Lecture 20

8. shell potential

\[ V(r) = -V_0 \cdot R \cdot S(r - R) \]

Schrodinger equation

\[
\left( -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{E}{r^2} - \frac{2\lambda V_0 R S(R - r) + \frac{k^2}{h^2}}{R^2} \right) \psi(r) = 0
\]

\[ E = -\frac{k^2}{2\mu} \]

For \( r < R \) and \( r > R \) \( V = 0 \) so the solution resembles the origin

\[ \psi_e(r) = A J_e(i \frac{k_r}{\mu}) \quad r < R \]

and the solution that falls off as \( r \to \infty \)

\[ \psi_e(r) = B H_e^{(1)}(i \frac{k_r}{\mu}) \]

we expect the solution to be continuous at \( R = R \). This requires

\[ \psi_e(r) = C \left\{ \begin{array}{ll}
J_e(i \frac{k_r}{\mu}) & r < R \\
H_e^{(1)}(i \frac{k_r}{\mu}) & r > R
\end{array} \right. \]

It turns out that the singularity nature of \( V(r) \) implies that the derivative of the wave function is discontinuous. This can be seen by integrating the differential equation from \( R-e \) to \( R+e \) assuming \( \psi(r) \) is continuous at \( r=R \):

\[
-\int_{R-e}^{R+e} \frac{d^2}{dr^2} \psi_e(r) \, dr - \frac{2}{i\hbar} \int_{R-e}^{R+e} \frac{d\psi_e}{dr} \, dr + \frac{\hbar^2}{2m} \int_{R-e}^{R+e} \psi_e(r) \, dr
\]

\[
- \frac{2\mu V_0 R}{\hbar^2} \psi_e(R) + \frac{\hbar^2}{2m} \int_{R-e}^{R+e} \psi_e(r) \, dr = 0
\]

as \( e \to 0 \) only the first and fourth terms survive:

\[
- \frac{d^2}{dr^2} \psi_e(R+e) + \frac{d\psi_e}{dr}(R-e) = \frac{2\mu V_0 R}{\hbar^2} \psi_e(R)
\]

as \( e \to 0 \) this becomes:

\[
- C \cdot \frac{\hbar^2}{i\hbar} \left( \psi_e^{(1)}(r) j_e(iKR) - \psi_e^{(1)}(iKR) j_e(iKR) \right) = \frac{2\mu V_0 R}{\hbar^2} C \psi_e^{(1)}(iKR) j_e(iKR)
\]

This gives an equation for the values of \( K \) that lead to a bound state.

The left-hand side can be simplified because it is the Wronskian of the Schrödinger equation.
to evaluate this let \( \psi_1(r) \) and \( \psi_2(r) \) be independent solutions of the Schrödinger equation

\[
-\psi_1'' - \frac{2}{r} \psi_1' + \frac{E(r+1)}{r^2} \psi_1 + \frac{k^2}{\hbar^2} \psi_1 = 0
\]

\[
-\psi_2'' - \frac{2}{r} \psi_2' + \frac{E(r+1)}{r^2} \psi_2 + \frac{k^2}{\hbar^2} \psi_2
\]

multiply the first equation by \( \psi_2 \)

the second equation by \( \psi_1 \) and subtract

\[
-\psi_1'' \psi_2 + \psi_2'' \psi_1 - \frac{2}{r} (\psi_1' \psi_2 - \psi_2' \psi_1) = 0
\]

\[
-\frac{d}{dr} (\psi_1' \psi_2 - \psi_2' \psi_1) = -\frac{2}{r} (\psi_1' \psi_2 - \psi_2' \psi_1)
\]

\[
\frac{d}{dr} \frac{(\psi_1' \psi_2 - \psi_1' \psi_1)}{(\psi_1' \psi_2 - \psi_1' \psi_1)} = -\frac{2}{r}
\]

integrating

\[
\ln (\psi_1' \psi_2 - \psi_2' \psi_1) = -2 \ln r + C
\]

\[
\psi_1' \psi_2 - \psi_2' \psi_1 = \frac{\text{const}}{r^2}
\]

\[
\frac{iK}{\hbar} \left( \eta_2^{(1)} (iK\eta^2)^{\frac{1}{2}} \right) = \frac{C}{r^2}
\]

