4. gyakorlat (okt. 1)

1. Determine the total cross-section for the following potential:

$$V(r) = \begin{cases} \infty, \text{ if } r \le R \\ 0, \text{ if } r > R \end{cases} \tag{1}$$

As a quick revision of the theoretical lecture we briefly summarize:

We search for the solution in case of spherically symmetric potentials, so we can write up the radial Schrödinger equation

$$\psi_{lm}(E,\mathbf{r}) = \frac{R_l(E,r)}{r} Y_l^m(\vartheta,\varphi)$$
$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r) - E\right) R_l(E,r) = 0$$

We can further expand every solution in terms of these radial solutions:

$$\psi(E,\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lm}\frac{R_l(E,r)}{r} Y_l^m(\vartheta,\varphi)$$

Starting from the solution of the free case

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2\right) R_l(r) = 0, \;\; k^2 = \frac{2mE}{\hbar^2}$$
$$R_l^{\text{reg}}(r) = r j_l(kr)$$
$$R_l^{\text{irreg}}(r) = r n_l(kr)$$

With which we get the linear combination for $V = 0$, i.e.: corresponding to the investigation far from the target:

$$\psi(\mathbf{r}) = \sum_{lm}\left[A_{lm} j_l(kr) - B_{lm} n_l(kr)\right] Y_l^m(\vartheta,\varphi)$$
$$\psi(\mathbf{r}) = \sum_{lm}\frac{1}{kr}\left[A_{lm}\sin(kr - l\pi/2) + B_{lm}\cos(kr - l\pi/2)\right] Y_l^m(\vartheta,\varphi)$$

Writing the coefficients as $A_{lm} = C_{lm}\cos\delta_{lm}$, $A_{lm} = C_{lm}\sin\delta_{lm}$ and again assuming the approximating form valid far from the target we write the trial wave-function:

$$\psi(\mathbf{r}) = \sum_{lm}\frac{C_{lm}}{kr}\sin(kr - l\pi/2 + \delta_{lm}) Y_l^m(\vartheta,\varphi)$$
$$\psi(\mathbf{r}) = A(e^{ikz} + \psi_s(\mathbf{r})) = \sum_l \frac{A}{kr}\sqrt{4\pi(2l+1)}\, i^l \sin(kr - l\pi/2) Y_l^0(\vartheta) + A f(\vartheta,\varphi)\frac{e^{ikr}}{r}$$

Where the δ_{lm}-s are the phase shifts induced by the target! After some calculation we get:

$$C_{lm} = \delta_{m,0} e^{i\delta_{l,0}} i^l \sqrt{4\pi(2l+1)}$$
$$f(\vartheta) = \sum_l \frac{\sqrt{4\pi(2l+1)}}{k} e^{i\delta_l}\sin\delta_l Y_l^0(\vartheta)$$
$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l$$

Now in the case of the "hard ball" we show how the phase shifts can be determined using the our knowledge of the form of the potential $V(r)$.

First write the asymptotic expansion of the radial solution of Schrödinger equation

$$R_l(r\to\infty) = A_l(k)rj_l(kr) - B_l(k)rn_l(kr) \approx \frac{A_l(k)}{k}\sin(kr-l\pi/2) + \frac{B_l(k)}{k}\cos(kr-l\pi/2) = \frac{C_l(k)}{k}\sin(kr-l\pi/2+\delta_l(k))$$

Or generally with the Bessel and Neumann functions:

$$R_l(r) = \frac{C_l(k)}{k}\left[\cos\delta_l(k)j_l(kr) - \sin\delta_l(k)n_l(kr)\right]$$

Now we are in the position of exploiting the fact that the potential enters the system with only a boudnary condition, that is the ball cannot be penetrated by the wave-function:

$$\psi(R) = 0 \to R_l(R) = 0 \to \cos\delta_l(k)j_l(kR) = \sin\delta_l(k)n_l(kR) \to \tan\delta_l(k) = \frac{j_l(kR)}{n_l(kR)}$$

We have an easy case for $l=0$, as $j_0(x) = \frac{\sin x}{x}$, $n_0(x) = \frac{\cos x}{x}$:

$$\tan\delta_0(k) = \tan(kR) \to \delta_0(k) = kR$$

Nevertheless, things gets less compact, as the general expression $\delta_l(k) = \mathrm{arctg}\left(\frac{j_l(kR)}{n_l(kR)}\right)$ is in general a hopelessly complicated function of k and so will be the case for the final expressin for σ_{tot} as well! So consider limiting cases!

