Lect 12 Analytic properties of Scattering amplitude and Levinson theorem

Radial Solutions: So far, we solve the radial equations using $u(r, k) = r R(r, k)$ as a standing-wave like solution. $u(r, k)$ is an even function of $k$ because the radial equation only involves $k^2$. We next consider the traveling wave solutions (thus $k$ can take both positive and negative values). Consider a solution of the radial Eq with the following boundary condition

$$\phi_+(k, r) \rightarrow i^l e^{-i kr}$$

The solution $\phi_+(k, r)$ is irregular at the origin, $R \phi_+(k, r) \sim k^{l+1} e^{-i kr}$.

Another solution $\phi_-(k, r) \rightarrow i^l e^{i kr}$, which is also irregular at the $r \to 0$.

The standing wave solution can be written as linear combinations of $\phi_+(k, r)$ and $\phi_-(k, r)$, as

$$u_0(k, r) = \frac{i^l}{k} k^{l+1} \left( \tilde{f}_+(-k) \phi_+(k, r) - (-1)^l \tilde{f}_-(k) \phi_-(k, r) \right)$$

this solution satisfies the boundary condition at the origin

$$\lim_{r \to 0} \frac{r^{l+1}}{(2l+1)!!}$$

which is independent of $k$. In this case, complex analysis theorem (Poincare) shows that $u_0(k, r)$ is an entire function of $k$. 

At \( r \to \infty \), \( U_e(k, r) \) approaches

\[
U_e(k, r) \underbrace{\to} \lim_{r \to \infty} \frac{1}{2} \left( \frac{i}{k} \right)^l [ \tilde{f}_e(-k) e^{-i kr} - (-)^l \tilde{f}_e(k) e^{i kr} ]
\]

Discussion:

(1) The radial equation is real, thus \( \phi_e^*(k, r) \) should also be a solution, and thus proportional to \( \phi_e(-k, r) \). More carefully, we have

\[
\left[ \phi_e(-k, r) \right]^* = (-)^l \phi_e(k, r).
\]

If \( k \) is complex for later convenience, we have

\[
\left[ \phi_e(-k^*, r) \right]^* = (-)^l \phi_e(k, r),
\]

for real values of \( k \).

(2) For the function \( [U_e(k, r)]^* = U_e(k, r) \), we want it to be real.

And also for complex \( k \), we want \( [U_e(k^*, r)]^* = U_e(k, r) \).

For this requirement, we need to assign relation between \( \tilde{f}_e(k) \) and \( \tilde{f}_e(-k) \).

\[
U_e(k, r) = -\frac{i}{2} (k^*)^{-l-1} \left[ \tilde{f}_e^*(k) \phi_e^*(k, r) - (-)^l \tilde{f}_e^*(k) \phi_e^*(-k, r) \right]
\]

\[
= -\frac{i}{2} (k^*)^{-l-1} \left[ \tilde{f}_e^*(-k) (-)^l \phi_e(-k^*, r) - \tilde{f}_e^*(k) \phi_e(k^*, r) \right]
\]

\[
= U_e(k^*, r) = \frac{i}{2} (k^*)^{-l-1} \left[ \tilde{f}_e(-k^*) \phi_e(k^*, r) - (-)^l \tilde{f}_e(k^*) \phi_e(-k^*, r) \right]
\]

\[
\implies \tilde{f}_e(-k^*) = \tilde{f}_e(k^*)
\]
$\text{3. If we compare the solution } u_e(kr) \xrightarrow{r \to \infty} \frac{1}{|k|^{2H}} \left( \tilde{f}_e(k) e^{-ikr} - (-)^H \tilde{f}_e(k) e^{ikr} \right) \\
with asymptotic solution } q_e(kr) \xrightarrow{r \to \infty} \frac{i}{\sqrt{k}} e^{ikr} \left( e^{-ikr} - e^{ikr} \right) \\
\text{They should equal up to a constant factor. } \\
\Rightarrow S_e(k) = e^{2i \delta_e} = 1 + 2ikf_e(k) = \frac{\tilde{f}_e(k)}{\tilde{f}_e(-k)} \\
\text{scattering matrix } \\
\text{Scattering amplitude (not Jost) } \\
f_e(k) = \frac{\sqrt{4\pi(2\ell+1)}}{k} \frac{e^{2i \delta_e} - 1}{2i \delta_e} = \frac{\sqrt{4\pi(2\ell+1)}}{k} \cot \delta_e - i \\
\text{if } k \text{ is real } \Rightarrow \frac{\tilde{f}_e(k)}{\tilde{f}_e(-k)} = \frac{\tilde{f}_e(k)}{\tilde{f}_e(-k)} = e^{2i \delta_e} \\
\Rightarrow |S_e(k)| = 1 \text{ is satisfied as required by the unitarity. } \\
\Rightarrow \tilde{f}_e(k) = |f_e(k)| e^{i \delta_e}, \text{ the phase of the Jost function. } \\
is just the phase shift. } \\
\text{4. In other word, } \tilde{f}_e(k) \text{ is the amplitude for the basis of the modified } \\
\text{propagating wave } \phi_e(k, r). \\
\text{}\tilde{f}_e(k) e^{i \ell k r} \quad \text{as } (r \to \infty)
Bound states.

