Diagonalization vs partial waves PhL 1.11.11

The word "diagonalization" refers to a certain matrix K_{nm} in the discussion below. This matrix is "the matrix elements" of an operator K which here is an integral operator. The term "partial waves" here refers to expanding a function on sines and cosines (or corresponding exponentials) which then are "partial waves" of the SO(2) group. At the end we mention partial waves of SO(3). A "partial wave" refers in general to the projection of a function onto some basis functions which are in fact EF's of some other operator(s) [J_z for SO(2), and J^2, J_z for SO(3)] . We show that SO(2) diagonalization of a convolution form integral equation causes K_{nm} to be diagonal and this happens when all the functions are expanded on their SO(2) partial waves. Sometimes I forget that in "group diagonalization", there is in fact a certain matrix that becomes diagonal (or at least achieves block form diagonal). See elsewhere for more details.

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Overview (2/3 page, written 1.16.11)

Given an arbitrary complete set of states |n> and eigenfunctions $\varphi_n(x)$ on (a,b), a 1D integral equation

$$f(x) = \int_a^b dy/C\ k(x,y)\ g(y)$$

can be converted to a matrix equation $f_m = \Sigma_{n=0}^{\infty} K_{mn}\ g_n$ where f_m is the projection of f(y) etc and where the matrix $K_{nm} = \langle n|K|m\rangle$ is in general fully populated and not diagonal. In the special case that k(x,y) = r(x-y), this conclusion still obtains. However, if this r(x) is *periodic on the interval (a,b),* then we can *select* for our set $\varphi_n(x)$ the functions $\exp(ik_nx)$ where $k_n=2\pi n/(b-a)$ which happen to be the 1D representations of the group SO(2). With this selection for $\varphi_n(x)$, the matrix K_{nm} becomes diagonal and the matrix equation becomes $f_m = K_{mm}g_m$ which is trival to solve for g_m. This basis $\varphi_n(x)$ is in this case the set of eigenfunctions of K, and the $r_n = K_{nn}$ are the eigenvalues. Sections A and B just fill out this paragraph.

A. Discussion

Section 1 gives the QM notation for how this all works, and talks about a certain constant C.

Section 2 notes the fairly obvious fact that if the $\varphi_n(x)$ are EF's of K, then K_{nm} is diagonal. But of course you don't in general know the EF's of K, so this is just an academic statement.

Section 3 notes that k(x,y)=r(x-y) in general does not make K_{nm} be diagonal.

Section 4 notes that if k(x,y)= r(x-y) AND r(x) is periodic in (a,b), for general $\varphi_n(x)$ again nothing has been simplified. K_{nm} is shown in equation (*) and is in general not diagonal.

Section 5 notes that if k(x,y)= r(x-y) AND r(x) is periodic in (a,b) AND you take $\varphi_n(x) = \exp(ik_nx)$ where $k_n=2\pi n/(b-a)$, then K_{nm} becomes diagonal. We don't consider the infinite interval case in this doc, but we know exactly how to handle it.

B. Summary of what happened above.

This long section just reviews with numbered items what we showed above.

A. Discussion

1. Suppose we have a 1D integral equation on some interval (a,b)

$$f(y) = \int_a^b dx/C\ k(y,x)\ g(x)$$

where C is some arbitrary constant. Suppose we have a set of orthonormal eigenfunctions $\varphi_n(x) = \langle n|x\rangle$ on this interval (a,b). Assume that the eigenfunctions can be labeled by n = 0,1,2,.... This means that

completeness	orthogonality
$\int_a^b dx/C\ \ |x\rangle\langle x| = 1$	$\langle x|x'\rangle = C\ \delta(x-x')$
$\Sigma_{n=0}^{\infty}\ |n\rangle\langle n| = 1$	$\langle n|m\rangle = \delta_{nm}$

In what follows, we will always have the |n> states be orthonormal, so $\langle n|m\rangle = \delta_{nm}$. But we are free to normalize the coordinate representation states |x> any way we want, and we have chosen to add the constant C which is the same as the C appearing in the integral equation. Normally people use C = 1, but we shall use C = C. Note then that we write

$$1 = \langle n|n\rangle = \langle n| \int_a^b dx/C\ |x\rangle\langle x|n\rangle = \int_a^b dx/C\ \langle n|x\rangle\langle x|n\rangle = \int_a^b dx/C\ \varphi_n(x)^*\ \varphi_n(x)$$