a.) Investigate the low energy limit and

b.) the high energy limit

Solution:

In the low energy regime we have $k^2 = \frac{2mE}{\hbar^2} \ll 1$ as small parameter. So let us expand the spherical functions:

$$\begin{aligned} j_l(kR) &= \frac{(kR)^l}{(2l+1)!!} + \mathrm{o}\left((kR)^{l+2}\right) \\ n_l(kR) &= \frac{2l-1)!!}{(kR)^{l+1}} + \mathrm{o}\left((kR)^{-l+1}\right) \\ \tan\delta_l(k) &= \frac{(kR)^{2l+1}}{(2l-1)!!(2l+1)!!} + \mathrm{o}\left((kR)^{2l+3}\right) \end{aligned}$$

From here we can again compute up to leading order the $\sin\delta_l(k)$ appearing in the calculation of the total cross-section:

$$\sin^2\delta_l(k) = \frac{\tan^2\delta_l(k)}{1+\tan^2\delta_l(k)} = \frac{(kR)^{4l+2}}{((2l-1)!!(2l+1)!!)^2} + \mathrm{o}\left((kR^{4l+6})\right)$$

Now the total cross section in leading order, first comptuting the contributions for each l:

$$\begin{aligned} &\sigma_l(k) = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(k) = \frac{4\pi(2l+1)}{((2l+1)!!(2l-1)!!)^2}k^{4l}R^{4l+2} + \mathrm{o}\left((kR)^{4l+4}\right) \to 4\pi R^2\delta_{l,0} \\ &\to \sigma_{\mathrm{tot}}(k) = \sum_l \sigma_l(k) \approx 4\pi R^2 \end{aligned}$$

Similarly to the above discussion we consider the high energy limit, where $k \gg 1$, i.e.: with small parameter $\frac{1}{k}$:

$$j_l(kr) \approx \frac{\sin(kr - l\pi/2)}{kr}$$
$$n_l(kr) \approx -\frac{\cos(kr - l\pi/2)}{kr}$$

Using this it is easy to express the tangent function

$$\tan \delta_l(k) = -\tan(kR - l\pi/2) \to \delta_l(k) = -kR + l\pi/2$$

Now using the formula for the total cross section, where we can tell an upper boundary on the summation on physically motivated grounds, that is classically the scattering of a particle is parametrized with the impact parameter a and so with an angular momentum $L = pa$ and so with energy $E = L^2/2ma^2$, qunatum mechanics enters via the possbile values of L we get $E = \hbar^2 l(l+1)/2ma^2$, now again classically arguing, partial waves' contributions are only relevant if $a < R$ giving the bound $l(l+1) < 2mER^2/\hbar^2 = R^2k^2$, which reads for large k, $l < kR$

$$\sigma_{\text{tot}}(k) = \frac{4\pi}{k^2}\sum_{l=0}^{kR}(2l+1)\sin^2(l\pi/2 - kR)$$

We can group all 2 successive terms in the sum giving $2\cos^2(l\pi/2 - kR) + (2l+1)$ giving for the summation in total, where now summation will be understood for only every even l

$$\frac{4\pi}{k^2}\sum_{l=0}^{kR}\cos^2(kR) + (2l+1)/2 = \frac{4\pi R}{k}\cos^2(kR) + \frac{2\pi}{k^2}(kR+1)kR + \frac{2\pi R}{k} \to 2\pi R^2$$

Determine the total cross-section for the following potential (soft ball/ sphere)

$$V(r) = \begin{cases} V_0, \text{ if } r \leq R \\ 0, \text{ if } r > R \end{cases} \tag{2}$$

Let us first discuss the $V_0 < 0$ case! Inside the ball we can only have the regular solution, $R_l(r < R) = rj_l(\kappa r)$, $\kappa^2 = k^2 - \frac{2mV_0}{\hbar^2}$, $k^2 = \frac{2mE}{\hbar^2}$, while outside we can have a general superposition, $R_l(r > R) = a_l r j_l(kr) + b_l r n_l(kr) \to \tan\delta_l = b_l/a_l$.

