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physics606 – Advanced Quantum Theory

Problem Set ~~9~~ 10

Martin Ueding
mu@martin-ueding.de

Lino Lemmer
l2@uni-bonn.de

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Group 2 – Dilege Gülmez

problem number	achieved points	possible points
1	11	15
2	13	13
total	24	28

1 Scattering on a hard sphere

1.1 Phase shift

Problem statement

Write down the radial wave function.

Inside the sphere, the potential is infinite, so it is exactly zero for any angular momentum l:

$$R_l^<(r) = 0.$$

The part outside the sphere is independent of the potential,

$$R_l^>(r) = \frac{1}{2}\left[h_l^*(kr) + e^{2i\delta_l} h_l(kr)\right],$$

where $h_l := h_l^{(1)}$ (Schwabl 2007, (18.59)).

Problem statement

Use the continuity of the wave function at $r = r_0$ together with the asymptotic expression for the wave function at $r \to \infty$ to show that

$$\tan(\delta_l) = \frac{j_l(kr_0)}{n_l(kr_0)}.$$

At the boundary r_0 the wave function ψ has to be both continuous and differentiable. Both criteria can be checked at the same time by the virtue of the logarithmic derivative, which is defined in (Schwabl 2007, (18.60)) as

$$\alpha_l := \left.\frac{\mathrm{d}\log\left(R_l^<(r)\right)}{\mathrm{d}r}\right|_{r=r_0} = \left.\frac{1}{R_l^<(r)}\frac{\mathrm{d}R_l^<(r)}{\mathrm{d}r}\right|_{r=r_0}. \checkmark$$

As mentioned before, the wave function ψ and its radial part R will be zero within this sphere of radius r_0. Also, since the potential makes an infinite jump, R will not be differentiable, just like the energy eigenfunctions of the infinite potential well. Both factors in the logarithmic derivative will be infinite, such that $\alpha_l = \infty$ is result. The logarithmic derivative of the inner and outer solutions have to match up. This leads to (ibid., (18.61)):

$$\frac{1}{R_l^>(r)}\frac{\mathrm{d}R_l^>(r)}{\mathrm{d}r} \stackrel{!}{=} \alpha_l. \checkmark$$

The spherical Hankel functions can be split up into spherical Bessel j_l and spherical von Neumann n_l functions. Then the previous equation can be transformed into (ibid., (18.62)):

$$\mathrm{e}^{2\mathrm{i}\delta_l} - 1 = 2\left.\frac{\frac{\mathrm{d}j_l}{\mathrm{d}r} - \alpha_l j_l}{\alpha_l h_l - \frac{\mathrm{d}h_l}{\mathrm{d}r}}\right|_{r=r_0}. \checkmark$$

Solving for δ_l gives (ibid., (18.62)):

$$\tan(\delta_l) = \left.\frac{\frac{\mathrm{d}j_l}{\mathrm{d}r} - \alpha_l j_l}{\frac{\mathrm{d}n_l}{\mathrm{d}r} - \alpha_l n_l}\right|_{r=r_0}.$$

Since α_l is infinite, the remainder of this fraction is

$$\tan(\delta_l) = \frac{j_l(kr_0)}{n_l(kr_0)}, \checkmark$$

which is also the result mentioned for the hard sphere in (ibid., (18.63)).

1.2 Negative shift

Problem statement

Use the explicit expressions for $j_0(x)$ and $n_0(x)$ to show that $\delta_0 = -kr_0$.

The first order of those spherical functions are given by (Weisstein 2014a,b):

$$j_0(x) = \frac{\sin(x)}{x}, \quad n_0(x) = -\frac{\cos(x)}{x}.$$

Inserting this into the previous expression for the phase shift gives us

$$\tan(\delta_l) = -\frac{\sin(kr_0)}{\cos(kr_0)}$$

which simplifies to $\delta_l = -kr_0$. The minus sign can be put into both sine and cosine, then the tangent can be inverted.

