Sturm-Liouville 3D problems PhL 11.20.10

This most related to Stak Chap 6, potential theory and spherical coordinates.

Overview: 1
Question #1 : 5
A. The internal Laplace EF's of a Sphere and connection to the internal Spherical Atoms 6
(1) The internal eigenfunctions of the $L = -\nabla^2$ for a sphere 6
(2) Where do the internal spherical atoms fit in? 7
B. The sphere internal eigenfunctions as a complete set. 8
C. Is there a 3D Sturm-Liouville theorem? 9
D. The Laplacian in different coordinate systems 11
(1) Cartesian vs spherical. 11
(2) Conical vs spherical 12
E. What about the "n subspace" business. 13
(1) in the sphere problem sense 13
(2) in the sphere problem small r limit sense 14
F. More on completeness of the spherical atoms 15
G. What about the Helmholtz Operator? 16

Overview (4 1/2 pages, circa 11.20.10)

In this document I consider several different but related topics. I will review them each, one at a time. There are many claims that I make just as conjectures which I think are correct. This doc is not one in which I attempt to do things with any sense of full rigor. Just getting the ideas *stated* is work enough for me. The raw notes below are not in a very good order, so the overview reorders them somewhat.

The 3D Sturm Liouville (SL) Problem

I was wondering about what I call "the 3D Sturm-Liouville problem" (which of course means nD). The question is: if you have some nD diff operator L, and you solve $Lu_\lambda = \lambda u_\lambda$ for the eigenfunctions u_λ (assuming the BC that $u_\lambda = 0$ on some enclosing surface σ), are the eigenfunctions u_λ an orthogonal and complete basis for the space of L_2 functions which meet the BC's ?

I knew the answer to this question in the 1D world, since that problem was treated in detail by Stak in his Vol I. The answer there is "yes", as long as L is formally self-adjoint, meaning it has a certain "form". There is some subtlety in the 1D case which distinguishes the "regular" problem from the "singular" problem, but this is I think completely understood at least by somebody. It involves a reinterpretation of the meaning of the BC's, and you have details like Weyl's Theorem and limit circle limit point stuff.

Stak has very little to say on this nD subject, but he *does* say a small amount which I located below. I think this is the answer, and it has three parts.

The *first part* is that L has to be formally self-adjoint. To see what that means, consider the following. In nD, here is the "allowed form" for L of order p, (Stak II p 3)

$Lf = \Sigma_{|k|<p}\, a_k(x)\, D^k[f(x)]$ k represents a set $k_1,k_2...k_n$ such that D^k means $\partial_1^{k1}\partial_2^{k2}...\partial_n^{kn}$

and |k| means $\Sigma_i\, k_i$ so that |k|<p means that in any given term, if you add up all the orders of all the derivatives, you cannot exceed the order p. For p = 2, a term $\partial_1^2\partial_2$ would be a violation, for example. You can compute L* by "throwing over" all the derivatives and ignoring parts, and you find this expression for the L* (the adjoint of L)

$L^*f = \Sigma_{|k|<p}\, (-1)^{|k|} D^k[a_k(x)\, f(x)]$ Stak II p 9 5.12

So the first nD Sturm-Liouville condition you need is that L = L*. The "form" allowed by this condition is obviously more complex that in the n= 1D case of order p=2 which we studied in Vol I.

A *second condition* concerns "the parts". In order to obtain orthogonal eigenfunctions (required to have a complete basis) and real eigenvalues, the parts must vanish. Regardless of whether L is self-adjoint, having the parts vanish means we will have (L*v,u) = (v,Lu). Then if in addition L is formally self-adjoint, we will have (Lv,u) = (v,Lu) and this is the condition we need to prove things like real eigenvalues and orthogonality. In general, Green tells us that

$\int dV\, (vLu - vL^*u) = \int d\mathbf{S}.\mathbf{J}$ = "the parts" = (v,Lu) – (L*v,u) // $vLu - uL^*v = \nabla\bullet\mathbf{J}$

where the current **J** is something you can compute with some effort from L by throwing over those terms, and I recall computing this for several different L's. In the case of $L = \nabla^2$, the parts has this form

$\int d\mathbf{S}.\mathbf{J} = \int_\sigma (v\partial_n u - u\partial_n v)dS$ // n here means normal, not same as number of variables

and we obtain our desired result that "parts = 0" because u and v are in our class of functions within L_2 that vanish on σ. You see here that we *could* have "Neumann BC eigenfunctions" where $\partial_n u = 0$ on σ. So at least for L = Laplace, if we are dealing with a Green's Function g, or if we are dealing with the actual eigenfunctions u_λ, we know the "parts" will vanish because g or u_λ requires vanishing of something on the boundary σ (usually it is g, sometimes $\partial_u g$, and probably radiative works here just as well.)

With the above conditions met, we at least have real eigenvalues and orthogonal eigenfunctions, but we don't yet have completeness of these eigenfunctions for the function class of interest. This is our *third condition*. To get this third step, we have to convert the PDE into an integral equation and show that the kernel in this integral equation is symmetric and completely continuous. The kernel is in fact the Green's Function so you have to go compute g and see whether it meets these conditions. It is always symmetric, but the big question is whether it is completely continuous. I think if it is Hilbert-Schmidt, that will do the trick. But we are talking n dimensions here and Stak has little to say about nD integral equation theory.

In the case of $L = \nabla^2$, all three conditions are met. Self adjointness is obvious in Cartesian coordinates. The parts vanish as shown above. And Stak just tells us that the third condition is met. I suspect these three conditions are also met for Helmholtz $L = \nabla^2 + k^2$. It is again obviously self adjoint, and k^2 creates no new parts when it is "thrown over", so it is only the third issue that is uncertain.

So the conclusion is this: If we have a candidate nD Sturm-Liouville problem with some L and σ, then the eigenfunctions of $Lu_\lambda = \lambda u_\lambda$ will form an orthogonal, complete set for the space of functions vanishing on σ, and the eigenvalues will be real, provided the three conditions mentioned above are met.

If these three conditions are met, the next problem is finding the eigenfunctions. That is normally done by going to a coordinate system in which the boundary surface σ aligns with one of the coordinate level surfaces. For the eigenfunctions of a sphere, for example, we use spherical coordinates.

