Quantum Mechanics 3 - Class Exercise 4

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The Born Approximation for Partial Waves

In class you derived the Lippmann-Schwinger equation.

$$\psi_k(\vec{r}) = \frac{1}{L^{3/2}}\left[e^{ikz} - \frac{2mL^{3/2}}{\hbar^2}\int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} V(\vec{r}')\psi_k(\vec{r}')\right]. \tag{1}$$

Also, you proved

$$e^{ikz} = \sum_{\ell=0}^{\infty}(2\ell+1)\, i^{\ell} j_\ell(kr)\, P_\ell(\cos\theta). \tag{2}$$

Let us now expand the wave-function in a similar manner.

$$\psi_k(\vec{r}) = \frac{1}{L^{3/2}}\sum_{\ell=0}^{\infty}(2\ell+1)\, i^{\ell} R_\ell(r)\, P_\ell(\cos\theta). \tag{3}$$

For a spherical symmetric potential, By plugging Eq. (2) and Eq. (3) to Eq. (1) one can obtain

$$R_\ell(r) = j_\ell(kr) - \frac{2imk}{\hbar^2}\int_0^\infty dr' r'^2 V(r')\, j_\ell(kr_<)\, h_\ell^{(1)}(kr_>)\, R_\ell(r'), \tag{4}$$

where $r_< = \min\{r, r'\}$, $r_> = \max\{r, r'\}$.

Exercise: prove Eq. (4)!
You will need to use the spherical harmonics expansion

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} = ik\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} j_\ell(kr_<)\, h_\ell^{(1)}(kr_>)\, Y_{\ell m}(\theta,\phi)\, Y^*_{\ell m}(\theta',\phi'). \tag{5}$$

We now apply the far field approximation — we assume that the potential vanishes for $r' > a$ and our observation point is at $r \gg r'$. In that case $r_> = r$ and $r_< = r'$.

$$\begin{aligned} R_\ell(r) &\approx j_\ell(kr) - \frac{2imk}{\hbar^2} h_\ell^{(1)}(kr)\int_0^a dr' r'^2 V(r')\, j_\ell(kr')\, R_\ell(r') \\ &\approx j_\ell(kr) - (-i)^\ell \frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int_0^a dr' r'^2 V(r')\, j_\ell(kr')\, R_\ell(r'), \end{aligned} \tag{6}$$

where in the second line I used the asymptotic behavior of the Hankel function,

$$h_{\ell}^{(1)}(kr) \underset{kr\to\infty}{\longrightarrow} -\frac{i}{kr}\mathrm{e}^{i(kr-\ell\pi/2)} = (-i)^{\ell+1}\frac{\mathrm{e}^{ikr}}{kr}. \tag{7}$$

Next, we plug the expression of $R_{\ell}(r)$ from Eq. (6) back in Eq. (3). This gives

$$\psi_k(\vec{r}) = \frac{1}{L^{3/2}}\left[\mathrm{e}^{ikz} - \frac{\mathrm{e}^{ikr}}{r}\frac{2m}{\hbar^2}\sum_{\ell=0}^{\infty}(2\ell+1)P_{\ell}(\cos\theta)\int_0^a dr' r'^2 V(r') j_{\ell}(kr') R_{\ell}(r')\right]. \tag{8}$$

Recall that in the far field approximation we can write

$$\psi_k(\vec{r}) = \frac{1}{L^{3/2}}\left[\mathrm{e}^{ikz} + f_k(\theta,\phi)\frac{\mathrm{e}^{ikr}}{r}\right], \tag{9}$$

and in the case of spherical symmetry you showed in class that

$$f_k(\theta,\phi) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\mathrm{e}^{i\delta_{\ell}}\sin\delta_{\ell}P_{\ell}(\cos\theta), \tag{10}$$

Thus we identify

$$\mathrm{e}^{i\delta_{\ell}}\sin\delta_{\ell} = -\frac{2mk}{\hbar^2}\int_0^a dr r^2 V(r) j_{\ell}(kr) R_{\ell}(r). \tag{11}$$

Finally, we consider weak scattering, i.e. Born approximation. We take on the LHS $\delta_{\ell} \ll 1$ and on the RHS we approximate $R_{\ell}(r) \approx j_{\ell}(kr)$. This yields

$$\boxed{\delta_{\ell}(k) \approx -\frac{2mk}{\hbar^2}\int_0^a dr r^2 V(r) j_{\ell}^2(kr)}. \tag{12}$$

Question 1

In the low energy limit where $ka \ll 1$, show that $|\delta_0| \gg |\delta_{\ell}| \quad \forall \ell > 0$, i.e. the dominant scattering is s-wave (no angular momentum, $\ell = 0$) scattering. Do so in the Born approximation.