Problem statement

Why is the phase shift negative here?

The shift is negative since the wave is scattered on a repulsive potential.

1.3 Expansion for small arguments

Problem statement

Use the expansions of j_l and n_l at small argument to show that $\delta_l \propto [kr_0]^{2l+1}$, just as for scattering on a spherical potential well.

In the ninth exercise, we derived this approximation, it was also given as a control result:

$$j_l(x) = x^l \frac{2^l l!}{[2l+1]!} + \mathcal{O}(x^{l+2}).$$

The von Neumann functions have a similar representation using repeated differentiation (Wikipedia 2014):

$$j_l(x) = [-x]^l \left[\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right]^l \frac{\sin(x)}{x}, \quad n_l(x) = -[-x]^l \left[\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right]^l \frac{\cos(x)}{x}.$$

The derivation is similar. We expand the cosine in terms of its power series:

$$n_l(x) = -\sum_{n=0}^{l} \frac{[-1]^n}{[2n]!}[-x]^l \left[\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right]^l x^{2n-1}.$$

Now we drop all but the lowest power, which comes at $n = 0$. This is the same as just using the first order expansion of the cosine.

$$\approx -[-x]^l \left[\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right]^l x^{-1}.$$

Assuming that $l \geq 1$, we can perform the derivatives and obtain

$$= -[2l-1]!!\, x^{-1-l}.$$ ✓

Then we simply have

$$\frac{j_l(x)}{n_l(x)} \propto \frac{x^l}{x^{-1-l}} = x^{2l+1}.$$ ✓

However, this is $\tan(\delta_l)$, not δ_l itself. Do we make the approximation $\tan(x) = x + \mathcal{O}(x^3)$ here as well? ✓

for small kr_0

1.4 Asymptotic expansion

Problem statement

Use the asymptotic expressions for j_l and n_l for large arguments to show that

$$\lim_{kr_0 \to \infty} \delta_l(k) = -kr_0 + \frac{l\pi}{2}.$$

(Wikipedia 2014) gives the following large argument expressions for the non-spherical functions:

$$J_\nu(x) = \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right), \quad N_\nu(x) = \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right).$$

The relation to the spherical ones is given by

$$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x), \quad n_l(x) = \sqrt{\frac{\pi}{2x}} N_{l+1/2}(x).$$

We now plug this together and get

$$j_l(x) = \frac{1}{x} \cos\left(x - \frac{l\pi}{2}\right), \quad n_l(x) = \frac{1}{x} \sin\left(x - \frac{l\pi}{2}\right).$$

The ratio gives us

$$\tan(\delta_l) = \tan\left(kr_0 - \frac{l\pi}{2}\right) \iff \delta_l = kr_0 - \frac{l\pi}{2}.$$ ✓ due to the defn. you have used there is a sign difference

The problem is that the sign is wrong.

$j_l \to \frac{1}{kr} \sin(x - l\frac{\pi}{2})$

$n_l \to -\frac{1}{kr} \cos(\ )$

1.5 Total cross section

We start with equation (Schwabl 2007, (18.40)):

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{kr_0} [2l+1] \sin(\delta_l)^2 .$$

Now we insert the result of δ_l from the previous part.

$$= \frac{4\pi}{k^2} \sum_{l=0}^{kr_0} [2l+1] \sin\left(-kr_0 + \frac{l\pi}{2}\right)^2 \quad ✓$$

→ for even l $\sin^2 -kr_0$
odd l $\cos^2 -kr_0$

We now split the sum into even and odd values of l, introducing m.

$$= \frac{4\pi}{k^2} \sum_{m=0}^{kr_0/2} \left[[2[2m]+1] \sin\left(-kr_0 + \frac{2m\pi}{2}\right)^2 + [2[2m+1]+1] \sin\left(-kr_0 + \frac{[2m+1]\pi}{2}\right)^2 \right]$$

$$= \frac{4\pi}{k^2} \sum_{m=0}^{kr_0/2} \left[[4m+1] \sin(-kr_0 + m\pi)^2 + [4m+3] \sin\left(-kr_0 + \frac{[2m+1]}{2}\pi\right)^2 \right]$$