We can ask what happens if we simply drop the σ surface requirement in our nD SL problem so the spatial region becomes infinite, and we retain our requirement perhaps that a function be finite at the origin. An example of this situation would be an analysis of the nullspace of ∇^2 as considered below in this overview where $u_{nm} = r^n Y_{nm}(\theta,\varphi)$ do form a complete orthogonal basis for this nullspace.

In conical coordinates we instead get $v_{np} = r^n E_{np}(\mu) E_{np}(\nu)$. In the spherical case, we can decompose the SL problem into a 1D expo r problem times two distinct oscillatory 1D SL problems. The φ problem quantizes m, then the θ problem in turn quantizes n. However, in the conical case, the two quantum numbers n and p are coupled together across the μ problem and the ν problem. We cannot factor the μ,ν problem into a product of two 1D SL problems as we could with the θ,φ problems. Thus, we have in effect a single 2D SL problem in μ,ν that has to be considered as a single entity, and that determines the values of m and n. Stakgold never discusses such a situation, mainly because he sticks all the time to Cartesian coordinates. But there is stuff out there on this subject. Hobson solves this problem by using the $N^{(n)}$ subspace idea mentioned below. Comparison with the sphericals world suggests n = integers, and then you find the p values using the various recursor rollup equations that truncate series.

A particular 3D Sturm Liouville Problem: the interior sphere Laplace problem

I show in the raw notes below how you solve this problem in spherical coordinates. If the sphere has radius a, here are the eigenfunctions and the eigenvalues:

$$u_{mnk}(r,\theta,\varphi) = C_{nmk}\ (\sqrt{a/r}\ )\ J_{n+1/2}(\beta_k^{n+1/2} r/a)\ Y_{nm}(\theta,\varphi) \qquad \lambda_{nk} = (\beta_k^{n+1/2}/a)^2$$

where C_{nmk} is adjusted to make these functions orthonormal. Based on the discussion above, this set of eigenfunctions is orthogonal and complete for expanding any reasonable 3D L_2 function which is finite at r=0 and which vanishes on a sphere of radius a. The eigenvalues are real and positive, and $\beta_k^{n+1/2}$ are the zeros, enumerated by index k = 1,2,3.. , of the function $J_{n+1/2}(z)$. And $J_{n+1/2}(z)/\sqrt{z}$ are the spherical Bessel functions, so called due to the above fact! They are associated with the so-called Fourier-Bessel transform.

I point out that if you consider a region $r \leq R$ where $R << a$, the above eigenfunctions reduce to

$$u_{mnk}(r,\theta,\varphi) \sim r^n Y_{nm}(\theta,\varphi)$$

which are the familiar interior spherical atoms which are finite at r = 0. I show how in this limit all the eigenvalues move into the origin, and the above atoms solve $\nabla^2 u_\lambda = \lambda u_\lambda = 0$. These atoms are then "the limits near the origin of a set of eigenfunctions which are orthogonal and complete in the full sphere, but the atoms themselves, just being limits, do not have these properties in the full sphere! "

Another 3D Sturm Liouville Problem: the "interior" Laplace problem with no BC

Here we just drop the condition that the eigenfunctions vanish on our spherical σ. Our eigenfunctions for $\nabla^2 u_\lambda = \lambda u_\lambda$ then have this form, where λ can be any real positive value you want.

$$u_{n,m,\beta}(r,\theta,\varphi) = C'_{nm\beta}\ (\sqrt{1/r}\ )\ J_{n+1/2}(\beta r)\ Y_{nm}(\theta,\varphi) \qquad\qquad (\beta)^2 = \lambda a^2$$

The spectrum for λ is the entire positive real axis. I think these eigenfunctions will be orthogonal in the sense of the Hankel transform, and the associated expansion theorem will be this

$$f(r,\theta,\varphi) = \Sigma_{nm}\ Y_{nm}(\theta,\varphi)\ \int_0^\infty d\beta\ (\sqrt{1/r}\ )\ J_{n+1/2}(\beta r)\ f_{nm}(\beta)$$

where f(r,θ,φ) is now any reasonable L_2 function which is finite at the origin. I have not studied this situation very much, so these claims might be wrong, they are just conjectures on my part.

Clearly there are corresponding versions of the above situations where we have functions which vanish at r = ∞ and then we will have atoms r^{-n-1} and probably Bessel functions of the $H^{(1)}_{n+1/2}(\beta r)$ form. I have not pursued this subject at all in this doc.

Changes of coordinate system

I claim without strong proof that equations like $\nabla^2 u = 0$ and $\nabla^2 u_\lambda = \lambda u_\lambda$ are true in all coordinate systems if they are true in one, even for non-orthogonal coordinate systems. So if you find the eigenfunctions on one system, you simply convert that to other coordinate systems by replacing the variables appropriately. As example, if we convert our sphere eigenfunctions to Cartesian or conical coordinates, we get

$$U_{mnk}(x,y,z) = C_{nmk}\ (\sqrt{a/\sqrt{x^2+y^2+z^2}}\ )\ J_{n+1/2}(\beta_k{}^{n+1/2}\sqrt{x^2+y^2+z^2}\ /a)\ Y_{nm}(\theta[x,y,z],\varphi[x,y,z])$$

$$U'_{mnk}(r,\mu,\nu) = C_{nmk}\ (\sqrt{a/r}\ )\ J_{n+1/2}(\beta_k{}^{n+1/2} r/a)\ Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\}\ )$$

The spherical atoms and the n subspace business.

I claim that we can regard the spherical atoms $u_{nm} = r^n\ Y_{nm}(\theta,\varphi)$ as a complete orthogonal basis for the set of L_2 functions which satisfy the Laplace equation and which are finite at r = 0. This function space is the finite-at-r=0 portion of the nullspace N of the Laplace equation $\nabla^2 u = 0$. We can regard the u_{nm} atoms as the set of eigenfunctions having λ = 0 for our eigenvalue equation $\nabla^2 u_\lambda = \lambda u_\lambda$. We know from somewhere that the manifold of a particular eigenvalue is a true subspace and we can find an orthogonal basis for such a subspace, and the atoms are it. The orthogonality integral can run over all space so we do have a divergent normalization factor, but for the orthogonal part we see that $(u_{mn}, u_{m'n'}) = \delta_{mm'}\delta_{nn}\ N_{nm}$ entirely due to the angular part of the atom. Notice that apart from the r=0 condition, we have no bounding surface σ involved in this paragraph. We might put in a radial cutoff R so that N_{nm} would be finite.

