So far in the notes we have examined the properties of the Lippmann–Schwinger equation without worrying about how to solve it for the exact scattering solution $\psi_{\vec{k}}(\vec{r})$. In fact, in most cases an exact or analytic solution is not possible, and we must resort to approximate or numerical methods.

To explore some of these, we first write the L-S eqn in ket form,

$$|\psi_{\vec{k}}\rangle = |\phi_{\vec{k}}\rangle + G_{0+}(E)V|\psi_{\vec{k}}\rangle,$$

where $|\phi_{\vec{k}}\rangle$ was just called $|\vec{k}\rangle$ in lecture (it is the incident plane wave). Moving terms containing $|\psi_{\vec{k}}\rangle$ to one side, we have

$$\left[1 - G_{0+}(E)V\right]|\psi_{\vec{k}}\rangle = |\phi_{\vec{k}}\rangle,$$

or

$$\boxed{|\psi_{\vec{k}}\rangle = \Omega_+(E)|\phi_{\vec{k}}\rangle}$$

where $\Omega_+(E)$, called the <u>Møller wave operator</u>, is given by

$$\Omega_+(E) = \left[1 - G_{0+}(E)V\right]^{-1}.$$

It is the operator that maps a plane wave $|\phi_{\vec{k}}\rangle$ (the incident wave) into the exact scattering solution $|\psi_{\vec{k}}\rangle$. Obviously if we can find convenient expressions or approximations for $\Omega_+(E)$ it will help solve the scattering problem. Incidentally, we will define a closely related operator,

$$\Omega(z) = [1 - G_0(z)V]^{-1},$$

where z is a complex energy and where

(so $\Omega_+(E) = \lim_{\epsilon \to 0} \Omega(E+i\epsilon)$)

$$G_0(z) = \frac{1}{z - H_0}$$

is the resolvent for the unperturbed system.

One way to approximate $\Omega(z)$ is to expand it in a power series in V, the operator equivalent of the expansion

$$\frac{1}{1-x} = 1 + x + x^2 + \dots$$

Thus, we have

$$\Omega(z) = 1 + G_0(z)V + G_0(z)V\,G_0(z)V + \dots$$

which expresses $\Omega(z)$ in terms of things we know how to compute. Now setting $z = E + i\epsilon$, taking $\epsilon \to 0$ to get $\Omega_+(E)$, and applying to $|\phi_{\vec{k}}\rangle$, we get a series,

$$\boxed{|\psi_{\vec{k}}\rangle = |\phi_{\vec{k}}\rangle + G_{0+}(E)V|\phi_{\vec{k}}\rangle + G_{0+}(E)V\,G_{0+}(E)V|\phi_{\vec{k}}\rangle + \dots}$$

This series for the exact wave field is called the Born series. It is obviously a kind of power series expansion of $|\psi_{\vec{k}}\rangle$ in powers of V. It may not converge or even be useful (it depends on V and E), but sometimes it is useful. If the series is truncated at order V^n, we obtain the n-th Born approximation to the exact wave field.

We can also get a Born series for the scattering amplitude, using Eq. (31.95). This gives

$$f(\vec{k},\vec{k}') = -(2\pi)^2 \frac{m}{\hbar^2}\left[\langle \vec{k}' | V | \vec{k} \rangle + \langle \vec{k}' | V G_{0+}(E) V | \vec{k} \rangle + \dots \right]$$

where now we write simply $|\vec{k}\rangle$ in place of $|\phi_{\vec{k}}\rangle$. ~~this not dead~~ Again, truncating at order V^n gives the n-th Born approximation to the scattering amplitude. Notice that in the first Born approximation, the scattering amplitude is proportional to the Fourier transform of the potential, evaluated at $\vec{k}'-\vec{k}$:

$$\langle \vec{k}' | V | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} \tilde{V}(\vec{k}'-\vec{k}),$$

where we use the convention (29.59) for the F.T. Thus

$$f(\vec{k},\vec{k}') = -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,\tilde{V}(\vec{k}'-\vec{k})$$

and

$$\frac{d\sigma}{d\Omega} = 2\pi \frac{m^2}{\hbar^4} \left| \tilde{V}(\vec{k}'-\vec{k}) \right|^2 .$$

This agrees with the result (29.61) obtained earlier by time-dependent perturbation theory. Indeed, the Dyson series for $W(t) = U_0(t)^{+} U(t)$ is closely related to the Born series for $\Omega(z)$. (Both are power series expansions in powers of V.)