Solution

We use Eq. (12) and apply the small argument limit for $j_{\ell}(kr)$.

$$\begin{aligned}
\delta_{\ell}(k) &= -\frac{2mk}{\hbar^2}\int_0^a dr r^2 V(r) j_{\ell}^2(kr) \approx -\frac{2mk}{\hbar^2}\int_0^a dr r^2 V(r)\left[\frac{(kr)^{\ell}}{(2\ell+1)!!}\right]^2 \\
&= -\frac{2mk^{2\ell+1}}{\hbar^2[(2\ell+1)!!]^2}\int_0^a dr r^{2\ell+2}V(r) = -\frac{2ma^2(ka)^{2\ell+1}}{\hbar^2[(2\ell+1)!!]^2}\int_0^1 dx x^{2\ell+2}V(ax).
\end{aligned} \tag{13}$$

Thus

$$\left|\frac{\delta_{\ell}(k)}{\delta_0(k)}\right| = \frac{(ka)^{2\ell}}{[(2\ell+1)!!]^2}\left|\frac{\int_0^1 dx x^{2\ell+2}V(ax)}{\int_0^1 dx x^2 V(ax)}\right| \underbrace{\ll}_{ka\ll 1} 1 \tag{14}$$

Question 2

In the Born approximation, reconstruct the potential $V(r)$ given that the s-wave phase shift is constant, i.e. $\delta_0(k) = \delta_0 = \text{const}$.

Solution

Let us write Eq. (12) with $\ell = 0$.[1]

$$\delta_0 = -\frac{2mk}{\hbar^2}\int_0^\infty dr r^2 V(r) \underbrace{\frac{\sin^2(kr)}{k^2r^2}}_{j_0^2(kr)} = -\frac{2m}{k\hbar^2}\int_0^\infty dr V(r)\sin^2(kr) = -\frac{2m}{k^2\hbar^2}\int_0^\infty dx V\left(\frac{x}{k}\right)\sin^2(x), \quad (15)$$

where $x \equiv kr$. We now apply derivatives on both sides of the equation with respect to k and demand the LHS to vanish.

$$0 = -\frac{2m}{\hbar^2}\int_0^\infty dx \left[\frac{1}{k^2}\frac{d}{dk}V\left(\frac{x}{k}\right) - \frac{2}{k^3}V\left(\frac{x}{k}\right)\right]\sin^2(x). \quad (16)$$

This equation is satisfied only when the expression in brackets is zero. Thus

$$\frac{2}{k}V(r) = \frac{dV(r)}{dk} = \frac{dV(r)}{dr}\frac{dr}{dk} = -\frac{dV(r)}{dr}\frac{x}{k^2} \quad (17)$$

$$\Longrightarrow \frac{dV(r)}{dr} = -\frac{2k}{x}V(r) = -\frac{2}{r}V(r). \quad (18)$$

The solution for this differential equation is $V(r) = A/r^2$, where A is a constant of integration. We can find A by plugging our solution in Eq. (15).

$$\delta_0 = -\frac{2mA}{\hbar^2}\underbrace{\int_0^\infty dx \frac{\sin^2(x)}{x^2}}_{\pi/2} = -\frac{\pi m A}{\hbar^2} \Longrightarrow A = -\frac{\hbar^2\delta_0}{\pi m}. \quad (19)$$

So the desired potential is[2]

$$\boxed{V(r) = -\frac{\hbar^2\delta_0}{\pi m r^2}}. \quad (20)$$

[1] I know what you are thinking: why is the integral's upper limit in Eq. (15) is ∞ and not a? You will see by the end of the calculation the that potential we get is attenuated like $\mathcal{O}\left(r^{-2}\right)$. Therefore, there is an effective region where $\hbar^2k^2/2m \gg V(r)$ and the far field approximation we made in Eq. (6) still holds.

[2] Notice that for this potential δ_ℓ does not depend on k even for $\ell > 0$ (it is however depend on the value of ℓ).

Question 3

For the finite repulsive potential ($V_0 > 0$)

$$V(r) = \begin{cases} V_0 & r < a \\ 0 & r > a \end{cases}, \tag{21}$$

find the phase shift δ_0 for s-waves with $E > V_0$.