The first sine will always be a sine for any value of m. The square will take care of the sign, so we can just write this as a pure sine of the first summand. The second sine will always be a cosine. ✓

$$= \frac{4\pi}{k^2} \sum_{m=0}^{kr_0/2} \left[[4m+1] \sin(kr_0)^2 + [4m+3] \cos(kr_0)^2 \right]$$

?

We combine sine and cosine.

$$= \frac{4\pi}{k^2} \sum_{m=0}^{kr_0/2} [8m+4]$$

The sum can now be evaluated and gives

$$= \frac{4\pi}{k^2} \left[[kr_0]^2 + 4kr_0 + 4 \right].$$

We simplify more and only keep the leading term in k since k is supposed to be large.

$$= \cancel{4}\,2\,\pi r_0^2$$

So this is a factor 4 larger than the geometrical cross section.

2 Scattering length

2.1 Relation to scattering length

We start with equation (3) from the problem set:

$$\tan(\delta_0) = -kr_0 \frac{\alpha_0}{1+\alpha_0}.$$

Then we invert this equation.

$$\iff \cot(\delta_0) = -\frac{1}{kr_0 \frac{\alpha_0}{1+\alpha_0}}$$

Now we multiply with k on both sides.

$$\iff k\cot(\delta_0) = -\frac{1}{r_0 \frac{\alpha_0}{1+\alpha_0}}$$

As a last step, we identify $R_0 = r_0 \frac{\alpha_0}{1+\alpha_0}$.

$$\iff k\cot(\delta_0) = -\frac{1}{R_0} \quad \checkmark$$

2.2

Problem statement

Show that

$$e^{2i\delta_0} = \frac{2i}{\cot(\delta_0) - i} = \frac{2kR_0}{i - kR_0} = -2ikR_0 + \mathcal{O}(k^2).$$

The correct version of the first equality is given in (Schwabl 2007, (18.95)) and has an additional term compared to the one from the problem set[1]:

$$e^{2i\delta_0} \underbrace{-1} = \frac{2i}{\cot(\delta_0) - i}.$$

With that, this is rather straightforward. We define $w := e^{i\delta_0}$ to write less stuff. The derivation is just the simplification backwards:

$$\exp(2i\delta_0) \neq w^2 - 1$$

[1] Regarding the version from the evening of Wednesday, 2014-12-10.

Expand.

$$= \frac{w^{-1}[w^2-1]}{w^{-1}}$$

Factor out.

$$= \frac{w-w^{-1}}{w^{-1}}$$

Introduce factor of 2.

$$= 2\frac{w-w^{-1}}{2w^{-1}}$$

Make this into a more complex double fraction.

$$= 2\frac{1}{\frac{2w^{-1}}{w-w^{-1}}}$$

Invent more terms.

$$= \frac{2}{\frac{w-w^{-1}-w+w^{-1}}{w-w^{-1}}}$$

Separate fractions.

$$= \frac{2}{\frac{w+w^{-1}}{w-w^{-1}}-1}$$

Introduce a factor of i.

$$= \frac{2\mathrm{i}}{\mathrm{i}\frac{w+w^{-1}}{w-w^{-1}}-\mathrm{i}}$$

Write said factor as another double fraction.

$$= \frac{2\mathrm{i}}{\frac{1/2}{1/[2\mathrm{i}]}\frac{w+w^{-1}}{w-w^{-1}}-\mathrm{i}}$$

Recognize cosine and sine.

$$= \frac{2\mathrm{i}}{\frac{\cos(\delta_0)}{\sin(\delta_0)-\mathrm{i}}}$$

Compress this into a cotangent.

$$= \frac{2\mathrm{i}}{\cot(\delta_0) - \mathrm{i}}$$

That was the first part.

