Inverse Scattering PhL 1.22.05

1. The relation between QM, EM and acoustic scattering. What is V(r) for acoustic case?

In **quantum mechanics** (QM), we have the Schrodinger Equation (SE) $H\psi=E\psi$ where $H = -\nabla^2 + V$ where V is some potential usually isolated to a region in space. We have various methods for solving scattering problems in quantum mechanics off potentials, often of the form V(r). We also have $E = id/dt$ which is a first order time derivative, so we have a parabolic ODE. If we assume sine time dependence, we find that E is replaced with a number, the energy eigenvalue, which we can write as k^2 of non-relativistic. Our equation now looks like $(-\nabla^2 + V)\psi = k^2\psi$ or $\mathbf{(\nabla^2 + k^2)\psi = V\psi}$. In free space, V = 0 and we get the Helmholtz equation. In QM, we think of ψ as being a complex valued function.

In **mechanical wave theory** (strings, for example, our sound), we have a classical wave equation as for example on page 54 of the Berkeley waves book, $\nabla^2\psi = \psi_{tt}$ which is hyperbolic. If we assume sine time dependence, then ψ_{tt} becomes $-k^2\psi$ and we then have $\mathbf{(\nabla^2 + k^2)\psi = 0.}$ Again, this is the Helmholtz equation, but now we think of ψ as being real-valued, like the physical displacement of a vibrating string.

In **E&M** wave theory we have Helmholtz equations for the E and B field components.

Question: I am familiar with the idea of a potential V in QM, how we add it to a Hamiltonian H_0 to get the full Hamiltonian H. How does this work in "mechanical wave theory" ? You might for example put a bead on a string and scatter off it.

Answer: In the mechanical wave scattering picture, I think it works like this. You have $(\nabla^2 + k^2)\psi$ where k might be a function of the density n(x), so we usually see this as $(\nabla^2 + k^2n(x))\psi$. This n(x) is like the index of refraction in E&M in that it is just telling us about the speed of propagation as a function of x. Then the idea is that a variation in n(x) causes scattering. Again, n(x) may not be the actual gm/cm^2 "density" of the medium at some point, but it is the "acoustic density" which controls the sound speed.

Now suppose you have a spherical scattering object in which the speed of sound differs from that of the embedding medium. Then you have this situation:

$(\nabla^2 + k^2n_0(x))\psi = 0$ outside
$(\nabla^2 + k^2n(x))\psi = 0$ inside

and you have to match boundary conditions at the surface. We can then write both equations as follows: Let $\delta n(x) = n(x) - n_0(x)$, and define $V(x) = -\delta n(x)$. Then we get

$(\nabla^2 + k^2n_0(x))\psi = 0$ outside
$(\nabla^2 + k^2n_0(x))\psi = V(x)\psi(x)$ inside

So we can then restate this as

$(\nabla^2 + k^2n_0(x))\psi = V(x)\psi(x)$ everywhere

where $V(x)= 0$ outside, and $V(x)= - \delta n(x)$ inside.

So, this shows that with this "interpretation" of the potential $V(x)$, the scattering problem for acoustic scattering is the same as the QM scattering problem in the presence of a potential. However, in QM the ψ will be complex, but in acoustic ψ is the wave density of a pressure wave (longitudinal only) and is therefore real.

2. The Lippman-Schwinger equation

See Exhibit 1. We start with the above potential-driven wave equation $(\nabla^2 + k^2)\psi = V(x)\psi(x)$ where we have now "scaled out" the $n_0(x)$ by assuming it is constant outside, so now $n(x) = n_0(x) - \delta n(x) = 1 - \delta n(x)$. We can compute the Green's Function $G(x,x')$ of the operator $(\nabla^2 + k^2)$ by driving with a delta function, and then we have this integral equation for scattering with an incident plane wave

$$\psi_k(x) = e^{ikx} + \int dx' \, G_k(x,x') \, V(x') \, \psi_k(x') \qquad \text{// Lippman-Schwinger equation}$$

which is an integral equation for ψ_k where k is our wave number (we have removed time from the problem in the usual Fourier manner). To prove the above equation, apply $D = (\nabla^2 + k^2)$ to both sides. On the left we get $V(x)\psi_k$, and on the right we get 0 from the plane wave term, and then $DG = \delta$ and we then get $V(x)\psi_k$ on the right as well.

So the L-S is just an integral equation statement of our problem. It also appears in (37.13) page 319 of Schiff. We can now insert our potential to get

$$\psi_k(x) = e^{ikx} + \int dx' \, G_k(x,x') \, [\, n_0(x') - n(x')] \, \psi_k(x')$$

where the integration is then only over the region D where the densities don't cancel.

We see something of this form in Exhibit 2, but there is some kind of scaling by $-k^2$ of the integral part that I don't understand. In this exhibit, the Green's function is called $\Phi(x,x')$. I note the familiar 3D result which is $G = \exp(ikr)/r$ but the 2D result is also stated which is $H_0^{(1)}(kr)$, something new to me.