We can regard the u_{nm} as vectors which span the Hilbert Space N. We can group these vectors into groups where we have a particular n and we let m run over its 2n+1 values. Such a group of vectors we claim spans a space we call $N^{(n)}$. Since vectors in different subspaces are orthogonal (as was just

pointed out), w can write $N = \Sigma_n N^{(n)}$ as a direct sum or block form decomposition, and we refer to the subspace $N^{(n)}$ as "the n subspace business".

We do an "application" of this concept. In conical coordinates, the atoms are $v_{np} = r^n E_{np}(\mu) E_{np}(\nu)$. If we consider all 2n+1 values of p, then we get a set of vectors which spans the same function subspace $N^{(n)}$ that is spanned by the spherical atoms $u_{nm} = r^n Y_{nm}(\theta,\varphi)$. This means that either of these angular functions is a linear combination of the other, a fact used by Hobson.

Helmholtz Equation

I show that the *atoms* for this equation have the form

$$J_{n+1/2}(\kappa r)\, Y_{nm}(\theta,\varphi) \;\rightarrow\; r^n\, Y_{nm}(\theta,\varphi) \qquad\qquad J_{-(n+1/2)}(\kappa r)\, Y_{nm}(\theta,\varphi) \rightarrow\; r^{-n-1}\, Y_{nm}(\theta,\varphi)$$

where the arrows show limits as $\kappa \rightarrow 0$. I then show that the eigenfunctions of the sphere are exactly the same as for the Laplace equation. The only difference is that the eigenvalues λ are shifted by $-\kappa^2$.

Question #1 :

Consider the 3D equation $\nabla^2 u = 0$ in spherical coordinates. I want to claim somehow that this ODE has the form $Lu = 0$ where $L = -\nabla^2$ is self-adjoint. The solutions u must be in the nullspace of L. Let's call this nullspace $\mathcal{N}$. I think it is a subspace of the space of all 3D L_2 functions which I will call $\mathcal{H}$. I suppose we have to define a region of space when we say these things, but how about the entire 3D space as the region. My feeling is that the set of atoms $r^n Y_{nm}(\theta,\varphi)$ form a complete basis for $\mathcal{N}$. Is this true?

One argument might be that we have a general Sturm-Liouville theorem which says that if L is a self-adjoint operator, then its eigenfunctions form a complete set on the region of interest. There are two problems at issue here:

(1) I only recall Stak stating this theorem in 1D, not 3D or nD.
(2) I don't know the eigenvalues of the operator $L^2 = -\nabla^2$ on all space, do I? That is, the spectrum.
(3) I am trying to claim maybe that $\lambda = 0$ is the only eigenvalue, and then $Lu = \lambda u = 0$ is an eigenvalue problem, and that $r^n Y_{nm}(\theta,\varphi)$ are the eigenfunctions.

Everything seems wobbly here. The only boundary condition I can think of in 3D is that the functions of interest in space $\mathcal{N}$ must be finite at the origin, hence I have excluded r^{-n-1}. I guess we have to arrange for our region $\mathcal{R}$ to have some boundary σ which we might take as a large sphere of radius a. Then at least we have something that corresponds to the two homo BC's at the endpoints of a 1D interval.

Did Stak address all my questions and issues here and I have just forgotten?

Maybe there *is* no 3D Sturm-Liouville implication from Stak and I am just imagining it. That would explain why I don't remember seeing it. In the above we have

$$L_n(r)\, u_{mnk}(r,\theta,\varphi) = \lambda_{n,k}\, r^2\, u_{mnk}(r,\theta,\varphi)$$

Now what can we say about completeness of these u functions? Treated just as function of r, where we regard θ,φ,n,m as fixed values, the $u_{mnk}(r,\theta,\varphi)$ form a complete set on the interval (0,a) and the set index is k. We know that treated as a function of θ or of φ alone, we again have a complete set on the related interval. We recall the Courant Hilbert idea that therefore the product is a complete set in the r,θ,φ space with these multiple intervals. But "a complete set for what? "

A. The internal Laplace EF's of a Sphere and connection to the internal Spherical Atoms

(1) The internal eigenfunctions of the $L = -\nabla^2$ for a sphere.

Start here and seek a separated form for these eigenfunctions

$$-\nabla^2 u = \lambda u$$

$$-[\nabla_r^2 - (1/r^2)L_{\theta\varphi}^2]\, u = \lambda u \qquad u = R(r)A(\theta,\varphi)$$

$$-[\nabla_r^2 - (1/r^2)L_{\theta\varphi}^2]\, R(r)A(\theta,\varphi) = \lambda\, R(r)A(\theta,\varphi)$$

$$\nabla_r^2\, R(r)\, A(\theta,\varphi) - (1/r^2)\, R(r)\, L_{\theta\varphi}^2 A(\theta,\varphi) = -\lambda\, R(r)A(\theta,\varphi)$$

$$[\nabla_r^2 + \lambda]R(r)\, A(\theta,\varphi) - (1/r^2)\, R(r)\, L_{\theta\varphi}^2 A(\theta,\varphi) = 0$$

$$r^2[\nabla_r^2 + \lambda]R(r)\, A(\theta,\varphi) - R(r)\, L_{\theta\varphi}^2 A(\theta,\varphi) = 0$$

$$r^2[\nabla_r^2 + \lambda]R(r)/R(r) - L_{\theta\varphi}^2 A(\theta,\varphi) = 0$$

This implies two separate equations with a separation constant μ so we write

$$r^2[\nabla_r^2 + \lambda]R(r)/R(r) = \mu \qquad L_{\theta\varphi}^2 A(\theta,\varphi)/A(\theta,\varphi) = \mu$$