Then we do some expansions like so (we show the corresponding projections on the far right)

$$f(x) = \Sigma_{n=0}^{\infty}\ f_n\varphi_n(x) \quad \text{ie} \quad \langle x|f\rangle = \Sigma_{n=0}^{\infty}\ \langle x|n\rangle\langle n|f\rangle \quad f_n = \int_a^b dx/C\ \varphi_n(x)^*\ f(x)$$

$$g(x) = \Sigma_{n=0}^{\infty}\ g_n\varphi_n(x) \quad \text{ie} \quad \langle x|g\rangle = \Sigma_{n=0}^{\infty}\ \langle x|n\rangle\langle n|g\rangle \quad g_n = \int_a^b dx/C\ \varphi_n(x)^*\ g(x)$$

Now use QM notation to write the integral equation as

$$\langle y|f\rangle = \int_a^b dx/C\ \langle y|K|x\rangle\langle x|g\rangle = \langle y|K|g\rangle \Rightarrow \quad |f\rangle = K|g\rangle$$

Then process this last result:

$$|f\rangle = K|g\rangle = \Sigma_{n=0}^{\infty}\ K|n\rangle\langle n|\ g\rangle$$

$$\langle m|f\rangle = \langle m|K|g\rangle = \Sigma_{n=0}^{\infty}\ \langle m|K|n\rangle\langle n|\ g\rangle$$

$$f_m = \Sigma_{n=0}^{\infty} K_{mn}\, g_n$$

In this way we have converted our equation f = Kg from coordinate space to eigenfunction space. For some random kernel k(y,x) and some random set $\varphi_n(x)$ on (a,b), K_{nm} is not going to be a diagonal matrix.

We can write

$$K_{mn} = \langle m|K|n\rangle = \langle m \int_a^b dx/C\ |x\rangle\langle x|K| \int_a^b dy/C\ |y\rangle\langle y|n\rangle$$

$$= \int_a^b dx/C \int_a^b dy/C\ \varphi_m(x)^*\ \langle x|K|y\rangle\ \varphi_n(y)$$

$$= \int_a^b dx/C \int_a^b dy/C\ \varphi_m(x)^*\ K(x,y)\ \varphi_n(y)$$

2. But suppose we can find eigenvalues and eigenfunctions of the operator K which form a complete set, $K|n\rangle = \lambda_n|n\rangle$, and suppose we take these (orthonormalized) to be our set $\varphi_n(x)$. Then we have

$$K_{mn} = \langle m|K|n\rangle = \langle m|\lambda_n|n\rangle = \lambda_n\langle m|n\rangle = \lambda_n\, \delta_{m,n}$$

so with this special set of $\varphi_n(x)$, K_{mn} is a diagonal matrix, and our integral equation becomes

$$f_m = \Sigma_{n=0}^{\infty} K_{mn}\, g_n = \Sigma_{n=0}^{\infty} \lambda_n\, \delta_{m,n}\, g_n = \lambda_m\, g_m$$

In a sense, we could say I think that we have "diagonalized" our integral equation. The solution is then

$$g_n = f_n/\lambda_n$$

$$g(x) = \Sigma_{n=0}^{\infty}\, g_n\varphi_n(x) = \Sigma_{n=0}^{\infty}\, (f_n/\lambda_n)\varphi_n(x)$$

so barring that some $\lambda_m = 0$, we have the problem completely solved. The Catch 22 here is of course that it may be extremely difficult to find and enumerate the eigenfunctions of K, and if K is not Hilbert-Schmidt, the eigenfunctions may not form a complete set. Stakgold has lots to say about this integral equation example and the solution outlined here.

3. How is the above discussion affected if k(x,y) = r(x-y) so the integral equation then is of "convolution form" ? Since this is just a special case, everything above still applies. We would then have for some general $\varphi_n(x)$ set

$$K_{mn} = \langle m|K|n\rangle = \int_a^b dx/C \int_a^b dy/C\ \varphi_m(x)^*\ r(x-y)\ \varphi_n(y)$$

Nothing is really any simpler than it was before. K_{mn} is still in general non-diagonal for some general set $\varphi_n(x)$ you pick.