We did not deal with the <u>conditions of validity</u> of the first Born approximation when discussing time-dependent perturbation theory. That was because it is easier to see the nature of the approximation when looking at the Born series.

Let us take the first Born approximation for the solution $|\psi_{\vec{k}}\rangle$ and compare it to the L-S eqn:

$$|\psi_{\vec{k}}\rangle \approx |\vec{k}\rangle + G_{0+}(E)V|\vec{k}\rangle \qquad \text{(1st Born)}$$

$$|\psi_{\vec{k}}\rangle = |\vec{k}\rangle + G_{0+}(E)V|\psi_{\vec{k}}\rangle \qquad \text{(LS eqn).}$$

The second term is multiplied by the potential V, so we see that the Born approximation will be good if $|\psi_{\vec{k}}\rangle \approx |\vec{k}\rangle$ in the regions of space where the potential is large. This leads to the <u>intuitive conditions of validity</u> of the Born approximation:

Born appx. good if

1) V is weak

or 2) E is large.

Because in the high energy limit, the particles blast through the potential without deflecting very much, and the exact wave fn $\psi_{\vec{k}}(\vec{r}) \approx \phi_{\vec{k}}(\vec{r})$ in the middle of the potential.

Now a more quantitative condition of validity of the Born approximation. Since we require $\psi_{\vec{k}}(\vec{r}) \approx \phi_{\vec{k}}(\vec{r})$, define

$$C = \frac{\phi_{\vec{k}}(\vec{r}) - \psi_{\vec{k}}(\vec{r})}{\phi_{\vec{k}}(\vec{r})}, \qquad \text{(dim-less)}$$

which we want to be small. This depends on $\vec{r}$, but let's evaluate at $\vec{r}=0$ for a typical (hopefully) point inside the scatterer. Then C depends only on $\vec{k}$. Using the Lipmann-Schwinger eqn, we get (evaluating kernel of integral transform at $\vec{r}=0$):

$$C(\vec{k}) = \frac{1}{2\pi}\frac{m}{\hbar^2}\int d^3\vec{r}\,' \frac{e^{ikr'}}{r'} V(\vec{r}\,')\, \psi_{\vec{k}}(\vec{r}\,') \times (2\pi)^{3/2}.$$

Since this is only an estimate, replace $\psi_{\vec{k}}(\vec{r}\,')$ by $\phi_{\vec{k}}(\vec{r}\,')$,

$$C(\vec{k}) = \frac{1}{2\pi}\frac{m}{\hbar^2}\int d^3\vec{r}\, \frac{e^{ikr}}{r} V(\vec{r})\, e^{i\vec{k}\cdot\vec{r}},$$

dropping primes on the dummy variable of integration. If $V(\vec{r}) = V(r)$ is central force, then we can do the angular integration, obtaining

$$C(\vec{k}) = \frac{2m}{\hbar^2}\frac{1}{k}\int_0^\infty dr\, e^{ikr} \sin kr\, V(r). \qquad (\ll 1 \text{ demand})$$

This integral is small if $V(r)$ is small, or if k is large, confirming our intuition about the validity of the Born appx. Note when k gets large, $C(k) \to 0$ both because of $1/k$ and because the integrand oscillates more and more rapidly as $k \to$ large.

~~[illegible]~~ In case of Yukawa potential (Sec. 29.13), let $a = 1/\kappa$ = range of potential. Then when $ka \ll 1$, the integral above gives

$$C(\vec{k}) = \frac{2m}{\hbar^2}\frac{1}{k}\int_0^\infty r\,dr \;\; kr \;\; \frac{Ae^{-r/a}}{r} = \frac{2mAa}{\hbar^2} \ll 1.$$

This is the condition that the Yukawa potential should be so weak that it does not support any bound states.

The conditions of validity of the Born approximation are not met for <u>any</u> value of k in the limit $a \to \infty$ $(\kappa \to 0)$, in which limit the Yukawa potential becomes the Coulomb potential.