We solve the angle equation and we find that $A(\theta,\varphi) = Y_{nm}(\theta,\varphi)$ with $\mu = n(n+1)$ and m = -n..n are the only possible solutions. Our radial equation is then

$$r^2[\nabla_r^2 + \lambda]R(r)/R(r) = n(n+1)$$

$$r^2[\nabla_r^2 + \lambda]R(r) = n(n+1)\, R(r)$$

$$-r^2\nabla_r^2\, R(r) + n(n+1)\, R(r) = \lambda\, r^2 R(r) \qquad (*)$$

The next step is to rescale the argument here so that $\xi = (r/a)$ in which case we get

$$-\xi^2\nabla_\xi^2\, R(\xi) + n(n+1)\, R(\xi) = (\lambda\, a^2)\, \xi^2\, R(\xi) = \lambda'\, \xi^2\, R(\xi) \qquad \lambda = \lambda'/a^2$$

$$[\ -\xi^2\nabla_\xi^2 + n(n+1)\ ]\ R(\xi) = \lambda'\ \xi^2\ R(\xi)$$

where we take note of the weight function ξ^2 on the right. The solutions of this radial eigenvalue equation and the eigenvalues are given by

$$R_{n,k}(\xi) = (\sqrt{1/\xi}\ )\ J_{n+1/2}(\beta_k^{n+1}\xi) \qquad \lambda'_{n,k} = (\beta_k^{n+1/1})^2$$

and you can see that R vanishes at $\xi = 1$ which means r = a. Therefore, the eigenvalues of the original 3D equation are

$$\lambda_{n,k} = \lambda'/a^2 = (\beta_k^{n+1/1}/a)^2$$

Therefore we have that

$$-\nabla^2 u = \lambda u$$

or

$$-\nabla^2\ u_{mnk}(r,\theta,\varphi) = (\beta_k^{n+1/1}/a)^2\ u$$

So, to summarize, the eigenfunctions and eigenvalues of the Laplacian inside a sphere are:

$$-\nabla^2\ u_{mnk}(r,\theta,\varphi) = (\beta_k^{n+1/1}/a)^2\ u \qquad \lambda_{nk} = (\beta_k^{n+1/1}/a)^2$$

$$u_{mnk}(r,\theta,\varphi) = C_{nmk}\ (\sqrt{a/r}\ )\ J_{n+1/2}(\beta_k^{n+1/2}r/a)\ Y_{nm}(\theta,\varphi) \qquad \text{// Stak p 145 H}$$

(2) Where do the internal spherical atoms fit in?

Now suppose we examine our $R_{n,k}(r)$ in a region $r \le \varepsilon$ where $\varepsilon << a$. *In this region* for fixed n,k we can take the small argument limit of the J function $J_n(x) = x^n 2^{-n}\ /\Gamma(n+1)$ (Jackson p 72 green). $R_{n,k}$ is not normalized to begin with, so we will just ignore constants. What we find then is that

$$R_{nk} \sim r^n$$

So if we consider in some sense the limit that $a \to \infty$, then any finite region of space is "near the origin" relative to a, and then we would expect to have $R_{nk} = r^n$ as the radial eigenfunctions in that region. Our eigenfunctions are now

$$u_{mnk}(r,\theta,\varphi) = r^n\ Y_{nm}(\theta,\varphi) \qquad \text{for } r << a$$

But we must still have

$$-\nabla^2\ u_{mnk}(r,\theta,\varphi) = (\beta_k^{n+1/1}/a)^2\ u$$

But in our same limit $a\to\infty$ for fixed n,k the RHS vanishes, and we find that we have

$u_{mnk}(r,\theta,\varphi) = r^n Y_{nm}(\theta,\varphi)$ for $r << a$

$\nabla^2 u_{mnk}(r,\theta,\varphi) = 0$ for $r << a$

Now if we regard any physical problem we have to be in some finite region of space with $r << a$, then we have found that our spherical atoms are solutions of the Laplace equation. Of course we can show the above result directly to be true regardless of any constant "a". But what we have shown is this:

"The spherical atoms are the limits for $r << a$ of the internal eigenfunctions of a sphere of radius a".

In some sense then you can regard the spherical atoms as the internal eigenfunctions of a sphere of infinite radius in the limit that you only work in some finite space $r << \infty$. Then the fact that these eigenfunctions diverge as r^n does not bother us.

Now as we go to the limit, what is happening? The eigenvalues $\lambda = (\beta_k^{n+1/1}/a)^2$ are all moving toward $\lambda = 0$, then are "moving in" all together. In the limit, the only eigenvalue is $\lambda = 0$ and it has an infinite multiplicity. This is a little iffy of course since the β_k can be infinitely large, but let's ignore that. So we might try to make this claim:

Claim: The eigenvalue equation $\nabla^2 u = 0$ is an eigenvalue equation where the only eigenvalue is $\lambda = 0$, and this λ has an infinite multiplicity, and the eigenfunctions are $u_{mn}(r,\theta,\varphi) = r^n Y_{nm}(\theta,\varphi)$ which are the internal spherical atoms.

But what are the *boundary conditions* for this eigenvalue problem? Finite at $r = 0$, yes. Certainly not finite or vanishing at $r = \infty$. So really, we can't fit this problem into our framework. We need some bounding surface σ which would be a sphere I suppose. But what is our boundary condition on that surface? On the unit sphere, each "eigenfunction" $r^n Y_{nm}(\theta,\varphi)$ has a different value, namely, $Y_{nm}(\theta,\varphi)$. But boundary conditions cannot be functions of the eigenfunction enumeration index. We can say that $r^n Y_{nm}(\theta,\varphi)$ is the unique solution to the internal Dirichlet problem where $Y_{nm}(\theta,\varphi)$ is prescribed on the bounding unit sphere. But there are no "eigenfunctions" here, there is no "completeness of the eigenfunctions" here. The whole notion of "eigenfunction" in the 3D world at least requires that $V = 0$ on some bounding surface, that is what we mean by eigenfunctions. But the functions $r^n Y_{nm}(\theta,\varphi)$ don't vanish on any bounding surface.

Therefore, the Claim made above is not really supportable in the usual Stakgold context.