4. Suppose we now add the extra condition that r(x) is periodic on the interval (a,b). Does that make things any simpler? To make things easier, assume that a = 0 so we then have

$$K_{mn} = \int_0^b dx/C \int_0^b dy/C\ \varphi_m(x)^*\ r(x-y)\ \varphi_n(y)$$

$$r(x+b) = r(x)$$

If some f(x) is periodic in this way, then we know that for any real α,

$$\int_\alpha^{b+\alpha} dx\ f(x) = \int_0^b dx\ f(x)$$

Suppose in our K_{mn} integral we define x' = x-y, does that help?

$$K_{mn} = \int_0^b dy/C \int_0^b dx/C\ \varphi_m(x)^*\ r(x-y)\ \varphi_n(y)$$

$$= \int_0^b dy/C\ \varphi_n(y) \int_{-y}^{b-y} dx'/C\ \varphi_m(x'+y)^*\ r(x')$$

Officially the functions $\varphi_n(x)$ are defined only on the interval (a,b), but we can replicate what we see in this interval across the entire x axis, and thus cause this extended $\varphi_n(x)$ to be periodic with period b. Then the dx' integrand shown above would be periodic with period b and we could say

$$= \int_0^b dy/C\ \varphi_n(y) \int_0^b dx'/C\ \varphi_m(x'+y)^*\ r(x')$$

$$= \int_0^b dx/C \int_0^b dy/C\ \varphi_m(x+y)^*\ r(x)\ \varphi_n(y) \qquad (*)$$

but this does not seem to be a simplification for arbitrary $\varphi_n(x)$.

5. Let's now further assume that b = 2π, and write coordinates as if they were angles. At the same time, we shall now set C = 2π, since we can set it to whatever we want. Then we have

$$K_{mn} = \int_0^{2\pi} d\theta'/2\pi \int_0^{2\pi} d\theta/2\pi\ \varphi_m(\theta)^*\ r(\theta-\theta')\ \varphi_n(\theta')$$

For general a and b, we could scale things to obtain the above form.

We now continue our list of assumptions by assuming now that the eigenfunctions $\varphi_m(\theta)$ are those associated with the group SO(2), so that $\varphi_m(\theta) = e^{-in\theta}$ now for n = all integers (making a slight change to what we assumed above about n). This is well known to be a complete set of basis functions.

These eigenfunctions have "the group property" which is this

$$\varphi_m(\theta)\varphi_m(\theta') = \varphi_m(\theta+\theta')$$

Now let's look at our K_{nm} integral in the form (*) above

$$K_{mn} = \int_0^{2\pi} d\theta/2\pi \int_0^{2\pi} d\theta'/2\pi\, \varphi_m(\theta+\theta')^*\, r(\theta)\, \varphi_n(\theta')$$

$$= \int_0^{2\pi} d\theta/2\pi \int_0^{2\pi} d\theta'/2\pi\, \varphi_m(\theta)^*\varphi_m(\theta')^*\, r(\theta)\, \varphi_n(\theta')$$

$$= \int_0^{2\pi} d\theta/2\pi\, \varphi_m(\theta)^*\, r(\theta) \int_0^{2\pi} d\theta'/2\pi\, \varphi_m(\theta')^*\, \varphi_n(\theta')$$

$$= \int_0^{2\pi} d\theta/2\pi\, \varphi_m(\theta)^*\, r(\theta)\, \delta_{m,n}$$

$$= \delta_{m,n} \int_0^{2\pi} d\theta/2\pi\, \varphi_m(\theta)^*\, r(\theta) = \delta_{m,n} \langle m|r\rangle = \delta_{m,n}\, r_m$$

where we now define r_m in the obvious manner (just as we did for f and g above)

$$r_m = \langle m|r\rangle = \langle m| \int_0^{2\pi} d\theta/2\pi\, |\theta\rangle\langle\theta|r\rangle = \int_0^{2\pi} d\theta/2\pi\, \langle m|\theta\rangle\langle\theta|r\rangle = \int_0^{2\pi} d\theta/2\pi\, \varphi_m(\theta)^*\, r(\theta)$$

Suddenly K_{mn} is diagonal! This means that the r_m and $\varphi_m(\theta)$are the eigenvalues and eigenfunctions of the operator K. (Above we referred with the eigenvalues as λ_m). Our $\varphi_n(\theta)$-space integral equation is then

$$f_m = \Sigma_{n=0}^{\infty} K_{mn}\, g_n = \Sigma_{n=0}^{\infty} \delta_{m,n}\, r_m\, g_n = r_m g_m$$

which we write again

$$f_n = r_n\, g_n$$

The solution to our problem is then

$$g_n = f_n / r_n$$

$$g(\theta) = \Sigma_n\, g_n \varphi_n(\theta) = \Sigma_n\, (f_n/r_n) e^{-in\theta}$$

so barring that one of the $r_n = 0$, we have a complete solution to our problem.