To find \( C \) we can use the asymptotic expansions of \( \eta, \eta' \) near the origin.
\[ J_e (\rho) \rightarrow \frac{\rho^\ell}{(2\ell+1)!!} \quad \nabla_e (\rho) = -\frac{(2\ell-1)!}{\rho^{2\ell+1}} \]

\[ h_e (\rho) \rightarrow J_e (\rho) + i \nabla_e (\rho) = \frac{\rho^\ell}{(2\ell+1)!!} - i\frac{(2\ell-1)!}{\rho^{2\ell+1}} \]

\[ \nabla_e \left( \frac{\rho^\ell}{(2\ell+1)!!} \right) = -i \frac{(2\ell-1)!}{\rho^{2\ell+1}} \]

\[ J_e = \frac{\ell \rho^{\ell-1}}{(2\ell+1)!!} \quad \nabla_e = -i \frac{(2\ell-1)!}{\rho^{2\ell+2}} \]

\[ h_e^{(\ell)} (\rho) J_e (\rho) = h_e^{(\ell)} (\rho) J_e (\rho) \rightarrow \]

\[ i (2\ell+1) \frac{(2\ell-1)!}{\rho^{2\ell+2}} \frac{\rho^\ell}{(2\ell+1)!!} - i(2\ell-1)!! \ell \rho^{\ell-1} \frac{\rho^\ell}{(2\ell+1)!!} \]

\[ \frac{1}{2\ell+1} \cdot \frac{1}{\rho^2} (\ell+1 + \ell) = \frac{1}{\rho^2} \]

\[ i \frac{\lambda}{\hbar} \left( h_e^{(\ell)} \left( \frac{\lambda \kappa R}{\hbar} \right) J_e \left( \frac{\lambda \kappa R}{\hbar} \right) - h_e^{(\ell)} \left( \frac{\lambda \kappa R}{\hbar} \right) J_e \left( \frac{\lambda \kappa R}{\hbar} \right) \right) = \frac{i \lambda}{\hbar} \frac{1}{\rho^2} = -\frac{\lambda}{\hbar} \frac{1}{\rho^2} \]

Using this in the boundary condition

\[ \frac{\lambda}{\hbar} \left( \frac{\hbar}{\lambda \kappa R} \right)^2 = \frac{2 V R}{\hbar^2} h_e^{(\ell)} \left( \frac{\lambda \kappa R}{\hbar} \right) J_e \left( \frac{\lambda \kappa R}{\hbar} \right) \]

\[ -\frac{\hbar}{\lambda \kappa R^2} = \frac{2 V R}{\hbar^2} h_e^{(\ell)} \left( \frac{\lambda \kappa R}{\hbar} \right) J_e \left( \frac{\lambda \kappa R}{\hbar} \right) \]
Consider \( l = 0 \)

\[
\hat{H}_0^{(1)}(\rho) = \frac{\sin \rho}{\rho} - i \frac{\cos \rho}{\rho} = -i \frac{\rho}{\rho} \\
\hat{J}_0(\rho) = \frac{\sin \rho}{\rho} \\
pos \left( \frac{iKR}{\hbar} \right) \hat{H}_0 \left( \frac{iKR}{\hbar} \right) = \\
\frac{\sinh \left( \frac{KR}{\hbar} \right)}{\frac{KR}{\hbar}} \cdot (-i) \frac{e^{-\frac{KR}{\hbar}}}{iKR} = -\frac{\hbar}{KR^2} \sinh \left( \frac{KR}{\hbar} \right) e^{-\frac{KR}{\hbar}} \\
-\frac{\hbar}{KR^2} = \frac{2\mu \nu \sigma R}{\hbar^2} \cdot \left( -\frac{\hbar}{KR^2} \right) \sinh \left( \frac{KR}{\hbar} \right) e^{-\frac{KR}{\hbar}} \\
\frac{\hbar}{KR^2} \frac{\hbar^2 \nu \sigma R^2}{2\mu \nu \sigma R} = \frac{1}{2} ( 1 - e^{-2KR/\hbar} ) \\
\frac{\hbar}{\mu \nu \sigma R} \kappa = 1 - e^{-2KR/\hbar} \\
e^{-2KR/\hbar} = 1 - \frac{\hbar \kappa}{\mu \nu \sigma R}
\]

This leads to a bound state with \( l = 0 \).
Scattering

Probability of a transition from an initial state to a final state

\[ P = \left| \langle \Psi_f(t) | \Psi_i(t) \rangle \right|^2 \]

since

\[ \hat{H} = -i\hbar \frac{\partial}{\partial t} \]

\[ \Psi(t) = e^{-i\hat{H}t/\hbar} \Psi(t) = e^{-i\hat{H}t/\hbar} \Psi(0) \]

\[ P = \left| \left< \Psi_f(t) | U(t)U^+(t) | \Psi_i(t) \right> \right|^2 = \\
   \left| \left< \Psi_f(t) | \Psi_i(t) \right> \right|^2 \]

Unitarity of time evolution means that this probability can be evaluated at any common time.