The real answer here is that the spherical atoms are *limits* of the eigenfunctions of the finite grounded sphere problem. In this limit, they still form a complete set, but only for functions which are finite at the origin and vanish on the sphere of radius a, and of course only near the origin. This does not include all reasonable functions of the form $f(r,\theta,\varphi)$. In fact, it includes only those functions of the form $f(r,\theta,\varphi)$ which satisfy the Laplace equation! So $f = r^2$ is not included in this set!

B. The sphere internal eigenfunctions as a complete set.

We showed how these eigenfunctions arise above, and we had

$$-\nabla^2 u_{mnk}(r,\theta,\varphi) = \lambda_{nk} u_{mnk}(r,\theta,\varphi) \qquad \lambda_{nk} = (\beta_k^{n+1/1}/a)^2$$

$$u_{mnk}(r,\theta,\varphi) = C_{nmk} \ (\sqrt{a/r}\ ) J_{n+1/2}(\beta_k^{n+1/2} r/a) Y_{nm}(\theta,\varphi) \qquad \text{// Stak p 145 H}$$

We like to think of the set of eigenfunctions $u_{mnk}(r,\theta,\varphi)$ as a "complete set". We now ask: a complete set for what? Before answering, we examine this simple 1D example:

Example: Go back to square 1 and think $L = -\partial_x^2$ and EV equation is $Lu = \lambda u$ with BC $u=0$ at $x=0$ and $x=a$. We find then that $u_n = \sin(nx\pi/a)$ with $n = 1,2,3...$ since $\partial_x^2 u = -(n\pi/a)^2 u$ so $Lu = (n\pi/a)^2 u$ and $\lambda_n = (n\pi/a)^2$. The functions $u_n(x) = \sin(nx\pi/a)$ then form a complete set for what? Well, consider

$$f(x) = \Sigma_{n=1}^{\infty} f_n \sin(nx\pi/a) \qquad \Rightarrow \qquad Lf(u) = \Sigma_{n=1}^{\infty} f_n \lambda_n \neq 0$$

so certainly they don't form a complete set for "f(x) such that Lf = 0". The answer is that the $u_n(x)$ form a complete set for L_2 functions f(x) which meet the boundary conditions (and are reasonable). That is all. There is no extra requirement that f(x) be in some subspace of some differential operator.

So, we ask again: *for what* are the functions $u_{mnk}(r,\theta,\varphi)$ a complete set? They form a complete set for L_2 functions inside a sphere which are finite at the sphere's origin, and which vanish on the boundary of the sphere. Period. These functions $u_{mnk}(r,\theta,\varphi)$ don't satisfy the Laplace equation.

C. Is there a 3D Sturm-Liouville theorem?

Let's try to think of this as a 3D SL problem:

$$-\nabla^2 u_{mnk}(r,\theta,\varphi) = \lambda_{nk} u_{mnk}(r,\theta,\varphi) \qquad \lambda_{nk} = (\beta_k^{n+1/1}/a)^2$$

Is the operator $L = -\nabla^2$ self-adjoint in some 3D sense? We would want I think to show that

$$(w,Lv) = (Lw,v)$$

where w,v are in our space of functions which meet our two boundary conditions at r=0 and r=a. To show this, we have to show that "the parts" vanish. They will probably involve either w or v on the spherical surface, so they *will* vanish, so it is a question of whether L* = L. To checks this out, suppose we expand

$$w(r,\theta,\varphi) = \Sigma_{mnk} w_{mnk} u_{mnk}(r,\theta,\varphi)$$

$$v(r,\theta,\varphi) = \Sigma_{mnk} v_{mnk} u_{mnk}(r,\theta,\varphi)$$

Then we have

$$(w,Lv) = \int r^2 dr\, d\Omega(\Sigma_{m'n'k'} w_{m'n'k'} u_{m'n'k'}(r,\theta,\varphi)) \Sigma_{mnk} \lambda_{nk} v_{mnk} u_{mnk}(r,\theta,\varphi)$$

$$= \Sigma_{m'n'k'} \Sigma_{mnk} w_{m'n'k'} \lambda_{nk} v_{mnk} \int r^2 dr\, d\Omega\, u_{m'n'k'}(r,\theta,\varphi)\, u_{mnk}(r,\theta,\varphi)$$

$$= \Sigma_{m'n'k'} \Sigma_{mnk} w_{m'n'k'} \lambda_{nk} v_{mnk} \delta_{m'm} \delta_{n'n} \delta_{k'k} N_{nmk}$$

$$= \Sigma_{mnk} w_{mnk} v_{mnk} \lambda_{nk} N_{nmk}$$

If we compute (Lw,v) = (v,Lw) [real space for now] , we get the same answer. So I think we know at least that L is formally self-adjoint, so L* = L. [Of course this begs the question really.]

So here we have a self-adjoint operator in 3D, and we have its eigenfunctions forming a complete set for functions inside a sphere which are finite at the origin and which vanish on the boundary.

Is this a generalizable fact? Any 3D self-adjoint differential operator defines a 3D Sturm-Liouville problem which in turn has a complete set of 3D eigenfunctions? That SL problem involves Lu = λu as the eigenvalue equation and u are the corresponding eigenvalues.

Stak vol II p 9 does talk about L and L* and the idea that you might have L=L* as formally self-adjoint, and the discussion is in terms of multiple variables. He notes that ∇^2 is formally self-adjoint, though he writes it in Cartesian coordinates, so the discussion is I guess limited to Cartesians. Stak is then off doing distribution theory, but he finally returns on page 39 where he writes again a general L and its L*, and he writes this Green's Theorem result

$$\int dV\, (vLu - uL^*v) = \int d\mathbf{S}.\mathbf{J} \qquad\qquad vLu - uL^*v = \nabla \bullet \mathbf{J}$$

where we are now looking at "the parts" I mentioned above. For $L = \nabla^2$ he shows that the RHS is this

$$\int d\mathbf{S}.\mathbf{J} = \int_\sigma (v\partial_n u - u\partial_n v) dS$$

so my conjecture that this vanishes in our space of functions which vanish on a sphere is correct. Stak deals with many other subjects in this Chapter 5, but never talks about the possible completeness of a set of nD eigenfunctions. That subject simply does not arise in Chap 5 as far as I can see paging through the chapter.

