Lect 12 Analytic properties of Scattering amplitude and Levinson theorem

§ Radial Solutions: so far, we solve the radial equations using $u_\ell(k,r) = r R_\ell(k,r)$ as a standing-wave like solution. $u_\ell(k,r)$ is an even function of k because the radial equation only involves k^2. We next conside 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

$$\phi_\ell(k,r) \xrightarrow[r\to\infty]{} i^\ell e^{-ikr}.$$

The solution $\phi_\ell(k,r)$ is irregular at the origin, proportional to $r\, n_\ell(kr) \sim k^{-(\ell+1)} r^{-\ell}$

Another solution $\phi_\ell(-k,r) \xrightarrow[r\to\infty]{} i^\ell e^{ikr}$, which is also irregular at the $r\to 0$.

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

Jost function of k.

$$u_\ell(k,r) = \frac{i}{2} k^{-(\ell+1)} \left[\tilde{f}_\ell(-k)\, \phi_\ell(k,r) - (-)^\ell \tilde{f}_\ell(k)\, \phi_\ell(-k,r) \right]$$

this solution satisfies the boundary condition at the origin

$$\boxed{u_\ell(k,r) \xrightarrow[r\to 0]{} \frac{r^{\ell+1}}{(2\ell+1)!!}},$$

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

(At $r \to \infty$, $u_\ell(k,r)$ approaches

$$u_\ell(k,r) \xrightarrow[r\to\infty]{} \frac{1}{2}\left(\frac{i}{k}\right)^{\ell+1} [\, \tilde{f}_\ell(-k)\, e^{-ikr} - (-)^\ell \tilde{f}_\ell(k)\, e^{ikr}) .$$

(*) Discussion:

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

$$[\phi_\ell(-k,r)]^* = (-)^\ell \phi_\ell(k,r) .$$

for real values of k.

if k is complex for later convenience, we have

$$[\phi_\ell(-k^*,r)]^* = (-)^\ell \phi_\ell(k,r) .$$

2. For the function $\underbrace{[u_\ell(k,r)]^* = u_\ell(k,r)}_{\text{we want it is real}}$,

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

For this requirment, we need to assign relation between $\tilde{f}_\ell(k)$ and $\tilde{f}_\ell(-k)$.

$$u_\ell^*(k,r) = \frac{-i}{2}(k^*)^{-\ell-1}[\, \tilde{f}_\ell^*(-k)\, \phi_\ell^*(k,r) - (-)^\ell \tilde{f}_\ell^*(k)\, \phi_\ell^*(-k,r)]$$

$$= \frac{-i}{2}(k^*)^{-\ell-1}[\, \tilde{f}_\ell^*(-k)\,(-)^\ell \phi_\ell(-k^*,r) - \underbrace{\tilde{f}_\ell^*(k)}_{(-)^\ell(-)^\ell} \phi_\ell(k^*,r)]$$

$$= u_\ell(k^*,r) = \frac{i}{2}(k^*)^{-\ell-1}[\, \tilde{f}_\ell(-k^*)\, \phi_\ell(k^*,r) - (-)^\ell \tilde{f}_\ell(k^*)\, \phi_\ell(-k^*,r)]$$

$$\Rightarrow \boxed{\tilde{f}_\ell(-k^*) = \tilde{f}_\ell^*(k)}$$

$\Rightarrow$ for real value of k $\Rightarrow$ $\tilde{f}_l(-k) = \tilde{f}^*(k)$.

③ If we compare the solution $u_l(k,r) \xrightarrow{r\to\infty} \frac{1}{2}\left(\frac{i}{k}\right)^{l+1}\left(\tilde{f}_l(-k)\, e^{-ikr} - (-)^l \tilde{f}_l(k)\, e^{ikr}\right)$

with asymtotic solution $rR_l(kr) \xrightarrow[r\to\infty]{} \frac{i^{l+1}}{2k} e^{i\delta_l}\left[e^{-ikr-i\delta_l} - (-)^l e^{ikr+i\delta_l}\right]$

They should equal up to a const ~~after~~ factor.