For scattering

\[ |\Psi_f(t)\rangle \quad \text{looks like free particles in the asymptotic future} \]

\[ |\Psi_i(t)\rangle \quad \text{looks like free particles in the asymptotic past} \]
The problem is that there is no common time when \( |\psi_1(t)\rangle \) and \( |\psi_2(t)\rangle \) have simple forms.

To construct these states:

\[ |\psi_{so}(t)\rangle = \text{free particle state where both particles have mean position } 0, \text{ and mean momenta pointing toward detector} \]

\[ |\psi_{so}(t)\rangle = \text{free particle states where both particles have mean position } 0 \text{ and the target with mean momentum } 0, \text{ projectile with mean momentum } p \text{ beam} \]

For example:

\[ \langle r_1 r_2 | \Phi \rangle = \frac{1}{(2\pi k)^3} \int e^{-i \left( \vec{p}_1 \cdot \vec{r}_1 + \vec{p}_2 \cdot \vec{r}_2 \right) / 2m^2} \left( (\vec{p}_1 - \vec{\mu})^2 / 2A_1 - (\vec{p}_2 - \vec{\mu}_2)^2 / 2A_2 \right) \]

where \( N \) is a normalization constant.
Thus we can define initial and final wave packets by

\[
\lim_{t \to +\infty} \| \Psi_s(t) \rangle - \Psi_{s_0}(t) \rangle \| = 0
\]

\[
\lim_{t \to -\infty} \| \Psi_{s_0}(t) \rangle - \Psi_{s_0}(t) \rangle \| = 0
\]

or

\[
\lim_{t \to +\infty} \| U(t) \Psi_s(0) \rangle - U_0(t) \Psi_{s_0}(0) \rangle \| = 0
\]

\[
\lim_{t \to -\infty} \| U(t) \Psi_{s_0}(0) \rangle - U_0(t) \Psi_{s_0}(0) \rangle \| = 0
\]

using \( \| U^+(t) \| = \| U(t) \| \) for unitary \( U(t) \)

Gives

\[
\lim_{t \to +\infty} \| \Psi_s(0) \rangle - U(-t) U_0(t) \Psi_{s_0}(0) \rangle \| = 0
\]

\[
\lim_{t \to +\infty} \| \Psi_{s_0}(0) \rangle - U(-t) U_0(t) \Psi_{s_0}(0) \rangle \| = 0
\]

These are called scattering asymptotic conditions -

* The replace the initial conditions
* Express solutions of the Schrödinger equation with interaction in terms of free particle wave packets
* The gives the initial and final state solutions of the Schrödinger equation at a common time.

We define

\[
\Omega_\pm = \lim_{t \to \pm \infty} U(-t) U_0(t) \\
= \lim_{t \to \pm \infty} e^\frac{iHt}{\hbar} e^{-\frac{iH_0t}{\hbar}}
\]

Properties

\[
|\psi_f(0)\rangle = \Omega_+ |\psi_{\delta 0}(\cdot)\rangle \\
|\psi_i(0)\rangle = \Omega_- |\psi_{\theta 0}(\cdot)\rangle
\]

Note

\[
\Omega_\pm = \\
= \lim_{s \to \pm \infty} e^\frac{iHs}{\hbar} e^{-\frac{iH_0s}{\hbar}}
\]

or

\[
U(t) \Omega_\pm = \Omega_\pm U_0(t)
\]
mis means

\[ \Omega(t) |\psi_0(0)\rangle = U(t) |\psi_0(0)\rangle = U(t) \Omega |\psi_0(0)\rangle = U(t) 1 |\psi(0)\rangle \]

so \( \Omega(t) \) transforms the free state at any time to the corresponding interacting state.

