R}^2 = f_1\, f_2\, R^2$
$(a\, \mathcal{R}^{\,2})^2/\, [a\, sh(\xi_1)\, \mathcal{R}^{\,2}] = g_3R^2$

or

$a\, sh(\xi_1)\, \mathcal{R}^2 = f_1\, f_2\, R^2$
$a\mathcal{R}^2/\, sh(\xi_1) = g_3R^2$.

The obvious choice is $R = \mathcal{R}$ and then

$a\, sh(\xi_1) = f_1(1)\, f_2(2)$
$a/sh(\xi_1) = g_3(12)$.

These imply that

$f_1(1) = a\, sh(\xi_1)$ $f_2(2) = 1$ $g_3(12) = a/sh(\xi_1)$ $R = \mathcal{R}$

and this agrees with the "blue data" above collected from earlier work. Done with Step 1.

<u>Step (2)</u> These items are taken from Condition 2 above

$M_1 = 1$
$M_2 = 1$
$M_3 = g_3(12) /(f_1(1)f_2(2)) \quad = a/sh(\xi_1) / [a\ sh(\xi_1)] = 1/ sh^2(\xi_1)$

<u>Step (3)</u> This slightly painful calculation was done back in Section 3 with results

$Q = a^2R^4 \qquad k_1^2 = (1/4)$

Note that $Q = h_1^2 = (aR^2)^2$.

<u>Step (4)</u>

$S = h_1^2/Q = 1$

<u>Step (5)</u>

$$\Phi = \begin{pmatrix} a(1) & -1 & c(1) \\ d(2) & 1 & f(2) \\ \alpha & 0 & 1 \end{pmatrix}$$

$$- g_3(12) = c(1)[f_1(1)f_2(2)] + f(2)[f_1(1)f_2(2)]$$

This last equation becomes

$$- a/sh(\xi_1) = c(1)[\ a\ sh(\xi_1)] + f(2)[\ a\ sh(\xi_1)]$$

or

$$- 1 = c(1)[\ sh^2(\xi_1)] + f(2)[\ sh^2(\xi_1)] \ .$$

A solution is $c(1) = -1/sh^2(\xi_1)$ and $f(2) = 0$. The Φ matrix at this point is then

$$\Phi = \begin{pmatrix} a(1) & -1 & c(1) \\ d(2) & 1 & f(2) \\ \alpha & 0 & 1 \end{pmatrix} = \begin{pmatrix} a(1) & -1 & -1/sh^2(\xi_1) \\ d(2) & 1 & 0 \\ \alpha & 0 & 1 \end{pmatrix}$$

<u>Step (6)</u>

$$1/Q(12) = (1/h_1^2) [\ a(1) + d(2)\ ] + \alpha\ (1/h_3^2)$$

which says

$$1 = [\ a(1) + d(2)\ ] + \alpha\ (Q/h_3^2) \ .$$

Pick $a(1) = 1$ and $d(2) = 0$ and $g(3) = \alpha = 0$ to get the final matrix

$$\Phi = \begin{pmatrix} a(1) & -1 & -1/sh^2(\xi_1) \\ d(2) & 1 & 0 \\ \alpha & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -1 & -1/sh^2(\xi_1) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

All these results agree with those found earlier and with Moon and Spencer p 112-113.

The 11 separable rotational systems of Moon and Spencer

Moon and Spencer in their fourth chapter (called Section IV) review a set of 11 rotational systems which can be R-separated. Evidently, if one tries to rotate the 21 conformal map 2D systems of their second chapter, 10 of them fail to meet one or more of our three Conditions.

The hardest Step is computing Q, and perhaps there is a more elegant way to do than by brute force from (3.9). (Of course Maple is happy to compute Q if it is given the f_n, h_n and R.) In particular, it is not obvious why Q comes out being a constant times a power of R. The fact seems to arise since R is always a power of some "atom" as shown in this partial table from Moon and Spencer Section III:

	q (atom)	h_1^2	R	Q	
tangent sphere	$\xi_1^2+\xi_2^2$	q^{-2}	$q^{-1/2}$	q^{-2}	
cardioid	$\xi_1^2+\xi_2^2$	q^{-3}	q^{-1}	q^{-4}	
bispherical	$ch\xi_1-\cos\xi_2$	a^2q^{-2}	$q^{-1/2}$	a^2q^{-2}	
toroidal	$ch\xi_1-\cos\xi_2$	a^2q^{-2}	$q^{-1/2}$	a^2q^{-2}	// differ in h_3
inverse prolate	$ch^2\xi_1-\sin^2\xi_2$	see M&S	$q^{-1/2}$	q^{-2}	

The atom appears first in the scale factors and then propagates to R through our Step 1. The fact that Q and the scale factors are both powers of the same atom is what allows Condition 3 to be met with $\alpha = 0$,

$$1/Q(12) = (1/h_1^2)\,[\,a(1) + d(2)\,] + \alpha\,(1/h_3^2)\,.$$

Notice how this is satisfied in the cardioid case

$$q^4 = q^3\,[\,a(1) + d(2)\,]$$

where then $[\,a(1) + d(2)\,]$ is taken to be the atom itself, q, to get $q^4 = q^4$. In most other cases the two powers match and we just take a(1) = 1 and d(2) = 0.

11. Separation of the Schrodinger equation.

(a) Schrodinger meets Helmholtz

The time-*dependent* Schrodinger equation of non-relativistic (no spin) quantum mechanics has this form for a single point particle existing in 3D space under the influence of a potential V,

$$\mathcal{H}\Psi = i\hbar\partial_t\Psi \qquad \Psi = \Psi(\mathbf{r},t) \tag{11.1}$$

where

$$\mathcal{H} = KE + PE = p^2/2m + V = (-i\hbar\nabla)^2/2m + V = -(\hbar^2/em)\nabla^2 + V \quad . \tag{11.2}$$

$\mathcal{H}$ is the Hamiltonian, the sum of kinetic and potential energy for the particle. Here we have used the quantum mechanical "rabbit in the hat" fact that $\mathbf{p} = -i\hbar\nabla$, which is to say, the classical particle momentum $\mathbf{p}$ is represented by operator $-i\hbar\nabla$ in "coordinate space" $\mathbf{r}$. This results in $\mathcal{H}$ being a differential operator as shown. The solution $\Psi(\mathbf{r},t)$ is called a wavefunction, and the probability of the particle being in some small volume d^3r at time t is $|\Psi(\mathbf{r},t)|^2d^3r$.

Assuming a monochromatic time dependence for Ψ,

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r})\, e^{-i\omega t} \qquad \Rightarrow \qquad \partial_t\Psi(\mathbf{r},t) = (-i\omega)\,\Psi(\mathbf{r},t) \tag{11.3}$$

equation (11.1) becomes

$$\mathcal{H}\Psi = i\hbar((-i\omega)\,\Psi(\mathbf{r},t) = \hbar\omega\,\Psi(\mathbf{r},t) \quad .$$

Defining $E \equiv \hbar\omega$, one finds

$$\mathcal{H}\Psi = E\Psi \qquad\qquad E = \hbar\omega \quad .$$

Assuming that $V(\mathbf{x},t) = V(\mathbf{x})$, then $\mathcal{H}$ does not involve t, and the above equation becomes

$$\mathcal{H}\psi_E(\mathbf{r}) = E\psi_E(\mathbf{r}) \tag{11.4}$$

which is known as the time-*independent* Schrodinger equation. The energies E and solutions ψ_E are thus the eigenvalues and eigenfunctions of the differential operator $\mathcal{H}$ subject to some kind of boundary conditions. It is traditional to refer to these eigenfunctions as "eigenstates" or just "states", while the eigenvalues are called "eigenenergies" or "energy levels". The continuous energy E of a classical particle ends up being "quantized" into these allowed eigenenergies. Of course the spectrum of E depends on the boundary conditions of the particular problem and might be discrete, continuous, or both.

Putting (11.2) into (11.4),

$$(-\hbar^2\nabla^2/2m + V)\psi = E\psi$$
$$(\nabla^2 - 2mV/\hbar)\psi = -2mE/\hbar\psi$$
$$(\nabla^2 + 2Em/\hbar - 2mV/\hbar)\psi = 0 \,.$$

One can now define a scaled potential φ and replace constant E with constant K_1^2

$$\varphi \equiv -(2m/\hbar)V \qquad K_1^2 \equiv (2m/\hbar)E \tag{11.5}$$

to get

$$(\nabla^2 + K_1^2 + \varphi)\psi = 0 \,. \tag{11.6}$$

And so the Schrodinger equation has become our Helmholtz equation *with the addition* of the scaled potential term φ.

(b) Separation of the Schrodinger Equation in Curvilinear coordinates

The previous section showed that the Schrodinger equation can be written as

$$(\nabla^2 + [K_1^2 + \varphi(123)])\,\psi(123) = 0 \,. \qquad \textit{(11.6)}$$

Tracing through our "processing of the Helmholtz equation" in Sections 3 and 4, we find that the K_1^2 term just "sits there" all the way through, and we end up with this new version of (4.4) in which K_1^2 is replaced by $K_1^2 + \varphi$,

$$-\Sigma_n(1/h_n^2)q_n + k_1^2/Q + K_1^2 + \varphi = 0 \,. \tag{11.7}$$

This suggests, following Morse and Feshbach, that the most general form for φ which would allow separation is this

$$\varphi(123) = \Sigma_n\, s_n(n)/h_n^2 \,, \tag{11.8}$$

and putting (11.8) into (11.7) gives

$$-\Sigma_n(1/h_n^2)(q_n-s_n) + k_1^2/Q + K_1^2 + \varphi = 0 \,. \tag{11.9}$$

We shall now modify (4.5) and introduce the Stäckel matrix this new way (a new LHS)

$$q_n-s_n = [\,\kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)] \qquad n = 1,2,3 \tag{11.10}$$

and then (11.9) becomes (multiplying through by Q)

$$- \Sigma_n (Q/h_n^2) [\kappa_1^2 \Phi_{n1}(n) + k_2^2 \Phi_{n2}(n) + k_3^2 \Phi_{n3}(n)] + k_1^2 + QK_1^2 = 0 \quad (11.11)$$

which is *identical* to equation (4.9) and (5.1). One therefore solves for the Stäckel matrix exactly as before. Recall that the problem of finding the Stäckel matrix Φ is based only on this equation.

What about the separated equations? The most general self-adjoint form is still as in (4.2),

$$L_n X_n = (1/f_n)\partial_n[f_n(\partial_n X_n)] + q_n X_n = 0 \quad \textit{(4.2)}$$

and replacing q_n from (11.10) gives

$$L_n X_n = (1/f_n)\partial_n[f_n(\partial_n X_n)] + [\kappa_1^2 \Phi_{n1}(n) + k_2^2 \Phi_{n2}(n) + k_3^2 \Phi_{n3}(n) + s_n(n)] X_n = 0 \quad (11.12)$$

which is the same as before but with the extra potential function $s_n(\xi_n)$ as shown.

Summary: In order to achieve separation of the Schrodinger Equation, the potential must have the restricted form $\varphi = \Sigma_n s_n(n)/h_n^2$ shown in (11.8). This leads to the exact same Stäckel matrix problem we had before, and the separated equations are the same as before but with an added s_n term from the potential. Since the Schrodinger E parameter is normally not 0, and since $K_1^2 \equiv (2m/\hbar)E$, the Stäckel matrix problem is that for the pure Helmholtz equation with $K_1^2 \neq 0$. We know from above that we can only achieve simple-separation (R = 1, Problem A) for the Helmholtz equation, and that only happens in the 11 classical curvilinear systems. In their review of these 11 classical systems on pages 656-666, for each system Morse and Feshbach state the most general form the potential can have ("General form for V").

(c) Central potentials and the hydrogen atom problem

The most famous instance of the Schrodinger Equation separation discussed here occurs in spherical coordinates where the potential V(r,θ,φ) is taken as V(r), known as a central potential. This potential meets the requirement of (11.8) where $h_1 = 1$, $s_1(1) = V(r)$, and $s_2(2)=s_3(3)=0$ where 123 = rθφ. Thus, only the separated equation for r (the "radial equation", (11.12) for n=1) has a modification from the pure Helmholtz case. If the spatial region includes all 4π steradians of angle, then the θ and φ separated equations yield the usual spherical harmonics $Y_{\ell m}(\theta,\varphi)$ in which the two separation constants k_2^2 and k_3^2 have been shuffled into ℓ and m, both forced to certain integer values: $\ell = 0,1,2...$ (to make $Y_{\ell m}$ finite at θ = π) and m = $-\ell..\ell$ (to make $Y_{\ell m}$ the same at φ = 0 and 2π) . When dimensionless separation constants get forced to certain discrete values, those values are traditionally called "quantum numbers".

A particular example is the hydrogen atom problem where $V(r) = -|e|^2/r$ and the solution is then the solution to the radial equation R(r) times the spherical harmonics. Only ℓ appears in the radial function along with $K_1^2 \sim E_n$. Specifically, one finds this wavefunction solution to the hydrogen atom problem,

$$\psi(r,\theta,\varphi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi)$$

where (see Schiff p 93)

$R_{n\ell}(r)$ = constant * $\rho^\ell L^{2\ell+1}{}_{n+\ell}(\rho)\, e^{-\rho/2}$ $\rho = (2/n)(r/a_0)$ $L^p{}_q$ = associated Laguerre
$a_0 = \hbar^2/(\mu e^2)$ = Bohr radius μ = "reduced mass" of electron $|e|$ = charge on electron
$E_n = -e^2/(2a_0)/n^2$ = eigenstate energies $n = 1,2,3...$ $\ell = 0,1...(n-1)$

A third quantum number n has appeared, and it arises from the need for the wave function ψ to be normalizable such that $\int d^3r\, |\psi(r,\theta,\varphi)|^2 = 1$, meaning the probability of finding the electron *somewhere* in all space must be 1. This requirement in turn creates a need for the power series expansion for the function L to truncate at some maximum power, and that power is related to n. Then function L becomes a polynomial, known as an associated Laguerre polynomial. The exponential factor $e^{-\rho/2}$ can then overwhelm the polynomial at large $r \sim \rho$ no matter how large n gets, providing normalization.

We can look quickly at a few solutions: (= states = orbitals)

With n=1 we have ℓ=m=0 and the energy E_1 is the most negative of all the E_n. This spherically symmetric state is called 1S and is the hydrogen atom "ground state".