Now we turn to the relation between the exact and unperturbed Green's operators. So far in setting up the LS eqn. we have only used the unperturbed Green's operators $G_{0+}(E)$, but as we have remarked the exact Green's operator (or resolvent) contains all the information we would ever want to know about the system. The unperturbed and exact resolvents $G_0(z)$ and $G(z)$ satisfy a number of relations. Remind you,

$$G_0(z) = \frac{1}{z - H_0}, \qquad G(z) = \frac{1}{z-H}$$

where z is a complexified energy. Setting $z = E \pm i\epsilon$ and taking $\epsilon \to 0$ gives $G_{0\pm}(E)$ or $G_\pm(E)$.

Here is an example of the identities we can derive:

$$z - H_0 = z - H_0 - V + V = z - H + V = \begin{cases} (z-H)(1 + G(z)V) \\ (1 + V\,G(z))\,(z-H) \end{cases}$$

where in the last step we have factored $z-H$ out to the left or right. Now multiply the first from the left by $G(z)$ and the second from the right, and we get

$$\left.\begin{aligned} 1 + G(z)V &= G(z)\,(z - H_0) \\ 1 + V\,G(z) &= (z-H_0)\,G(z) \end{aligned}\right\}.$$

Now multiply the first from the right by $G_0(z)$ and the 2nd from the left by $G_0(z)$, and we get

$$\left.\begin{aligned} G(z) &= G_0(z) + G(z)VG_0(z) \\ G(z) &= G_0(z) + G_0(z)VG(z) \end{aligned}\right\}$$

two different but equal expressions for $G(z)$ (the order of the factors in the last term can be reversed without effect).

The second of these equations can be regarded as an operator version of the LS eqn, in which $G(z)$ is the unknown instead of $|\psi_{\vec{k}}\rangle$. To see this, just write the equations side by side:

$$\left.\begin{aligned} G(z) &= G_0(z) + G_0(z)VG(z) \\ |\psi_{\vec{k}}^{(+)}\rangle &= |\vec{k}\rangle + G_0(z)V|\psi_{\vec{k}}\rangle \end{aligned}\right\}.$$

And we can solve this "operator LS eqn" just as we did the ket LS eqn, just bring the terms involving $G(z)$ over to one side,

$$[1 - G_0(z)V]\,G(z) = G_0(z),$$

or

$$\boxed{G(z) = \Omega(z)G_0(z).}$$

Thus $G(z)$ can also be expanded in a Born series,

$$G(z) = G_0(z) + G_0(z)VG_0(z) + G_0(z)VG_0(z)VG_0(z) + \ldots$$

This is a perturbation expansion (Born series) for the exact resolvent. If we set $z = E + i\epsilon$ and take $\lim \epsilon \to 0$, we get a Born series for $G_+(E)$ in terms of $G_{0+}(E)$ and V.

The Møller wave operator not only maps $|\vec{k}\rangle$ into $|\psi_{\vec{k}}\rangle$, it also maps $G_{0+}(E)$ into $G_+(E)$.

Another useful identity comes from examing the operator $1 - G_0(z)V$, whose inverse is the Møller wave operator. That is,

$$1 - G_0(z)V = 1 - \frac{1}{z-H_0}V = \frac{1}{z-H_0}\left(z-H_0-V\right) = \frac{1}{z-H_0}(z-H).$$

So,

$$\Omega(z) = \left[1 - G_0(z)V\right]^{-1} = \left[\frac{1}{z-H_0}(z-H)\right]^{-1} = G(z)(z-H_0).$$

But this is

$$G(z)(z-H_0) = 1 + G(z)V$$

(see p. 7). In summary,

$$\Omega(z) = \left[1 - G_0(z)V\right]^{-1} = 1 + G(z)V,$$

or, at real energies,

$$\Omega_+(E) = 1 + G_+(E)V,$$

so

means $|\vec{k}\rangle$.

$$|\psi_{\vec{k}}\rangle = \left[1 + G_+(E)V\right]|\Phi_{\vec{k}}\rangle.$$

We see that if we know $G_+(E)$ we can find $\Omega_+(E)$ and thereby find the exact scattering wave functions. This is another example of how knowing $G_+(E)$ (or $G(z)$) implies knowing everything about a system.