\[ \frac{d}{dt} \left( U(t) \Omega - \Omega U(t) \right) = 0 \quad t=0 \]

\[ i \hbar \Omega(t) = \Omega t \frac{i \hbar}{\hbar} \]

or

\[ \hbar \Omega(t) = \Omega(t) H_0 \]

mis means that if \( H_0 |\psi_0\rangle = E |\psi_0\rangle \)

then

\[ H(t) |\psi(t)\rangle = \Omega(t) H_0 |\psi_0\rangle = E \Omega(t) |\psi_0\rangle \]

so \( \Omega(t) |\psi_0\rangle \) is an eigenstate of \( H(t) \) with the same energy as \( |\psi_0(0)\rangle \).
This is not surprising — it says that the conserved energy of the system is the same as the energy of the correspondingly asymptotically separated free particles.

Now we can compute $P$:

$$ P = | \langle \psi_f (0) | \psi_i (0) \rangle |^2 = $$

$$ = | \langle \psi_{d0} (0) | \Omega^+ + \Omega^- | \psi_{f0} (0) \rangle |^2 $$

The operator

$$ S = \Omega^+ + \Omega^- $$

is called the scattering operator.

$\therefore P = | \langle \psi_{f0} (0) | S | \psi_{f0} (0) \rangle |^2 $
This allows us to compute the scattering probability using me will understood free wave packets.

The physics associated with the potential is in 

Remarks - even though \( U(t) \) and \( U_0(t) \) are unitary - \( \mathcal{S}_\pm \) are not necessarily unitary.

\[ H_0 \text{ has eigenvalues } \varepsilon_0 > 0 \]
\[ \mathcal{S}_\pm |E\rangle \text{ has eigenvalues of } H \]
with the same energy.

\[ H |1B\rangle = -E_0 |1B\rangle \quad , \quad E_0 < 0 \]

\[ 0 = \langle 1B | (H-H) \mathcal{S}_\pm |E_0\rangle = \]
\[ = (E_0-E_0) \langle 1B | \mathcal{S}_\pm |E_0\rangle \]
\[ #0 \text{ this must be } 0 \]

\[ \Rightarrow \text{ the range of } \mathcal{S}_\pm \text{ is orthogonal to all bound states.} \]
Existence of the limit

\[
\lim_{t \to \pm \infty} e^{-\frac{iHt}{\hbar}} e^{\frac{iH\tau}{\hbar}} |\psi_0\rangle =
\]

\[
|\psi_0\rangle + \lim_{\tau \to \infty} \int_{-\infty}^{\infty} \frac{d\tau'}{2\pi} \left( e^{iH\tau'/\hbar} - e^{-iH\tau'/\hbar} \right) |\psi_0\rangle d\tau =
\]

\[
|\psi_0\rangle + \frac{i}{\hbar} \lim_{\tau \to \infty} \int_{-\infty}^{\infty} e^{iH\tau'/\hbar} V e^{-iH\tau'/\hbar} |\psi_0\rangle d\tau
\]

we need to show

\[
\lim_{t \to \infty} \| \int_{-\infty}^{t} e^{iH\tau'/\hbar} V e^{-iH\tau'/\hbar} |\psi_0\rangle d\tau \| \leq \int_{-\infty}^{\infty} \| e^{iH\tau'/\hbar} V e^{-iH\tau'/\hbar} |\psi_0\rangle \| d\tau \leq \int_{-\infty}^{\infty} \| V e^{-iH\tau'/\hbar} |\psi_0\rangle \| d\tau < \infty
\]

This can be checked for various \( V \) when \( |\psi_0\rangle \) is a minimal uncorrelated state. If \( V \) falls off faster than \( \frac{1}{t} \) and is not singular \( \Rightarrow \) the integrand \( \sim t^{-3}\hbar \) for large \( t \) which converges.
while $P$ is a proper quantum observable - we do not prepare the system in a wave packet that we control. Instead we compare the incident particles run it time to the rate of collecting particles in a detector.

It turns out that we can use $S$ to determine the experimentally observable quantities.