With n = 2 we get ℓ = 0,1. The ℓ=0 (m=0) case gives a spherically symmetric state (called 2S) while the ℓ=1 cases with m = -1,0,1 are usually linearly combined into three perpendicular dumbbell shaped states called $2P_{x,y,z}$. All four n=2 states have the same energy E_2 in this non-relativistic model.

12. Separation in Ellipsoidal Coordinates

The ellipsoidal coordinate system is the most complicated of the classical curvilinear systems and provides a good exercise in applying the apparatus of the previous sections. We shall make use of some of the equivalence operations of Section 6, and shall end up with three separated equations. The good news is that the three separated equations turn out to be identical, a fact traceable to cyclic symmetry of this system. The bad news is that all of the Stäckel matrix elements are non-zero, so the two separation constants are fully entangled into each separated equation, precluding a simple 1D Sturm-Liouville type solution except in very simplest cases, one of which is quoted below.

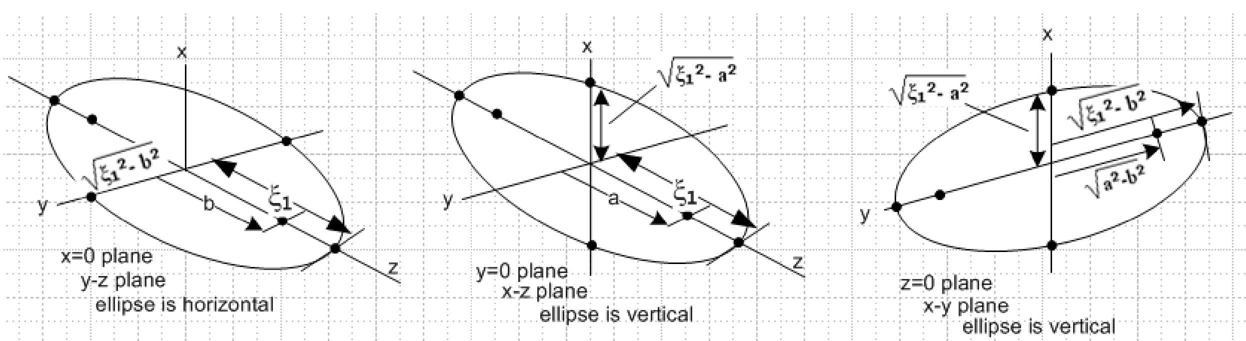
This section is not meant to be a complete monograph on ellipsoidal coordinates. Enough facts are given to hopefully make the reader comfortable with this system and to support the calculations below. See Morse and Feshbach for full details.

(a) Some details about ellipsoidal coordinates

Conveniently, our generic variable names ξ_1, ξ_2, ξ_3 match the notation of Morse and Feshbach's ellipsoidal coordinate discussion. In this system the level surfaces (ξ_n=constant) are ellipsoids and certain hyperboloids. The ellipsoids are the surfaces of constant ξ_1 and have this equation in Cartesian space,

$$x^2/(\xi_1^2 - a^2) + y^2/(\xi_1^2 - b^2) + z^2/(\xi_1^2) = 1 \quad , \tag{12.1}$$

which is an ellipsoid centered at the origin. The largest semimajor axis of this ellipsoid is obviously ξ_1, and the other two semimajor axes $\sqrt{\xi_1^2 - a^2}$ and $\sqrt{\xi_1^2 - b^2}$ are smaller. The quantities a and b are focal distances associated with the x and y directions. Here are crude pictures showing slices of this ellipsoid in the x=0, y=0 and then z=0 plane:



Assuming an eye position such that the +x axis is "up", as these pictures are drawn, then the left and middle pictures show that

b is the focal distance of the horizontal ellipse = the intersection of the ellipsoid with the x=0 plane.
a is the focal distance of the vertical ellipse = the intersection of the ellipsoid with the y=0 plane.

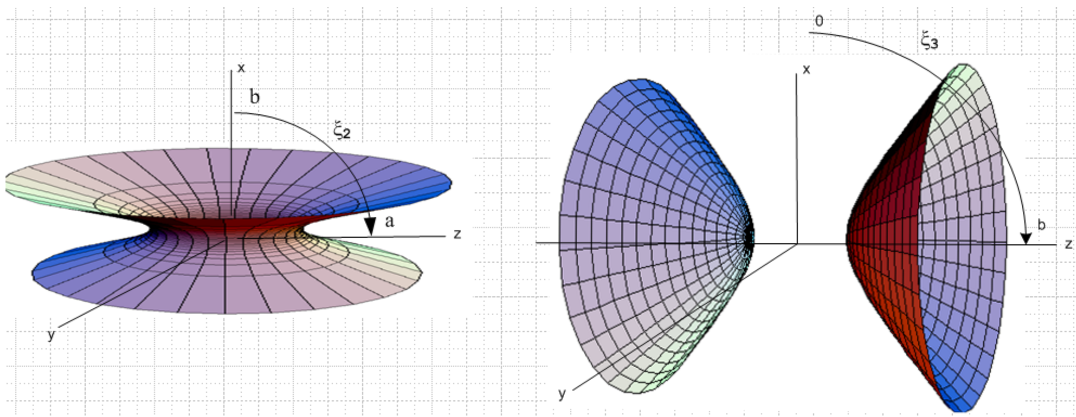
Notice that both these focal distances are along the z axis. The right picture then shows the other vertical slice ellipse= the intersection of the ellipsoid with the z=0 plane. It will be assumed that a > b.

Sweeping ξ_1 through some range produces a *family* of ellipsoids, each labeled by its value of ξ_1, the longest semimajor axis length. All these ellipsoids have the same a and b focal distances. For this reason, such a family of ellipsoids is called "confocal".

As ξ_1 gets very large, the ellipsoid gets long in the z direction, and has the shape of a cigar whose cross section is elliptical. The lower limit for ξ_1 is a, since a semimajor axis cannot be smaller than a focal distance (and a is the larger of the two focal distances). If $\xi_1 = a + \varepsilon$, the ellipsoid is crushed vertically, lies close to the x=0 plane, and looks a thin elliptical cookie.

The upshot is that one must have $a < \xi_1 < \infty$.

The other two surface families (those of constant ξ_2 and constant ξ_3) are types of infinite hyperboloids. Here are some graphs showing one surface of constant ξ_2 (left) and one of constant ξ_3 (right),



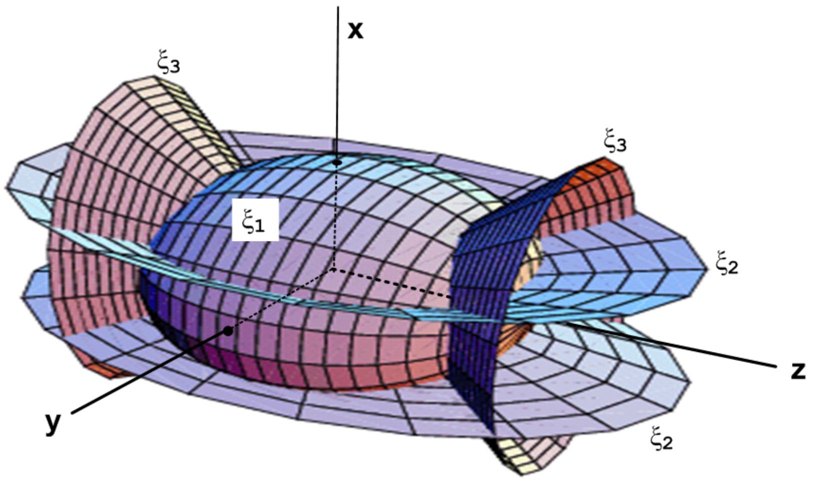
These hyperboloids are not surfaces of revolution, they are generally asymmetric, though these pictures don't make that clear. The surface on the left is called a one-sheeted hyperboloid and the one on the right two-sheeted. The pictures show that the coordinates ξ_2 and ξ_3 also have certain legal ranges, and these ranges can be summarized as follows:

$$0 \le \xi_3 \le b \le \xi_2 \le a \le \xi_1 \tag{12.2}$$

These hyperboloid families are also "confocal" in the sense noted above.

Replacing ξ_1 in (12.1) by ξ_2 or ξ_3 gives the other two level-surface equations. It is the fact that one or two of the terms in (12.1) then change sign, according to 12.2, that causes these surfaces to be the one and two sheeted hyperboloids. In fact, the three coordinates ξ_n^2 for n=1,2,3 can be regarded as the three solutions of equation (12.1) written with $\xi_1 \rightarrow \xi_n$ and treated as a cubic equation in ξ_n^2. One could in this manner find (ξ_1,ξ_2,ξ_3) for a given (x,y,z), though the expressions are quite ugly. It is much easier to go the other direction using (12.3) below.

The ellipsoid family intersects these two hyperboloid families such that everything is at right angles -- this is an *orthogonal* coordinate system! Here is an attempt to show one member of each surface family in the same drawing: (We call this picture "the Q Bomb", in fond memory of *The Mouse that Roared*.)



Examination of the Q Bomb shows that the surfaces labeled by ξ_1, ξ_2, ξ_3 intersect at 8 places in Cartesian space. These locations are given by $(\pm x, \pm y, \pm z)$ where

$$
\begin{aligned}
x^2 &= (\xi_1^2-a^2)(\xi_2^2-a^2)(\xi_3^2-a^2)/[\,a^2(a^2-b^2)] && = + - - / + = + \\
y^2 &= (\xi_1^2-b^2)(\xi_2^2-b^2)(\xi_3^2-b^2)/[\,b^2(b^2-a^2)] && = + + - / - = + \qquad // = x^2(a \leftrightarrow b) \\
z &= \xi_1\xi_2\xi_3/(ab) && = + + + / + = +
\end{aligned}
\tag{12.3}
$$

The quantities on the RHS's of these equations are all positive.

(b) Notation and comparison to that of Morse and Feshbach

Right off the bat we are going to make a notational change to our separation machinery. Recall that in Step 1 of our solution method we are supposed to analyze equations (3.5),

$$
\begin{aligned}
(H/h_1^2) &= f_1(1)g_1(23)\, R^2 \\
(H/h_2^2) &= f_2(2)g_2(31)\, R^2 \\
(H/h_3^2) &= f_3(3)g_3(12)\, R^2 \quad .
\end{aligned}
\tag{3.5}
$$

We replace $f_n(n)$ by $F_n(n)$, in order to use $f_n(n)$ for another purpose, so the new equations (3.5) read,

$$
\begin{aligned}
(H/h_1^2) &= F_1(1)g_1(23)\, R^2 \\
(H/h_2^2) &= F_2(2)g_2(31)\, R^2 \\
(H/h_3^2) &= F_3(3)g_3(12)\, R^2 \quad ,
\end{aligned}
\tag{3.5}
$$

and of course we make this same change in all our separation equations where the $f_n(n)$ appear. The reason for doing this is to try and maintain compatibility with the notation of Morse and Feshbach regarding ellipsoidal coordinate separation, so we will use f_n for *their* purpose (see Morse and Feshbach p 512 5.1.35), which purpose is the following set of definitions:

$$
\begin{aligned}
f_1^2 &\equiv (\xi_1^2-a^2)(\xi_1^2-b^2) = ++ \ = + & \qquad G_1 &\equiv (\xi_2^2-\xi_3^2) \ = + \\
f_2^2 &\equiv (\xi_2^2-a^2)(\xi_2^2-b^2) = -+ \ = - & \qquad G_2 &\equiv (\xi_3^2-\xi_1^2) \ = - \\
f_3^2 &\equiv (\xi_3^2-a^2)(\xi_3^2-b^2) = -- \ = + & \qquad G_3 &\equiv (\xi_1^2-\xi_2^2) \ = +
\end{aligned} \qquad (12.4)
$$

These G_n functions have nothing to do with G_n functions we used in Sections 8, 9 and 10. What we have here are $G_n(\neq n)$ type functions, such as $G_1(23)$. [G_n is another Morse and Feshbach notation, p 512 5.1.37.]

Running down the lines above, everything is seen to be nice and cyclic. *However*, the inequality chain in (12.2) gives expression signs as shown to the right above. One implication is that f_2 must be imaginary, and then we have to worry about branches and factors of ±i and such things. We don't *like* having imaginary stuff floating around unnecessarily, so we now introduce some new italicized capital F and G functions as follows (notice the minus signs in front of f_2^2 and G_2)

$$
\begin{aligned}
F_1^2 &\equiv +(\xi_1^2-a^2)(\xi_1^2-b^2) = f_1^2 & \qquad \mathcal{G}_1 &\equiv +(\xi_2^2-\xi_3^2) = G_1 \\
F_2^2 &\equiv -(\xi_2^2-a^2)(\xi_2^2-b^2) = -f_2^2 & \qquad \mathcal{G}_2 &\equiv -(\xi_3^2-\xi_1^2) = -G_2 \\
F_3^2 &\equiv +(\xi_3^2-a^2)(\xi_3^2-b^2) = f_3^2 & \qquad \mathcal{G}_3 &\equiv +(\xi_1^2-\xi_2^2) = G_3 \ .
\end{aligned} \qquad (12.5)
$$

All the F_n^2 and $\mathcal{G}_n$ quantities are positive and have unambiguous square roots. Note by the way that both functions f_n and F_n are of the functional form type $f_n(n)$ and $F_n(n)$.