The subject does come up later in Chapter 6 on page 136 which is about such eigenfunctions, but this discussion is just for $L = -\nabla^2$. He shows that eigenvalues are real and positive, and that eigenfunctions of different eigenvalues are orthogonal.

And now finally he gets to our subject. Are the eigenfunctions a complete set, he asks? Using the Green's function g(x|ξ) he converts the EV equation to an integral equation of one of our standard forms, see 6.86 page 138. In this case, the kernel g(x|ξ) implies an integral operator G which is symmetric and completely continuous. In the integral equations chapter, we showed that such integral operators do in fact have complete sets of eigenfunctions.

So the 3D Sturm-Liouville idea is this:

" If your operator L has a Green's function g which implies an integral operator G which is symmetric and which is completely continuous, then the eigenfunctions of Lu=λu do form a complete set for your space of interest."

So this is not as simple as the 1D SL situation where L = self-adjoint => complete set. But at least we have a statement of the 3D theorem. And we know that for $L = -\nabla^2$, we do get a complete set.

If someone hands you some general operator L, it might take you a while to figure out whether its eigenfunctions form a complete set! You would have to compute g, compute G, and then remember what completely continuous means. Maybe you could show G was H-S and that would be good enough.

D. The Laplacian in different coordinate systems.

Another question them comes to mind just for $L = -\nabla^2$. Are the eigenfunctions a complete set in any coordinate system? I think this is the answer: If we say $\nabla^2 u_\lambda = \lambda u_\lambda$ then this equation should be true in any coordinate system you want. As a Hilbert-space statement, $Lu_\lambda = \lambda u_\lambda$, there is no reference to any particular coordinate system. Think $L\,|\lambda\rangle = \lambda|\lambda\rangle$ in the abstract Hilbert space where we don't refer to how points in space are represented.

So, suppose you can find a coordinate system in which you can solve $\nabla^2 u_\lambda = \lambda u_\lambda$. In our case, we were able to solve this in the spherical system and we had

$$-\nabla^2\, u_{mnk}(r,\theta,\varphi) = \lambda_{nk}\, u_{mnk}(r,\theta,\varphi) \qquad \lambda_{nk} = (\beta_k^{n+1/2}/a)^2$$

$$u_{mnk}(r,\theta,\varphi) = C_{nmk}\ (\sqrt{a/r}\,)\, J_{n+1/2}(\beta_k^{n+1/2} r/a)\, Y_{nm}(\theta,\varphi) \qquad \text{// Stak p 145 H}$$

I think if you replace r,θ,φ with some u,v,w of another coordinate system, your functions will still be eigenfunctions with the same eigenvalues. You will have

$$-\nabla_{u,v,w}^2\, U_{mnk}(u,v,w) = \lambda_{nk}\, U_{mnk}(u,v,w)$$

where

$$U_{mnk}(u,v,w) = u_{mnk}(r[u,v,w],\, \theta[u,v,w],\, \varphi[u,v,w])$$

The functions are likely to be unpleasant.

(1) Cartesian vs spherical.

If we take u,v,w = Cartesian we have $r = \sqrt{x^2+y^2+z^2}$ and our solutions would be

$$U_{mnk}(x,y,z) = C_{nmk}\ \left(\sqrt{a/\sqrt{x^2+y^2+z^2}}\,\right) J_{n+1/2}(\beta_k^{n+1/2}\sqrt{x^2+y^2+z^2}/a)\, Y_{nm}(\theta[x,y,z],\varphi[x,y,z])$$

I now know exactly how to write $Y_{nm}(\theta[x,y,z],\varphi[x,y,z])$ which is really $Y_{nm}(z,\tan^{-1}(y/x))$. I know this because I wrote a doc on writing the spherical harmonics in Cartesian coordinate!

$$P_n^m(\cos\theta)\,[\cos(m\varphi), \sin(m\varphi)] \;=\; (1/r)^n\;[\; C_n(x,y,z;\, n,m),\; S_n(x,y,z;\, n,m)\;]$$

So the eigenfunctions of a sphere in Cartesians is not too bad, just a bit messy.

(2) Conical vs spherical.

Now suppose we let u,v,w = r,μ,ν which is meant to be the conical system. Then our eigenfunctions are these:

$$U_{mnk}(r,\mu,\nu) = C_{nmk}\;(\sqrt{a/r}\,)\,J_{n+1/2}(\beta_k^{\,n+1/2} r/a)\;Y_{nm}(\theta[r,\mu,\nu],\,\varphi[r,\mu,\nu])$$

But we know that we have this connection between spherical coordinates and conical ones,

$$\Rightarrow\; \cos\theta = \mu\nu/(kh)$$
$$\sin\theta\,\cos\varphi = \sqrt{\mu^2 - h^2}\,\sqrt{h^2 - \nu^2}\,/\,(hs)$$
$$\sin\theta\,\sin\varphi = \sqrt{k^2 - \mu^2}\,\sqrt{k^2 - \nu^2}\,/(ks)$$

$$\tan\varphi = \{\,(h/k)\,\sqrt{k^2 - \mu^2}\,\sqrt{k^2 - \nu^2}\,/[\sqrt{\mu^2 - h^2}\,\sqrt{h^2 - \nu^2}\,]\} \;=\; \{...\}$$

so the above really becomes

$$U_{mnk}(r,\mu,\nu) = C_{nmk}\;(\sqrt{a/r}\,)\,J_{n+1/2}(\beta_k^{\,n+1/2} r/a)\;Y_{nm}(\theta[\mu,\nu],\,\varphi[\mu,\nu])$$

and more specifically

$$U_{mnk}(r,\mu,\nu) = C_{nmk}\;(\sqrt{a/r}\,)\,J_{n+1/2}(\beta_k^{\,n+1/2} r/a)\;Y_{nm}(\mu\nu/(kh),\,\tan^{-1}\{...\}\,)$$

If we work in the same limit described above in section X, we find this limit

$$U_{mnk}(r,\mu,\nu) \sim\; r^n\,Y_{nm}(\mu\nu/(kh),\,\tan^{-1}\{...\}\,) \qquad \text{where m takes 2n+1 values}$$