From here, the next part is a bit easier:

$$\frac{2\mathrm{i}}{\cot(\delta_0) - \mathrm{i}} = \frac{2\mathrm{i}}{-\frac{1}{kR_0} - \mathrm{i}}$$

Combine the fractions.

$$= -\frac{2\mathrm{i}}{\frac{1+\mathrm{i}kR_0}{kR_0}}$$

Simplify the double fraction.

$$= -\frac{2\mathrm{i}kR_0}{1 + \mathrm{i}kR_0}$$

Introduce a $-\mathrm{i}$ in the denominator.

$$= -\frac{2\mathrm{i}kR_0}{[-\mathrm{i}][\mathrm{i} - kR_0]}$$

Cancel $-\mathrm{i}$.

$$= \frac{2kR_0}{\mathrm{i} - kR_0}$$

That is the second part.

The last part is a Taylor expansion around $k = 0$. The steps are:

$$f(k) := \frac{2kR_0}{\mathrm{i} - kR_0}$$
$$f(0) = 0$$
$$f'(k) = \frac{2R_0[\mathrm{i} - kR_0] - 2kR_0[-R_0]}{[\mathrm{i} - kR_0]^2}$$
$$f'(0) = -2\mathrm{i}R_0$$

So the approximation is

$$\frac{2kR_0}{\mathrm{i} - kR_0} = -2\mathrm{i}kR_0 + \mathcal{O}(k^2).$$

2.3 S-wave amplitude

Using the equation from (Schwabl 2007, (18.96)),

$$f_0 = \frac{2kR_0}{\mathrm{i} - kR_0} \frac{1}{2\mathrm{i}k},$$

we find using the approximation that we have just derived that

$$f_0 \approx -R_0.$$

Since the total cross section for S-wave scattering is given by

$$\sigma = \int \mathrm{d}\Omega \, |f_0|^2,$$

we obtain the desired result of

$$\sigma = 4\pi R_0^2.$$

2.4 Wavefunction outside

In this problem, a second R_0 comes up. Until now, $R_0 \in \mathbb{R}$ was the scattering length. Now this second R_0 is an element of the mapping $\mathbb{R} \to \mathbb{R}$. It stands for the radial part of the S-wave function. It is the special case $l = 1$ of $R_l(r)$. As a rule of thumb, every $R_0(r)$ means the radial wave function, R_0 without function arguments means the scattering length. Luckily, this problem does not ask anything about the function R_0 itself, so the notation would be impossible.

Anyway, to the problem at hand, I digress. We are given another form of the wave function outside of the sphere. We had a version by Schwabl. This one here is

$$R_0(r) \propto \cos(\delta_0) j_0(kr) - \sin(\delta_0) n_0(kr).$$

Now we factor out a factor of cosine and hide it in the proportionality since it does not depend on the radius r.

$$\propto j_0(kr) - \tan(\delta_0) n_0(kr)$$

Here we use equation (4) from the problem set to replace the tangent. Keep in mind that this R_0 is not the same as the other one.

$$= j_0(kr) + kR_0 n_0(kr)$$

Next are the approximations for the Bessel and von Neumann functions. For the zeroth order, they are quite simple, just 1 and $-1/[kr]$.

$$= 1 - \frac{R_0}{r}$$

We change the order of the summands and again use the proportionality here.

$$\propto \frac{R_0}{r} - 1$$

Now we just multiply both sides with the radius r.

$$rR_0(r) \propto R_0 - r$$

So this gives us a proportionality between the two R_0.

References

Schwabl, Franz (2007). *Quantenmechanik*. 7. Berlin: Springer-Verlag. ISBN: 978-3-540-73674-5.

Weisstein, Eric W. (2014a). *Spherical Bessel Function of the First Kind*. URL: http://mathworld.wolfram.com/SphericalBesselFunctionoftheFirstKind.html.

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