Finally we are ready to write down the ellipsoidal scale factors h_n. In terms of the f_i and G_i functions one finds these unpleasant looking forms (e.g., Morse and Feshbach page 663),

$$
\begin{aligned}
h_1^2 &= -G_2G_3/f_1^2 & \qquad h_1 &= \sqrt{-G_2G_3/f_1^2} \\
h_2^2 &= -G_3G_1/f_2^2 & \qquad h_2 &= \sqrt{-G_3G_1/f_2^2} \\
h_3^2 &= -G_1G_2/f_3^2 & \qquad h_3 &= \sqrt{-G_1G_2/f_3^2} & \qquad H = h_1h_2h_3 = \sqrt{-G_2^2G_2^2G_3^2/(f_1^2 f_2^2 f_3^2)}
\end{aligned} \qquad (12.6)
$$

We hope the reader feels as uncomfortable as the writer about scale factors that are not obviously positive real numbers (though of course they are). We prefer to write the above our using our non-Morse and Feshbach symbols which are all positive quantities,

$$
\begin{aligned}
h_1^2 &= \mathcal{G}_2\mathcal{G}_3/F_1^2 & \qquad h_1 &= \sqrt{\mathcal{G}_2\mathcal{G}_3}\ /\ F_1 & \qquad &\Rightarrow \qquad h_n^2 = \mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(\mathcal{G}_nF_n^2) \\
h_2^2 &= \mathcal{G}_3\mathcal{G}_1/F_2^2 & \qquad h_2 &= \sqrt{\mathcal{G}_3\mathcal{G}_1}\ /\ F_2 \\
h_3^2 &= \mathcal{G}_1\mathcal{G}_2/F_3^2 & \qquad h_3 &= \sqrt{\mathcal{G}_1\mathcal{G}_2}\ /\ F_3 & \qquad &H = h_1h_2h_3 = \mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(F_1F_2F_3)z
\end{aligned}
$$

$$
\begin{aligned}
(H/h_1^2) &= [\mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(F_1F_2F_3)]\ /\ [\mathcal{G}_2\mathcal{G}_3/F_1^2\ ] = \mathcal{G}_1F_1/(F_2F_3) \\
(H/h_2^2) &= [\mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(F_1F_2F_3)]\ /\ [\mathcal{G}_3\mathcal{G}_1/F_3^2\ ] = \mathcal{G}_2F_2/(F_3F_1) \\
(H/h_3^2) &= [\mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(F_1F_2F_3)]\ /\ [\mathcal{G}_1\mathcal{G}_2/F_3^2\ ] = \mathcal{G}_3F_3/(F_1F_2) \ .
\end{aligned} \qquad (12.7)
$$

All the equation sets in (12.7) are cyclic.

(c) Running through the Steps of Section 7 (b)

Step (1) As noted above, the first task is to solve (3.5) for the 7 functions F_n, g_n and R

$$(H/h_1^2) = F_1(1)g_1(23)\, R^2$$
$$(H/h_2^2) = F_2(2)g_2(31)\, R^2 \qquad \Rightarrow \qquad (H/h_n^2) = F_n g_n R^2$$
$$(H/h_3^2) = F_3(3)g_3(12)\, R^2 \qquad (3.5)$$

We know the ellipsoidal system is a classical system that allows simple-separation for Helmholtz so R=1. The left sides of the three equations above are provided in (12.7) to give

$$\mathcal{G}_1(23)\mathcal{F}_1/ (\mathcal{F}_2\mathcal{F}_3) = F_1(1)g_1(23)$$
$$\mathcal{G}_2(23)\mathcal{F}_2/ (\mathcal{F}_3\mathcal{F}_1) = F_2(2)g_2(31)$$
$$\mathcal{G}_3(23)\mathcal{F}_3/ (\mathcal{F}_1\mathcal{F}_2) = F_3(3)g_3(12) .$$

A visual "functional form inspection" of these (again cyclic) equations tells us what we need to know:

$$F_1 = \mathcal{F}_1 \qquad g_1(23) = \mathcal{G}_1(23)/(\mathcal{F}_2\mathcal{F}_3)$$
$$F_2 = \mathcal{F}_2 \qquad g_2(31) = \mathcal{G}_2(31)/(\mathcal{F}_3\mathcal{F}_1) \qquad \Rightarrow \quad g_n = \mathcal{G}_n\mathcal{F}_n/(\mathcal{F}_1\mathcal{F}_2\mathcal{F}_3)$$
$$F_3 = \mathcal{F}_3 \qquad g_3(12) = \mathcal{G}_3(12)/(\mathcal{F}_1\mathcal{F}_2) \qquad (12.8)$$

So the $\mathcal{F}$ functions turn out to be exactly our separation functions F, and we can now dispense with the $\mathcal{F}$. We can now collect our "data" from (12.7) and (12.8) into one place, using $(-1)^{n-1}$ to handle the minus signs for the case n=2,

$$h_n^2 = \mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(\mathcal{G}_n F_n^2) \qquad H = \mathcal{G}_1\mathcal{G}_2\mathcal{G}_3/(F_1F_2F_3) \qquad \mathcal{G}_n = (-1)^{n-1}G_n$$

$$F_n^2 \equiv (-1)^{n-1} (\xi_n^2-a^2)(\xi_n^2-b^2) \qquad g_n = \mathcal{G}_n F_n/(F_1F_2F_3) \qquad (12.9)$$

$$H/h_n^2 = \mathcal{G}_n F_n^2/(F_1F_2F_3) \qquad g_n/H = \mathcal{G}_n F_n/ (\mathcal{G}_1\mathcal{G}_2\mathcal{G}_3)$$

Step (2) The three first-column cofactors of Φ are, from (5.8) and (12.9),

$$M_n = g_nF_n/(F_1F_2F_3) = \{G_nF_n/(F_1F_2F_3)\}\, F_n/(F_1F_2F_3) = G_n\, F_n^2/ (F_1^2F_2^2F_3^2)$$

or

$$M_1 = G_1/ (F_2^2F_3^2) = - G_1/(f_2^2f_3^2)$$
$$M_2 = G_2/ (F_3^2F_1^2) = - G_2/(f_3^2f_1^2)$$
$$M_3 = G_3/ (F_1^2F_2^2) = - G_3/(f_1^2f_2^2) \qquad (12.10)$$

Step (3) R=1 => Q = 1.

Step (4) Knowing Q, one can compute S from the Robertson condition,

$$S(\Phi) = H / (F_1F_2F_3QR^2) \qquad \text{"Robertson condition"} \qquad \mathit{(5.7)}$$

$$= H / (F_1F_2F_3) = [G_1G_2G_3/(F_1F_2F_3)] / (F_1F_2F_3)$$

$$= G_1G_2G_3 / (F_1^2F_2^2F_3^2) = G_1G_2G_3/(f_1^2f_2^2f_3^2) \qquad (12.11)$$

Step (5) The next step is to find the rightmost two columns of the Stäckel matrix,

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \qquad S = \det(\Phi) \qquad \mathit{(7.1)}$$

One can do this by solving the following equation set, using the M_n found in Step (2),

$$M_1 = e(2)i(3)-f(2)h(3)$$
$$-M_2 = b(1)i(3)-c(1)h(3)$$
$$M_3 = b(1)f(2)-c(1)e(2) \qquad \mathit{(7.2)}$$

$$G_1(23)/F_2^2F_3^2 = e(2)i(3)-f(2)h(3)$$
$$-G_2(31)/F_3^2F_1^2 = b(1)i(3)-c(1)h(3)$$
$$G_3(12)/F_1^2F_2^2 = b(1)f(2)-c(1)e(2)$$

$$G_1(23)/F_2^2F_3^2 = e(2)i(3)-f(2)h(3)$$
$$G_2(31)/F_3^2F_1^2 = b(1)i(3)-c(1)h(3)$$
$$G_3(12)/F_1^2F_2^2 = b(1)f(2)-c(1)e(2)$$

$$(\xi_2^2- \xi_3^2)/F_2^2F_3^2 = e(2)i(3)-f(2)h(3)$$
$$(\xi_3^2- \xi_1^2)/F_3^2F_1^2 = b(1)i(3)-c(1)h(3)$$
$$(\xi_1^2- \xi_2^2)/F_1^2F_2^2 = b(1)f(2)-c(1)e(2) \;.$$

Unlike all our previous examples, *both* terms on the RHS's of these equations are activated and come into play. Looking at the first equation, one can try the following choices,

$e(2) = s\xi_2^2/F_2^2 \qquad i(3) = s/F_3^2 \qquad\qquad f(2) = t/F_2^2 \qquad h(3) = t\,\xi_3^2/F_3^2$

where s and t are signs ±1 to be determined below. The second and third equations then become

$$(\xi_3^2 - \xi_1^2)/F_3^2F_1^2 = b(1) * s/F_3^2 - c(1) * t\,\xi_3^2/F_3^2$$
$$(\xi_1^2 - \xi_2^2)/F_1^2F_2^2 = b(1) * t/F_2^2 - c(1) * s\xi_2^2/F_2^2 \quad .$$

Try $b(1) = u\xi_1^2/F_1^2$ and $c(1) = v/F_1^2$ where u and v are two new signs,

$$(\xi_3^2 - \xi_1^2)/F_3^2F_1^2 = u\xi_1^2/F_1^2 * s/F_3^2 - v/F_1^2 * t\,\xi_3^2/F_3^2$$
$$(\xi_1^2 - \xi_2^2)/F_1^2F_2^2 = u\xi_1^2/F_1^2 * t/F_2^2 - v/F_1^2 * s\xi_2^2/F_2^2$$

$$(\xi_3^2 - \xi_1^2)/F_3^2F_1^2 = us\xi_1^2/F_1^2F_3^2 - vt\,\xi_3^2/F_3^2F_1^2$$
$$(\xi_1^2 - \xi_2^2)/F_1^2F_2^2 = ut\,\xi_1^2/F_1^2F_2^2 - vs\,\xi_2^2/F_1^2/F_2^2$$

$$us = -1 \qquad -vt = 1$$
$$ut = 1 \qquad vs = 1 \quad .$$

Picking one sign s = +1 we find

$$u = -1 \qquad -vt = 1$$
$$ut = 1 \qquad v = 1$$

then

$$u = -1 \qquad -t = 1$$
$$-t = 1 \qquad v = 1$$

and everything works. The solution is this

$$b(1) = u\xi_1^2/F_1^2 \qquad c(1) = v/F_1^2$$
$$e(2) = s\xi_2^2/F_2^2 \qquad f(2) = t/F_2^2$$
$$h(3) = t\,\xi_3^2/F_3^2 \qquad i(3) = s/F_3^2$$

$$b(1) = -\xi_1^2/F_1^2 = -\xi_1^2/f_1^2 \qquad c(1) = 1/F_1^2 = 1/f_1^2$$
$$e(2) = \xi_2^2/F_2^2 = -\xi_2^2/f_2^2 \qquad f(2) = -1/F_2^2 = 1/f_2^2$$
$$h(3) = -\xi_3^2/F_3^2 = -\xi_3^2/f_3^2 \qquad i(3) = 1/F_3^2 = 1/f_3^2$$

and we now have the rightmost two columns of the Stäckel matrix

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} = \begin{pmatrix} a(1) & -\xi_1^2/f_1^2 & 1/f_1^2 \\ d(2) & -\xi_2^2/f_2^2 & 1/f_2^2 \\ g(3) & -\xi_3^2/f_3^2 & 1/f_3^2 \end{pmatrix} \approx \begin{pmatrix} a(1) & 1/f_1^2 & \xi_1^2/f_1^2 \\ d(2) & 1/f_2^2 & \xi_2^2/f_2^2 \\ g(3) & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix} \qquad (12.12)$$

To get to the rightmost form, we have used the Section 6 equivalence rule which allows us to swap the last two columns and then negate one of them.

<u>Step (6)</u> Find the first column of the Stäckel matrix by solving (7.6) :

$$1/Q = a(1)\,(1/h_1^2) + d(2)\,(1/h_2^2) + g(3)\,(1/h_3^2) \qquad (7.6)$$

$$1 = a(1)\,F_1^2/\,G_2G_3 + d(2)\,F_2^2/\,G_3G_1 + g(3)\,F_3^2/\,G_1G_2$$

$$G_1G_2G_3 = a(1)\,G_1\;F_1^2 + d(2)\,G_2F_2^2 + g(3)\,G_3F_3^2$$

$$-\,G_1G_2G_3 = a(1)\,G_1\;f_1^2 + d(2)\,G_2f_2^2 + g(3)\,G_3f_3^2$$

This formidable-looking equation has at least two solutions. The first is this

$$\begin{aligned} a(1) &= \xi_1^4/f_1^2 \\ d(2) &= \xi_2^4/f_2^2 \\ g(3) &= \xi_3^4/f_3^2 \end{aligned} \qquad (12.13)$$

which we can verify by showing that

$$-\,G_1G_2G_3 = a(1)\,G_1\;f_1^2 + d(2)\,G_2f_2^2 + g(3)\,G_3f_3^2$$

$$-\,G_1G_2G_3 = \xi_1^4G_1 + \xi_2^4G_2 + \xi_3^4G_3 \qquad ? \qquad (12.14)$$

$$-\,(\xi_2^2 - \xi_3^2)\,(\xi_3^2 - \xi_1^2)\,(\xi_1^2 - \xi_2^2) \;=\; \xi_1^4(\xi_2^2 - \xi_3^2) + \xi_2^4(\xi_3^2 - \xi_1^2) + \xi_3^4(\xi_1^2 - \xi_2^2) \qquad ?$$

$$-\,(x_2 - x_3)\,(x_3 - x_1)\,(x_1 - x_2) \;=\; x_1^2(x_2 - x_3) + x_2^2\,(x_3 - x_1) + x_3^2\,(x_1 - x_2) \qquad ?$$

Expansion of both sides into 6 terms shows this last equation is true, so the question marks can be removed.

The other solution is this,

$$\begin{aligned} a(1) &= 1 \\ d(2) &= 1 \\ g(3) &= 1 \end{aligned} \qquad (12.15)$$

which can be verified by showing that

$$-\,G_1G_2G_3 = a(1)\,G_1\;f_1^2 + d(2)\,G_2f_2^2 + g(3)\,G_3f_3^2$$

$$-\,G_1G_2G_3 = G_1\;f_1^2 + G_2f_2^2 + G_3f_3^2 \qquad ?$$

$$-\,(\xi_2^2 - \xi_3^2)\,(\xi_3^2 - \xi_1^2)\,(\xi_1^2 - \xi_2^2) \;=\; (\xi_2^2 - \xi_3^2)\;(\xi_1^2 - a^2)(\xi_1^2 - b^2) + \text{cyclic} \qquad ? \qquad (12.16)$$

It seems hard to imagine how (12.16) can be true since the RHS depends on a and b while the LHS does not! But let's examine the coefficient of a^2 on the RHS

$$\text{coeff}(a^2) = - (\xi_2^2 - \xi_3^2)(\xi_1^2 - b^2) + \text{cyclic}$$

$$= - [\xi_1^2(\xi_2^2 - \xi_3^2) + \text{cyclic}] + b^2[(\xi_2^2 - \xi_3^2) + \text{cyclic}] \quad .$$

But both square brackets vanish due to the following two trivial theorems valid for any function f

$$f(1)[f(2) - f(3)] + \text{cyclic} = 0 \qquad \text{// makes first [] = 0 in the line above}$$
$$[f(2) - f(3)] + \text{cyclic} = 0 \qquad \text{// makes second [] = 0 in the line above} \quad . \qquad (12.17)$$

Thus coeff(a^2) = 0 and similarly coeff(b^2) = 0 . In other words, the RHS of (12.16) depends on neither a^2 nor b^2, despite appearances. Thus one can select any value of a^2 or b^2 to evaluate the RHS. If one takes $a^2 = \xi_2^2$ and $b^2 = \xi_3^2$, then both the terms that make up "+ cyclic" in (12.16) vanish because each of those terms then has a zero factor. Then the RHS of (12.16) becomes

$$(\xi_2^2 - \xi_3^2)(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2) = (\xi_2^2 - \xi_3^2)(\xi_1^2 - \xi_3^2)(\xi_1^2 - \xi_2^2) = - (\xi_2^2 - \xi_3^2)(\xi_3^2 - \xi_1^2)(\xi_1^2 - \xi_2^2)$$

But this matches the LHS of (12.16), so we can erase the question marks above.