$$\Rightarrow \quad S_l(k) = e^{2i\delta_l} = 1 + \frac{2ik f_l(k)}{\sqrt{4\pi(2l+1)}} = \frac{\tilde{f}_l(k)}{\tilde{f}_l(-k)}$$

scattering matrix

scattering aplitude (not Jost)

$$f_l(k) = \frac{\sqrt{4\pi(2l+1)}}{k}\,\frac{e^{2i\delta_l}-1}{2i} = \frac{\sqrt{4\pi(2l+1)}}{k}\,\frac{1}{\cot\delta_l - i}$$

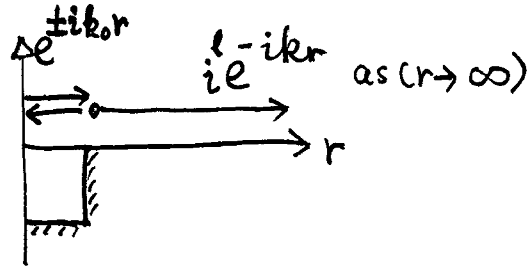
if k is real $\Rightarrow$ $\dfrac{\tilde{f}_l(k)}{\tilde{f}_l(-k)} = \dfrac{\tilde{f}_l(k)}{\tilde{f}^*_l(k)} = e^{2i\delta_l}$

$\Rightarrow$ $|S_l(k)| = 1$ is satisfied as required by the unitarity.

$\Rightarrow$ $\tilde{f}_l(k) = |f_l(k)|\, e^{i\delta_l}$, the phase of the Jost function.

is just the phase shift.

④ In other word, $\tilde{f}_l(k)$ is the amplitude for the basis of the modified propogating wave $\phi_l(k,r)$.



§ Bound states.

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

$$u_l(i\chi, r) \xrightarrow{r\to+\infty} \frac{1}{2}\left(\frac{i}{i\chi}\right)^{l+1} \tilde{f}_l(-i\chi)\, e^{\chi r} - \frac{1}{2}\left(\frac{i}{i\chi}\right)^{l+1} (-)^l\, \tilde{f}_l(i\chi)\, e^{-\chi r}$$

we need $f_l(-i\chi) = 0$ for $\chi > 0$. $\Rightarrow$

$$u_l(i\chi, r) \xrightarrow{r\to+\infty} \frac{1}{2}(-\chi)^{-l-1}\, \tilde{f}_l(i\chi)\, e^{-\chi r}$$

Similarly, we have $u_l(-i\chi, r) = u^*(i\chi, r)$

$$\xrightarrow{r\to+\infty} \frac{1}{2}(-\chi)^{l-1}\, \tilde{f}_l^*(i\chi)\, e^{-\chi r} = \frac{1}{2}(-\chi)^{l-1}\, \tilde{f}_l(i\chi)\, e^{-\chi r}$$

according to $\tilde{f}_l(-k^*) = \tilde{f}_l^*(k) \Rightarrow \tilde{f}_l^*(i\chi) = \tilde{f}_l(i\chi)$

$\Rightarrow$ The zero of the Jost function on the negative imaginary axis corresponds to a bound state. We need $\begin{cases} \tilde{f}_l(-i\chi) = 0 \\ \tilde{f}_l(i\chi) \neq 0 \end{cases}$

According to, $\tilde{S}_l(k) = \dfrac{\tilde{f}_l(k)}{\tilde{f}_l(-k)}$ $\Rightarrow$ $S(k)$ has a pole at $k = i\chi$, and a zero at $k = -i\chi$.

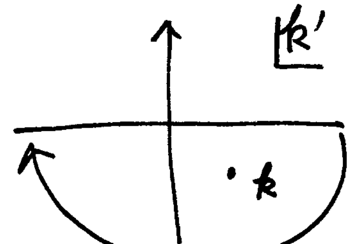
§ Dispersion relation for the Jost function $\tilde{f}_\ell(k)$

It can be derived, that on the real axis, and the lower half plane $\tilde{f}_\ell(k)$ is analytical, and as $|k|\to\infty$,

$$\tilde{f}_\ell(k) \xrightarrow[|k|\to\infty]{} 1 - i\frac{m}{k\hbar^2}\underbrace{\int_0^\infty V(r)\,dr}_{\text{assuming intergral converges.}} \quad \text{for } \operatorname{Im} k \le 0$$

$$\Rightarrow \delta_\ell(k) \xrightarrow[|k|\to+\infty]{} -\frac{m}{k\hbar^2}\int_0^\infty V(r)\,dr.$$