If we substitute this into the expression for the scattering amplitude, we find

$$f(\vec{k},\vec{k}') = -(2\pi)^2 \frac{m}{\hbar^2} \langle \vec{k}' | T(E) | \vec{k} \rangle ,$$

where

$$T(E) = V + V\, G_+(E)\, V .$$

The scattering amplitude can be expressed in terms of the matrix elements of the T (or transition) operator between plane wave states (the incident and scattered). This is particularly useful for finding the signatures of various conservation laws (parity, time-reversal, ...), or the violation of them, on the observable scattering cross section. This subject is discussed in the Notes and also in Sakurai.

Now we turn to the optical theorem. First, an almost one-line proof for central force potentials, using the method of phase shifts. We have:

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)\, e^{i\delta_l} \sin\delta_l \; P_l(\cos\theta)$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l .$$

Evaluate $f(\theta)$ in the forward direction, $\theta = 0$, where $P_l(1) = 1$:

$$f(0) = \frac{1}{k} \sum_l (2l+1) \sin\delta_l \,(\cos\delta_l + i \sin\delta_l),$$

so

$$\frac{4\pi}{k} \operatorname{Im} f(0) = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l = \sigma .$$

In summary,

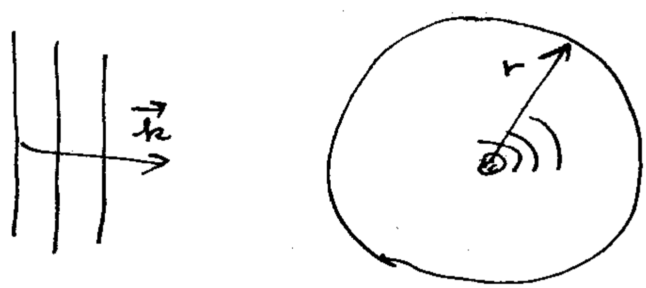
$$\boxed{\sigma = \frac{4\pi}{k} \operatorname{Im} f(0)} \qquad \text{(Optical theorem).}$$

This is easy, but it doesn't give any insight into the meaning. (The total cross section is proportional to the Im part of the scattering amplitude in the forward direction).

Now a longer proof that carries more insight. Also generalizes to non-central force potentials. We consider the probability current,

$$\vec{J} = \frac{-i\hbar}{2m} \psi^* \nabla \psi + \text{c.c.}$$

in QM (scalar particle). For an scattering soln. $H|\psi\rangle = E|\psi\rangle$ it satisfies $\nabla \cdot \vec{J} = 0$, hence its integral over any closed surface is 0. We will integrate it over a large sphere of radius r centered on the scatterer, and take $r \to \infty$.



So,

$$0 = \int_{\text{sphere}} \vec{J} \cdot d\vec{a} = r^2 \int J_r \, d\Omega \qquad J_r = \hat{r} \cdot \vec{J}.$$

Since we are in the asymptotic regime, we can take the asymptotic form of ψ,

normaliz. const.

$$\psi(\vec{r}) = A\left[e^{i\vec{k}\cdot\vec{r}} + f(\theta,\phi)\,\frac{e^{ikr}}{r}\right] + \text{higher order terms.}$$

With $\vec{k} = k\hat{z}$, we have $\vec{k}\cdot\vec{r} = kz = kr\cos\theta$. Then

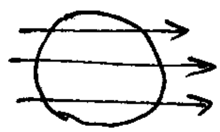
$$\vec{J} = \frac{|A|^2 v}{2}\left[e^{-ikr\cos\theta} + f^*\,\frac{e^{-ikr}}{r}\right]\left[e^{ikr\cos\theta}\,\hat{z} + \frac{f}{r}\,e^{ikr}\,\hat{r}\right] + \text{c.c.},$$

where we drop terms that $\to 0$ faster than $1/r^2$, since they won't contribute to the integral. $\vec{J}$ breaks up into the incident, scattered, and cross-term (X) or interference currents, $\vec{J}_{inc}$, $\vec{J}_{sc}$, $\vec{J}_X$. Here