Installing the first solution (12.13) gives this for the full Stäckel matrix,

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \approx \begin{pmatrix} a(1) & 1/f_1^2 & \xi_1^2/f_1^2 \\ d(2) & 1/f_2^2 & \xi_2^2/f_2^2 \\ g(3) & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix} \approx \begin{pmatrix} \xi_1^4/f_1^2 & 1/f_1^2 & \xi_1^2/f_1^2 \\ \xi_2^4/f_2^2 & 1/f_2^2 & \xi_2^2/f_2^2 \\ \xi_3^4/f_3^2 & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix}$$

$$\text{where} \qquad f_1^2 \equiv (\xi_1^2 - a^2)(\xi_1^2 - b^2) \qquad (12.18)$$
$$f_2^2 \equiv (\xi_2^2 - a^2)(\xi_2^2 - b^2)$$
$$f_3^2 \equiv (\xi_3^2 - a^2)(\xi_3^2 - b^2)$$

Let's calculate the first column cofactors of this result. They are (cofactor = $(-1)^{n+1}$ minor)

$$M_1 = (1/f_2^2)(\xi_3^2/f_3^2) - (\xi_2^2/f_2^2)(1/f_3^2) = (\xi_3^2 - \xi_2^2) / f_2^2 f_3^2 = (- G_1/ f_2^2 f_3^2)$$
$$M_2 = (1/f_3^2)(\xi_1^2/f_1^2) - (\xi_3^2/f_3^2)(1/f_1^2) = (\xi_1^2 - \xi_3^2) / f_3^2 f_1^2 = (- G_2/ f_3^2 f_1^2)$$
$$M_3 = (1/f_1^2)(\xi_2^2/f_2^2) - (\xi_1^2/f_1^2)(1/f_2^2) = (\xi_2^2 - \xi_1^2) / f_1^2 f_2^2 = (- G_3/ f_2^2 f_3^2)$$

and these results agree with (12.10) in Step 2 above. The determinant should be

$$S = (\xi_1^4/f_1^2)M_1 + (\xi_2^4/f_2^2)M_2 + (\xi_3^4/f_3^2)M_3$$

$$= (\xi_1^4/f_1^2)(- G_1/ f_2^2 f_3^2) + (\xi_2^4/f_2^2)(- G_2/ f_3^2 f_1^2) + (\xi_3^4/f_3^2)(- G_3/ f_2^2 f_3^2)$$

$$= - \{ \xi_1^4 G_1 + \xi_2^4 G_2 + \xi_3^4 G_3 \} /(f_1^2 f_2^2 f_3^2) \; .$$

But we showed in (12.14) that $\{ \xi_1^4 G_1 + \xi_2^4 G_2 + \xi_3^4 G_3\} = -G_1G_2G_3$ so we find that

$$S = G_1G_2G_3/ (f_1^2 f_2^2 f_3^2)$$

which agrees with Step 4 result (12.11) above. So we *know* this Stäckel matrix is valid.

Our result (12.18) agrees with Moon and Spencer page 41, but the agreement is a bit hard to see because Moon and Spencer use the following mapping of our symbols which then hides the cyclic nature of things: $a\to c$, $\xi_1, \xi_2, \xi_3 \to \eta, \theta, \lambda$.

Step (7) Finally we get to do a Step 7! First, we will use our second solution (12.15) for the Stäckel first column and write

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \approx \begin{pmatrix} a(1) & 1/f_1^2 & \xi_1^2/f_1^2 \\ d(2) & 1/f_2^2 & \xi_2^2/f_2^2 \\ g(3) & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix} \approx \begin{pmatrix} 1 & 1/f_1^2 & \xi_1^2/f_1^2 \\ 1 & 1/f_2^2 & \xi_2^2/f_2^2 \\ 1 & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix} \qquad (12.19)$$

which by itself is not such a bad Stäckel matrix. But there is a simpler form that Morse and Feshbach quote and we will use our Section 6 equivalence rules to "get to it".

In the (12.19) Φ matrix above add $(-b^2)$ times the second column to the third column. The new third column top row entry is

$$\xi_1^2/f_1^2 - b^2/f_1^2 = (\xi_1^2-b^2)/f_1^2 = (\xi_1^2-b^2)/ [(\xi_1^2-a^2)(\xi_1^2-b^2)] = 1/(\xi_1^2-a^2)$$

and the equivalent Φ matrix is now

$$\Phi \approx \begin{pmatrix} 1 & 1/f_1^2 & 1/(\xi_1^2-a^2) \\ 1 & 1/f_2^2 & 1/(\xi_2^2-a^2) \\ 1 & 1/f_3^2 & 1/(\xi_3^2-a^2) \end{pmatrix} \qquad (12.20)$$

Now add $-(a^2-b^2)^{-1}$ times the third column to the second column. The new second column top row entry is

$$1/f_1^2 - 1/[(\xi_1^2-a^2) (a^2-b^2)] = 1/[(\xi_1^2-a^2)(\xi_1^2-b^2)] - 1/[(\xi_1^2-a^2) (a^2-b^2)]$$

$$= 1/(\xi_1^2-a^2) * \{ 1/(\xi_1^2-b^2) - 1/(a^2-b^2) \} =$$

$$= 1/(\xi_1^2-a^2) * \{ (a^2-b^2) - (\xi_1^2-b^2)/ \}/ [(\xi_1^2-b^2) (a^2-b^2)]$$

$$= 1/(\xi_1^2-a^2) * \{ (a^2- \xi_1^2)\}/ [(\xi_1^2-b^2) (a^2-b^2)]$$

$$= -1/ [(\xi_1^2-b^2) (a^2-b^2)] .$$

The new equivalent Φ matrix is then

$$\Phi \approx \begin{pmatrix} 1 & -1/[(\xi_1^2-b^2)(a^2-b^2)] & 1/(\xi_1^2-a^2) \\ 1 & -1/[(\xi_2^2-b^2)(a^2-b^2)] & 1/(\xi_2^2-a^2) \\ 1 & -1/[(\xi_3^2-b^2)(a^2-b^2)] & 1/(\xi_3^2-a^2) \end{pmatrix}$$

Now we reuse another one of our rules: swap the last two columns and then negate one of them,

$$\Phi \approx \begin{pmatrix} 1 & 1/(\xi_1^2-a^2) & 1/[(\xi_1^2-b^2)(a^2-b^2)] \\ 1 & 1/(\xi_2^2-a^2) & 1/[(\xi_2^2-b^2)(a^2-b^2)] \\ 1 & 1/(\xi_3^2-a^2) & 1/[(\xi_3^2-b^2)(a^2-b^2)] \end{pmatrix} \qquad S = \det(\Phi) \qquad (12.21)$$

and this form agrees with Morse and Feshbach page 663:

$$S = \begin{vmatrix} 1 & \dfrac{1}{(\xi_1^2 - a^2)} & \dfrac{1}{(\xi_1^2 - b^2)(a^2 - b^2)} \\ 1 & \dfrac{1}{(\xi_2^2 - a^2)} & \dfrac{1}{(\xi_2^2 - b^2)(a^2 - b^2)} \\ 1 & \dfrac{1}{(\xi_3^2 - a^2)} & \dfrac{1}{(\xi_3^2 - b^2)(a^2 - b^2)} \end{vmatrix}$$

(d) Summary of Results

Step 1: The functional-form solution to (3.5) is :

$$F_1 = F_1 \qquad g_1 = G_1/(F_2F_3)$$
$$F_2 = F_2 \qquad g_2 = G_2/(F_3F_1)$$
$$F_3 = F_3 \qquad g_3 = G_3/(F_1F_2)$$

Step 2: The first column cofactors are

$$M_1 = - G_1/f_2^2f_3^2$$
$$M_2 = - G_2/f_3^2f_1^2$$
$$M_3 = - G_3/f_1^2f_2^2$$

Step 3: Q = 1 since R = 1

Step 4: $S \equiv \det(\Phi) = G_1G_2G_3/(f_1^2f_2^2f_3^2)$

Step (5): Use the cofactor information to obtain the rightmost two columns of a Φ matrix and get

$$\Phi = \begin{pmatrix} a(1) & b(1) & c(1) \\ d(2) & e(2) & f(2) \\ g(3) & h(3) & i(3) \end{pmatrix} \approx \begin{pmatrix} a(1) & 1/f_1^2 & \xi_1^2/f_1^2 \\ d(2) & 1/f_2^2 & \xi_2^2/f_2^2 \\ g(3) & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix}$$

Step 6: Obtain two alternative solutions for the first column entries:

$a(1) = \xi_1^4/f_1^2$ $a(1) = 1$
$d(2) = \xi_2^4/f_2^2$ $d(2) = 1$
$g(3) = \xi_3^4/f_3^2$ $g(3) = 1$

Use the first solution to obtain the Φ matrix of Moon and Spencer:

$$\Phi \approx \begin{pmatrix} \xi_1^4/f_1^2 & 1/f_1^2 & \xi_1^2/f_1^2 \\ \xi_2^4/f_2^2 & 1/f_2^2 & \xi_2^2/f_2^2 \\ \xi_3^4/f_3^2 & 1/f_3^2 & \xi_3^2/f_3^2 \end{pmatrix} \qquad \text{// Moon and Spencer page 41}$$

(12.18)

Step 7: Use the second solution and do some equivalence operations to obtain the Φ matrix of Morse and Feshbach:

$$\Phi \approx \begin{pmatrix} 1 & 1/(\xi_1^2-a^2) & 1/[(\xi_1^2-b^2)(a^2-b^2)] \\ 1 & 1/(\xi_2^2-a^2) & 1/[(\xi_2^2-b^2)(a^2-b^2)] \\ 1 & 1/(\xi_3^2-a^2) & 1/[(\xi_3^2-b^2)(a^2-b^2)] \end{pmatrix} \qquad \text{// Morse and Feshbach page 663}$$

(12.19)

Notice that in all our Stäckel matrices, the three rows are identical except for the coordinate label.

(e) The separated solutions: Lamé functions

Any of these Stäckel matrices may be used to obtain the separated equations of the Helmholtz equation, which are (4.8) with $\kappa_1 = K_1$. Thus,

$$(\nabla^2+K_1^2)\psi = 0 \qquad \psi = X_1X_2X_3$$

$$L_nX_n = (1/F_n)\partial_n[F_n(\partial_nX_n)] + [\, K_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n)]X_n = 0 \qquad n = 1,2,3$$

or

$$L_iX_i = (1/f_i)\partial_i[f_i(\partial_iX_i)] + [\, K_1^2\Phi_{i1}(\xi_i) + k_2^2\Phi_{i2}(\xi_i) + k_3^2\Phi_{i3}(\xi_i)]X_i = 0 \quad i = 1,2,3 \qquad (12.22)$$

In the second line, we can think of $f_2 = +i\, F_2$ and then the +i's cancel up and down. (We have changed the index from n to i, because n will have a completely new meaning below.)

Because the three functions in each row of Φ are different and non-zero, one finds that the separation constants k_2^2 and k_3^2 are "fully entangled" in each separated equation. Also, and most impressively, we find that each of the separated equations *is the same equation,* and so has the same solutions, because the three rows of Φ are the same apart from the coordinate.

Using the Morse and Feshbach (12.19) form of the Φ matrix, one can install the Φ functions into (12.22) to get

$$L_iX_i = (1/f_i)\partial_i[f_i(\partial_iX_i)] + \{\, K_1^2 + k_2^2/(\xi_i^2-a^2) + k_3^2/[(\xi_i^2-b^2)(a^2-b^2)] \,\}\, X_i = 0 \qquad (12.23)$$

where $f_i^2 \equiv (\xi_i^2-a^2)(\xi_i^2-b^2)$

which appears as in Morse and Feshbach (5.1.37) with $K_1^2 \to k_1^2$.

The solutions X_i are Lamé functions, and the "ellipsoidal harmonics" are products of three Lamé functions

$$\psi = X_1X_2X_3 \sim [E_n^p(\xi_1),F_n^p(\xi_1)]\,[E_n^p(\xi_2),F_n^p(\xi_2)]\,[E_n^p(\xi_3),F_n^p(\xi_3)] \qquad (12.24)$$

where E and F are first and second kind Lamé functions, somewhat analogous to the Legendre P and Q functions. The two separation constants k_2^2 and k_3^2 have now been shuffled into the function parameters n and p which one sees are fully cross-linked between the three factors of each harmonic.

The n values get quantized to be integers n = 0,1,2,3... and for each value of n, there are certain peculiar quantized values of p for which normalizable solutions exist. Moreover, solutions E_n^p can be partitioned into four classes called K_n^p, L_n^p, M_n^p, N_n^p which have these forms (each series truncates)

$$K_{n,p}(x) = 1\,[\,x^n + \alpha x^{n-2} + \beta x^{n-4} + ..\,]$$
$$L_{n,p}(x) = \sqrt{x^2 - b^2}\,[\,x^{n-1} + \alpha x^{n-3} + \beta x^{n-5} + ..]$$
$$M_{n,p}(x) = \sqrt{x^2 - a^2}\,[\,x^{n-1} + \alpha x^{n-3} + \beta x^{n-5} + ..]$$
$$N_{n,p}(x) = \sqrt{x^2 - b^2}\,\sqrt{x^2 - a^2}\,[\,x^{n-2} + \alpha x^{n-4} + \beta x^{n-6} + ..]$$

where α,β are generic constants, different on each line. These E_n^p functions are all quite simple, having the usual Frobenius form $(x-x_0)^r\,\Sigma_j\,A_jx^j$ where x_0 is a regular singular point of the ODE. In our case, r = 1/2 and the regular singular points are ±a and ±b.