B. Summary of what happened above.

1. We first considered an integral equation with some arbitrary kernel

$$f(y) = \int_a^b k(y,x)\, g(x)\, dx/C$$

We would like to solve this integral equation for g(x), given k and f.

2. There are an infinite number of complete sets of eigenfunctions $\varphi_n(x)$ on the interval (a,b) -- each would correspond to some self-adjoint differential operator L_x with some boundary conditions at a and b, a so-called Sturm-Liouville problem. If we re-express the integral equation in the |n> basis instead of the |x> basis, where $\langle x|n\rangle = \varphi_n(x)$, we obtain

$$f_m = \Sigma_{n=0}^{\infty}{}_n\, K_{mn}\, g_n$$

where

$$K_{mn} = \langle m|K|n\rangle = \int_a^b dx/C \int_a^b dy/C\, \varphi_m(x)^*\, K(x,y)\, \varphi_n(y)$$

$$f_n = \int_a^b dx/C\, \varphi_n(x)^*\, f(x) \qquad f(x) = \Sigma_{n=0}^{\infty}\, f_n \varphi_n(x)$$

$$g_n = \int_a^b dx/C\, \varphi_n(x)^*\, g(x) \qquad g(x) = \Sigma_{n=0}^{\infty}\, g_n \varphi_n(x)$$

We have assumed that the eigenfunctions $\varphi_n(x)$ can be labeled by n = 0,1,2... but some other infinite numbering system might be appropriate depending on the Sturm-Liouville problem. It might come out that we want n = all integers from $-\infty$ to $+\infty$ including 0, for example.

3. For some general k(y,x) kernel and some randomly chosen complete set $\varphi_n(x)$ on (a,b), the matrix K_{mn} will not be diagonal. The integral equation has now become a matrix/vector equation which we could write as

$$\mathbf{f} = K\, \mathbf{g}$$

so we have a linear algebra situation, except the vectors have an infinite number of components and K is an ∞ x ∞ matrix. Perhaps if we keep only the first 50 components and the upper left 50 x 50 part of the matrix K, we can use linear algebra to solve the above equation for

$$\mathbf{g} = K^{-1}\mathbf{f}$$

and our problem will then be approximately solved if we can show that higher components make very small contributions.

4. For certain kernels k(y,x) the corresponding Hilbert Space operator K will have eigenvectors and eigenfunctions which form a complete set which we could then *use* as our $\varphi_n(x)$. This is of course a very special set of basis functions, and it might be very difficult to find out what the $\varphi_n(x)$ are. If k(x,y) is symmetric k(x,y) = k(y,x), and if the double integral of k^2 over the (a,b) x (a,b) square is finite, then K is a Hilbert-Schmidt integral operator and such a complete set of $\varphi_n(x)$ is known to exist. There will be some eigenvalues λ_n such that $K|n\rangle = \lambda_n|n\rangle$. In this very special basis, the matrix K_{nm} is trivially diagonal, having the form $K_{nm} = \lambda_n \delta_{n,m}$. The matrix equation $\mathbf{f} = K\,\mathbf{g}$ then becomes $f_n = \lambda_n g_n$ and our problem is completely solved, barring technical difficulties, since we then have $g_n = f_n/\lambda_n$ and we then put these coefficients into our expansion for g(x). The big problem here is that, even assuming k(y,x) has the required properties, it is usually very hard to find the λ_n and $\varphi_n(x)$ and one can only do that by some numeric approximation method.

5. If it happens that the kernel has the "convolution form" k(x,y) = r(x-y), *in general* there is no simplification of the problem outlined above. For a general set $\varphi_n(x)$, K_{nm} won't be diagonal. And K will have some eigenfunctions which will likely still be hard to find. The Love Equation is an example.

6. However, if k(x,y) = r(x-y) *and* if r(x) is periodic *with a period equal to the interval width b-a,* then all of a sudden the problem becomes simple. Assuming a and b are finite, the fact that r(x) is periodic means it can be expanded in a complex Fourier Series,

$$r(x) = \Sigma_n\, r_n\, \varphi_n(x) \qquad \text{// expansion}$$

$$r_n = \int_a^b dx/C\; r(x)\, \varphi_n(x)^* \qquad \text{// inversion} \qquad C = (b-a)$$

where $\varphi_n(x) = e^{-inx[2\pi/(b-a)]}$

and we note in passing that

$$\langle n|n\rangle = \int_a^b dx/C\, \langle n|x\rangle\langle x|n\rangle = \int_a^b dx/C\, e^{+inx[2\pi/(b-a)]}\, e^{-inx[2\pi/(b-a)]} = \int_a^b dx/C = 1$$

