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

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

such that the wavefunction is normalizable

$$\int d^3r\, |\psi(\vec{r})|^2 < \infty .$$

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

$$E \equiv -\frac{\hbar^2 \kappa^2}{2m} \quad \text{with } \kappa^2 > 0.$$

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

$$U(r) = \frac{2m}{\hbar^2} V(r), \text{ so}$$

Schrödinger's equation becomes

$$(\nabla^2 - \varkappa^2)\psi(\vec{r}) = U(r)\psi(\vec{r}).$$

with $\int d^3r\, |\psi(\vec{r})|^2 < \infty$. To convert this to an integral equation, we now need the Green function for the differential operator $(\nabla^2 - \varkappa^2)$. In the scattering case G_+ was the Green function for $(\nabla^2 + k^2)$ with outgoing spherical wave asymptotic condition. By letting $k = i\varkappa$ in G_+ we will find the Green function we need (as well instead of an oscillatory outgoing asymptotic wave, it will become exponentially damped, $e^{ikr} = e^{-\varkappa r}$ yielding the normalizability we need in the bound state case.

So $(\nabla^2 + k^2)\, G_+(\vec{r}, \vec{r}\,')$ (let $k = i\varkappa$)

$$= (\nabla^2 - \varkappa^2)\left[\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} 4\pi G_+^l(r, r'; k = i\varkappa)\, Y_l^{m*}(\theta', \varphi')\, Y_l^m(\theta, \varphi)\right]$$

$$= \delta^3(\vec{r} - \vec{r}\,')$$

Where now

$$G_+^\ell(r,r';k=i\varkappa)=\frac{\varkappa}{4\pi}\,j_\ell(i\varkappa r_<)\,h_\ell(i\varkappa r_>).$$

At the same time we have that there are no normalizable solutions to the free equation

$$(\nabla^2-\varkappa^2)\,\psi^{in}(\vec r)=0$$

and $\int d^3r\,|\psi^{in}(\vec r)|^2<\infty \Rightarrow \psi^{in}(\vec r)=0$, (i.e. there is no potential to provide a bound state).

Thus the Lippman-Schwinger boundstate integral equation becomes a homogeneous integral equation

$$\psi(\vec r)=\varkappa\int d^3r'\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} j_\ell(i\varkappa r_<)\,h_\ell(i\varkappa r_>)\times$$

$$\times\, Y_\ell^{m*}(\theta',\varphi')\,Y_\ell^m(\theta,\varphi)\;U(r')\,\psi(\vec r').$$

For a central potential we have

$$\psi(\vec r)=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} R_\ell(r;\varkappa)\,Y_\ell^m(\theta,\varphi)$$

where $R_\ell(r;\kappa)$ depends on the energy eigenvalue κ. Substituting into the integral equations yields

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} R_\ell(r;\kappa)\,Y_\ell^m(\theta,\varphi)$$

$$= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\sum_{\ell'=0}^{\infty}\sum_{m'=-\ell'}^{+\ell'} \kappa\int_0^\infty dr'\,r'^2\, j_\ell(i\kappa r_<)\,h_\ell(i\kappa r_>)$$

$$\times\, Y_\ell^m(\theta,\varphi)\,U(r')\,R_{\ell'}(r',\kappa)\,\times$$

$$\times\,\underbrace{\int_{4\pi} d\Omega'\, Y_\ell^{m*}(\theta',\varphi')\,Y_{\ell'}^{m'}(\theta',\varphi')}_{=\,\delta_{\ell\ell'}\delta_{mm'}}$$

$$= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} Y_\ell^m(\theta,\varphi)\,\kappa\int_0^\infty dr'\,r'^2\, j_\ell(i\kappa r_<)\,h_\ell(i\kappa r_>)$$

$$\times\, U(r')\,R_\ell(r',\kappa)\,.$$

Since the $Y_\ell^m(\theta,\varphi)$ are independent, we find an integral equation for each ℓ for R_ℓ:

$$\boxed{R_\ell(r;\varkappa) = \varkappa \int_0^\infty dr' r'^2 \, j_\ell(i\varkappa r_<) h_\ell(i\varkappa r_>) \times \times U(r') R_\ell(r';\varkappa).}$$

Knowing the large r behavior of the spherical Hankel function

$$h_\ell(i\varkappa r) \underset{r\to\infty}{\sim} \frac{1}{i\varkappa r} e^{-\varkappa r} e^{-i(\ell+1)\frac{\pi}{2}}$$

we can check the asymptotic behavior of $R_\ell(r;\varkappa)$ to see that it is normalizable.

As $r\to\infty$, $r_> = r$ and $r_< = r'$ in the integrand above, so

$$R_\ell(r;\varkappa) \underset{r\to\infty}{\sim} \varkappa h_\ell(i\varkappa r) \int_0^\infty dr' r'^2 j_\ell(i\varkappa r') \times \times U(r') R_\ell(r';\varkappa)$$

$$\sim \frac{e^{-\varkappa r}}{r} e^{-i(\ell+2)\frac{\pi}{2}} \times \times \int_0^\infty dr' r'^2 j_\ell(i\varkappa r') U(r') R_\ell(r';\varkappa).$$

For $\underline{\kappa > 0}$, $R_\ell(r;\kappa) \to 0$ as $r \to \infty$ rapidly enough to guarantee that $\psi(\vec{r})$ is normalizable.