The functions may be simple, but the theory underlying them is quite complicated, though each element of the theory is reasonably straightforward. Here are a few E_n^p functions taken from Byerly for n = 0,1,2 and 3 (a,b are here c,b):

$E_0(x)$

$$K_0(x) = 1$$
$$L_0(x) = 0$$
$$M_0(x) = 0$$
$$N_0(x) = 0$$

$E_1(x)$

$$K_1(x) = x$$
$$L_1(x) = \sqrt{x^2 - b^2}$$
$$M_1(x) = \sqrt{x^2 - c^2}$$
$$N_1(x) = 0$$

$E_2(x)$

$$K_2^{p_1}(x) = x^2 - \tfrac{1}{3}\left[b^2 + c^2 - \sqrt{(b^2+c^2)^2 - 3b^2c^2}\right]$$
$$K_2^{p_2}(x) = x^2 - \tfrac{1}{3}\left[b^2 + c^2 + \sqrt{(b^2+c^2)^2 - 3b^2c^2}\right]$$
$$L_2(x) = x\sqrt{x^2 - b^2}$$
$$M_2(x) = x\sqrt{x^2 - c^2}$$
$$N_2(x) = \sqrt{(x^2 - b^2)(x^2 - c^2)}$$

$E_3(x)$

$$K_3^{p_1}(x) = x^3 - \frac{x}{5}\left[2(b^2+c^2) - \sqrt{4(b^2+c^2)^2 - 15b^2c^2}\right]$$
$$K_3^{p_2}(x) = x^3 - \frac{x}{5}\left[2(b^2+c^2) + \sqrt{4(b^2+c^2)^2 - 15b^2c^2}\right]$$
$$L_3^{q_1}(x) = \sqrt{x^2 - b^2}\left[x^2 - \tfrac{1}{5}\left(b^2 + 2c^2 - \sqrt{(b^2+2c^2)^2 - 5b^2c^2}\right)\right]$$
$$L_3^{q_2}(x) = \sqrt{x^2 - b^2}\left[x^2 - \tfrac{1}{5}\left(b^2 + 2c^2 + \sqrt{(b^2+2c^2)^2 - 5b^2c^2}\right)\right]$$
$$M_3^{r_1}(x) = \sqrt{x^2 - c^2}\left[x^2 - \tfrac{1}{5}\left(2b^2 + c^2 - \sqrt{(2b^2+c^2)^2 - 5b^2c^2}\right)\right]$$
$$M_3^{r_2}(x) = \sqrt{x^2 - c^2}\left[x^2 - \tfrac{1}{5}\left(2b^2 + c^2 + \sqrt{(2b^2+c^2)^2 - 5b^2c^2}\right)\right]$$
$$N_3(x) = x\sqrt{(x^2 - b^2)(x^2 - c^2)}$$

Notice in Byerly's table that there are always (2n+1) solutions for a given n. Hobson considers *conical* coordinates (r,μ,ν) and shows that the harmonics in that system are $r^n\ E_n^p(\mu)E_n^p(\nu)$ which can be compared to $r^n\ Y_{nm}(\theta,\varphi)$ in spherical coordinates. The linearly independent functions $E_n^p(\mu)\ E_n^p(\nu)$ for fixed n are thus linear combinations of the (2n+1) $Y_{nm}(\theta,\varphi)$, and that is why there are (2n+1) E_n^p functions. The label n is of course the quantum number associated with angular momentum. If one writes the angular momentum operator L^2 in these two coordinate systems, one finds that $E_n^p(\mu)\ E_n^p(\nu)$ and $Y_{nm}(\theta,\varphi)$ are both eigenfunctions of L^2 with eigenvalue n(n+1).

A classic problem in ellipsoidal coordinates is determining the electrostatic potential outside a charged metal ellipsoid having label ξ_1= c and potential V_0. The solution is this (see Morse and Feshbach p 1308 10.3.91)

$$\psi = \text{constant} * [F_0{}^0(\xi_1)]\,[E_0{}^0(\xi_2)]\,[E_0{}^0(\xi_3)] = \text{constant} * [F_0{}^0(\xi_1)]\,[1]\,[1]$$

$$= \text{constant} * F_0{}^0(\xi_1) = \text{constant} * sn^{-1}(1/\xi_1,b/a) = V_0\, sn^{-1}(1/\xi_1,b/a)/\, sn^{-1}(1/c,b/a) \qquad (12.25)$$

where the sn^{-1} is an inverse Jacobi function which is equal to the elliptic integral of the first kind,

$$sn^{-1}(x,k) = F(\sin^{-1}x,k) = F(\sin^{-1}x \mid m) = F(\sin^{-1}x \setminus \alpha) \qquad k = \sin\alpha \qquad m = k^2 \ .$$

Taking the limit c→a, ψ becomes the potential of a charged thin metal elliptical plate, and then taking b→a ψ is the potential a charged metal disk. These three problems, especially the first two, are quite difficult to solve in any other coordinate system.

The reader interested in learning about Lamé functions luckily has a very excellent source: the 43-page final chapter of a 1931 book by E.W. Hobson. Even in 2011 this chapter is crisp and clear, though there are a few typos. The latter part of the chapter deals with the issue of expressing the ellipsoidal harmonics in Cartesian coordinates.

(f) Comment on a missing minus sign on page 512 of Morse and Feshbach

Looking back at the start of Section 3, we had (take $K_1{}^2 \rightarrow k_1{}^2$ for this subsection)

$$(\nabla^2+k_1{}^2)\psi = 0$$
$$\Sigma_n(1/H)\partial_n[(H/h_n{}^2)(\partial_n\psi)] + k_1{}^2\psi = 0 \qquad H \equiv h_1h_2h_3 \qquad (3.1)$$

For cases with R=1 we know from (3.5) that $(H/h_n{}^2) = F_ng_n$, so (3.1) may be written

$$\Sigma_n\,(g_n/H)\,\partial_n[F_n(\partial_n\psi)] + k_1{}^2\psi = 0 \ . \qquad (12.26)$$

From (12.9),

$$g_n/H = \mathcal{G}_nF_n/\,(\mathcal{G}_1\mathcal{G}_2\mathcal{G}_3) = -\,\mathcal{G}_nF_n/\,(G_1G_2G_3)$$

and then (12.26) becomes

$$-\,\Sigma_n\,\mathcal{G}_nF_n/\,(G_1G_2G_3)\,\partial_n[F_n(\partial_n\psi)] + k_1{}^2\psi = 0 \ . \qquad (12.27)$$

From (12.5) make these replacements in (12.27),

$$\mathcal{G}_1F_1 \ .... \ F_1 \ \rightarrow \ G_1f_1 .... \ f_1$$
$$\mathcal{G}_2F_2 \ .... \ F_2 \ \rightarrow \ (-G_2)(\pm if_2) .... \ (\pm if_2) = G_2f_2 .... \ f_2$$
$$\mathcal{G}_3F_3 \ .... \ F_3 \ \rightarrow \ G_3f_3 .... \ f_3$$

to get

$$-\Sigma_n G_n f_n/(G_1G_2G_3)\,\partial_n[f_n(\partial_n\psi)] + k_1^2\psi = 0 \tag{12.28}$$

where notice the minus sign on the LHS. We now compare (12.28) with Morse and Feshbach p 512 (5.1.37),

$$\sum_n \frac{G_n f_n}{(\xi_1^2-\xi_2^2)(\xi_2^2-\xi_3^2)(\xi_3^2-\xi_1^2)} \frac{\partial}{\partial \xi_n}\left[f_n \frac{\partial\psi}{\partial\xi_n}\right] + k_1^2\psi = 0;$$

$$G_1 = (\xi_2^2 - \xi_3^2);\quad G_2 = (\xi_3^2-\xi_1^2);\quad G_3 = (\xi_1^2-\xi_2^2)$$

and we see that Morse and Feshbach should have a minus sign to the left of the large Σ in the above equation. Their G_n are the same as ours in (12.4), defined cyclically. There is no disagreement about the sign of k_1^2 as this Morse and Feshbach quote from p 509 shows

§5.1] *Separable Coordinates* 509

The Stäckel Determinant. The general technique for separating our standard three-dimensional partial differential equation

$$\nabla^2\psi + k_1^2\psi = 0$$

This rare Morse and Feshbach sign error created much confusion for the author until it was detected.

13. Stäckel Theory in N dimensions

Altered Development Equations

The generalization of the above analysis from N = 3 to N = N is completely straightforward, one can just march down the development and make the necessary alterations. It seemed best not to do this initially to keep things simple. Rather than create new equation numbers, we show the old ones and the reader can assume that future references to these numbers in this section imply use of the equations as modified here. We start at the beginning,

$$(\nabla^2+K_1^2)\psi = 0$$

$$H^{-1}\{ \partial_1[(H/h_1^2)(\partial_1\psi)] + \text{cyclic}\} + K_1^2\psi = 0 \qquad H \equiv h_1h_2h_3...h_N$$

$$H^{-1} \Sigma_{n=1}^N \partial_n[(H/h_n^2)(\partial_n\psi)] + K_1^2\psi = 0 \tag{3.1}$$

$$\psi = X_1X_2X_3...X_N/R \ . \tag{3.2}$$

The "+ cyclic" notation now brings in N-1 other terms obtained by cyclic permutation of the first term. Continuing on, we find

$$(H/[R^2h_n^2]) = f_n(n)g_n(\neq n) \qquad n = 1,2,3...N \tag{3.5}$$

$$(1/R)\, \Sigma_{n=1}^N \left[(1/[h_n^2X_n])\, (1/f_n)\partial_n[f_n \{ R(\partial_nX_n) - X_n(\partial_nR) \}] + K_1^2 = 0 \right. \tag{3.6}$$

$$\Sigma_{n=1}^N (1/[h_n^2f_nR])\, \partial_n\{f_n(\partial_nR)\} \equiv - k_1^2/Q(123) \tag{3.9}$$

$$\Sigma_{n=1}^N (1/[h_n^2X_n])\, (1/f_n)\partial_n[f_n(\partial_nX_n)] + k_1^2/Q + K_1^2 = 0 \tag{3.10}$$

$$-\Sigma_{n=1}^N (1/h_n^2)q_n + k_1^2/Q + K_1^2 = 0 \ . \tag{4.4}$$

The Stäckel matrix is now an NxN matrix defined in the obvious manner, and one has

$$q_n(n) = [\, \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n) + ... + k_N^2\Phi_{nN}(n)] \qquad n = 1,2,3..N \tag{4.5}$$

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [\, \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n) + k_3^2\Phi_{n3}(n) + ... + k_N^2\Phi_{nN}(n)]X_n = 0$$

This represents a set of N separated equations, n = 1,2....N (4.8)

There are now N-1 separation constants k_2^2, k_3^2....k_N^2, each a real number (possibly negative).

Recall that κ_1^2 is a stand-in for either the Helmholtz parameter K_1^2 for Problem B (R-separation), or the constant k_1^2 associated with Q for Problem A (simple-separation).

The matrix equation (5.3) is the same, but the matrices are NxN. The solution of this equation is still the Cofactor condition as in (5.6a),

$$M_n(\Phi)/S(\Phi) = (Q/h_n^2) \qquad n=1,2,3..N \qquad \text{" Cofactor condition"} \tag{5.6a}$$

The Robertson condition is slightly generalized now and says

$S(\Phi) = H / (f_1 f_2 f_3 ... f_N \ QR^2)$ "Robertson condition" *(5.7)*

and then (5.8a) is similarly generalized

$$M_n = g_n f_n / (f_1 f_2 f_3 ... f_N) \qquad (5.8a)$$

$$1/Q = \Sigma_{n=1}^{N} (1/h_n^2) \Phi_{n1}(n) \qquad (5.10)$$

Problem B recast at the end of Section 5 is this. Given

$S(\Phi) = H / (f_1 f_2 f_3 ... f_N QR^2)$ // Robertson
$M_n(\Phi) = S(\Phi) (Q/h_n^2)$ // Cofactor *(5.11)*

how *exactly* do we find the N^2 elements of Φ ?

Equivalence Rules

The equivalence rules of Section 6 are slightly modified and their derivation just slightly more complicated. It helps to have a 4x4 example for illustration:

$$\Phi = \begin{pmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & \ell \\ m & n & o & p \end{pmatrix}$$

Suppose we multiply one of the last N-1 columns by α and another by $1/\alpha$. For example, doing this for the 2nd and 4th columns gives

$$\Phi = \begin{pmatrix} a & \alpha b & c & d/\alpha \\ e & \alpha f & g & h/\alpha \\ i & \alpha j & k & \ell/\alpha \\ m & \alpha n & o & p/\alpha \end{pmatrix}$$

We know that if we take a matrix and multiply any column (or row) by a scalar α, the determinant gets multiplied by α. So here we have done that once with α and once with $1/\alpha$ so the determinant S is unchanged. Now consider the cofactor of a first column element. This cofactor is a signed minor with the sign fixed by position of the element, and the minor is the *determinant* of a 3x3 matrix. By the same argument just stated, this determinant is unaltered by having one column scaled by α and another by $1/\alpha$. Therefore, the cofactors of the elements of the first column are unaltered by our scaling process. Therefore this process generates an equivalent Stäckel matrix. So we modify Rule (1) to read

(1) multiply one of the last N-1 columns by any (nonzero) constant α,
and multiply another of the last N-1 columns by $1/\alpha$. *(6.1)*

Now what happens if we swap a pair of columns among the last N-1 columns and then negate one of them? We know that this action does not change the overall determinant S, but by the *same argument* it does not change any of the 3x3 minors involved in the four cofactors of the first column elements. Thus, this action creates an equivalent Stäckel matrix. So we have Rule (2)

(2) swap any pair of the last N-1 columns of Φ and then negate either of these columns. *(6.2)*

Finally, what happens if we add a multiple of one of the last N-1 columns to another of the last N-1 columns. For example, let's add λ times the last column to the second last:

$$\Phi = \begin{pmatrix} a & b & c+\lambda d & d \\ e & f & g+\lambda h & h \\ i & j & k+\lambda \ell & \ell \\ m & n & o+\lambda p & p \end{pmatrix}$$

We know $S = \det\Phi$ is unchanged. And once again, this operation does not change any of the minors of the first column elements. So again we have an equivalence operation. Adding a multiple of one of the last N-1 columns to the first is also OK since it changes neither S nor the M_n cofactors. Rule (3) becomes:

(3) add any multiple of one of the last N-1 columns to a different column. *(6.3)*

Summary of Stäckel Matrix Equivalence Operations for NxN matrices

(1) multiply one of the last N-1 columns by any (nonzero) constant α,
and multiply another of the last N-1 columns by $1/\alpha$. *(6.1)*

(2) swap any pair of the last N-1 columns and then negate either of these columns. *(6.2)*

(3) add any multiple of one of the last N-1 columns to a different column. *(6.3)*

Conditions

We generalize Section 7 (a):

Condition (1) Equations (3.5) must be solvable for the 2N+1 functions f_n, g_n and R. If some f_n is a constant, set that constant to 1. For Problem A, set R=1.