Thus $\tilde{f}_\ell(k)-1$ is analytic and decay as $1/k$ in the lower half plane. By Cauchy's theorem



$$\tilde{f}_\ell(k)-1 = -\frac{1}{2\pi i}\int_C \frac{\tilde{f}_\ell(k')-1}{k'-k+i\eta}\,dk' \qquad (\operatorname{Im} k\le 0)$$

i.e.

now let us set k at the real axis

$$\int_C = P\int_{-\infty}^{+\infty} + \underbrace{\text{semi-circle small}}_{\searrow\ -\pi i[\tilde{f}_\ell(k')-1]} + \underbrace{\int \text{big semi-circle}}_{\searrow\ 0}$$

$\leftarrow$ half of the value of the integral

$$\Rightarrow \tilde{f}_\ell(k)-1 = \frac{i}{\pi}P\int_{-\infty}^{+\infty} dk' \frac{f_\ell(k')-1}{k'-k}, \text{ where } P\text{: principle value.}$$

$$\Rightarrow \left.\begin{aligned} \mathrm{Re}[\tilde{f}_e(k)-1] &= \frac{-1}{\pi} P\int_{-\infty}^{+\infty} \frac{\mathrm{Im}[\tilde{f}_e(k)-1]}{k'-k}\,dk' \\ \mathrm{Im}[\tilde{f}_e(k)-1] &= \frac{+1}{\pi} P\int_{-\infty}^{+\infty} \frac{\mathrm{Re}[\hat{f}_e(k)-1]}{k'-k}\,dk' \end{aligned}\right\} \text{Kramers-Kronig relation.}$$

(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 uper half plane, we also have

$$\varepsilon(\omega) - 1 = \frac{1}{i\pi} P\int_{-\infty}^{+\infty} \frac{\varepsilon(\omega')-1}{\omega'-\omega}\,d\omega$$

$$\Rightarrow \boxed{\begin{aligned} \mathrm{Re}[\varepsilon(\omega)-1] &= \frac{1}{\pi} P\int_{-\infty}^{+\infty} \frac{\mathrm{Im}(\varepsilon(\omega')-1)}{\omega'-\omega}\,d\omega \\ \mathrm{Im}[\varepsilon(\omega)-1] &= \frac{-1}{\pi} P\int_{-\infty}^{+\infty} \frac{\mathrm{Re}(\varepsilon(\omega')-1)}{\omega'-\omega}\,d\omega \end{aligned}}$$

$$\varepsilon(\omega) - 1 = 4\pi i \frac{\sigma(\omega)}{\omega} = 4\pi\chi(\omega)$$

conductivity polarizibility

$$\Rightarrow \mathrm{Re}\,\sigma(\omega) = \omega\,\mathrm{Im}\,\chi(\omega)$$

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

§ Levinson theorem

We build up the connetion 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

$$\tilde{f}_l(-k^*) = \tilde{f}_l^*(k) \quad \text{and} \quad \tilde{f}_l(k) = |\tilde{f}_l(k)|\, e^{i\delta_l(k)}$$

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

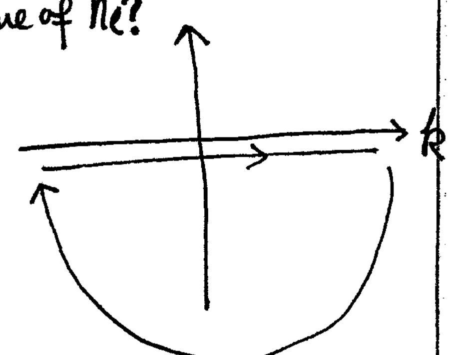
this $\delta_l(-k) = -\delta(k)$ for $k \neq 0$, this means that $\delta_l(k)$ is discontinous at $k = 0$.

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

$$\delta_l(0^+) - \delta_l(0^-) = 2n_l\pi \Rightarrow \delta_l(0) = n_l\pi \quad \text{if } f_l(0) \neq 0.$$

Q: what's the value of n_l?

