7.2.2. Bound States and the Lippman–Schwinger Integral Equation

The Lippman–Schwinger equation can also be used to study bound states. In this case, we are interested in the Schrödinger equation solutions

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r}) \]

such that the wavefunction is normalizable

\[ \int d^3r |\psi(\mathbf{r})|^2 < \infty \]

Further, if the zero of energy is such that \( V(\mathbf{r}) \to 0 \) as \( \mathbf{r} \to \infty \), then we have that the bound state energies are negative

\[ E = -\frac{\hbar^2 k^2}{2m} \quad \text{with} \quad k^2 > 0. \]

To simplify the discussion consider the central potential case \( V(\mathbf{r}) = V(r) \) with

\[ V(r) = \frac{2m}{\hbar^2} V(r), \]

Schrödinger's equation becomes
\[(\nabla^2 - \kappa^2)A(r) = U(r)A(r)\]

with \(\int d^3r |A(r)|^2 < \infty\). To convert this to an integral equation, we need the Green function for the differential operator \((\nabla^2 - \kappa^2)\).

The scattering case \(G_+\) was the Green function for \((\nabla^2 + k^2)\) with outgoing spherical wave asymptotic condition. By letting \(k = i\kappa\) in \(G_+\) we will find the Green function we need as well.

Instead of an oscillatory outgoing asymptotic wave, we will demand exponentially damped \(e^{-kr}\) yielding the normalizability we need at the bound state case.

So \((\nabla^2 + k^2)G_+(r, r')\) \((\text{let } k = i\kappa)\)

\[= (\nabla^2 - \kappa^2)\left[ \sum_{l=0}^{\infty} \sum_{m= -l}^{l} (2l+1) G_l^m(r, r'; k = i\kappa) Y_l^m(\theta, \phi) Y_l^m(\theta, \phi) \right] \]

\[= \delta^3(r - r')\]
Where now
\[ G^2_{\pm}(r, r'; k = i\lambda) = \frac{Z}{4\pi} J_\ell(i\lambda r) H_{\ell}(i\lambda r'). \]

At the same time we have that there are no normalizable solutions to the free equation
\[ (\nabla^2 - k^2) 4^{\text{in}}(r) = 0 \]
and
\[ \int d^3x |4^{\text{in}}(r)|^2 < \infty \Rightarrow 2^{\text{in}}(r) = 0, \]
(i.e. there is no potential to provide a bound state).

Then the Lippman-Schwinger bound state integral equation becomes a homogeneous integral equation
\[ 4(r) = 2 \int d^3r' \sum_\ell \sum_{m=\ell} J_\ell(i\lambda r) H_{\ell}(i\lambda r') \times \]
\[ \times Y_{\ell m}^*(\theta', \varphi') Y_{\ell m}(\theta, \varphi) U(r') 2(r'). \]

For a central potential we have
\[ 4(r) = \sum_\ell \sum_{m=-\ell}^{\ell} R_{\ell}(r; x) Y_{\ell m}^*(\theta, \varphi) \]
\[ \times Y_{\ell m}(\theta, \varphi) \]
where $R_\ell(r, x)$ depends on the energy eigenvalue $\ell$. Substituting into the integral equations yields

$$
\frac{\partial^2}{\partial t^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} R_\ell(r, x) Y_\ell^m(\theta, \phi) d\theta d\phi
$$

$$
= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \int_0^\infty dr' r'^2 j_l(i x r) h_{l'}(i x r')
$$

$$
\times Y_\ell^m(\theta, \phi) W(r') R_{\ell'}(r', x)
$$

$$
\times \int d\theta' d\phi' Y_{\ell'}^{m'}(\theta', \phi') Y_\ell^m(\theta, \phi)
$$

$$
= \delta_{\ell, \ell'} \delta_{mm'}
$$

$$
= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_\ell^m(\theta, \phi) \int_0^\infty dr' r'^2 j_l(i x r) h_{l'}(i x r')
$$

$$
\times W(r') R_{\ell'}(r', x)
$$

Since the $Y_\ell^m(\theta, \phi)$ are independent, we find an integral equation for each $l$ and $R_\ell$. 

For each $l$ and $R_\ell$: 

\[ R_{\ell}(r; x) = x \int_0^\infty dr' r'^2 j_{\ell}(ixr') h_{\ell}(ixr') x \times U(r') \Re(r' ; x). \]

Knowing the large \( r \) behavior of the spherical Hankel function,
\[ h_{\ell}(ixr) \sim \frac{1}{ixr} e^{-ixr} \quad \text{as} \quad r \to \infty, \]
we can check the asymptotic behavior of \( R_{\ell}(r; x) \) to see that it is normalizable.

As \( r \to \infty \), \( r_1 = r \) and \( r_2 = r' \) in the integrand above, so
\[ R_{\ell}(r; x) \sim 2x h_{\ell}(ixr) \int_0^\infty dr' r'^2 j_{\ell}(ixr') x \times \Re(r') \Re(r' ; x) \]
\[ \sim \left( \frac{e^{-ixr} e^{-ic \ell r}}{r} \right) \int_0^\infty dr' r'^2 j_{\ell}(ixr') U(r') \Re(r' ; x). \]
For $x > 0$, $R_{\ell} (r; x) \to 0$ as $r \to \infty$ rapidly. Energy is nonzero for guarantee that $\tilde{Z} (r)$ is normalizable.