$(H/h_1^2) = f_1(1)g_1(\neq 1)\, R^2$ $\qquad H = h_1h_2h_3...h_N$
$(H/h_2^2) = f_2(2)g_2(\neq 2)\, R^2$
....
$(H/h_N^2) = f_N(N)g_N(\neq N)\, R^2$ *(3.5)*

Assuming equations (3.5) can be solved, compute the M_n cofactors as follows from (5.8a)

$M_n(\neq n) = g_n f_n / (f_1 f_2 ... f_N)$ $\qquad$ $n = 1,2...N$ $\qquad$ *(5.8a)*

Condition (2) Equations (7.2) must have a solution. This is a set of N functional-form conditions, where the M_n are as given above,

$$\begin{aligned} M_1(\neq 1) &= ... \\ -M_2(\neq 2) &= ... \\ M_3(\neq 3) &= ... \\ -M_4(\neq 4) &= ... \end{aligned} \qquad (7.2)$$

where the RHS's of these equations are the appropriate (N-1)x(N-1) minors. So the RHS of each equation has N-1 terms each of which is the product of N-1 Φ elements. We can write these expressions using the totally antisymmetric ε tensor having N indices:

$$\det(\Phi) = \Sigma_{nabc..}\ \varepsilon_{nabc..}\ \Phi_{n1}\ \Phi_{a2}\ \Phi_{b3}\ \Phi_{c4} ....$$

$$= \Sigma_n\ \Phi_{n1} [\ \Sigma_{abc..}\ \varepsilon_{nabc..}\ \Phi_{a2}\ \Phi_{b3}\ \Phi_{c4}....\ ]$$

$$= \Sigma_n\ \Phi_{n1} M_n$$

so that the above equations are these, where there are indeed N-1 Φ factors in each term,

$$M_n(\neq n) = \Sigma_{abc..}\ \varepsilon_{nabc..}\ \Phi_{a2}(a)\ \Phi_{b3}(b)\ \Phi_{c4}(c).... \qquad n = 1,2...N \quad .$$

As noted earlier, it is not obvious that, given the M_n as stated in Condition 1, the non-first-column Φ_{nm} elements can be found to satisfy these N conditions due to the functional form restriction *and* due to correlations between the equations since each Φ_{nm} appears in N-1 equations.

Condition (3) If conditions (1) and (2) are met, we then do the work of computing Q and k_1^2 from (3.9),

$$\Sigma_{n=1}^{N} (1/[h_n^2 f_n R])\ \partial_n\{f_n(\partial_n R)\} \ = - k_1^2/Q(123..N) \quad . \qquad (3.9)$$

For Problem A, Q = 1 and $k_1^2 = 0$ and no work is needed. Then with this Q expression, equation (7.6) must have a solution for the first column Φ elements,

$$1/Q = \Phi_{11}(1)\ (1/h_1^2) + \Phi_{21}(2)\ (1/h_2^2) + ... +\ \Phi_{2N}(N)\ (1/h_N^2) \qquad (7.6)$$

and this is another functional-form condition.

Steps

We generalize Section 7 (b):

Step 0: Write down the h_n for the curvilinear system of interest and compute $H = h_1h_2h_3 .. h_n$. Perhaps write down other useful facts concerning the system of interest.

Step (1) As noted above, the first task is to solve (3.5) for the 2N+1 functions f_n, g_n and R

$$(H/h_1^2) = f_1(1)g_1(\neq 1)\, R^2 \qquad\qquad H = h_1h_2h_3...h_N$$
$$(H/h_2^2) = f_2(2)g_2(\neq 2)\, R^2$$
$$....$$
$$(H/h_N^2) = f_N(N)g_N(\neq N)\, R^2 \qquad (3.5)$$

This task is pretty much just one of "inspection" when the LHS's of (3.5) are inserted (assuming Condition 1 that a solution exists!)

Step (2) Write down the N first-column cofactors from (5.8b),

$$M_n(\neq n) = g_nf_n /(f_1f_2...f_N) \qquad\qquad n = 1,2...N$$

Step (3) If Problem A, Q = 1. Otherwise compute Q and k_1^2 from (3.9),

$$\Sigma_{n=1}^N (1/[h_n^2f_nR])\, \partial_n\{f_n(\partial_nR)\} \quad = - k_1^2/Q(123) \qquad (3.9)$$

Step (4) Knowing Q, compute S from the Robertson condition,

$$S(\Phi) = H / (f_1f_2f_3...f_N\ QR^2) \qquad \text{"Robertson condition"} \qquad (5.7)$$

Step (5) Find the rightmost N-1 columns of the Stäckel matrix by solving the following N functional-form equations for a viable set of N*(N-1) Φ_{nm} elements (see Condition 2 above)

$$g_n(\neq n)f_n(n) /(f_1(1)f_2(2)...f_N(N)) = \Sigma_{abc..}\, \varepsilon_{nabc..}\ \Phi_{a2}(a)\, \Phi_{b3}(b)\, \Phi_{c4}(c).... \qquad n = 1,2....N$$

Step (6) Find the first column of the Stäckel matrix by solving (7.6) or (5.9)

$$1/Q(12...N) = \Phi_{11}(1)\, (1/h_1^2) + \Phi_{21}(2)\, (1/h_2^2) + ... + \Phi_{2N}(N)\, (1/h_N^2) \qquad (7.6)$$

which is of course another functional-form equation.

Step (7) At this point, we may want to apply some of our Section 6 equivalence operations to obtain a Stäckel matrix Φ that is of the simplest possible form, or of a form that matches the literature.

Examples? N=2 examples are given in the next section. We shall not work out any examples here for N>3, but two candidates would be "hyper-ellipsoidal coordinates in N dimensions" and "hyper-spherical coordinates in N dimensions". In the first case the confocal hypersurface families would have N-1 focal distances a_1, $a_2 \ldots\ldots a_{N-1}$ and things are just a generalization of what appears in Section 12. For example, the inequality chain (12.2) would be

$$0 \le \xi_N \le a_{N-1} \le \xi_{N-1} \ldots\ldots a_2 \le \xi_2 \le a_1 \le \xi_1 \quad .$$

For hyper-spherical coordinates ξ_1 would be the radial coordinate r, then ξ_2 through ξ_{N-1} are polar angles θ_1 through θ_{N-2}, and finally ξ_N is an azimuth φ. It seems likely to the author that both these N dimensional coordinate systems will be separable, but that is just a conjecture.

Non-Euclidian Stäckel Theory? For an orthogonal non-Euclidian curvilinear coordinate system one has a diagonal metric tensor which contains elements of both signs. This means that some of the h_n^2 (squared scale factors) are negative and H might be negative. These facts should not affect the development as presented above in this section.

14. Stäckel Theory in N=2 dimensions

As noted earlier, Moon and Spencer deal with various 3D cylindrical systems each with its own 2D orthogonal system in the ξ_1,ξ_2 coordinates. Moon and Spencer then state the nature of the Helmholtz and Laplace solution functions in various scenarios, *one* of which is that the solution has no z dependence due to an "extrusion symmetry" of the problem. This scenario yields separated equations for ξ_1,ξ_2 which agree with those we find below using the 2D Stäckel method, so Moon and Spencer provide a catalog of 2D separated equations, even though they don't explicitly state the 2D Stäckel matrices.

It should be realized that the 2x2 Stäckel matrix is *not* in general the "upper right 2x2 piece" of the 3x3 Stäckel matrix for the corresponding cylindrical system. We cannot just "delete" the 3 coordinate in a naive way, because in the 3x3 case ∂_z^2 is an active part of ∇^2. This fact will be demonstrated in the second Example below.

We assume at first arbitrary h_1 and h_2 and then later specialize to $h_1= h_2$. There will be only one separation constant, k_2^2.

We shall now restate the Conditions and Steps as given in Sections 7(a) and 7(b) for our case N = 2.

Conditions

Condition (1) Equations (3.5) must be solvable for the 5 functions f_n, g_n and R. If some f_n is a constant, set that constant to 1. For Problem A, set R=1.

$$(h_2/h_1) = f_1(1)g_1(2)\, R^2 \qquad\qquad H = h_1h_2$$
$$(h_1/h_2) = f_2(2)g_2(1)\, R^2 \qquad (3.5)$$

Assuming (3.5) can be solved, compute the M_n as follows :

$$M_1 = g_1 /f_2$$
$$M_2 = g_2 /f_1 \qquad (5.8b)$$

Condition (2) Equations (7.2) must have a solution. For N = 2 each first column cofactor is just a signed multiple of an element in the second column, so then

$$\Phi = \begin{pmatrix} a(1) & b(1) \\ c(2) & d(2) \end{pmatrix} \qquad S = \det(\Phi)$$

$$M_1 = d(2) \qquad => \qquad d(2) = M_1 = g_1 /f_2$$
$$M_2 = -b(1) \qquad => \qquad b(1) = -M_2 = - g_2 /f_1$$

Thus Condition 2 is satisfied in any N=2 system so we can ignore it, and we know that Φ has the form

$$\Phi = \begin{pmatrix} a(1) & b(1) \\ c(2) & d(2) \end{pmatrix} = \begin{pmatrix} a(1) & - g_2 /f_1 \\ c(2) & g_1 /f_2 \end{pmatrix}$$

Condition (3) If condition (1) is met, compute Q and k_1^2 from (3.9),

$$\Sigma_{n=1}^2 (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} \;\; = - k_1^2/Q(12) \qquad (3.9)$$

For Problem A, set Q = 1 and $k_1^2 = 0$ and no work is needed. Then with this Q expression, equation (7.6) must have a solution for a and c

$$1/Q = a(1)\,(1/h_1^2) + c(2)\,(1/h_2^2) \qquad (7.6)$$

Steps

Step (0) Write down the h_1 and h_2.

Step (1) As noted above, the first task is to solve (3.5) for the 5 functions f_n, g_n and R

$$(h_2/h_1) = f_1(1)g_1(2)\, R^2$$
$$(h_1/h_2) = f_2(2)g_2(1)\, R^2 \qquad (3.5)$$

This task is pretty much just one of "inspection" when the LHS's of (3.5) are inserted.

Step (2) Write down the two first-column cofactors from (5.8b)

$$M_1 = g_1/f_2$$
$$M_2 = g_2/f_1 \qquad (5.8b)$$

Step (3) If Problem A, Q = 1. Otherwise compute Q and k_1^2 from (3.9),

$$\Sigma_{n=1}^2 (1/[h_n^2 f_n R])\, \partial_n\{f_n(\partial_n R)\} \;\; = - k_1^2/Q(12) \qquad (3.9)$$

Step (4) Knowing Q, compute S from the Robertson condition,

$$S(\Phi) = (h_1 h_2) / (f_1 f_2 Q R^2) \qquad (5.7)$$

Step (5) We did this in Condition 2 above and found $\Phi = \begin{pmatrix} a(1) & -g_2/f_1 \\ c(2) & g_1/f_2 \end{pmatrix}$.

Step (6) Find the first column of the Stäckel matrix by solving (7.6) or (5.9)

$$1/Q = a(1)\,(1/h_1^2) + c(2)\,(1/h_2^2) \qquad (7.6)$$

or

$$S = a(1)\, M_1 + c(2)\, M_2 \qquad (5.9)$$

Step (7) The only equivalence rule that survives for N = 2 is to add a multiple of the second column to the first column.

Example: Polar Coordinates $(\xi_1, \xi_2) = (r,\theta)$

Step 0: $h_1 = 1 \quad h_2 = \xi_1$

Step (1) We know R = 1 so get

$$(h_2/h_1) = f_1(1)g_1(2)\, R^2$$
$$(h_1/h_2) = f_2(2)g_2(1)\, R^2 \tag{3.5}$$

$$\xi_1 = f_1(1)g_1(2) \quad \Rightarrow \quad f_1 = \xi_1 \quad g_1 = 1$$
$$1/\xi_1 = f_2(2)g_2(1) \quad \Rightarrow \quad f_2 = 1 \quad g_2 = 1/\xi_1$$

Step (2) Write down the two first-column cofactors from (5.8b),

$$M_1 = g_1/f_2 = 1/1 = 1$$
$$M_2 = g_2/f_1 = \xi_1^{-1}/\xi_1 = 1/\xi_1^2 \tag{5.8b}$$

Step (3) R = 1 => Q = 1

Step (4) Knowing Q, compute S from the Robertson condition

$$S(\Phi) = [\,(h_1h_2) / (f_1f_2)] \tag{5.7}$$

$$S(\Phi) = [\xi_1/\,\xi_1] = 1$$

Step (5) From Condition 3 above we found $\Phi = \begin{pmatrix} a(1) & -g_2/f_1 \\ c(2) & g_1/f_2 \end{pmatrix}$, therefore $\Phi = \begin{pmatrix} a(1) & -\xi_1^{-2} \\ c(2) & 1 \end{pmatrix}$

Step (6) We have to solve

$$S = a(1)\, M_1 + c(2)\, M_2 \tag{5.9}$$

$$1 = a(1)\, 1 + c(2)\, 1/\xi_1^2$$

This has a solution a(1) = 1 and c(2) = 0 so that

$$\Phi = \begin{pmatrix} a(1) & -\xi_1^{-2} \\ c(2) & 1 \end{pmatrix} = \begin{pmatrix} 1 & -\xi_1^{-2} \\ 0 & 1 \end{pmatrix}$$ // Stäckel matrix for polar coordinates.