Now let us calculate the countour 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_ℓ. The RHS

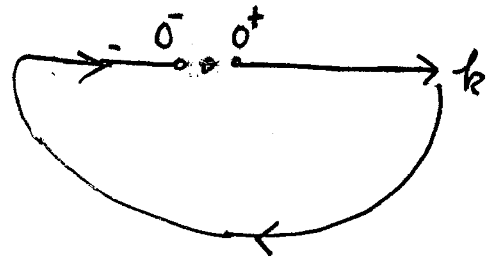
$$\ln \tilde{f}_\ell(k) = \ln|\tilde{f}_\ell(k)| + i\delta_\ell(k)$$

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

① Apparently, at the x-axis, $k \neq 0$, $\tilde{f}_\ell(k) \neq 0$, otherwise, $u_\ell(k,r) = 0$.

② Also, the bound state energy cannot go to $-\infty$, thus the zero of $\tilde{f}_\ell(k)$ cannot sit on the infinity semi-circle.

$$\Rightarrow \oint d\ln|\tilde{f}_\ell(k)| = 0$$



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

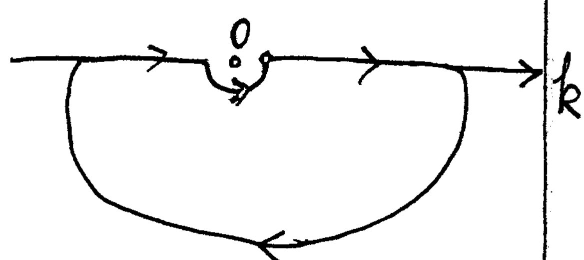
$$\oint d\delta_\ell(k) = \delta(0^-) - \delta(0^+) = -2\delta(0^+)$$

$$\Rightarrow -\frac{1}{2\pi i}\oint_c d\ln\tilde{f}_\ell(k) = \frac{-i}{\pi i}\delta(0^+) = n_\ell \Rightarrow \boxed{\delta(0^+) = n_\ell\pi.}$$

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

✱ What happens if $\tilde{f}_\ell(0) = 0$? In this case, it's phase δ_ℓ is ill-defined. We need to choose the countour with a semi-circle (small)

Again, we consider the integral



$$-\frac{1}{2\pi i}\int_c \frac{\tilde{f}'_\ell(k)}{\tilde{f}_\ell(k)}\,dk = -\frac{1}{2\pi i}\int_c d\ln\tilde{f}_\ell(k).$$

LHS: If $\ell=0$, then $\tilde{f}_\ell(0)=0$ does not represent a true bound state because the wavefunction leak outside. Thus LHS really represent the number of bound states n_ℓ. If $\ell \geq 1$, due to centrifugal potential $\frac{\ell(\ell+1)}{r^2}$, the zero-energy state really represents a bound state. It can be shown that the transmission probility to infinity is 0. The radial wavefunct $R_\ell(r) \sim r^{-(\ell+1)}$, and thus

$$\int_R^{+\infty} |R_\ell(r)|^2 r^2 dr \sim \int_R^{+\infty} r^{-2\ell-2} r^2 dr = \int_a^{+\infty} \frac{dr}{r^{-2\ell}}$$ which converge!

Thus although it's a power-law wave function, but is a bound state ($\ell=0$ does not work!). Thus at $\ell \geq 1$, the LHS $= n_\ell - 1$.

If $\tilde{f}_\ell(0)=0$, it can be shown (see Shiff texbook, cite Levinson),

then $f_\ell(k) \propto k^q$ where $q = \begin{cases} 1 & \text{for } \ell=0. \\ 2 & \text{for } \ell \neq 0. \end{cases}$

then the right hand side

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

$\Rightarrow$ $\delta_{\ell=0}(0^+) = \pi(n_0 + \frac{1}{2})$ if $\tilde{f}_0(0)=0$ and $\ell=0$

otherwise $\delta_\ell(0^+) = \pi n_\ell$, Levinson's theorem!