Now we exploit boundary conditions

$$j_l(\kappa R) = aj_l(kR) + bn_l(kR)$$

$$\kappa j_l'(\kappa R) = kaj_l'(kR) + bkj_l'(kR)$$

Which can be cast into a matrix equation:

$$\begin{pmatrix} j_l(kR) & n_l(kR) \\ kj_l'(kR) & kn_l'(kR) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} j_l(\kappa R) \\ \kappa j_l'(\kappa R) \end{pmatrix}$$

Using the general inversion of a 2×2 matrix we have $\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right)^{-1} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$ with the trivial substitutions we get that:

$$\tan\delta_l = \frac{j_l(kR)\kappa j_l'(\kappa R) - kj_l'(kR)j_l(\kappa R)}{kn_l'(kR)j_l(\kappa R) - n_l(kR)\kappa j_l'(\kappa R)}$$

Now consider the $l=0$ case with $j_0(x)=\frac{\sin x}{x}$ and $n_0(x)=\frac{\cos x}{x}$

$$\tan\delta_0 = -\frac{\sin(kR)\cos(\kappa R)/k - \cos(kR)\sin(\kappa R)/\kappa}{\sin(kR)\sin(\kappa R)/\kappa + \cos(kR)\cos(\kappa R)/k} = \frac{k\tan(\kappa R) - \kappa\tan(kR)}{k\tan(kR)\tan(\kappa R) + \kappa}$$

Now "as usual" let us investigate the low energy limit, with $k \ll 1$ and introduce $q^2 = -\frac{2mV_0}{\hbar^2}$, we have for the terms $k\tan(\kappa R) \approx -k\tan(qR)\,, -\kappa\tan(kR) \approx -\kappa kR\,, k\tan(kR)\tan(\kappa R) \sim k^2 \approx 0$, so in total we have

$$\tan\delta_0 \approx kR\left(\frac{1}{qR}\tan(qR) - 1\right)$$

for which the corresponding cross section:

$$\sigma_0(k) = \frac{4\pi}{k^2}\frac{\tan^2\delta_0}{\tan^2\delta_0 + 1} \approx \frac{4\pi}{k^2}\tan^2\delta_0 = 4\pi R^2\left(\frac{1}{qR}\tan(qR) - 1\right)^2$$

We have a resonance if this expression diverges, that is $\sqrt{-2mV_0/\hbar^2}R = (2n+1)\pi/2 \to V_0 = -\frac{\hbar^2\pi^2}{8mR^2}(2n+1)^2$.

Now we turn to the case of $V_0 > 0$, in this case we should write instead of all κ-s, $i\kappa$ as the expression under the square root becomes negative if $V_0 > E \to \frac{2m}{\hbar^2}(E - V_0) < 0$ and we get instead of the tangents $\frac{\tan(i\kappa R)}{i\kappa R} = \frac{\tanh(\kappa R)}{\kappa R}$. Now substituing it back to the leading order expression of $\sigma_0(k)$ we have

$$\sigma_0(k) \approx 4\pi R^2\left(\frac{1}{qR}\tanh(qR) - 1\right)^2$$

which visibly do not have any resonance, as $\tanh(x)$ is a bounded function! Nevertheless now we are in the position to recover the result obtained for the hard sphere via the limit $V_0 \to -\infty$ for which $\kappa \to \infty$, that is $\tanh(\kappa R) \to 1$ but this gets annullated by the denominator so we are left only with the second term in the bracket

$$\lim_{V_0 \to -\infty} \sigma_0(k) = 4\pi R^2$$

HW:

1. Determine the total cross section in case of a Dirac-delta potential

$$V(r) = K\delta(r - R)$$

Hints: Divide the space into two parts, $r < R$ and $r \geq R$ and use that the solution cannot be singular at $r = 0$ as we did for the soft ball, then exploit boundary conditions at $r = R$, that is the continuity of the wave function and the jump of its derivative due to the Dirac-delta (The radial equation is an effectice one-dimensional Schrödinger equation, so the jump is described in the same way as in the one-dimensional case)!

2. Consider an arbitrary scattering, spherically symmetric potential, $V(r)$ with a compact support of radius R and suppose that we know the solutions of the corresponding radial Schrödinger equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2 - \frac{2mV(r)}{\hbar^2}\right)R_l(r) = 0,\ \ k^2 = \frac{2mE}{\hbar^2}. \tag{3}$$

That is, we know $R_l(r) = a_l r\alpha_l(r) + b_l r\beta(r)$ with the properties, $\alpha_l(r \to 0) \sim r^l$, being regular in the origin and with $\beta_l(r \to 0) \sim r^{-(l+1)}$, being singular in the origin, for $r < R$. While for $r > R$, with $V(r) = 0$,y we have the "usual" free radial solutions, $R_l(r > R) = c_l r j_l(kr) + d_l r n_l(kr)$.
Use the boudnary conditions and the fact that the wave-fucntion cannot be singular at $r = 0$ for determining the a_l, b_l, c_l, d_l, coefficients and so the $\delta_l(k)$ phase shifts!