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

$$\boxed{\psi_\ell^{(+)}(r;z) = j_\ell(zr) - iz\int_0^\infty dr' r'^2 j_\ell(zr_<) \times h_\ell(zr_>) U(r') \psi_\ell^{(+)}(r';z)}.$$

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

$$j_\ell(zr) \underset{r\to\infty}{\sim} \frac{1}{2zr}\left[e^{i[zr-(\ell+1)\frac{\pi}{2}]} + e^{-i[zr-(\ell+1)\frac{\pi}{2}]}\right]$$

$$\underset{r\to\infty}{\sim} \frac{e^{|\mathrm{Im}\,z|r}}{2zr} .$$

For $\mathrm{Im}\,z \neq 0$, this grows exponentially as $r \to \infty$, and $\psi_\ell^{(+)}(r;z)$ defined by this 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 $\mathrm{Im}\,z > 0$. This follows from the behavior of the Hankel function again

$$h_\ell(zr) \underset{r\to\infty}{\sim} \frac{1}{zr} e^{i[zr-(\ell+1)\frac{\pi}{2}]}$$

$$\underset{r\to\infty}{\sim} \frac{e^{-(\mathrm{Im}\,z)r}}{zr} e^{i[(\mathrm{Re}\,z)r-(\ell+1)\frac{\pi}{2}]} .$$

Because $r_> > r_<$ (by definition), the exponential damping of $h_\ell(zr_>)$ dominates over the exponential growth of $j_\ell(zr_<)$ as long as $\underline{\text{Im}\, z > 0}$.

Thus we would like to eliminate the inhomogeneous term $j_\ell(zr)$ from the equation since it alone diverges as $r \to \infty$ for any $\text{Im}\, z \neq 0$. This can be done by multiplying the integral equation by $(z-z_0)$ and let $z \to z_0$

$$(z-z_0)\psi_\ell^{(+)}(r;z) = (z-z_0)j_\ell(r;z)$$

$$-iz\int_0^\infty dr' r'^2 j_\ell(zr_<)h_\ell(zr_>) \times$$

$$\times U(r')(z-z_0)\psi_\ell^{(+)}(r';z).$$

Since $j_\ell(r;z)$ is analytic at $z=z_0$, we have

$$\lim_{z\to z_0}(z-z_0)j_\ell(zr) = 0.$$

This implies

$$\lim_{z\to z_0}(z-z_0)\psi_\ell^{(+)}(r;z) = \lim_{z\to z_0}(-iz)\int_0^\infty dr' r'^2 j_\ell(zr_<) \times$$

$$\times h_\ell(zr_>)U(r')(z-z_0)\psi_\ell^{(+)}(r';z)$$

If $\psi_\ell^{(+)}(r;z)$ has a simple pole at $z=z_0$, that is,

$$\psi_\ell^{(+)}(r;z) = \frac{R_\ell(r;-iz_0)}{z-z_0} + \text{function regular at } z=z_0,$$

then

$$\lim_{z\to z_0} (z-z_0)\psi_\ell^{(+)}(r;z) = R_\ell(r;-iz_0)$$

and the integral equation reduces to

$$R_\ell(r;-iz_0) = -iz_0\int_0^\infty dr' r'^2 \, j_\ell(z_0 r_<)\, h_\ell(z_0 r_>) \times$$
$$\times U(r')\, R_\ell(r';-iz_0) .$$

But this is just the bound state L-S integral equation if we set $z_0 = i\chi$. Hence we can find the bound states of the potential $U(r)$ by studying the analytic structure of the L-S integral eq. wave function.

The bound state radial wavefunction is given by the Residue of the simple pole in the scattering wavefunction

$$\psi_\ell^{(+)}(r;k) = \frac{R_\ell(r;\chi)}{k-i\chi} + \begin{array}{c}\text{analytic function}\\ \text{in complex } k\text{-plane}\end{array}$$

The position of the pole occurs at the bound state energy E,

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

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

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

$$f^{(+)}(\vec{k},\vec{k}') = -\sum_{l=0}^{\infty}(2l+1)\int_0^\infty dr'\, r'^2 j_l(kr')U(r')\psi_l^{(+)}(r';k)P_l(\hat{k}\cdot\hat{k}')$$

$$= \sum_{l=0}^{\infty}(2l+1)\,\frac{e^{i\delta_l}\sin\delta_l}{k}P_l(\hat{k}\cdot\hat{k}') \text{ (page -1077-)}$$

Then if bound state poles occur in $\psi_l^{(+)}(r;k)$ at $k = i\varkappa$, $\varkappa > 0$, the poles should occur in $f(\vec{k},\vec{k}')$ and hence the phase shifts $\delta_l(k)$.