$$\vec{J}_{inc} = |A|^2 v\,\hat{z} = \text{const.},$$

so

$$\int_{\text{sphere}} \vec{J}_{inc}\cdot d\vec{a} = 0.$$



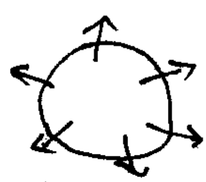
The incident flux goes right through the sphere. As for $\vec{J}_{sc}$,

$$\vec{J}_{sc} = |A|^2 v\,\frac{|f|^2}{r^2}\,\hat{r}, \qquad |f|^2 = \frac{d\sigma}{d\Omega}$$

so

$$\int_{\text{sphere}} \vec{J}_{sc}\cdot d\vec{a} = |A|^2 v \int d\Omega\,\frac{d\sigma}{d\Omega} = |A|^2 v\,\sigma.$$

This is the positive flux of scattered particles.



Of course it's proportional to σ; this is the def. of σ.

The scattered particles are coming out of the sphere, so there must be some net flux in. It must come from the cross terms.

$$\vec{J}_x = \frac{|A|^2 v}{2}\Big[e^{ikr(1-\cos\theta)} \frac{f}{r}\hat{r} + e^{-ikr(1-\cos\theta)} \frac{f^*}{r}\hat{z}$$

$$+ e^{-ikr(1-\cos\theta)} \frac{f^*}{r}\hat{r} + e^{ikr(1-\cos\theta)} \frac{f}{r}\hat{z}\Big\}$$

$$= \frac{|A|^2 v}{2} e^{ikr(1-\cos\theta)} \frac{f}{r}(\hat{r}+\hat{z}) + \text{c.c.}$$

So,

$$= r^2 \int d\Omega\, (\hat{r}\cdot\vec{J}_x)$$

$$\int_{\text{sphere}} \vec{J}_x \cdot d\vec{a} = \frac{|A|^2 v}{2} r \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; e^{ikr(1-\cos\theta)} f(\theta,\phi)(1+\cos\theta) + \text{c.c.}$$

where we use $(\hat{r}+\hat{z})\cdot\hat{r} = 1+\cos\theta$. We want this in the limit $r\to\infty$, which is tricky since the integral is multiplied by r but the integrand oscillates ever more rapidly as $r\to\infty$. It helps to clarify this if we ~~set~~ integrate by parts, using

$$\sin\theta\, d\theta\, e^{ikr(1-\cos\theta)} = \frac{1}{ikr}\, d\, e^{ikr(1-\cos\theta)}.$$

So,

$$\int_{\text{sphere}} \vec{J}_x \cdot d\vec{a} = \frac{|A|^2 v}{2}\frac{r}{ikr}\int_0^{2\pi} d\phi \Big[e^{ikr(1-\cos\theta)} f(\theta,\phi)(1+\cos\theta)\Big|_0^{\pi}$$

$$- \int_0^{\pi} d\theta\, e^{ikr(1-\cos\theta)} \frac{\partial}{\partial\theta}\left[f(\theta,\phi)(1+\cos\theta)\right]\Big\} + \text{c.c.}$$

The r's out front cancel and the remaining integral still has the oscillating integrand, so it goes to 0 as $r \to \infty$, and we just have the 1st term,

$$e^{i(kr)(1-\cos\theta)} f(\theta,\phi)(1+\cos\theta)\Big|_0^\pi = 0 - 2f(0,\phi).$$

But $f(0,\phi)$ is f at the north pole, where it doesn't depend on ϕ. Just call it $f(0)$. So the ϕ integral can be done, and gives 2π.

Thus,

$$\int_{\text{sphere}} \vec{J}_x \cdot d\vec{a} = \frac{|A|^2 v}{2} \frac{2\pi}{k} \left[-\frac{2f(0)}{i} + \frac{2f(0)^*}{i} \right]$$

$$= -|A|^2 v \frac{4\pi}{k} \operatorname{Im} f(0).$$

Putting it together, $\int \vec{J} \cdot d\vec{a} = 0 \quad \Rightarrow$

$$\boxed{\sigma = \frac{4\pi}{k} \operatorname{Im} f(0)}$$

We see that the scattered flux is compensated by an inward coming flux from down the + z-axis, coming from the interference between the incident and scattered wave. This flux cancels out some of the incident flux, creating the ~~shadow~~ shadow downstream from the scatterer. More later...