$k^2 < 0$, but real $\Rightarrow k = \pm ix$, where $x > 0$. we have

$$u_k(ix, r) \overset{r \to +\infty}{\longrightarrow} \frac{1}{a} \left( \frac{i}{ix} \right)^{l+1} \tilde{f}_e(-ix) e^{xr}$$

$$- \frac{1}{a} \left( \frac{i}{ix} \right)^{l+1} (r^l \tilde{f}_e(ix)) e^{-xr}$$

we need $\tilde{f}_e(-ix) = 0$ for $x > 0$. $\Rightarrow$

$$u_k(ix, r) \overset{r \to +\infty}{\longrightarrow} \frac{1}{a} (-x)^{-l-1} \tilde{f}_e(ix) e^{-xr}$$

Similarly, we have $u_k(-ix, r) = u_k^*(ix, r)$

$$\overset{r \to +\infty}{\longrightarrow} \frac{1}{2} (-x)^{l-1} \tilde{f}_e^*(ix) e^{xr} = \frac{1}{a} (-x)^{l+1} \tilde{f}_e(ix) e^{xr}$$

according to $\tilde{f}_e(-ik^*) = \tilde{f}_e^*(k) \Rightarrow \tilde{f}_e^*(ix) = \tilde{f}_e(ix)$

$\Rightarrow$ The zero of the Jost function on the negative imaginary axis corresponds to a bound state. We need $\tilde{f}_e(-ix) = 0$

$$\begin{cases} \tilde{f}_e(-ix) = 0 \\ \tilde{f}_e^*(ix) \neq 0 \end{cases}$$

According to, $\tilde{S}_e(k) = \frac{\tilde{f}_e^*(k)}{\tilde{f}_e(-k)} \Rightarrow $ $S(k)$ has a pole at

$k = ix$, and a zero at $k = -ix$. 
Dispersion relation for the Jost function \( \tilde{f}_e(k) \)

It can be derived that on the real axis, and the lower half plane
\( \tilde{f}_e(k) \) is analytical, and as \( |k| \to \infty \),
\[
\tilde{f}_e(k) \xrightarrow{|k| \to \infty} 1 - i \frac{m}{k^2} \int_{0}^{\infty} V(r) \, dr \quad \text{for } \text{Im} \, k \leq 0
\]
assuming integral converges.

\[
\Rightarrow \tilde{f}_e(k) \xrightarrow{|k| \to \infty} - \frac{m}{k^2} \int_{0}^{\infty} V(r) \, dr.
\]
Thus \( \tilde{f}_e(k) - 1 \) is analytical and decay as \( \frac{1}{k} \) in the lower half plane. By Cauchy's theorem,
\[
\tilde{f}_e(k) - 1 = - \frac{1}{2\pi i} \oint \frac{\tilde{f}_e(k') - 1}{k' - k + i\epsilon} \, dk' \quad (\text{Im} \, k \leq 0)
\]
i.e.

Now let us set \( k \) at the real axis
\[
\oint_c = P \int_{-\infty}^{+\infty} + \text{semi-circle small} \\
+ \int \text{big semi-circle}
\]
\[
\tilde{f}_e(k) - 1 = \frac{i}{\pi} P \int_{-\infty}^{+\infty} \frac{\tilde{f}_e(k') - 1}{k' - k} \, dk' , \quad \text{where } P: \text{principle value}
\]
\[
\Rightarrow \quad \text{Re}[\tilde{f}(k') - 1] = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\text{Im}[\tilde{f}(k') - 1]}{k' - k} \, dk',
\]
\[
\text{Im}[\tilde{f}(k') - 1] = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\text{Re}[\tilde{f}(k') - 1]}{k' - k} \, dk'.
\]

(You can also prove it by using \( \frac{1}{k' - k + i\eta} = P \frac{1}{k' - k} - i\pi \delta(k' - k) \)).