So we have that the L-S equation for the bound state radial function $R_{\ell} (r; x)$ is obtained from the L-S scattering equation and $\tilde{Z}^{(4)} (r)$ by letting $k \to i \kappa$ with $x > 0$ and neglecting the $2^{(\text{in})} (r) = j_{\ell} (kr)$ free solution. This line of reasoning suggests that we consider the scattering L-S equation for complex values of $k$. Thus consider $\tilde{Z}^{(4)} (r; z)$ with $z \in \mathbb{C}$ and the L-S equation

\[
\tilde{Z}^{(4)} (r; z) = j_{\ell} (z r) - i z \int_0^\infty dr' r'^2 j_{\ell} (z r') \times
\]

\[
\times [he (z r')] U (r) \tilde{Z}^{(4)} (r'; z).
\]

For asymptotic values of $r$, we have that the spherical Bessel function

\[
he (z r) \ll r^{2 \ell + \frac{1}{2}}.
\]
\[ j_1(2r) \sim \frac{1}{2\pi} \left[ e^{i[2r - (l+1)\frac{\pi}{2}]} - e^{-i[2r - (l+1)\frac{\pi}{2}]} \right] \]
\[ \sim \frac{|\Im z|}{r} e^{-\frac{\pi}{2r}} \]

For \( |\Im z| \neq 0 \), this grows exponentially as \( r \to \infty \), and \( 2j_1^4(z, 2) \) defined by their integral equation is not normalizable.

On the other hand, the scattered wave function given by the integral term is well defined as \( r \to \infty \) as long as \( \Im z > 0 \). This follows from the behavior of the Hankel function again:
\[ h_1(2r) \sim \frac{1}{2\pi} e^{i[2r - (l+1)\frac{\pi}{2}]} \]
\[ \sim \frac{|\Im z|}{r} e^{-(\Re z)\frac{\pi}{2r} - (l+1)\frac{\pi^2}{2r}} e^{-\frac{\pi}{2r}} \]

Because \( r > r_0 \) (by definition), the exponential damping of \( h_1(2r) \) dominates over the exponential
growth of $J_e(zr^2)$ as long as $\text{Im} z > 0$.

Thus we would like to eliminate the inhomogeneous term $\tilde{J}_k(z_r)$ from the equation since it alone diverges at $r \to \infty$ for any $\text{Im} z \neq 0$. This can be done by multiplying the integral equation by $J_e(z_r)$ and let $z \to z_0$

$$(z-z_0) \tilde{J}_k^{(4)}(r;z) = (z-z_0) J_e(r;z)$$

$$-iz \int_{0}^{\infty} dr' r'^2 J_e(zr') h_0(zr') \times$$

$$\times \mathcal{U}(r') (z-z_0) \tilde{J}_k^{(4)}(r';z).$$

Since $J_e(r;z)$ is analytic at $z = z_0$, we have

$$\lim_{z \to z_0} (z-z_0) J_e(z_r) = 0.$$ 

This implies

$$\lim_{z \to z_0} (z-z_0) \tilde{J}_k^{(4)}(r;z) = \lim_{z \to z_0} (-iz \int_{0}^{\infty} dr' r'^2 J_e(zr') \times$$

$$\times h_0(zr') \mathcal{U}(r') (z-z_0) \tilde{J}_k^{(4)}(r';z))$$
If \( \psi^{(4)}_{l}(r; z) \) has a simple pole at \( z = z_0 \), then

\[
\psi^{(4)}_{l}(r; z) = \frac{\text{Re}(r; -iz_0)}{z - z_0} + \text{regular at } z = z_0
\]

and the integral equation reduces to

\[
\text{Re}(r; -iz_0) = -iz_0 \int dr' r'^2 j_l(2r) h_0(2r_0') \times
\]
\[
\times U(r') \text{Re}(r'; -iz_0)
\]

But this is just the bound state L-S integral equation if we set \( z_0 = iX \). Hence, we have found the bound states of the potential \( U(r) \) by studying the analytic structure of the L-S integral \( p \)-wave function. The bound state radial wave function is given by the residues of the simple pole in the scattering wave function.

\[
\psi^{(4)}_{l}(r; k) = \frac{\text{Re}(r; X)}{k - iX} + \text{analytic function in complex } k \text{ plane}
\]
The position of the pole occurs at the bound state energy $E$, 

$$k = iX = i\sqrt{\frac{2m|E|}{\hbar^2}} \quad \text{with} \quad E = -|E|.$$ 

For the wavefunction to be normalizable, we had that $X > 0$. Thus, the bound state poles of the scattering wavefunction lie on the positive imaginary axis in the complex $k$-plane.

Since the scattering amplitude is given by (page -1065-) 

$$f^{(4)}(r, k) = -\sum_{l=0}^{\infty} (2l+1)\int dr' r'^2 J_l(kr') \phi_l(r', k) \frac{\rho_l(k)}{k}$$ 

$$= \sum_{l=0}^{\infty} (2l+1) \frac{e^{ikr} \sin(kr)}{k} \phi_l(k)$$ (page -1077-) 

Then if bound state poles occur in $\phi_l^+(r; k)$ at $k = iX$, $X > 0$, the poles should occur in $f(t, k)$ and hence the phase shifts $\delta_l(k)$. 