§ Effective interaction range

Let us consider an explicit example of the Jost function

$$\tilde{f}_0(k) = \frac{k + i\chi}{k - i\alpha}$$ which has the right asymptotic behavior

$\tilde{f}_0(k) - 1 \xrightarrow{k\to\infty} 1/k$. It has zero at $k = -i\chi$ corresponding to bond states with energy $-\frac{\hbar^2\chi^2}{2m}$.

$$\tilde{f}_0(k) = \left(\frac{k^2+\chi^2}{k^2+\alpha^2}\right)^{1/2} e^{i\delta_0(k)}$$, the phase shift $\delta_0(k) = \tan^{-1}\frac{\chi}{k} + \tan^{-1}\frac{\alpha}{k}$

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

$$k \operatorname{ctg}\delta_0(k) = k\,\frac{k^2-\chi\alpha}{k(\chi+\alpha)} = -\frac{\chi\alpha}{\chi+\alpha} + \frac{k^2}{\chi+\alpha}$$

For the low energy scattering if we expand to second order of k^2

$$\boxed{k \operatorname{ctg}\delta_0(k) = -\frac{1}{a} + \frac{1}{2}r_0 k^2},$$ where r_0 is called interaction range.

$$\Rightarrow \quad r_0 = \frac{2}{\chi+\alpha}$$, r_0 is usually small, so α needs to be large.

$$\boxed{\frac{1}{a} = \frac{\chi\alpha}{\chi+\alpha} = \chi\left(1 - \frac{\chi}{\chi+\alpha}\right) = \chi - \frac{r_0}{2}\chi^2}$$

correct to the second order of k^2

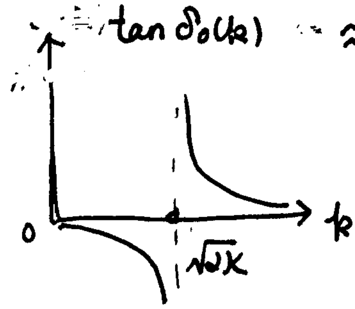
Conside the situation where α is fixed, but $\varkappa$ decreases to zero and becomes negative. At $\varkappa = 0$, $f_0(0) = 0$, there is a zero energy resonance and the scattering length a divergers. For $\varkappa$ is negative, there is no true bound state, and the scattering length is negative.

For all the three cases, $\delta_0(k)$ increases from zero as k decreases from $+\infty$.

with a bound state,

$\varkappa > 0$

$\tan\delta_0(k) \approx k/(\frac{k^2}{\alpha} - \varkappa)$



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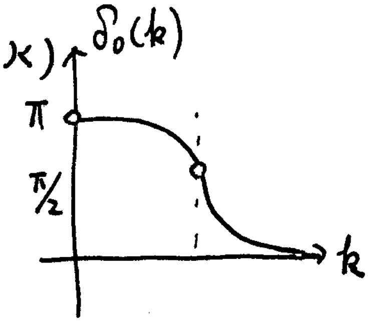
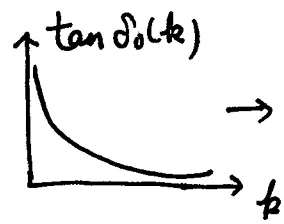


zero energy resonance

$\varkappa = 0$,

$$\tan\delta_0(k) = \frac{k\alpha}{k^2} = \frac{\alpha}{k}$$



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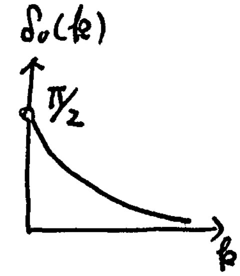
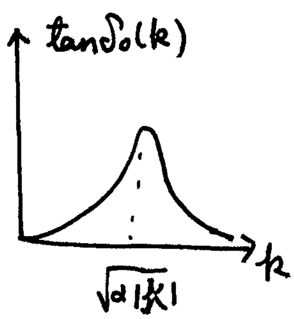


no-bound state

$\varkappa < 0$

$$\tan\delta_0(k) = \frac{1}{\frac{k}{\alpha} + \frac{|\varkappa|}{k}}$$



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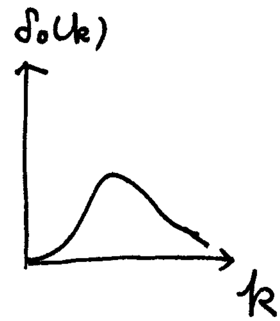

all agree with Levinson theorem.