Solution

For a spherical potential, the radial part of the wave-function satisfies

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(E - V(r)) - \frac{\ell(\ell+1)}{r^2}\right] rR_\ell(r) = 0 \tag{22}$$

For s-waves we set $\ell = 0$. We define

$$u(r) \equiv rR_0(r) \qquad k^2 \equiv \frac{2mE}{\hbar^2} \qquad K^2 \equiv \frac{2m(E - V_0)}{\hbar^2}, \tag{23}$$

and the differential equation becomes

$$\begin{cases} u'' + K^2 u = 0 & r < a \\ u'' + k^2 u = 0 & r > a \end{cases}. \tag{24}$$

The solutions are combinations of sin's and cos's. For $r < a$ we can exclude the cos part, otherwise R_0 diverges at $r = 0$ and so $u(r) \propto \sin(Kr)$. For $r > a$, where the potential vanishes, you showed in class that $u(r) \propto \sin(kr + \delta_0)$. Thus

$$u(r) = \begin{cases} A\sin(Kr) & r < a \\ B\sin(kr + \delta_0) & r > a \end{cases}. \tag{25}$$

We require continuity at $r = a$,

$$A\sin(Ka) = B\sin(ka + \delta_0), \tag{26}$$

and we require also continuity of the derivative at $r = a$,

$$AK\cos(Ka) = Bk\cos(ka + \delta_0). \tag{27}$$

Division of Eq. (26) by Eq. (27) yields

$$\frac{\tan(Ka)}{K} = \frac{\tan(ka + \delta_0)}{k}, \tag{28}$$

from which we can extract the phase shift,

$$\boxed{\delta_0 = -ka + \tan^{-1}\left[\frac{k}{K}\tan(Ka)\right]}. \tag{29}$$

Let's do a sanity check. For $V_0 \to \infty$, $K = i\kappa$ where $\kappa \to \infty$, and $\tan(Ka)/K = \tanh(\kappa a)/\kappa \to 0$. Therefore $\delta_0 = -ka$ which is exactly the result you obtained in class. Now let's consider the other limit of $V_0 \ll E$. We calculate first the argument of $\tan^{-1}$ to first order in V_0/E.

$$\begin{aligned} \frac{k}{K}\tan(Ka) &= \frac{k}{K}\tan\left(ka\frac{K}{k}\right) = \frac{1}{\sqrt{1-\frac{V_0}{E}}}\tan\left(ka\sqrt{1-\frac{V_0}{E}}\right) \approx \left(1-\frac{V_0}{2E}\right)\tan\left(ka\left(1-\frac{V_0}{2E}\right)\right) \\ &\approx \left(1-\frac{V_0}{2E}\right)\left[\tan(ka) - \frac{1}{\cos^2(ka)}\frac{kaV_0}{2E}\right] \approx \tan(ka) - \frac{V_0}{2E}\left[\tan(ka) + \frac{ka}{\cos^2(ka)}\right] \end{aligned} \tag{30}$$

We now calculate the $\tan^{-1}$ itself to first order of V_0/E.[3]

$$\begin{aligned} \tan^{-1}\left[\frac{k}{K}\tan(Ka)\right] &\approx \tan^{-1}[\tan(ka)] - \frac{1}{1+\tan^2(ka)}\frac{V_0}{2E}\left[\tan(ka) + \frac{ka}{\cos^2(ka)}\right] \\ &= ka - \cos^2(ka)\frac{V_0}{2E}\left[\tan(ka) + \frac{ka}{\cos^2(ka)}\right] \quad (31) \\ &= ka - \frac{V_0}{2E}\left(\frac{1}{2}\sin(2ka) + ka\right). \quad (32) \end{aligned}$$

Thus, to first order in V_0/E,

$$\delta_0 = -ka + \tan^{-1}\left[\frac{k}{K}\tan(Ka)\right] \approx -\frac{V_0}{2E}\left(\frac{1}{2}\sin(2ka) + ka\right). \tag{33}$$

This result should be identical to what the Born approximation (Eq. 12) predicts.

$$\begin{aligned} \delta_0 &= -\frac{2mk}{\hbar^2}\int_0^a dr r^2 V(r) j_0^2(kr) = -\frac{2mkV_0}{\hbar^2}\int_0^a dr r^2 \frac{\sin^2(kr)}{k^2r^2} = -\frac{2mV_0}{\hbar^2 k}\int_0^a dr \sin^2(kr) \\ &= -\frac{2mV_0}{\hbar^2k^2}\int_0^{ka} dx \sin^2(x) = -\frac{V_0}{E}\int_0^{ka} dx \frac{1-\cos(2x)}{2} = -\frac{V_0}{2E}\left(ka + \frac{1}{2}\sin(2ka)\right). \end{aligned} \tag{34}$$

[3] Remember: $\tan^{-1}(x_0 + \Delta x) \approx \tan^{-1}(x_0) + \Delta x/\left(1 + x_0^2\right)$.