The separated equations are (since simple-separation, $\kappa_1^2 = K_1^2$ = the Helmholtz parameter)

$$L_nX_n = (1/f_n)\partial_n[f_n(\partial_nX_n)] + [K_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n)\,]X_n = 0 \tag{4.8}$$

$$(1/f_1)\partial_1[f_1(\partial_1X_1)] + [K_1^2 1 + k_2^2(-\xi_1^{-2})\,]X_1 = 0$$
$$(1/f_2)\partial_2[f_2(\partial_2X_2)] + [K_1^2 0 + k_2^2 1\,]X_2 = 0$$

$$(1/\xi_1)\partial_1[\xi_1(\partial_1 X_1)] + [K_1^2 - k_2^2/\xi_1^2\,]X_1 = 0$$
$$(\partial_2^2 X_2) + [\,k_2^2\,]X_2 = 0$$

$$(1/r)\partial_r[r(\partial_r R)] + [K_1^2 - k_2^2/r^2\,]R = 0 \qquad \text{or} \qquad -(rR')' + k_2^2\,(R/r) - K_1^2 rR = 0$$
$$(\partial_\theta^2\Theta) + [\,k_2^2\,]\Theta = 0$$

$$r^2R'' + rR' + [\,r^2 K_1^2 - k_2^2\,]R = 0 \qquad R = X_1 \qquad (14.1)$$
$$\Theta'' + [\,k_2^2\,]\Theta = 0 \qquad \Theta = X_2$$

These agree with Moon and Spencer p 16 ("For φ independent of z") with $K_1^2 \to \kappa^2$ and $k_2^2 \to \alpha_2$.

To simplify notation a bit, we define

$a^2 = K_1^2$= the Helmholtz parameter // $= -\alpha^2$
$b^2 = k_2^2$ = the separation constant // $= -\beta^2$

We then rewrite the above pair of separated equations as

$$r^2R'' + rR' + [\,r^2 a^2 - b^2\,]R = 0 \qquad \text{or} \qquad -(rR')' + b^2\,(R/r) - a^2rR = 0 \qquad (14.2)$$
$$\Theta'' + b^2\Theta = 0$$

This radial equation is a scaled Bessel equation with solution of the type $J_b(ar)$. Consider now various situations:

$a^2 > 0$	a = real	
$a^2 < 0$	$a = i\alpha$ = imaginary,	α real
$b^2 > 0$	b = real	
$b^2 < 0$	$b = i\beta$ = imaginary,	β real

With these symbols, one can write the separated solution in a variety of ways. Here are the possible "atomic forms" (they cannot be called harmonics because they are Helmholtz solutions, not Laplace solutions)

$$\psi \sim X_1X_2 \sim [J_b(ar), Y_b(ar)]\ \ [\sin(b\theta),\cos(b\theta)] \qquad a = \text{real} \qquad b = \text{real} \qquad (14.3a)$$

$$\psi \sim X_1X_2 \sim [I_b(\alpha r), K_b(\alpha r)]\ \ [\sin(b\theta),\cos(b\theta)] \qquad a = \text{imaginary} \qquad b = \text{real} \qquad (14.3b)$$

$$\psi \sim X_1X_2 \sim [J_{i\beta}(ar), Y_{i\beta}(ar)]\ \ [\sinh(\beta\theta),\cosh(\beta\theta)] \qquad a = \text{real} \qquad b = \text{imaginary} \qquad (14.3c)$$

$$\psi \sim X_1X_2 \sim [I_{i\beta}(\alpha r), K_{i\beta}(\alpha r)]\ \ [\sinh(\beta\theta),\cosh(\beta\theta)] \qquad a = \text{imaginary} \qquad b = \text{imaginary} \qquad (14.3d)$$

Using Sturm-Liouville to solve a specific Helmholtz problem in polar coordinates

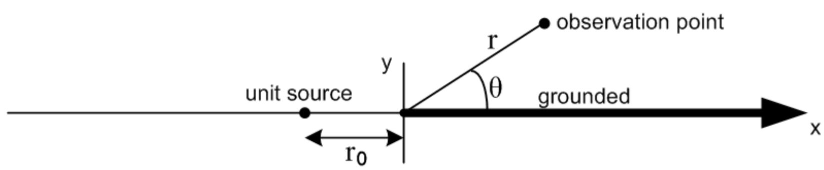
A prototype problem in 2D polar coordinates is to find the Helmholtz Green's Function for an infinite 2D wedge-shaped region with vertex at the origin. If this is a normal "Dirichlet" Green's Function, then the solution must vanish on both faces of the wedge, say θ=0 and θ=ψ, and the point source lies somewhere inside the wedge at r',θ'. This then turns the Θ equation above into a simple 1D Sturm Liouville problem and we find that the separation constant called b^2 gets quantized to specific values b_n^2 where $b_n = n\pi/\psi$, n = 0,1,2... The complete set of eigenfunctions associated with this SL problem is { $\sin(b_n\theta)$, n = 1.2.3...} and the "transform" associated with this Sturm Liouville problem is the Fourier Sine Series transform. If we start off assuming that the Helmholtz parameter a^2 is negative, then we can try to find a solution using atoms in (14.3b) where a = iα, and we try this "Smythian form",

$$g(r,\theta|r',\theta') = \Sigma_{n=1}^{\infty} C_n(r',\theta') \sin(b_n\theta)\, I_b(\alpha r_<)\, K_b(\alpha r_>) \qquad r_< = \min(r,r') \quad r_> = \max(r,r')$$

where C_n is a coefficient to be determined. One can in fact solve for C_n to obtain this result (see Stakgold vol 2 p 273 (7.174)),

$$g(r,\theta|r',\theta') = \Sigma_{n=1}^{\infty} (2/\psi) \sin(n\pi\theta/\psi) \sin(n\pi\theta'/\psi)\, I_{n\pi/\psi}(\alpha r_<)\, K_{n\pi/\psi}(\alpha r_>) \ . \qquad (14.4)$$

An interesting special case is also treated by Stakgold. If one lets the wedge angle increase all the way to 2π, then the two wedge sides meet along the +x axis, and the problem is to find the Helmholtz Green's Function where this half line x>0 is "grounded", meaning g=0. He further places the Green's unit point source at location $x = -r_0$ on the x axis.



The reader can extrude this picture out of the plane of paper to find a 3D problem solvable by 2D methods in which there is an infinite line source lying off the edge of a grounded half plane. The solution to this special case is of course just the above formula with ψ = 2π and θ' = π, so we get [Stakgold vol 2 p 275 (7.183)]

$$g(r,\theta|r_0,\pi) = \Sigma_{n=1}^{\infty} (1/\pi) \sin(n\theta/2) \sin(n\pi/2)\, I_{n/2}(\alpha r_<)\, K_{n/2}(\alpha r_>) \ . \qquad (14.5)$$

Remember that α encodes the Helmholtz parameter according to $\alpha^2 = -K_1^2$ and for this problem we can assume that $K_1^2 < 0$ so $\alpha^2 > 0$, at least for a start, then we can analytically continue in α as needed.

Stakgold then proceeds to do this same special case problem by instead treating the *radial* R equation as a 1D Sturm-Liouville problem in r on the interval (0,∞). In this case, taking b = iβ and a = iα, we can use atomic form (14.3d) to set things up. In *this* Sturm-Liouville problem, it turns out that the complete set of eigenfunctions is { $K_{i\beta}(\alpha r)$, β = real values 0 to ∞ }. Looking at (14.3d) and looking at the symmetry of the problem relative to θ = π, we are led to *try* the following Smythian form (this form is symmetric under x axis reflection which takes θ → 2π-θ)

$$g(r,\theta|r_0,\pi) = \int_0^\infty d\beta\ K_{i\beta}(\alpha r)\ [F_\alpha(\beta, r_0)\ ch(\beta|\theta-\pi|) + G_\alpha(\beta, r_0)\ sh(\beta|\theta-\pi|)]$$

where now F_α and G_α are the unknown coefficients. As in the previous case, we are just expanding on the appropriate Sturm-Liouville basis functions, which for the r coordinate are $K_{i\beta}(\alpha r)$. It is then possible to find these coefficients and express the answer to this problem as follows:

$$g(r,\theta|r_0,\pi) = (1/\pi^2) \int_0^\infty d\beta\ K_{i\beta}(kr)\ K_{i\beta}(kr_0)\ sh(\beta\pi)\ \{\ th(\beta\pi)\ ch(\beta(|\theta-\pi|) - sh(\beta(|\theta-\pi|)\ \}\ . \qquad (14.6)$$

As must be the case for any Green's Function (as we are using them), g must be symmetric under the interchange $r \leftrightarrow r_0$ *and* $\theta \leftrightarrow \pi$. In this particular problem, g is symmetric under each of these swaps separately. Notice how all our previous g's have been symmetric as well.

An interesting exercise is to show that (14.5) and (14.6) are in fact the same. This can be done by rewriting (14.6) this way

$$g(r,\theta|r_0,\pi) = -(i/2\pi) \int_{-\infty}^\infty d\beta\ I_{-i\beta}(kr_<)\ K_{-i\beta}(kr_>)\ \{\ th(\beta\pi)\ ch(\beta(|\theta-\pi|) - sh(\beta(|\theta-\pi|)\ \}\ .$$

The contour can be closed up or down, and then as it is deformed, it picks up the pole residues of th($\beta\pi$) which are located where ch($\beta\pi$) = 0 = cos($i\beta\pi$), which are points on the imaginary β axis at $i\beta = \pm n/2$. This sum of residues becomes the sum shown in (14.5).

The point is that in polar coordinates, where there is one separation constant $b^2= -\beta^2$, it is possible to do the 1D Sturm-Liouville analysis in *either* of the separated functions. The transform associated with the complete set of functions just mentioned is known as the Kantorovich-Lebedev Transform. The functions $K_{i\beta}(\alpha r)$ are the usual modified Bessel functions (McDonald functions) but of imaginary order, and are in fact real and oscillatory for real argument αr (see Appendix A).

We want to emphasize a key point. In our first solution of the "half plane problem", the spectrum of β^2 was discrete, being $i\beta_n = b_n = n\pi/\psi$ with $\psi = 2\pi$. In our second solution, the spectrum of this *very same* separation constant β^2 was continuous with β being the continuum of the positive real axis.

The reader interested in studying this problem should be advised there are 5 typos in this section of Stakgold (1968) Volume 2 which we can just nail down right here :

p 273 middle of page should say "by $K_{i\gamma}(kr)$ and " , not "by r $K_{i\gamma}(kr)$ and"
bottom equation should contain sinh, not sin

p 275 the A+B equation should contain sinh, not sin
same for the following equation
the equation following that is wrong and should read

$$\tilde{v} = -\ \{\ \cosh[\gamma(\varphi-\pi)]\ /\ [\gamma\ \sinh(2\gamma\pi)]\}\ \ K_{i\gamma}(kr_0)$$

Only the first of these five errors is corrected in the 2000 SIAM edition of the book.

The special case $h_1 = h_2$

Step 0: Let $h_1^2 = h_2^2 \equiv \mathcal{R}^2$

Step (1)

$(h_2/h_1) = f_1(1)g_1(2)\, R^2$
$(h_1/h_2) = f_2(2)g_2(1)\, R^2$

$1 = f_1(1)g_1(2)\, R^2$
$1 = f_2(2)g_2(1)\, R^2$

An obvious solution is

$f_1 = 1 \qquad g_1 = 1 \qquad R = 1$
$f_2 = 1 \qquad g_2 = 1$

Step (2) Write down the two first-column cofactors from (5.8b)

$M_1 = g_1 / f_2 = 1$
$M_2 = g_2 / f_1 = 1$

Step (3) R = 1 => Q = 1

Step (4) Knowing Q, compute S from the Robertson condition

$S(\Phi) = (h_1 h_2) / (f_1 f_2)$ "Robertson condition" *(5.7)*

$S(\Phi) = (h_1^2) / (1*1) = \mathcal{R}^2$

Step (5) Find the rightmost column of the Stäckel matrix,

$d(2) = g_1 / f_2 = 1 \qquad b(1) = - g_2 / f_1 = - 1$

so that

$$\Phi = \begin{pmatrix} a(1) & b(1) \\ c(2) & d(2) \end{pmatrix} = \begin{pmatrix} a(1) & -1 \\ c(2) & 1 \end{pmatrix}$$

Step (6) We have now to solve

$S = a(1)\, M_1 + c(2)\, M_2$

or

$\mathcal{R}^2 = a(1) + c(2)$

This will *only be possible if* our 2D system is such that

$$\mathcal{R}^2 = \mathcal{R}_1^2(1) + \mathcal{R}_2^2(2)$$

in which case we have our final Stäckel matrix

$$\Phi = \begin{pmatrix} a(1) & b(1) \\ c(2) & d(2) \end{pmatrix} = \begin{pmatrix} \mathcal{R}_1^2 & -1 \\ \mathcal{R}_2^2 & 1 \end{pmatrix}$$

Step (7) The only equivalence rule that survives for N = 2 is to add a multiple of the second column to the first column.

Separated equations:

$$L_n X_n = (1/f_n)\partial_n[f_n(\partial_n X_n)] + [\ \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n)\ ]X_n = 0 \qquad (4.8)$$

$$(1/f_1)\partial_1[f_1(\partial_1 X_1)] + [\ \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n)\ ]X_1 = 0$$
$$(1/f_2)\partial_2[f_2(\partial_2 X_2)] + [\ \kappa_1^2\Phi_{n1}(n) + k_2^2\Phi_{n2}(n)\ ]X_2 = 0$$

$$(1/1)\partial_1[1(\partial_1 X_1)] + [\ \kappa_1^2\mathcal{R}_1^2 - k_2^2]X_1 = 0$$
$$(1/1)\partial_1[1(\partial_1 X_1)] + [\ \kappa_1^2\mathcal{R}_2^2 + k_2^2\ ]X_2 = 0$$

$$(\partial_1^2 X_1) + [\ \kappa_1^2\mathcal{R}_1^2 - k_2^2]X_1 = 0$$
$$(\partial_2^2 X_2) + [\ \kappa_1^2\mathcal{R}_2^2 + k_2^2\ ]X_2 = 0$$

Summary of 2D systems with $h_1 = h_2$

Define $\mathcal{R}^2 \equiv h_1^2 = h_2^2$. Separability is only possible if one can write $\mathcal{R}^2(12) = \mathcal{R}_1^2(1) + \mathcal{R}_2^2(2)$. In this case, we get simple-separation for the Helmholtz equation with this data

$f_1 = 1$	$g_1 = 1$	$R = 1$	$M_1 = 1$	$S = \mathcal{R}^2$
$f_2 = 1$	$g_2 = 1$	$Q = 1$	$M_2 = 1$	

$$\Phi = \begin{pmatrix} \mathcal{R}_1^2 & -1 \\ \mathcal{R}_2^2 & 1 \end{pmatrix}$$

$$(\partial_1^2 X_1) + [\ \kappa_1^2\mathcal{R}_1^2 - k_2^2]X_1 = 0$$
$$(\partial_2^2 X_2) + [\ \kappa_1^2\mathcal{R}_2^2 + k_2^2\ ]X_2 = 0$$

Example : elliptical coordinates

In this system one has

$$h_1^2 = h_2^2 = \mathcal{R}^2 = a^2(\text{ch}^2\xi_1 - \cos^2\xi_2)$$

so

$$\mathcal{R}_1^2(1) = a^2\text{ch}^2\xi_1$$
$$\mathcal{R}_2^2(2) = -a^2\cos^2\xi_2$$

$$\Phi = \begin{pmatrix} a^2\text{ch}^2\xi_1 & -1 \\ -a^2\cos^2\xi_2 & 1 \end{pmatrix} \approx \begin{pmatrix} a^2\text{sh}^2\xi_1 & -1 \\ -a^2\sin^2\xi_2 & 1 \end{pmatrix}$$

$$(\partial_1^2 X_1) + [\ \kappa_1^2 a^2\text{ch}^2\xi_1 - k_2^2]X_1 = 0$$
$$(\partial_2^2 X_2) + [-\kappa_1^2 a^2\cos^2\xi_2 + k_2^2\ ]X_2 = 0$$

We added a^2 times the last column to the first to get an equivalent form of Φ. The first form agrees with Moon and Spencer p 20 ("For φ independent of z") with $\kappa_1^2 \rightarrow \kappa^2$ and $k_2^2 \rightarrow \alpha_2$. The solutions to these equations are Mathieu functions.