This says that the solutions of the Laplace equations can be formed from these atoms in conical coordinates, so we can expand a Laplace-solving function f(r,μ,ν) in this manner, near the origin,

$$f(r,\mu,\nu) \;=\; \Sigma_n\, r^n\, \Sigma_m Y_{nm}(\mu\nu/(kh),\,\tan^{-1}\{...\}\,) f_{nm}$$

Hobson did the direct separation and found that

$$\text{atoms} \;=\; r^n\,E_{n,p}(\mu) E_{n,p}(\nu)$$

so he concludes that we can expand a Laplace-solving function f(r,μ,ν) in this manner, near the origin,

$$f(r,\mu,\nu) \;=\; \Sigma_n\, r^n\, \Sigma_p\, E_{n,p}(\mu) E_{n,p}(\nu)\, F_{np}$$

If we compare these two expansions we get

$$\Sigma_n r^n \Sigma_m Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\})f_{nm} = \Sigma_n r^n \Sigma_p E_{n,p}(\mu)E_{n,p}(\nu) F_{np}$$

or

$$\Sigma_n r^n \{ \Sigma_m Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\})f_{nm} - \Sigma_p E_{n,p}(\mu)E_{n,p}(\nu) F_{np} \} = 0$$

or

$$\Sigma_n r^n A_n(\mu,\nu) = 0$$

We know (see "Power series...doc") that if this true for a tiny but finite region of r, it implies $A_n(\mu,\nu)$ for all n. Thus we conclude that

$$\Sigma_m f_{nm} Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\}) = \Sigma_p F_{np} E_{n,p}(\mu)E_{n,p}(\nu)$$

We can construct a specific function of the form $f(r,\mu,\nu)$ setting $F_{np} = \delta_{p,p1}$ which says

$$\Sigma_m f_{nm} Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\}) = E_{n,p1}(\mu)E_{n,p1}(\nu)$$

If we just rename this arbitrary p1 to be p, we have

$$E_{n,p1}(\mu)E_{n,p1}(\nu) = \Sigma_m f_{nm} Y_{nm}(\mu\nu/(kh), \tan^{-1}\{...\})$$

which says that EE is a linear combination of spherical harmonics of degree n, expressed in μ,ν coordinates.

E. What about the "n subspace" business.

(1) in the sphere problem sense

For our sphere problem, the eigenfunctions $u_{nmk}(r,\theta,\varphi)$ form a complete basis for a subspace S of L_2 functions -- those that are finite at the origin and vanish at r = a. The functions $u_{nmk}(r,\theta,\varphi)$ are the basis vectors in this subspace S of L_2. (I am not sure the technical term "subspace" is correct here, but I will use it anyway for now.) Since k = 1,2,3....∞, and n = 1,2.3....∞ and m = -n....n, we really have a triply infinite basis.

Suppose we take a subset of these basis vectors where we specify n = 4 and k = 7, so we have $\{ u_{4m7}(r,\theta,\varphi) \}$ This is a set of 9 basis vectors. In some sense, these 9 vectors span a subspace of the subspace S. We might define it as $S^{(7,4)}$. More generally, we could talk about $S^{(k,n)}$ as being a subspace of S which is spanned by 2n+1 vectors. We should be able to write

$$S = \Sigma_{k,n} S^{(k,n)}$$

Eigenfunctions are orthogonal if they have $k \neq k'$ or $n \neq n'$ (recall above that Stak shows this). So this means somehow that the above thing is a direct sum or block form sum thing and I think somehow that

means the space = direct sum of subspaces idea is valid. So we can talk about $S^{(k,n)}$ as being a subspace of S which has the finite dimension 2n+1. So that is one meaning of "the n subspace business" alluded to in the section title above. But it is really an "n,k subspace business".

If we go to the small r region, the $u_{nmk}(r,\theta,\varphi)$ don't depend on k, so "there is no k" and we have just the spherical atoms, and we might like to write in this limit

$$S = \Sigma_n S^{(n)}$$

but we might worry that this $S^{(n)}$ think has $(2n+1) * \infty$ dimension.

(2) in the sphere problem small r limit sense

But we can start in a different manner. Suppose we define N to be the subspace of L_2 which is functions which are finite at r = 0 and which solve the Laplace equation. We think the atoms $r^n Y_{nm}$ are complete in this space, but I don't know how to justify that claim. We have not a boundary condition on a surface, it is a domain restriction for a differential operator equation Lu = 0. In fact, N is the nullspace of this operator L, and I think a null space is in fact a true subspace. Let's define $a_{nm}(r,\theta,\varphi) = r^n Y_{nm}(\theta,\varphi)$ and then a_{nm} are the basis vectors of this nullspace N. We really should include $b_{nm}(r,\theta,\varphi) = r^{-n-1} Y_{nm}(\theta,\varphi)$, but if we further restrict our domain to be functions finite at r=0, then that restricted nullspace N has only the a_{nm} as its basis vectors.

Now, can we state that the atoms are a complete basis for the nullspace of ∇^2 ? Remember that these atoms are not eigenfunctions of any eigenvalue problem that I can identify. I have to appeal to my limit of the sphere eigenfunctions in order to claim that the a_{nm} are in fact a complete basis in the nullspace. So I will use this appeal, and then declare that the atoms are a complete spanning set for the nullspace N of L_2 which includes the r=0 boundary condition restriction.

So, we move along now with this extra fact: the atoms $r^n Y_{nm}(\theta,\varphi)$ are a complete basis for the nullspace of ∇^2. In any event, whether or not this is true, we can take a subset of these vectors a_{4m} which set has 9 vectors in it. We can then write this subspace as $N^{(4)}$. Then we have this decomposition of the nullspace

$$N = \Sigma_n N^{(n)}$$

where $N^{(n)}$ is a real subspace which is spanned by the 2n+1 functions $r^n Y_{nm}(\theta,\varphi)$. Vectors for different n are orthogonal, so we think this is a valid direct sum subspace sum with block form in the matrix view.

So this $N^{(n)}$ is another interpretation of " the n subspace business" of our title mention.