3. The differential equation.

Our differential operator of interest is $L' = (\nabla^2 + k^2 - V(x))$ with $L'\psi = 0$ as shown above. In QM one would write $k^2 = E$, the energy. So maybe say $L = -\nabla^2 + V(x)$ and our equation is then $L\psi = k^2\psi$ as in (23) page 270 of Saxon. This is an eigenvalue problem. If $V(x) = V(r)$, a central potential, we can separate variables and get $\psi_{k\ell m} = R_\ell(r) \; Y_{\ell m}(\theta,\phi)$ where R satisfies a radial differential equation (49) Saxon page 275, all in 3D. We then redefine $R = u/r$ as in (53) and we get the ODE as in (54) page 276. This then is the equation we start with as (20.1,2) of Newton page 614. Newton uses ϕ instead of u.

The ODE with V=0 for $R_\ell(r)$ is the spherical Bessel ODE as given in A&S page 437, and the solutions are the $j_n(r)$ and $y_n(r)$. Recall that $j_n(r)$ is related to $J_{n+1.2}$, the half-order regular Bessel's. The $j_n(r)$ are called the spherical Bessel functions.

4. The Gel'fand-Leviton Equation (for doing the "inverse scattering problem")

Now we are looking at Newton page 614. We have (20.1) and (20.2) stating the ODE above, but this is the ODE for $u = \phi_1$, not R. Our GOAL is to somehow "deduce" V(r) backwards by looking at the scattered waves. Remember that $V(r) = n_0(r) - n(r)$. We have to think of an isolated spherically symmetric object as the scatterer to maintain the "central potential" idea. So at least this is "the first" problem we should look at.

The solution that GL (now known as GLM) propose is rather complicated and I will try to outline it here. We are going to somehow compute a function called K(r,r') *from which* we can deduce $\Delta V(r)$ which is the variation in our potential from some nominal potential $V_1(r)$, as shown in (20.14). So if we can find K, we can find ΔV and we are happy, we have solved "the inverse scattering problem".

What is this function K ? It is the solution to the integral equation $K = g - \int Kg$ where g is a certain other function. And just what is this function g? It is given by the expansion in (20.6) where you see our ϕ_1 function appearing twice, but there is some as-yet undetermined measure dh.

Now if we whip over to page 370 and look at (12.128a), we see a completeness relation for ϕ which I presume are the eigenvectors of some $L\phi = E\phi$ equation, and you recall from somewhere that in a completeness relation you have to sum over the entire "spectrum" of eigenvalues, and $\rho(E)$ is that spectrum. Recall such a spectrum often has a discrete (think bound states) and a continuous part (scattering states), this integral is often a mixed integral + sum as shown, eg, in (12.128).

Now flip to page 616 (20.16) and you see that ρ is the spectrum that goes with ϕ, and ρ' is that which goes with ϕ_1. Then (20.18) shows that our measure in the definition of g is just $h = \rho - \rho'$.

Well that's fine. Note that ϕ_1 is the solution of our ODE (20.1) with D_1, while ϕ is the solution of our ODE (20.12) with D, and the difference between D and D_1 is our ΔV. So if we somehow knew the complete solutions to these two problems, we would know ρ and ρ' and thus h. And in that case we would know the function g as shown in (20.3).

So things seem pretty circular here. We have { solution to D and ϕ } $\rightarrow \rho$ and { solution to D_1 and ϕ_1 } $\rightarrow \rho_1$, and then ρ, ρ_1 + { ϕ_1 } $\rightarrow$ g , and then you solve $K = g - \int Kg$ for K, and then from K you get your ΔV. I don't yet know how we do anything useful with this stuff.

Along the theoretical way we see some other facts. One is (20.9) that $D(r)K(r,r') = D_1(r')K(r,r')$. And then we have an integral equation (20.11) for ϕ which reads: $\phi = \phi_1 - \int K\phi_1$. Then in (20.15) we see that $K(r,r') = \int dh\, \phi\, \phi_1$ whereas recall that $g(r,r') = \int dh\, \phi_1\, \phi_1$.

Now let's jump over to page 624 where things seem to repeat the above discussion but in a simpler form. Here they set k = 1. D_1 is now defined a little differently in (20.41) so the eigenvalue equation for ϕ_1 looks like (20.42). But now instead of talking about ϕ_1, we denote that by $\phi^{(1)}$, because we need to make room for a partial wave index ℓ, so we how have $\phi_\ell^{(1)}$. It was there before as well, we just did not show it. The superscript (1) means without the scattering potential ΔV. Then in (20.43) we have the same expression for g(r,r') as before, but our spectral integral is now a sum over ℓ (the eigenvalue) and we have some kind of weight c_ℓ sitting in there playing the role of ρ_1. We now find that $D_1(r)g = D_1(r')g$, something not stated in the general section. Then comes our integral equation $K = g - \int Kg$, and then (20.48) defines D which now includes ΔV. Then we see how we are going to recover our ΔV from K.