Recall from Section 9 Example 1 the Stäckel matrix for elliptic cylinder coordinates

$$\Phi = \begin{pmatrix} 0 & -1 & -a^2\text{ch}^2(\xi_1) \\ 0 & 1 & a^2\cos^2(\xi_2) \\ 1 & 0 & 1 \end{pmatrix} \approx \begin{pmatrix} 0 & a^2\text{ch}^2(\xi_1) & -1 \\ 0 & -a^2\cos^2(\xi_2) & 1 \\ 1 & -1 & 0 \end{pmatrix}$$

where to get the second form we have swapped the last two columns and then negated the 2nd column. In this special form, it happens that the upper right 2x2 matrix of Φ_{3x3} is the same as our first Φ_{2x2} matrix, but it is pretty clear than one cannot just take any form of Φ_{3x3} and assume this will be the case!

Appendix A. Review of 1D Sturm-Liouville Theory; the Kantorovich-Lebedev transform

The requirements of a 1D Sturm-Liouville problem are these: [Stakgold vol 1 p 268 + p 295]

(1) $\mathcal{L}$ is a self-adjoint differential operator of the form $\mathcal{L}u = (pu')'+q$.

(2) $\mathcal{L}$ acts on L^2-normalizable (possibly complex) functions on some interval (a,b). L^2 is a Hilbert Space of such normalizable functions with scalar product (physics convention) $<f,g> = \int_a^b dx\, f^*(x)g(x)$.

(3) The eigenvalue problem is $\mathcal{L}\varphi_\lambda = s(x)\lambda\varphi_\lambda$ where s(x) is some weight function. The functions p,q,s are all real and "reasonable" (C_1), and p and s must be non-negative on (a,b). At each end of the interval we have an unmixed boundary condition such as $A\varphi_\lambda(a) + B\varphi_\lambda'(a) = 0$, where A and B are real. If either of the endpoints is "singular", such as $b=\infty$ or $p(b) = 0$, the boundary condition for that endpoint is replaced by a requirement that φ_λ be finite at that endpoint. This can happen in two ways called "limit circle" and "limit point" as discussed by Stakgold.

The eigenfunctions of such a problem form a complete set: the φ_λ span the infinite dimensional Hilbert Space of L^2 of functions on (a,b) which meet the boundary conditions. The spectrum of eigenvalues of λ can in general be "mixed", consisting of a point spectrum and a continuous spectrum, both on the positive real axis in the λ plane, though in practice one usually has *either* discrete or continuous. We will assume the general mixed case, so we shall write the eigenvalue problem on two lines

$$\mathcal{L}\varphi_\lambda(x) = \lambda\ s(x)\ \varphi_\lambda(x) \qquad // \text{ spectrum } \lambda_n = \text{continuous range of real values} \qquad (A.1)$$
$$\mathcal{L}\varphi_{\lambda i}(x) = \lambda_i\ s(x)\ \varphi_{\lambda i}(x) \qquad // \text{ spectrum } \lambda_{ni} = \text{discrete set of real values } i = 1,2,3....$$

The statements of completeness and orthonormality of the eigenfunctions are these

$$\Sigma_i\ \varphi_{\lambda i}^*(x)\varphi_{\lambda i}(\xi) + \int d\lambda\ \varphi_\lambda(x)^*\ \varphi_\lambda(\xi) = \delta(x-\xi)/s(x) \qquad // \text{ completeness} \qquad (A.2)$$

$$<\varphi_{\lambda i},s\varphi_{\lambda j}> = \delta_{i,j}$$
$$<\varphi_\lambda,s\varphi_{\lambda'}> = \delta(\lambda-\lambda')$$
$$<\varphi_\lambda,s\varphi_{\lambda n}> = 0 \qquad // \text{ orthogonality} \qquad (A.3)$$

where one should take note of the weight function s(x) in all equations.

Such relations immediately imply the existence of a "transform" which we write as

$$F_{\lambda i} \equiv \int_a^b dx\ s(x)\ \varphi_{\lambda i}^*(x)\ f(x)$$
$$F_\lambda \equiv \int_a^b dx\ s(x)\ \varphi_\lambda^*(x)\ f(x) \qquad // \text{ projections} \qquad (A.4)$$

$$f(x) = \Sigma_i\ F_{\lambda i}\ \varphi_{\lambda i}(x) + \int d\lambda\ F_\lambda\ \varphi_\lambda(x) \qquad // \text{ expansion} \qquad (A.5)$$

where we ignore issues of convergence of sums and integrals and assume f(x) is suitable such that its projections exist, and that the expansion converges. The above transform can easily be "verified" by inserting either line into the other and using the completeness and orthogonality given above.

The reader is reminded that every Sturm-Liouville problem is associated with its own private transform, though frequently occurring transforms have people's names attached to them such as Fourier Sine Series Transform, Fourier Integral Transform, Mellin Transform, Hankel Transform, and so on.

Having been explicit with the mixed spectrum, we now adopt a more compact notation where the reader understands that the spectrum can be discrete, continuous, or mixed:

$$F_{\lambda i} \equiv \int_a^b dx\, s(x)\, \varphi_{\lambda i}^*(x)\, f(x) \qquad \text{// projection}$$
$$f(x) = \Sigma_{\lambda i} F_{\lambda i}\, \varphi_{\lambda i}(x) \qquad \text{// expansion}$$

Here the λ_i in the projection includes discrete and continuous, and the notation $\Sigma_{\lambda i}$ implies a sum on the discrete part plus an integral on the continuous part. If we *knew* there was only a continuous spectrum, we might write this as

$$F(\lambda) \equiv \int_a^b dx\, s(x)\, \varphi_\lambda^*(x)\, f(x) \qquad \text{// projection}$$
$$f(x) = \int d\lambda\, F(\lambda)\, \varphi_\lambda(x) \qquad \text{// expansion}$$

but we shall retain the $F_{\lambda i}$ notation. The $F_{\lambda i}$ are sometimes called "the coefficients", or "the transform". Basically the variable x of f(x) is traded out for the variable λ_i of $F_{\lambda i}$, just as in a spatial Fourier transform the variable x is traded out for $\lambda = k^2$. One must be a little careful with the distinction between λ and a convenient variable used to label λ, in this case k. For example, $d\lambda = 2kdk$.

In the same vein, we can compact down our completeness and orthogonality this way

$$\Sigma_{\lambda i}\, \varphi_{\lambda i}^*(x)\varphi_{\lambda i}(\xi) = \delta(x-\xi)/s(x) \qquad \text{// completeness}$$
$$\int_a^b dx\, s(x)\, \varphi_{\lambda i}^*(x)\, \varphi_{\lambda i}'(x) = \delta_{\lambda i,\lambda i'} \qquad \text{// orthogonality}$$

The notations $\Sigma_{\lambda i}$ and $\delta_{\lambda i,\lambda i'}$ are just shorthands for the fuller equations. We can gather up the above results and summarize the 1D Sturm Liouville situation as follows:

$$\mathcal{L}\varphi_{\lambda i}(x) = \lambda_i\, s(x)\, \varphi_{\lambda i}(x) \qquad \text{// eigenvalue problem (with BC's) on (a,b)}$$

$$\Sigma_{\lambda i}\, \varphi_{\lambda i}^*(x)\varphi_{\lambda i}(\xi) = \delta(x-\xi)/s(x) \qquad \text{// completeness}$$
$$\int_a^b dx\, s(x)\, \varphi_{\lambda i}^*(x)\, \varphi_{\lambda i}'(x) = \delta_{\lambda i,\lambda i'} \qquad \text{// orthogonality}$$
$$F_{\lambda i} \equiv \int_a^b dx\, s(x)\, \varphi_{\lambda i}^*(x)\, f(x) \qquad \text{// transform projection}$$
$$f(x) = \Sigma_{\lambda i} F_{\lambda i}\, \varphi_{\lambda i}(x) \qquad \text{// transform expansion} \qquad (A.6)$$

We should mention that there is a standard technique used to find the eigenfunctions φ_λ. One first solves this Green's Function problem,

$$[\mathcal{L}_x - \lambda s(x)]\, g(x|\xi;\lambda) = \delta(x-\xi) \qquad (A.7)$$

using the usual method of finding a boundary-condition-matching homogeneous solution to the left and to the right of x = ξ, and then matching the jump condition in the first derivative at x = ξ.

$$g(x|\xi;\lambda) = A(\lambda)\, u_{left}(x_<)\, u_{right}(x_>) \qquad\qquad \Delta g'|^{x=\xi} = -1/p \ .$$

Once this $g(x|\xi;\lambda)$ is found, one can deduce the normalized eigenfunctions by matching the two sides of this equation, where C is a counterclockwise great circle contour in the λ plane,

$$-(1/2\pi i) \int_C d\lambda\, g(x|\xi;\lambda) = \Sigma_{\lambda n}\, \varphi_{\lambda n}{}^*(x)\varphi_{\lambda n}(\xi) + \int d\lambda\, \varphi_\lambda(x)^*\, \varphi_\lambda(\xi) \quad . \qquad (A.8)$$

If $g(x|\xi;\lambda)$ has a branch cut along the real axis, the contour wraps this cut and one obtains a real integral of the discontinuity of g across the cut, and that becomes the second term on the RHS. Again, care is needed to distinguish the use of λ on the LHS as a complex contour integral variable, and on the RHS as the variable of a real axis integration. Poles in $g(x|\xi;\lambda)$ give rise to the first term on the RHS. We would be remiss to omit the following standard expansion for $g(x|\xi;\lambda)$,

$$g(x|\xi;\lambda) = \Sigma_i\, \varphi_{\lambda i}\,(x)^*\, \varphi_{\lambda i}(\xi)/\,(\lambda_i-\lambda) + \int d\lambda'\, \varphi_\lambda(x)^*\, \varphi_{\lambda'}(\xi)/(\lambda'-\lambda)] \qquad (A.9)$$

In the second term it is the "continuum of poles" that creates the branch cut whose discontinuity is then picked up as the second term in (A.8).

As an example, here is the Sturm Liouville data for equation (14.2) on the interval (0,∞). This is the radial equation for separated polar coordinates. We used this data slightly in the discussion leading to (14.6) and it is the basis of the derivation of (14.6), which is somewhat involved. The spectrum in this case is purely continuous and eigenvalue $\lambda = \beta^2$ spans the entire positive real axis of the λ plane.

$$-(xu')' + \alpha^2 xu - \beta^2 x^{-1} u = 0 \quad \text{or} \quad Lu = \beta^2 x^{-1} u \quad \text{where } L = -(xu')' + \alpha^2 xu$$

$$\text{or} \quad L_\lambda u = 0 \quad \text{where } L_\lambda = L - \beta^2 x^{-1} \qquad \lambda = \beta^2 \qquad s(x) = x^{-1}$$

$$\varphi_\beta(x) = (1/\pi)\sqrt{sh(\pi\beta)}\ K_{i\beta}(\alpha x) \qquad \text{// eigenfunctions}$$

$$(2/\pi^2) \int_0^\infty d\beta\, \beta\, sh(\pi\beta)\, K_{i\beta}(\alpha x)\, K_{i\beta}(\alpha x') = x\, \delta(x-x') \qquad \text{// completeness}$$

$$\int_0^\infty dx\, x^{-1} K_{i\beta}(\alpha x)\, K_{i\beta'}(\alpha x) = \delta(\beta-\beta')\, \pi^2/[2\beta sh(\pi\beta)] \qquad \text{// orthogonality}$$

$$F_\alpha(\beta) \equiv \int_0^\infty dx\, x^{-1} f(x)\, K_{i\beta}(\alpha x) \qquad \text{// projection (KL)}$$

$$f(x) = (2/\pi^2) \int_0^\infty d\beta\, \beta\, sh(\pi\beta)\, K_{i\beta}(\alpha x)\, F_\alpha(\beta) \qquad \text{// expansion (KL)} \qquad (A.10)$$

As noted earlier, for this particular operator L, the transform is called the Kantorovich-Lebedev transform (see e.g. Stakgold vol 1 p 317 4.30). It is always possible to write the halves of a transform some other way by replacing f(x) = jobob(x) F(x).

The entire discussion of this Appendix can be generalized such that the transform projections are onto eigenfunctions of multiple operators, which functions are the unitary irreducible representation functions of a continuous group. The spherical harmonics are a well known example associated with the rotation group SO(3).

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I. Stakgold, *Boundary Value Problems of Mathematical Physics,* Volumes 1 and 2 (MacMillan, London, 1967). These are astoundingly good books, but the high level of detail (the subject *is* intrinsically complex) makes them hard to use in a normal "course", which is why the author later put out a condensed single-volume version *Green's Functions and Boundary Value Problems,* now in a third edition. The original two volumes were reprinted with some corrections in 2000 (SIAM, Philadelphia). The author is alive and well and working emeritus at UCSD http://ccom.ucsd.edu/people/faculty.php. P. Lucht has a list of errata.

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