Another application: the dielectric function \( \varepsilon(\omega) \) is analytic in the upper half plane, we also have
\[
\varepsilon(\omega) - 1 = \frac{1}{i\pi} P \int_{-\infty}^{+\infty} \frac{\varepsilon(\omega') - 1}{\omega' - \omega} \, d\omega
\]
\[
\Rightarrow \quad \text{Re}[\varepsilon(\omega) - 1] = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\text{Im}(\varepsilon(\omega') - 1)}{\omega' - \omega} \, d\omega
\]
\[
\text{Im}[\varepsilon(\omega) - 1] = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\text{Re}(\varepsilon(\omega') - 1)}{\omega' - \omega} \, d\omega
\]

\[
\varepsilon(\omega) - 1 = 4\pi i \frac{\sigma(\omega)}{\omega} = 4\pi \chi(\omega)
\]
\[
\text{real conductivity}
\]

\[
\Rightarrow \quad \text{Re} \sigma(\omega) = \omega \text{Im} \chi(\omega)
\]

If you measure the polarizability \( \text{Re} \chi(\omega) \), then through the \( K - K \) relation, you can obtain \( \text{Im} \chi(\omega) \), then you know the conductivity.

\[
\text{optical}
\]
We build up the connection between the number of bound states of a given $l$, and the phase shift $\delta_l(0)$ at the zero energy defined as $k \to 0$.

Let us assume $|\tilde{f}_l(0)| \neq 0$.

First, let us check the behavior of $\delta_l(k)$ as $k \to 0$. Due to

$$\tilde{f}_l(-k^*) = \tilde{f}_l^*(k)$$

and

$$\tilde{f}_l(k) = |\tilde{f}_l(k)| e^{i\delta_l(k)}$$

for $k$ on real axis $\Rightarrow \tilde{f}_l(-k) = \tilde{f}_l^*(k) = |\tilde{f}_l(k)| e^{-i\delta_l(k)}$

this $\delta_l(-k) = -\delta_l(k)$ for $k \neq 0$, this means that $\delta_l(k)$ is discontinuous at $k = 0$.

Also $\delta_l(k) \to 0$ for high energy scattering. To maintain the analyticity of $\tilde{f}_l(0)$ at $x$-axis and lower half plane, we need

$$\delta_l(0^+) - \delta_l(0^-) = 2N\pi \Rightarrow \delta_l(0) = N\pi$$

if $\tilde{f}_l(0) \neq 0$.

Q: What's the value of $N$?

Now let us calculate the contour integral

$$-\frac{1}{2\pi i} \int_{c} \frac{\tilde{f}_l'(k)}{\tilde{f}_l(k)} dk = -\frac{1}{2\pi i} \int_{c} d\ln \tilde{f}_l(k)$$

The integrand has simple poles at zeros of $\tilde{f}_l(k)$, i.e. bound states
The LHS just gives the number of bound states $N_e$. The RHS
\[ \ln \tilde{f}(k) = \ln |\tilde{f}(k)| + i \delta(k) \]

$\ln |\tilde{f}(k)|$ is continuous because $|\tilde{f}(k)|$ is nonzero along the contour.

\begin{itemize}
  \item Apparently, at the $x$-axis, $k = 0$, $\tilde{f}(k) \neq 0$, otherwise, $\tilde{U}(k,r) = 0$.
  \item Also, the bound state energy cannot go to $-\infty$, thus the zero of $\tilde{f}(k)$ cannot sit on the infinity semi-circle.
\end{itemize}

\[ \Rightarrow \oint \ln |\tilde{f}(k)| = 0 \]

$\delta(k)$ is also continuous, but multiple-valued

\[ \oint \delta(k) = \delta(0^-) - \delta(0^+) = -2\delta(0^+) \]

\[ \Rightarrow -\frac{1}{2\pi i} \oint_c \frac{d \ln \tilde{f}(k)}{\tilde{f}(k)} = -\frac{i}{\pi i} \delta(0^+) = n_e \Rightarrow \delta(0^+) = n_e \pi. \]

It's clear that $n_e$ is just the number of bound states.

* What happens if $\tilde{f}(0) = 0$? In this case, its phase $\delta(0)$ is ill-defined. We need to choose the contour with a semi-circle (small).