When we look in conical coordinates and see atoms $a'_{np}(r,\mu,\nu) = r^n E_{np}(\mu) E_{np}(\nu)$, we can consider just those atoms for a specific n, and claim that we have 2n+1 functions which span the same $N^{(n)}$ we talked about above. The subspace $N^{(n)}$ has dimension 2n+1 and consists of all vectors in N which are of the form r^n * something. So a vector r^5*something cannot possibly be a basis vector in $N^{(4)}$. Then since both the $r^n Y_{nm}(\theta,\varphi)$ and $r^n E_{np}(\mu) E_{np}(\nu)$ for fixed n are a complete set of basis vectors for $N^{(n)}$, they must

be linear combinations of each other, and this means the $Y_{nm}(\theta,\varphi)$ and $E_{np}(\mu)E_{np}(\nu)$ must be linear combinations of each other.

Elsewhere I have arrived at this same conclusion making use of the "angular momentum" phrase, but I don't think that is really necessary, I have not mentioned it here.

F. More on completeness of the spherical atoms

Perhaps we can claim that the spherical atoms form a complete basis for the eigenvalue problem $\nabla^2 u = 0$ where the infinite multiplicity eigenvalue is $\lambda = 0$ and where there ARE no boundary conditions at all. We do talk about Green's Functions $\nabla^2 g = \delta$ where we specify no boundary conditions at all. The Green's function here is 1/R and we then get the solution of $\nabla^2 u = \sigma$ as $u = \int dS\ 1/R\ \sigma = G\sigma$ where G is our operator. We know G is symmetric, maybe it is completely continuous. That would tell us that the atoms are a complete set. But how to we know the entire spectrum is $\lambda = 0$? Maybe there is some λ_1 such that we have $\nabla^2 u = \lambda_1 u$ and we have omitted this eigenfunction from our complete set. What happens when we seek a separated solution here with no boundary conditions? I think you would get to this point:

$$-r^2 \nabla_r^2 R(r) + n(n+1) R(r) = \lambda_1 r^2 R(r)$$

The solution of this equation must be

$$R_{n,\beta}(r) = (\sqrt{1/r}\,)\, J_{n+1/2}(\beta r) \qquad \text{where} \quad (\beta)^2 = \lambda_1 a^2$$

so this says that any positive real λ_1 would be an eigenvalue. So our complete set of eigenfunctions is

$$u_{n,m,\beta}(r,\theta,\varphi) = (\sqrt{1/r}\,)\, J_{n+1/2}(\beta r)\, Y_{nm}(\theta,\varphi) \qquad (\beta)^2 = \lambda_1 a^2$$

OK, then our claim would be this

$$f(r,\theta,\varphi) = \Sigma_{nm}\, Y_{nm}(\theta,\varphi) \int d\beta\ (\sqrt{1/r}\,)\, J_{n+1/2}(\beta r)\, f_{nm}(\beta)$$

and maybe this is a value Fourier expansion for any reasonable function f. Maybe use the Hankel transform to invert it.

But be that as it may, perhaps we can restrict our interest in the spectrum to just those eigenfunctions which have $\lambda = 0$. We often talk about the subspace associated with a particular eigenvalue, so this would be just such a subspace, and then we can forget about the other possible eigenvalues. In this subspace, we see that we take $\beta \to 0$ and our eigenfunctions become the atoms again.

Claim: the atoms $u_{nm} = r^n\, Y_{nm}(\theta,\varphi)$ form a complete basis for the $\lambda = 0$ *subspace* of the eigenvalue problem $\nabla^2 u = 0$ with no boundary conditions other than finite at r=0. This subspace is the nullspace N of ∇^2, and we showed above how we can decompose this way: $N = \Sigma_n\, N^{(n)}$. The subspace N is the set of all L_2 functions $f(r,\theta,\varphi)$ which are finite at r = 0 and which solve the Laplace equation.

I have shown elsewhere that there is a little restriction to the above which is this: The region R upon which your eigenvalue problem is defined must include a ball around the origin of your spherical system. This origin cannot, for example, be sitting on the surface of a piece of metal. Among other things we need that ball to get quantization of n and m to integers. I learned this while trying to do the charged disk problem with a spherical origin at the center of the disk, and it would not fly.

G. What about the Helmholtz Operator?

If we gaze at M&S page 27, we can learn about the atoms for the Helmholtz equation in spherical coordinates. Their p and q are the same n and m we have in the Laplace world, quantized the same way. The angular functions are still the $Y_{nm}(\theta,\varphi)$, but the radial functions are no longer r^n type. The show the radial functions being these

$$R(r) = 1/\sqrt{r}\ [\ A\ J_{n+1/2}(\kappa r) + B\ J_{-(n+1/2)}(\kappa r)\ ]$$

In the limit $\kappa \rightarrow 0$, we can see that this gives $A\ r^n + B\ r^{-n-1}$. So we have a big change going from Laplace to Helmholtz in terms of the atoms

$$r^n\ Y_{nm}(\theta,\varphi) \rightarrow J_{n+1/2}(\kappa r)\ Y_{nm}(\theta,\varphi)$$

Now, what happens to our eigenfunction problem for the sphere of radius a ? We want to solve this eigenvalue problem for the sphere

$$-[\nabla^2+\kappa^2]u = \lambda u$$

but we just rewrite this as

$$-\nabla^2 u = (\lambda+\kappa^2)u = \Lambda u \qquad\qquad \Lambda = \lambda+\kappa^2$$

Then we just read off the eigenfunctions replacing λ by $\lambda+\kappa^2$ and we get

$$u_{mnk}(r,\theta,\varphi) = C_{nmk}\ (\sqrt{a/r}\ )\ J_{n+1/2}(\beta_k^{n+1/2} r/a)\ Y_{nm}(\theta,\varphi) \qquad \lambda+\kappa^2 = (\beta_k^{n+1/1}/a)^2$$

The solutions are *exactly the same* as those for the Laplace problem. The only difference is that for Helmholtz, the eigenvalues are shifted to new values by subtracting κ^2

$$\lambda_{Laplace} = (\beta_k^{n+1/1}/a)^2$$

$$\lambda_{Helmholtz} = -\kappa^2 + (\beta_k^{n+1/1}/a)^2$$

At first I thought maybe those Bessel wave functions were going to appear here, but that is not the case.