It then follows, due to the obvious "group property" of these basis functions,

$$\varphi_n(x+x') = \varphi_n(x)\varphi_n(x'),$$

that the basis functions are in fact eigenfunctions of K with eigenvalues r_n. There are various ways to show this, here is one way. First, we have

$$k(y,x) = r(y-x) = \Sigma_n\, r_n\, \varphi_n(y-x) = \Sigma_n\, r_n\, \varphi_n(y)\varphi_n(-x) = \Sigma_n\, r_n\, \varphi_n(y)\varphi_n(x)^*$$

Second, we write

$$\tilde{K}\,\varphi_m(y) \equiv \langle y|K|m\rangle = \langle y|K \int_a^b dx/C|x\rangle\langle x \;|m\rangle = \int_a^b dx/C\, \langle y|K|x\rangle\langle x|m\rangle$$

$$= \int_a^b dx/C\ k(y,x)\ \varphi_m(x) \quad = \int_a^b dx/C\ r(y-x)\varphi_m(x)$$

so we can insert the first result into the second to get

$$\tilde{K}\ \varphi_m(y) = \int_a^b dx/C[\ \Sigma_n\ r_n\ \varphi_n(y)\ \varphi_n(x)^*]\varphi_m(x)$$

$$= \Sigma_n\ r_n\ \varphi_n(y)\ \int_a^b dx/C\ \varphi_n(x)^*\ \varphi_m(x)\ = \Sigma_n\ r_n\ \varphi_n(y)\langle n|m\rangle = \Sigma_n\ r_n\ \varphi_n(y)\delta_{n,m}$$

$$= r_m\ \varphi_m(y)$$

which we can write also $\langle y|K|m\rangle = r_m \langle y|m\rangle$ or just $K|m\rangle = r_m|m\rangle$. Thus, K is diagonal

$$K_{nm} = \langle n|\ K\ |m\rangle = r_m \langle n|m\rangle\ = r_m\ \delta_{n,m}$$

and then our matrix equation

$$\mathbf{f}\ = K\ \mathbf{g}$$

becomes just

$$f_m = r_m\ g_m$$

and the solution to our integral equation problem is then

$$g(x) = \Sigma_n\ g_n\ \varphi_n(x) \qquad \text{where } g_n = f_n/r_n$$

If a and/or b are infinite, we must modify the above analysis replacing Fourier Series by Fourier Transforms, but the general nature of the result comes out the same.

7. Let's now go back to the original integral equation

$$f(y) = \int_a^b\ dx/C\ \ k(y,x)\ g(x)$$

and let's go ahead and assume the convolution form for the kernel,

$$f(y) = \int_a^b\ dx/C\ \ r(y-x)\ g(x) \qquad\qquad y \text{ in } (a,b)$$

The whole problem is defined on the interval (a,b) of width L = b-a. Notice that, depending on the value of y and the location of the integration point x, the function r(x) is accessed from x = -L to x = +L, which is a width of 2L. If we wanted, we could take this 2L wide chunk of r(x) and replicate it along the entire x axis. Replacing the original r(x) with this replicated r(x) makes no difference since we only access (-L,L)

of this function. But this does make r(x) be periodic, but alas, the period is 2L, not L, so we don't get the massive simplification described above for some general r(x). Nevertheless, we could expand all the functions on a set of basis functions over the interval (-L,L) which has width 2L. We could even perhaps use our same complex Fourier Series basis functions, but geared to 2L. This will then lead to a matrix equation of the form $\mathbf{f} = K\,\mathbf{g}$ but K won't be diagonal and we will have to use some kind of approximation method. This is done in the Love numerical paper I downloaded.

We only get the massive simplification (diagonalization) when r(x) is periodic with period L = b-a.

When we say that we can "diagonalize" a convolution equation using some $\varphi_n(x)$, we have shown above that we are in fact "diagonalizing" matrix K_{mn} so the projected equation is not $\mathbf{f} = K\mathbf{g}$, but $f_m = r_m\, g_m$. The matrix in question is $\langle m|K|n\rangle$ where $|n\rangle$ are the SO(2) representation states. If we were to diagonalize using SO(3) instead of SO(2) as discussed here, the matrix K is then

$$K_{jm,j'm'} = \langle jm|\, K\, |j'm'\rangle = \delta_{j,j'}\langle jm|\, K\, |jm'\rangle$$

In this case the matrix $K_{jm,j'm'}$ is not completely diagonal, but has a block diagonal form where the size of each block is $(2j+1)^2$.