Continuing onto page 625, things continue to look familiar. We see that $D(r)K = D_1(r')K$ as before, and we see our statement that $\phi = \phi_1 - \int K\phi_1$ as before. Then (20.52) is our ODE with D and ϕ, and then below we have $K = \Sigma_\ell\, c_\ell\, \phi\, \phi_1$ again as before.

Now we arrive at some new stuff. We take (20.51) $\phi = \phi_1 - \int K\phi_1$ and jam in $K = \Sigma_{\ell'} c_{\ell} \phi_{\ell'}(r) \phi_{\ell'}^{(1)}(r')$ which seems to give

$$\phi_\ell = \phi_\ell^{(1)} - \int dr'\{\Sigma_{\ell'} c_{\ell'} \phi_{\ell'}(r) \phi_{\ell'}^{(1)}(r')\}\phi_\ell^{(1)}(r') = \phi_1 - \Sigma_{\ell'} c'_\ell \phi_{\ell'}(r)[\int dr'\{\phi_{\ell'}^{(1)}(r')\}\phi_\ell^{(1)}(r')]$$

and we now define

$$L_{\ell\ell'} = \int dr'\{\phi_{\ell'}^{(1)}(r')\}\phi_\ell^{(1)}(r') \quad \text{more accurately shown in (20.57)}$$

and this takes us to the form (20.56). So L is some integral of our unperturbed functions ϕ_1.

If there were no phase shifts, we would know our large-r solutions from the Bessel form of the equation where they are $j_\ell(r)$ which become $\sin(r - \pi\ell/2)$, but then we add in phase shifts δ_ℓ and $\delta_\ell^{(1)}$ as shown in (20.58) and from that we can compute $L_{\ell\ell'}(r=\infty)$ as shown.

At this point, things fade. I think in the end, the idea is that by measuring the phase shifts δ_ℓ , you can work backwards and compute the c_ℓ and then you know g, and then K, and then finally ΔV. Notice that neither g nor K is really a Green's function, they are just "supporting actors" each of two variables.

In any event, they are laying out a "plan" here for solving the inverse scattering problem.

5. The Born Approximation

Let's go to page 360 Saxon. We have our same Helmholtz equation driven by V(r) in (27), and below that the general form for the scattering in 3D. I think you would have to replace e^{ikr}/r with $H_0^{(1)}(kr)$ for 2D. Green's is defined in (28), and then (29) is our Lippman-Schwinger. Saxon computes G as in (31). Now you go to the far field zone and *simplify the phase* (as in Jackson and optics etc) and you can then pull out a factor e^{ikr}/r and by comparison you have your "far field scattering amplitude" f(**k**,**k'**) as in (33).

At this point we make the Born Approximation by replacing ψ in the f integral with ψ_0, the incident wave, which is saying that the scattered wave is weak compared to the incident. When we do that, our f becomes simply the Fourier Transform of V(**r**) but with **Δk** as the conjugate variable. This is all familiar from my last optics adventure. You can do an iteration then with this idea. Basically, Born means you are doing perturbation theory for your scattering solution. It may or may not be justified.

I remember Steve Johnson making comments about the Born approx and maybe how it is no good for his work.

Notes added 4.19.07

I read the above stuff today, the Born Approximation in Saxon is very good, as reviewed above. Here is the basic idea one more time of the framework in which you make the Born Approximation:

(1) you write your ODE (27) for your wavefunction in the presence of potential V(**r**) that is isolated to some region. It is Helmholtz driven by $V\psi$ on the right, driven by the potential. You know the free particle Green's function for this equation.

(2) you convert this to an integral equation for the wavefunction (29) or (32). The left side is the wavefunction, the right has the plane wave term plus an integral of the wavefunction where the kernel is the usual Greens' function plane wave.

(3) If you then go to "large r" you can make a simplification, pull the exp(ikr)/r out of the integral, and you can *identify* the remaining integral with f(**Δk**), which I guess we would call **the scattering amplitude**. This appears generally in (27b) and (33). But all you have at this point is a far field equation relating scattering amplitude f to the full solution wavefunction ψ integrated against the potential.

(4) You don't know ψ, so you do perturbation theory and put in the plane wave there since presume scattered field is weak, even inside the scattering region. This step is the **Born Approximation**. This gives you (34) which says that the f(**Δk**) is in fact the **3D Fourier Transform** of the potential V(**r**) [does not have to be a central potential] .

So I am used to computing f from a given potential like Yukawa or what have you.

I suppose if you measured f(**Δk**) in lots of places, you could do the inverse Fourier transform of f to get the potential, that would be one way to solve the "inverse scattering problem".

This latter is the general idea behind the transmission scattering method that Techniscan uses.