Again, we consider the integral
\[ -\frac{1}{2\pi i} \oint_c \frac{\tilde{f}'(k)}{\tilde{f}(k)} dk = -\frac{1}{2\pi i} \int_c d \ln \tilde{f}(k). \]
LHS: If $l=0$, then $\tilde{f}_e(0) = 0$ does not represent a true bound state because the wavefunction leaks outside. Thus LHS really represents the number of bound states $N_e$. If $l \geq 1$, due to centrifugal potential $\frac{l(l+1)}{r^2}$, the zero-energy state really represents a bound state. It can be shown that the transmission probability to infinity is 0. The radial wavefunction $R_e(r) \sim r^{-(l+1)}$, and thus

$$\int_{R}^{+\infty} r^2 |\psi|^2 \, dr \sim \int_{R}^{+\infty} r^{-2l-2} \, dr = \int_{0}^{+\infty} \frac{dr}{r^{2l}}$$

which converges.

Thus although it's a power-law wave function, but is a bound state ($l=0$ does not work!). Thus at $l \geq 1$, $\text{LHS} = N_e - 1$.

If $\tilde{f}_e(0) = 0$, it can be shown (see Shiff textbook, cite Levinson), then $f_e(k) \propto k^q$ where $q = 1$ for $l = 0$,

$$1/2 \text{ for } l \neq 0.$$  

then the right hand side

$$= \frac{1}{\pi} \delta(0^+) - \frac{q}{2} = \begin{cases} \frac{\delta(0^+)}{\pi} - \frac{1}{2} & \text{for } l = 0 \\
\frac{\delta(0^+)}{\pi} - 1 & \text{for } l \neq 0 \end{cases}$$

$$\delta_{l=0}(0^+) = \pi (n_0 + \frac{1}{2}) \text{ if } \tilde{f}_e(0) = 0 \text{ and } l = 0$$

otherwise $\delta_{l}(0^+) = \pi n_e$, Levinson's theorem!
§ Effective interaction range

Let us consider an explicit example of the Jost function

\[ \tilde{f}_0(k) = \frac{k + i\alpha}{k - i\alpha} \]

which has the right asymptotic behavior

\[ \tilde{f}_0(k) \rightarrow \frac{1}{k} \]

It has zero at \( k = -i\alpha \) corresponding to bound states with energy \( -\frac{\hbar^2 \alpha^2}{2m} \).

\[ \tilde{f}_0(k) = \left( \frac{k^2 + \alpha^2}{k^2 - \alpha^2} \right)^{1/2} e^{i\delta_0(k)} \]

the phase shift \( \delta_0(k) = \tan^{-1} \frac{k}{\alpha} + \tan^{-1} \frac{\alpha}{k} \)

\[ \Rightarrow \tan \delta_0(k) = \frac{k(k + \alpha)}{k^2 - \alpha^2} \]

\[ k \cot \delta_0(k) = k \left( \frac{k^2 - \alpha^2}{k(k + \alpha)} \right) = -\frac{\alpha^2}{k + \alpha} + \frac{k^2}{k + \alpha} \]

For the low-energy scattering if we expand to second order of \( k^2 \)

\[ k \cot \delta_0(k) = -\frac{1}{\alpha} + \frac{1}{2} \alpha \]

where \( \alpha \) is called interaction range.

\[ \Rightarrow \alpha = \frac{2}{k + \alpha} \]

\( \alpha \) is usually small, so \( \alpha \) needs to be large.

\[ \frac{1}{\alpha} = \frac{\alpha}{k + \alpha} = \frac{\alpha}{k} \left( 1 - \frac{k}{k + \alpha} \right) \]

\[ k \left( 1 - \frac{k}{k + \alpha} \right) = k - \frac{\alpha}{2} k^2 \]

correct to the second order of \( k^2 \).
Consider the situation where \( \alpha \) is fixed, but \( x \) decreases to zero and becomes negative. At \( x = 0 \), \( f_0(0) = 0 \), there is a zero energy resonance and the scattering length a diverges. For \( x \) is negative, there is no true bound state, and the scattering length is negative.

For all the three cases, \( \phi(0, k) \) increases from zero as \( k \) decreases from \(-\infty\).

- **Zero energy resonance**
  \[ x = 0, \quad \tan \delta_0(k) = \frac{k \alpha}{k^2} = \frac{\alpha}{k^2} \]

- **No-bound state**
  \[ x < 0, \quad \tan \delta_0(k) = \frac{1}{k + |x|} \]

All agree with Levinson theorem.