Question 3

For the spherical shell ($V_0 > 0$)

$$V(r) = \begin{cases} V_0 & a < r < b \\ 0 & \text{else} \end{cases}, \tag{35}$$

find

1. the phase shift δ_0 for s-waves with $E < V_0$.
2. bound states.

Solution to 1

This problem is very similar to the previous one, so we know how the solutions look like,

$$u(r) = \begin{cases} A\sin(kr) & r < a \\ B\cosh(Kr) + C\sinh(Kr) & a < r < b \\ D\sin(kr + \delta_0) & b < r \end{cases}. \tag{36}$$

Notice that the definition of K is slightly different than before because $E < V_0$, $K \equiv 2m(V_0 - E)/\hbar^2$. We have five unknowns: A, B, C, D, δ_0. One of the equations we have is the requirement that R_0 is normalized to 1. The other four equations are:

$$u(a^-) = u\left(a^+\right) \implies A\sin(ka) = B\cosh(Ka) + C\sinh(Ka) \tag{37}$$

$$u'(a^-) = u'\left(a^+\right) \implies Ak\cos(ka) = BK\sinh(Ka) + CK\cosh(Ka) \tag{38}$$

$$u(b^-) = u\left(b^+\right) \implies B\cosh(Kb) + C\sinh(Kb) = D\sin(kb + \delta_0) \tag{39}$$

$$u'(b^-) = u'\left(b^+\right) \implies BK\sinh(Kb) + CK\cosh(Kb) = Dk\cos(kb + \delta_0) \tag{40}$$

If we divide Eq. (37) by Eq. (38), and Eq. (39) by Eq. (40), we get

$$\frac{\tan(ka)}{k} = \frac{\frac{B}{C} + \tanh(Ka)}{\frac{B}{C}K\tanh(Ka) + K} \tag{41}$$

$$\frac{\tan(kb + \delta_0)}{k} = \frac{\frac{B}{C} + \tanh(Kb)}{\frac{B}{C}K\tanh(Kb) + K} \tag{42}$$

We can now extract B/C from Eq. (41) and then plug its expression in Eq. (42). The algebra is horrible and super boring so I only write here the the final result.

$$\boxed{\tan(kb + \delta_0) = \frac{k}{K}\frac{k\tanh(KR) + K\tan(ka)}{k + K\tan(ka)\tanh(KR)}, \qquad R \equiv b - a}. \tag{43}$$

Solution to 2

Recall that in the lecture you saw the expression for the cross section in terms of the phase shifts,

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell \underset{\text{s-waves}}{\approx} \frac{4\pi}{k^2} \sin^2 \delta_0. \tag{44}$$

The cross section reaches to a maximal value when the energy of the incoming particle matches the energy of a bound state. This happens at

$$\delta_0 = \pi \left(n + \frac{1}{2} \right). \tag{45}$$

For these values

$$\tan(kb + \delta_0) = \tan\left(kb + \pi \left(n + \frac{1}{2} \right) \right) = \tan\left(kb + \frac{\pi}{2} \right) = -\frac{1}{\tan(kb)}. \tag{46}$$

Moreover, true bound states can only exist for $V_0 \to \infty$, otherwise a trapped particle will eventually leak out via tunneling. In this limit $K \to \infty$ and $\tanh(KR) \to 1$. Therefore, we get from Eq. (43) that

$$-\frac{1}{\tan(kb)} = \frac{k}{K} \frac{k + K \tan(ka)}{k + K \tan(ka)}. \tag{47}$$

Which can also be written as

$$\tan(ka) = -\frac{k}{K} \frac{k \tan(kb) + K}{k \tan(kb) + K} = -\frac{k}{K} \underset{K \to \infty}{\longrightarrow} 0. \tag{48}$$

Thus $ka = \pi n$ where n is a positive integer, and the energy levels are

$$\boxed{E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}}. \tag{49}$$

Note: You might be wondering why I didn't cancel out the $k + K \tan(ka)$ terms in the numerator and denominator of Eq. (47). As you can see, this equation has two solutions: the first is $\tan(ka) = -k/K \to 0$ and the second is $\tan(kb) = -K/k \to -\infty$. However, from a physical point of view, a particle trapped in an infinite well shouldn't be concerned about what lies beyond the well. Therefore the solution $\tan(ka) = -k/K \to 0$ corresponds to bound states. The second solution, although it has nothing to do with bound states, does maximizes the cross section (for $V_0 \to \infty$).