We start with the formal expression for the transition amplitude

$$\langle \psi_{S_0}(c) | S | \psi_{I_0}(c) \rangle =$$

$$\lim_{t \to -\infty} \lim_{s \to -\infty} \langle \psi_{S_0}(c) | e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} e^{iH(t-s)/\hbar} | \psi_{I_0}(c) \rangle$$

$$\lim_{t \to -\infty} \langle \psi_{S_0}(c) | e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} \underbrace{\langle \psi_{S_0}(c) | e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} \langle \psi_{I_0}(c) | e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} \rangle}_{U_1(t,s)}$$

Let $s = -t$ and let $t \to -\infty$

$$\lim_{t \to -\infty} \langle \psi_{S_0}(c) | e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} e^{-iH(t-s)/\hbar} e^{-iH_s/\hbar} | \psi_{I_0}(c) \rangle.$$
\[ = \langle \psi_{f_0}(0) | \psi_{f_0}(0) \rangle \]
\[ + \int_{0}^{\alpha} \int_{0}^{\omega} \int_{0}^{\omega} \left\{ -\frac{1}{\hbar} \langle \psi_{f_0}(0) | E \rangle \langle E | V e^{-i \omega t} | E \rangle \langle E | \psi_{f_0}(0) \rangle \right. \]
\[ + \langle \psi_{f_0}(0) | E \rangle \langle E | V e^{-i \omega t} | E \rangle \langle E | \psi_{f_0}(0) \rangle \left. \right\} \]

To compute this we put in complete sets of energy eigenstates of \( H_0 \).

\[ = \langle \psi_{f_0}(0) | \psi_{f_0}(0) \rangle \]
\[ + \int_{0}^{\alpha} \int_{0}^{\omega} \int_{0}^{\omega} \left\{ -\frac{2i}{\hbar} (H - \frac{E + E'}{2} + i \hbar) \langle \psi_{f_0}(0) | E \rangle \langle E | V e^{-i \omega t} | E \rangle \langle E | \psi_{f_0}(0) \rangle \right. \]
\[ + \left. \langle \psi_{f_0}(0) | E \rangle \langle E | V e^{-i \omega t} | E \rangle \langle E | \psi_{f_0}(0) \rangle \right\} \]

In this form the order of integration matters – the \( E \) and \( E' \) integrals must be done first.
we note that the time evolved wave packets fall off for large \( t \).

we can choose \( \varepsilon \) small enough so \( e^{-\varepsilon t} \approx 1 \) when \( \psi_0(\varepsilon) \approx 0 \) and then fall off when \( \psi_0(\varepsilon) \approx 0 \).

It we insert this into our expression nothing changes except now it is possible to change the order of integration and do the \( t \) integral first.

\[
\begin{align*}
= & \left\langle \psi_{f_0}(\varepsilon) \mid \psi_{i_0}(\varepsilon) \right\rangle \\
- \frac{i}{\hbar} \int dE dE' \left\{ & \left\langle \psi_{f_0}(\varepsilon) \mid E \right\rangle \left\langle E \mid V \frac{1}{-2i} \frac{1}{H - \frac{E^2}{2} - i\varepsilon} 1E' \right\rangle \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right. \\
& \left. \left\langle \psi_{f_0}(\varepsilon) \mid E \right\rangle \left\langle E - \frac{\hbar}{-2i} \frac{1}{H - \frac{E^2}{2} + i\varepsilon} V1E' \right\rangle \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right\} \\
= & \left\langle \psi_{f_0}(\varepsilon) \mid \psi_{i_0}(\varepsilon) \right\rangle + \\
\frac{1}{2} \int \left\{ & \left\langle \psi_f(\varepsilon) \mid E \right\rangle \left\langle E \right\rangle \left( \frac{1}{(E^2 + E') - i\varepsilon} V1E' \times E' \right\rangle \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right. \\
& \left. \left\langle \psi_f(\varepsilon) \mid E \right\rangle \left\langle E \right\rangle V \frac{1}{(E^2 + E') - i\varepsilon} 1E' \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right\rangle \\
\frac{1}{2} \int \left\{ & \left\langle \psi_f(\varepsilon) \mid E \right\rangle \left\langle E \right\rangle \left( \frac{1}{(E^2 + E') - i\varepsilon} V1E' \times E' \right\rangle \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right. \\
& \left. \left\langle \psi_f(\varepsilon) \mid E \right\rangle \left\langle E \right\rangle \frac{1}{(E^2 + E') - i\varepsilon} 1E' \left\langle E' \mid \psi_{i_0}(\varepsilon) \right\rangle \right\rangle \\
\end{align*}
\]